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Topics from 20^{th} century physics.
An introductory course for students in mathematics

III. QUANTUM THEORY: CHAPTERS 7 - 9

– QUANTUM MECHANICS OF A SINGLE PARTICLE

7. HEISENBERG'S UNCERTAINTY RELATION

7.1. *Quantum mechanics of a particle: a summary*

This chapter begins the detailed discussion of the behaviour of a single particle in quantum mechanics. In this section we give a short review of basic material, some of which was discussed already in earlier sections. The Hilbert space of states $\mathcal{H}$ of a point particle in ordinary 3-dimensional space is $L^2(R^2, d\vec{x})$, the space of square integrable complex-valued functions on R^3. These functions will be denoted as $\psi(\vec{x})$, $\phi(\vec{x})$, etc., with $\vec{x} = (x_1, x_2, x_3)$, and are usually called 'wave functions'. The inner product on $\mathcal{H}$ is given by

$$(\psi_1, \psi_2) = \int_{-\infty}^{+\infty} \overline{\psi_1(\vec{x})} \psi_2(\vec{x})\, d\vec{x},$$

with $d\vec{x} = dx_1 dx_2 dx_3$. Note that the inner product is conjugate-linear in the *first* variable, the standard convention in physics. The basic observable quantities of the theory are *position* and *(linear) momentum*, represented by the selfadjoint operators Q_j and P_j defined, for $j = 1, 2, 3$, as

$$\begin{aligned} (Q_j\psi)(\vec{x}) &= x_j \psi(\vec{x}) \\ (P_j\psi)(\vec{x}) &= \frac{\hbar}{i} \frac{\partial}{\partial x_j} \psi(\vec{x}). \end{aligned}$$

These operators satisfy the *Heisenberg* or *canonical commutation relations*

$$\begin{aligned} [P_j, Q_k] &= \frac{\hbar}{i} \delta_{jk} \\ [P_j, P_k] &= 0 \\ [Q_j, Q_k] &= 0, \end{aligned}$$

for $j, k = 1, 2, 3$. Note that we consider these unbounded operators on the common dense domain $\mathcal{S}(R^3)$, the space of Schwartz functions, the C^∞ functions that, together with all their derivatives, go to zero at infinity faster than arbitrary inverse polynomials. By this choice we avoid the more obvious domain problems.

The most important physical observable of a particle is the *energy*. It is represented, according to the 'principle of canonical quantization', by an expression in the position and momentum operators Q_j and P_j which is the same as that for the energy of a classical particle. For a particle with mass m, moving under the influence of a force $\vec{F}$ derived from a potential V as $F_j = -\frac{\partial}{\partial x_j} V(\vec{x})$, the most common case, this gives

$$H\psi = \left(\frac{P^2}{2m} + V(\vec{Q}) \right) \psi,$$

or, more explicitly,

$$(H\psi)(\vec{x}) = -\frac{\hbar^2}{2m} (\Delta\psi)(\vec{x}) + V(\vec{x})\psi(\vec{x}),$$

with $P^2 = P_1^2 + P_2^2 + P_3^2$ and Δ the Laplace operator $\Delta = \frac{\partial^2}{\partial {x_1}^2} + \frac{\partial^2}{\partial {x_2}^2} + \frac{\partial^2}{\partial {x_3}^2}$. For $V = 0$ the particle is called *free*. In this case, again the most common one, the energy operator is also the *Hamiltonian*, the generator of the time evolution of the system. For this reason it is denoted as H.

In classical mechanics a rotating body has *angular momentum*: an important physical quantity the conservation of which explains why the axis of a gyroscope persists in a given initial position and also why one is able to ride a bicycle without falling over. A classical particle moving with linear momentum $\vec{p}$ has a vector $\vec{l}$ of angular momentum with respect to the origin $\vec{x} = \vec{0}$ of the coordinate system defined as

$$\vec{l} = \vec{x} \times \vec{p},$$

or in components

$$\begin{aligned} l_1 &= x_2 p_3 - x_3 p_2 \\ l_2 &= x_3 p_1 - x_1 p_3 \\ l_3 &= x_1 p_2 - x_2 p_1 . \end{aligned}$$

The 'canonical quantization principle' gives that the quantum mechanical description three *angular momentum operators* L_1, L_2, L_3, defined as

$$\begin{aligned} L_1 &= Q_2 P_3 - Q_3 P_2 \\ L_2 &= Q_3 P_1 - Q_1 P_3 \\ L_3 &= Q_1 P_2 - Q_2 P_1 . \end{aligned}$$

The L_k are differential operators, one has

$$L_1 = \frac{\hbar}{i}\left(x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2} \right),$$

and the two others by cyclic permutation of the indices. The three angular momentum operators do not commute. Their commutation relations can be worked out by using their explicit forms as differential operators, but can however more easily be found from the known commutation relations for the position and momentum operators. The result is

$$\begin{aligned} [L_1, L_2] &= i\hbar L_3 \\ [L_2, L_3] &= i\hbar L_1 \\ [L_3, L_1] &= i\hbar L_2 \end{aligned}$$

There is also the operator $L^2 = L_1^2 + L_2^2 + L_3^2$, representing the square of the absolute value of angular momentum. It commutes with all three components L_j. Angular momentum in quantum mechanics has very non-classical properties: its measurement gives only discrete discrete values; its three components are incommensurable. It is also strongly connected with symmetry aspects: the three operators L_j span a representation of the Lie algebra of $SO(3)$, the 3-dimensional rotation group. All this will be discussed later.

7.2. *More on position and momentum*

When discussing the properties of position, momentum and energy in quantum mechanics, it is an inessential but notationally very convenient simplification to do this first for a 1-dimensional particle, a simplification which would of course not make sense for the discussion of angular momentum.

For a 1-dimensional particle the state space $\mathcal{H}$ is the Hilbert space $L^2(R^1, dx)$, with inner product

$$(\psi_1, \psi_2) = \int_{-\infty}^{+\infty} \overline{\psi_1(x)}\psi_2(x)\, dx.$$

As basic observables one has the position and momentum operators Q and P, defined as

$$(Q\psi)(x) = x\psi(x)$$

and

$$(P\psi)(x) = \frac{\hbar}{i}\frac{d}{dx}\psi(x),$$

satisfying the Heisenberg commutation relation

$$[P, Q] = \frac{\hbar}{i}\, 1.$$

The energy operator is

$$H = \frac{P^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2},$$

for a free particle, and

$$H = \frac{P^2}{2m} + V(Q) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x),$$

for a particle moving in a potential V. We take the space of Schwartz functions $\mathcal{S}(R^1)$ as common dense domain on which the P and Q are essentially selfadjoint. The operator H is also essentially selfadjoint on this domain if the potential V is a bounded real function on R^1; it is a nontrivial mathematical problem to decide for which *unbounded* functions V this remains true.

A useful device is the *Fourier transform*

$$\hat{\psi}(p) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \psi(x) e^{-\frac{i}{\hbar}px}\, dx,$$

with the inverse transform

$$\psi(x) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \hat{\psi}(p) e^{+\frac{i}{\hbar}px}\, dp.$$

For the ψ and its Fourier transform $\hat{\psi}$ one has Plancherel's formula

$$\int_{-\infty}^{+\infty} |\psi(x)|^2\, dx = \int_{-\infty}^{+\infty} |\hat{\psi}(p)|^2\, dp.$$

The theory of Fourier transforms of functions of a single variable is a fairly subtle part of mathematical analysis. In this case technicalities can be avoided: as a linear transformation of the Hilbert space the Fourier transform makes sense as an integral which defines an invertible continuous linear map from $\mathcal{S}(R)$ onto itself and extends to a unitary operator on the full Hilbert space of all square integrable functions.

In our general outline of the formalism of quantum theory and its physical interpretation we mentioned already that the square of the absolute value of the wave function $\psi(x)$, provided that it is normalized to one, i.e. provided that its Hilbert space norm is one, is interpreted as the *probability density* for the position of the particle: the probability for finding the particle in an interval $[x_1, x_2]$ is given by the integral $\int_{x_1}^{x_2} |\psi(x)|^2 dx$. The mean value, the expectation, or *expectation value* as one says in the physics literature, is given by $(\overline{Q})_\psi = \int_{-\infty}^{+\infty} x|\psi(x)|^2 dx$, and, more generally, the n^{th} moment as $(\overline{Q^n})_\psi = \int_{-\infty}^{+\infty} x^n |\psi(x)|^2 dx$, in agreement with the general Hilbert space formula $(\overline{A^n})_\psi = (\psi, A^n \psi)$, for the measurement of an observable A in a state ψ.

The same operator formula holds for the expectation value and the n^{th} moments of the probability distribution for momentum measurements in the state $\psi(x)$: $(\overline{P^n})_\psi = (\psi, P\psi)$. We use this to calculate $(\overline{P^n})_\psi$ explicitly. We note first that Plancherel's formula can be generalized to

$$\int_{-\infty}^{+\infty} \psi_1^*(x)\psi_2(x)dx = \int_{-\infty}^{+\infty} \hat{\psi}_1^*(p)\hat{\psi}_2(p)dp,$$

for arbitrary functions ψ_1 and ψ_2 in $L^2(R^1, dx)$, and with $\hat{\psi}_1$ and $\hat{\psi}_2$ the Fourier transforms of ψ_1 and ψ_2. To prove this one uses a general expression for the inner product (ψ_1, ψ_2) in terms of $(\psi_1 \pm \psi_2, \psi_1 \pm \psi_2)$ and $(\psi_1 \pm i\psi_2, \psi_1 \pm i\psi_2)$.

We write, for a function $\psi(x)$ in $\mathcal{S}(R)$,

$$(P\psi)(x) = \frac{\hbar}{i}\frac{d}{dx}\left[\frac{1}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{+\infty} \hat{\psi}(p)e^{\frac{i}{\hbar}px}dp\right] =$$
$$= \frac{1}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{+\infty} p\hat{\psi}(p)e^{\frac{i}{\hbar}px}dp,$$

which implies $(\widehat{P\psi})(p) = p\hat{\psi}(p)$, and more generally $(\widehat{P^n\psi})(p) = p^n\hat{\psi}(p)$. Using the generalization of Plancherel's formula gives

$$(\overline{P^n})_\psi = (\psi, P^n\psi) = \int_{-\infty}^{+\infty} (P^n\psi)^*(x)\psi(x)dx =$$
$$= \int_{-\infty}^{+\infty} (\widehat{P^n\psi})^*(p)\hat{\psi}(p)dp = \int_{-\infty}^{+\infty} p^n|\hat{\psi}(p)|^2 dp,$$

which means that the function $|\hat{\psi}(p)|^2$ is the probability density for the measurement of momentum p.

The function $\psi_p(x) = e^{\frac{i}{\hbar}px}$ is a *plane wave* in (one-dimensional) space, with wave length $\lambda = 2\pi\hbar/p$. It is an eigenfunction of the momentum operator $P = \frac{\hbar}{i}\frac{\partial}{\partial x}$ for the eigenvalue p. Physicists therefore use such plane waves for the quantum mechanical description of a particle with sharp momentum p. This expresses one of the oldest and most influential general ideas of quantum mechanics, the *particle-wave duality*: a point particle of mass m and momentum $p = mv$ is described by a plane wave with wave lenght

$$\lambda = \frac{2\pi\hbar}{p}.$$

This λ is called the *De Broglie wave length* of the particle, after the French physicist Louis de Broglie, one of the pioneers of early quantum mechanics, who was the first to suggest this idea of a 'particle - wave duality', as was already mentioned in Section 2.1. of Chapter 2. The interpretation of the function $\psi_p(x) = e^{\frac{i}{\hbar}px}$ as a physical state is nevertheless incorrect. The general formalism of quantum theory tells us that a function $\psi(x)$, which is an eigenfunction of a selfadjoint operator A for an eigenvalue a, should be interpreted a physical state with a as a sharp value for the observable represented by A. However, the function $\psi(x)$ should be square integrable. The plane wave $\psi_p(x) = e^{\frac{i}{\hbar}px}$ is clearly *not* square integrable, it is not an element of the Hilbert space of physical states.

The Fourier transformation provides us with a mathematically more precise way of expressing the above physical idea. The intuitive meaning of the Fourier formula for the function $\psi(x)$ – the 'wave function' as it is called, not surprisingly in view of what has just been said – is that it gives $\psi(x)$ as a 'continuous superposition' of plane waves. To approximate the notion of a sharp momentum state we can use a superposition over a narrow p-interval ε around a p-value p_0, for instance

$$\psi_{p_0,\varepsilon}(x) = \varepsilon^{-\frac{1}{2}} \int_{p_0-\frac{1}{2}\varepsilon}^{p_0+\frac{1}{2}\varepsilon} e^{\frac{i}{\hbar}px}\, dp.$$

The constant $\varepsilon^{\frac{1}{2}}$ in front is such that $\psi_{p_0,\varepsilon}$ will be normalized to one. An elementary calculation gives

$$\psi_{p_0,\varepsilon}(x) = F_\varepsilon(x)\, e^{\frac{i}{\hbar}p_0x},$$

with

$$F_\varepsilon(x) = \varepsilon^{\frac{1}{2}} \frac{\sin \frac{\varepsilon}{2\hbar}x}{\frac{\varepsilon}{2\hbar}x}.$$

The function $\psi_{p_0,\varepsilon}(x)$ is a plane wave $\psi_{p_0}(x)$, multiplied with the real function $F_\varepsilon(x)$ which makes it square integrable. $F(x)$ has a maximum $\varepsilon^{\frac{1}{2}}$ in $x = 0$ and goes to 0 for x going to $\pm\infty$, oscillating with decreasing amplitude between the absolute value of the function $\frac{1}{x}$. For small ε, i.e. when the momentum lies within a narrow interval, the function flattens out in space, which means physically that the position of the particle becomes very unpredictable. For large

ε, i.e. for undeterminate momentum, $F_\varepsilon(x)$ becomes sharply peaked around $x = 0$, which means that the position of the particle becomes narrowly determined. This example shows us that we can have quantum mechanical states in which the position of the particle can be predicted with arbitrary precision, that we can also have states in which the momentum is as sharply defined as one wishes, but that we can *not* have both at the same time. This can be shown generally by means of an inequality for the standard deviations of the measurements of position and momentum which will be discussed in the next section.

The fact that one cannot simultaneously measure the position and velocity of a particle with arbitrary precision means that the particle can be observed at discrete times, but not over a *continuous* time interval. It cannot be followed in time; its *orbit* is not observable. There is an even stronger interpretation of this: *the classical notion of orbit of particle is meaningless in quantum mechanics*.

7.3. *The uncertainty relation of Heisenberg*

Consider for a moment an arbitrary quantum system with Hilbert space $\mathcal{H}$. Take two physical observables a and b, not necessarily commensurable, represented by two (not necessarily commuting) selfadjoint operators A and B. Let ψ be a state vector in $\mathcal{H}$, which should be such that $A\psi$, $A^2\psi$, $B\psi$, $B^2\psi$, $AB\psi$ and $BA\psi$ are well-defined. Denote in the usual way the mean values $\langle A\rangle_\psi = (\psi, A\psi)$ and $\langle B\rangle_\psi = (\psi, B\psi)$ as $\overline{a}$ and $\overline{b}$, and the standard deviations $\langle (A-\overline{a})^2\rangle^{1/2} = (\psi, (A-\overline{a})^2\psi)^{1/2}$ and $\langle (B-\overline{b})^2\rangle^{1/2} = (\psi, (B-\overline{b})^2\psi)^{1/2}$ as Δa and Δb. We then have

$$\begin{aligned} &|(\psi, [A,B]\psi)| = |(\psi, [A-\overline{a}, B-\overline{b}]\psi)| = \\ &= 2\,|Im\left((A-\overline{a})\psi, (B-\overline{b})\psi\right)| \,\leq\, 2\,|\left((A-\overline{a})\psi, (B-\overline{b})\psi\right)|. \end{aligned}$$

The inequality of Schwarz gives

$$\begin{aligned} &2\,|\left((A-\overline{a})\psi, (B-\overline{b})\psi\right)| \,\leq\, 2\,||(A-\overline{a})\psi||\,||(B-\overline{b})\psi|| = \\ &= 2\,(\psi, (A-\overline{a})^2\psi)^{1/2}\,(\psi, (B-\overline{b})^2\psi)^{1/2} = 2\,\Delta a\,\Delta b. \end{aligned}$$

The result is the *general uncertainty relation*, for the standard deviations of the observables a and b in the state ψ,

$$(\Delta a)_\psi\,(\Delta b)_\psi \,\geq\, \frac{1}{2}\,|(\psi, [A,B]\psi)|.$$

This is a restriction on the possibility of simultaneously measuring a and b. For commensurable a and b, when A and B commute, there is of course no restriction.

Return now to the case of a 1-dimensional particle and choose $A = P$ and $B = Q$. This gives immediately the *Heisenberg uncertainty relation*

$$\Delta p\,\Delta x \,\geq\, \frac{\hbar}{2}.$$

Note that we write Δx and Δp instead of Δx_ψ and Δp_ψ because the right-hand side no longer depends on the state vector ψ. The Heisenberg uncertainty relation is one of the centre pieces of elementary quantum mechanics, illustrating the fundamental incommensurability of position and momentum measurements.

7.4. *Minimal uncertainty states*

For an arbitrary state ψ the product of the standard deviations in position and momentum is always larger or equal than $\frac{1}{2}\hbar$. We are interested in states ψ for which this product is *minimal*, i.e. equal to $\frac{1}{2}\hbar$. Such *states of minimal uncertainty in position and momentum* will just be called *minimal states* or *minimal wave packets* in this section. Finding all minimal states is simplified by the following remarks:

a. Translating a wave function ψ over a distance a in space gives a new wave function $\psi_a(x) = \psi(x-a)$. Its probability density for measuring position is $\rho_a(x) = |\psi_a(x)|^2 = |\psi(x-a)|^2 = \rho(x-a)$, which gives a translated expectation value $(\overline{x})_a = \overline{x} + a$. Its standard deviation Δx clearly remains the same. The Fourier expression for the translated function ψ_a is

$$\psi_a(x) = \psi(x-a) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} \hat{\psi}(p) e^{\frac{i}{\hbar}p(x-a)} dp$$
$$= \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} \hat{\psi}_a(p) e^{\frac{i}{\hbar}px} dp,$$

with the new Fourier transform

$$\hat{\psi}_a(p) = e^{-\frac{i}{\hbar}pa} \hat{\psi}(p).$$

This is just multiplication of $\hat{\psi}(p)$ with a phase factor, which does not affect $\hat{\rho}(p) = |\hat{\psi}(p)|^2$, the probability density for the measurement of moment, and consequently leaves both the expectation value $\overline{p}$ and the standard deviation Δp unchanged. This means that translation in x carries minimal states into minimal states. Note that the above Fourier formula argument shows that translation in space of a wave function ψ over a distance a can be seen as the result of the action of the 1-parameter unitary group $U(a) = e^{-\frac{i}{\hbar}aP}$, or

$$\psi_a = e^{-\frac{i}{\hbar}aP} \psi.$$

b. A similar argument applies to a translation in momentum space, given in terms of the Fourier transform as $\hat{\psi}_b(p) = \hat{\psi}(p-b)$, for an arbitrary b in R^1. The mean value $\overline{p}$ changes into $\overline{p} + b$, but the standard deviation Δp remains the same. The wave function in x-space is multiplied by a phase factor,

$$\psi_b(x) = e^{\frac{i}{\hbar}bx} \psi(x),$$

so it is clear that neither $\overline{x}$ nor Δx changes. This means that translation in p also maps minimal states into minimal states. Note that these translations are the result of the action of a second 1-parameter group of unitary operators, n.l. the group $V(b) = e^{\frac{i}{\hbar}bQ}$, or

$$\psi_b = e^{\frac{i}{\hbar}bQ}\psi.$$

The remarks a. and b. together imply that it is sufficient to find the minimal states with $\overline{x} = 0$ and $\overline{p} = 0$; all others can be obtained from these by the action of the operators $U(a) = e^{-\frac{i}{\hbar}aP}$ and $V(b) = e^{\frac{i}{\hbar}bQ}$, for all possible real a and b.

The derivation of Heisenberg's uncertainty relation in Section 7.3 gives for a state ψ with $\Delta p = \Delta x = 0$ the relations

$$\hbar = |(\psi, [P, Q]\psi)| \leq 2|(P\psi, Q\psi)| \leq 2||P\psi||\,||Q\psi|| = 2\Delta p\,\Delta x.$$

For a minimal state, i.e. with $\Delta p\,\Delta x = \frac{1}{2}\hbar$, the Schwarz inequality in the middle becomes an equality. This is only possible if $P\psi = \lambda Q\psi$, for some complex number λ. One has on one hand $||P\psi|| = |\lambda|\,||O\psi||$, or $|\lambda| = \frac{\Delta p}{\Delta x}$, and on the other hand $\Delta p\,\Delta x = \frac{1}{2}\hbar = \frac{i}{2}(\psi, [P, Q]\psi) = \frac{i}{2}Im\,(P\psi, Q\psi) = (\Delta x)^2 Im\,\lambda$, which gives $Im\,\lambda = \frac{\Delta p}{\Delta x}$. Together this gives $\lambda = i\frac{\Delta p}{\Delta x}$. The minimal states with $\Delta p = \Delta x = 0$ are therefore normalized vectors ψ satisfying

$$P\psi = i\,\frac{\Delta p}{\Delta x}\,Q\psi,$$

i.e. solutions of the differential equation

$$\left(\frac{d}{dx} + \frac{1}{\hbar}\,\frac{\Delta p}{\Delta x}\,x\right)\psi(x) = 0.$$

The solutions of this equation are obtained by the substitution $y = x^{1/2}$, which leads to an even more elementary differential equation in y. One finds as general solution

$$\psi(x) = C\,e^{-\frac{\varrho}{2\hbar}x^2},$$

with the positive parameter $\varrho = \frac{\Delta p}{\Delta x}$. The constant C can be determined, up to an irrelevant phase factor, by the normalization condition $(\psi, \psi) = 1$. Using the well-known Gaussian integral $\int_{-\infty}^{+\infty} e^{-t^2}dt = \sqrt{\pi}$ one finds $C = \left(\frac{\varrho}{\pi\hbar}\right)^{1/4}$. With this we have a 1-parameter set of minimal states with $\Delta p = \Delta p = 0$. Their wave functions are

$$\psi_\varrho(x) = \left(\frac{\varrho}{\pi\hbar}\right)^{1/4}\,e^{-\frac{\varrho}{2\hbar}x^2},$$

with the positive parameter ϱ equal to the quotient $\frac{\Delta p}{\Delta x}$. The probability density for the measurement of position is

$$|\psi_\varrho(x)|^2 = \left(\frac{\varrho}{\pi\hbar}\right)^{\frac{1}{2}}\,e^{-\frac{\varrho}{\hbar}x^2} = \frac{1}{(2\pi)^{1/2}\Delta x}\,e^{-\frac{1}{2(\Delta x)^2}x^2},$$

a *normal* or *Gaussian* distribution centered at $x = 0$ and with standard deviation Δx. One can show that the Fourier transform of ψ_ϱ is

$$\hat{\psi}_\varrho(p) = \left(\frac{1}{\pi\hbar\varrho}\right)^{1/4}\,e^{-\frac{1}{2\varrho\hbar}x^2},$$

which leads to a probability density for the measurement of momentum

$$|\hat{\psi}_\varrho(p)|^2 = \left(\frac{1}{\pi\hbar\varrho}\right)^{1/2} e^{-\frac{1}{\varrho\hbar}p^2} = \frac{1}{(2\pi)^{1/2}\Delta p}\, e^{-\frac{1}{2(\Delta p)^2}p^2},$$

a Gaussian distribution centered at $p = 0$ and with standard deviation Δp.

The minimal states with arbitrary values for $\overline{p}$ and $\overline{x}$ are obtained from those with $\overline{p} = \overline{x} = 0$ by translations in position and momentum space. The result is a 3-parameter collection of wave functions

$$\psi_{\overline{p},\overline{x},\varrho}(x) = \left(\frac{\varrho}{\pi\hbar}\right)^{1/4} e^{\frac{i}{\hbar}\overline{p}(x-\overline{x})} e^{-\frac{\varrho}{2\hbar}(x-\overline{x})^2},$$

with Fourier transform

$$\hat{\psi}_{\overline{p},\overline{x},\varrho}(p) = \left(\frac{1}{\pi\hbar\varrho}\right)^{1/4} e^{-\frac{i}{\hbar}\overline{x}p}\, e^{-\frac{1}{2\hbar\varrho}(p-\overline{p})^2}.$$

The probability densities for position and momentum measurements are

$$|\psi_{\overline{p},\overline{x},\varrho}(x)|^2 = \left(\frac{\varrho}{\pi\hbar}\right)^{1/2} e^{-\frac{1}{\varrho\hbar}(x-\overline{x})^2} = \frac{1}{(2\pi)^{1/2}\Delta x}\, e^{-\frac{1}{2(\Delta x)^2}(x-\overline{x})^2}$$

$$|\hat{\psi}_{\overline{p}\overline{x},\varrho}(p)|^2 = \left(\frac{1}{\pi\hbar\varrho}\right)^{1/2} e^{-\frac{1}{\hbar\varrho}(p-\overline{p})^2} = \frac{1}{(2\pi)^{1/2}\Delta p}\, e^{-\frac{1}{2(\Delta p)^2}(p-\overline{p})^2},$$

again Gaussian distributions with standard deviations Δx and Δp, now centered at $x = \overline{x}$ and $p = \overline{p}$.

7.5. *Examples*

The numerical consequences of the uncertainty relation can be demonstrated in appropiately chosen concrete physical systems.

a. An example of a *microscopic* system:

The mass of an electron is roughly 9×10^{-31} kg. Assume that it moves with a velocity $v = 10^3$ m/s, so the momentum p is 9×10^{-28} kg.m/s. (We use KMS (kilogram - meter - second) units.) Suppose again an uncertainty in the momentum of 0.1 percent, so $\Delta p = 9 \times 10^{-31}$ kg.m/s. This gives for the uncertainty in the position a value $\Delta x = 4.5 \times 10^{-5}$ m. This may be a small lenght in the macroscopic world, but it is very large in the atomic contex, for instance in comparison with the size of the hydrogen atom, in a certain way defined by the radius of the inner electron orbit which is roughly 5×10^{-11} m. (With this 'orbit' we mean the space region in which the wave function of the electron in its state of lowest energy is appreciably different from 0. An orbit in the classical sense does not exist, as was discussed in 7.2.)

b. An example of a *macroscopic* system:

Think of a bullet with a size of a centimeter and mass of 10 grammes, moving with a velocity of 200 meters per second. (The velocity of sound in air at room temperature is 340 meters per second). The momentum $p = mv$ is 2 kg.m/s. Suppose that there a is an uncertainty in this momentum of $0,1$ percent, i.e. the standard deviation Δp is equal to 2×10^{-3} kg.m/s. Planck's constant $\hbar$ is 1.054×10^{-34} kg.m^2/s, so $\frac{1}{2}\hbar$ is roughly 5×10^{-35} kg.m^2/s. This gives the minimal uncertainty in the position of the bullet as $\Delta x = \frac{1}{2}\hbar/\Delta p = 2.5 \times 10^{-33}$ m, a value which is extremely small and would be totally unobservable in this context.

The last example illustrates an important general point in the application of quantum theory to physics. Quantum theory is considered to be valid for *all* physical phenomena. It is indispensable for understanding the world of atomic physics. However, in macroscopic physical situations its predictions can often not be distinguished experimentally from those of classical mechanics. In such cases the continued use of classical ideas is justified.

7.6. *The 3-dimensional case*

The basic formulas for the quantum mechanical description of a 3-dimensional particle were given in 7.1. In the subsequent sections we discussed the case of a particle in 1-dimensional space. This simplified our formulas, while nothing essential was lost. In this section we briefly review some of the remaining aspects of the 3-dimensional case and give – for the sake of completenesss – the 3-dimensional versions of the appropriate formulas.

The position operators Q_1, Q_2, Q_3 commute; they form a triple of *commensurable operators*, which means that they give a system of *stochastic variables* in the sense of ordinary probability theory: a normalized state vector ψ defines the *joint probability density*

$$\rho(x_1, x_2, x_3) = |\psi(x_1, x_2, x_3)|^2$$

for the three position variables x_1, x_2, x_3. The same is true for the three components of momentum, with a simultaneous probability density

$$\hat{\rho}(p_1, p_2, p_3) = |\hat{\psi}(p_1, p_2, p_3)|^2.$$

For this one needs the 3-dimensional Fourier transformation. The formulas for this transformation and its inverse are

$$\hat{\psi}(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{+\infty} \psi(\vec{x})\, e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{x}} d\vec{p}$$
$$\hat{\psi}(\vec{x}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{+\infty} \hat{\psi}(\vec{x})\, e^{\frac{i}{\hbar}\vec{p}\cdot\vec{x}} d\vec{x},$$

with the Plancherel formula

$$\int_{-\infty}^{+\infty} |\psi(\vec{x}|^2 d\vec{x} = \int_{-\infty}^{+\infty} |\hat{\psi}(\vec{p}|^2 d\vec{p}.$$

Each pair (P_j, Q_j), $j = 1, 2, 3$, consists of two *incommensurable* observables. There are no simultaneous probability distributions; instead we have, for $j = 1, 2, 3$, the *Heisenberg uncertainty relations*

$$\Delta p_j \, \Delta x_j \geq \frac{1}{2}\hbar.$$

The set of states of minimal uncertainty in position and momentum, states which satisfy

$$\Delta p_j \, \Delta x_j = \frac{1}{2}\hbar,$$

for $j = 1, 2, 3$, consists of all product wave functions

$$\psi_{\overline{p_1}, \overline{x_1}, \varrho_1}(x_1) \, \psi_{\overline{p_2}, \overline{x_2}, \varrho_2}(x_2) \, \psi_{\overline{p_3}, \overline{x_3}, \varrho_3}(x_3),$$

for abritrary expectation values $\overline{p_j}$, $\overline{x_j}$ and arbitrary positive values of the quotients $\varrho_j = \Delta p_j / \Delta x_j$, for $j = 1, 2, 3$.

8. TIME EVOLUTION OF WAVE FUNCTIONS

8.1. *Motion of a wave packet*

In the preceding chapter we discussed the quantum mechanical description of a free particle at a fixed time. In this section its time evolution will be studied. For simplicity we again consider first the case of a particle in 1-dimensional space. In general the time evolution of a state in quantum theory, from an initial time t_1 to a later time t_2, is given by a 1-parameter group of unitary operators $U(t) = e^{-\frac{i}{\hbar}tH}$ as

$$\psi(t_2) = e^{-\frac{i}{\hbar}(t_2 - t_1)H} \psi(t_1).$$

This means that state vectors, as functions of time, should be solutions of the 'abstract' Schrödinger equation

$$\frac{d}{dt}\psi(t) = -\frac{i}{\hbar} H \psi(t),$$

which in the special case of a 1-dimensional particle becomes the 'concrete' Schrödinger equation

$$\frac{\partial}{\partial t}\psi(x, t) = -\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x, t),$$

with the state vector now the 'wave function' $\psi(x, t)$. This differential equation is of course only defined for wave functions in the domain of the (unbounded) operator H, for instance for functions that are in $\mathcal{S}(R)$ as functions of x.

A state of a particle may have a wave function which is different from 0 only in a small region of space and which has a Fourier transform concentrated in a small momentum interval. It will have small standard deviations Δx and Δp from the average values $\overline{x}$ and $\overline{p}$ of position and momentum. Such a state can be called 'quasi classical'. It resembles a classical particle with well-defined position $x = \overline{x}$ and momentum $p = \overline{p}$. This is of course only approximately so, because Heisenberg's uncertainty relation tells us that Δx and Δp cannot be both arbitrary small; the product $\Delta p\,\Delta x$ has $\frac{1}{2}\hbar$ as lower limit. The minimal uncertainty states discussed in Section 7.4 are the best one can have in this respect.

In fact, even the time evolution of an *arbitrary* wave function has classical aspects. This is in particular true for the time dependence of the average values of position and momentum. One has for the expectation value of position

$$\begin{aligned}\frac{d\overline{x}(t)}{dt} &= \frac{d}{dt}(\psi(t), Q\psi(t)) = \\ &= (-\frac{i}{\hbar}H\psi(t), Q\psi(t)) + (\psi(t), -\frac{i}{\hbar}QH\psi(t)) = \\ &= \frac{i}{\hbar}(\psi(t), [H,Q]\psi(t)).\end{aligned}$$

Using the basic commutation relation $[P,Q] = \frac{i}{\hbar}1$, together with the fact that Q commutes with $V(Q)$, one finds

$$[H,Q] = [\frac{P^2}{2m} + V(Q), Q] = \frac{1}{2m}[P^2, Q] = \frac{\hbar}{im}P,$$

which gives finally

$$\frac{d\overline{x}(t)}{dt} = \frac{1}{m}(\psi(t), P\psi(t)) = \frac{1}{m}\overline{p}(t).$$

For $\overline{p}(t)$ one obtains in a similar manner

$$\frac{d\overline{p}(t)}{dt} = \frac{i}{\hbar}(\psi(t), [H,P]\psi(t)) = -(\psi(t), \frac{dV}{dQ}\psi(t)) = -\overline{\left[\frac{dV}{dQ}\right]},$$

in which $\frac{dV}{dQ}$ is the operator which multiplies a wave function with the function $\frac{dV(x)}{dx}$. The pair of first order equations

$$m\frac{d\overline{x}}{dt} = \overline{p}, \qquad \frac{d\overline{p}}{dt} = -\overline{\left[\frac{dV}{dx}\right]}$$

can be combined to single second order equation

$$m\frac{d^2\overline{x}}{dt^2} = -\overline{\left[\frac{dV}{dx}\right]},$$

which brings out even more clearly the analogy with the classical equations of motion. The time evolution of a wave function which is quasi-classical at an initial time will resemble in first approximation the motion of a classical particle with position $x = \overline{x}(t)$ and momentum $p = \overline{p}(t)$, at least for a certain initial period of time, because the wave packet will eventually spread out, and its quasi-classical character will then be lost.

8.2. *The free particle*

In this simple case the Schrödinger equation can be explicitly solved, i.e. the wave function at time t_2 can be expressed in the wave function at an earlier time t_1. For this one can use the Fourier transformation. We demonstrate this for the 1-dimensional case. Let the initial state at $t = t_1$ be given by the function $\psi(x, t_1)$, a function in which we assume to be in $\mathcal{S}(R^1)$ in the variable x. Its Fourier transform is

$$\hat{\psi}(p, t_1) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \psi(x, t_1)\, e^{-\frac{i}{\hbar}px}\, dx.$$

The Hamiltonian is a simple expression in the momentum operator P, so the action of the unitary evolution operator $e^{-\frac{i}{\hbar}tH}$ in terms of the Fourier transform is also simple and gives

$$\hat{\psi}(p, t_2) = e^{-\frac{i}{\hbar}(t_2 - t_1)\frac{p^2}{2m}}\, \hat{\psi}(p, t_1).$$

By using the inverse Fourier transformation finally one obtains the solution at $t = t_2$ as

$$\begin{aligned}
\psi(x, t_2) &= \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \hat{\psi}(p, t_2)\, e^{\frac{i}{\hbar}px}\, dp = \\
&= \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \hat{\psi}(p, t_1)\, e^{-\frac{i}{\hbar}(t_2 - t_1)\frac{p^2}{2m}}\, e^{\frac{i}{\hbar}px}\, dp = \\
&= \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp \int_{\infty}^{+\infty} dx'\, \psi(x', t_1) \left[e^{-\frac{i}{\hbar}p(x - x')}\, e^{-\frac{i}{\hbar}(t_2 - t_1)\frac{p^2}{2m}} \right].
\end{aligned}$$

This is a well-defined repeated integral which gives $\psi(x, t_2)$ as a function in $\mathcal{S}(R^1)$ for all $t_2 \geq t_1$. It is sometimes written as

$$\psi(x, t_2) = \int_{-\infty}^{+\infty} G(x, t_2; x', t_1)\psi(x', t_1)dx',$$

with

$$G(x, t_2; x', t_1) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{-\frac{i}{\hbar}p(x' - x)}\, e^{-\frac{i}{\hbar}(t_2 - t_1)\frac{p^2}{2m}}\, dp,$$

the *Green's function* or *evolution kernel* of the differential equation. This involves an interchange in the order of integrations which is strictly speaking not allowed and leads to an integral for G which is singular; the formula, which is very useful, can however be made rigorous by interpreting G as a *distribution* or *generalized function* in the sense of Laurent Schwartz, instead of a as function in the ordinary sense.

The analogous formula for the 3-dimensional case can be written down immediately as

$$\psi(\vec{x},t_2) = \frac{1}{(2\pi\hbar)^3}\int_{-\infty}^{+\infty} d\vec{p}\int_{-\infty}^{+\infty} d\vec{x}'\,\psi(\vec{x}',t_1)\left[e^{-\frac{i}{\hbar}\vec{p}\cdot(\vec{x}-\vec{x}')}\,e^{-\frac{i}{\hbar}(t_2-t_1)\frac{\vec{p}^2}{2m}}\right],$$

with the heuristic reformulation

$$\psi(\vec{x},t_2) = \int_{-\infty}^{+\infty} G(\vec{x},t_2;\vec{x}',t_1)\psi(\vec{x}',t_1)d\vec{x}',$$

with

$$G(\vec{x},t_2;\vec{x}',t_1) = \frac{1}{(2\pi\hbar)3}\int_{-\infty}^{+\infty} e^{-\frac{i}{\hbar}\vec{p}\cdot(\vec{x}'-\vec{x})}\,e^{-\frac{i}{\hbar}(t_2-t_1)\frac{\vec{p}^2}{2m}}\,d\vec{p}.$$

Note that the equations for the time evolution of average position and momentum are now precisely the classical equation for position and momentum, because $V(x) = 0$.

8.3. *A particle in a box*

Consider the quantum mechanical description of a 1-dimensional particle moving freely in a box of length a. The Hilbert space is $\mathcal{H} = L^2([0,a],dx)$. The position operator $Q : \psi(x) \mapsto x\psi(x)$ is now defined on all vectors in $\mathcal{H}$; it is a bounded operator with norm $||Q|| = a$. The momentum operator P, the differential operator $\frac{\hbar}{i}\frac{d}{dx}$, is well-defined on the linear subspace $\mathcal{D}^{(1)}$ of all differentiable functions ψ in $L^2([0,a],dx)$, with the derivative $\psi^{(1)}(x) = \frac{d}{dx}\psi(x)$ again in $L^2([0,a],dx)$, but it is clearly *not* symmetric on $\mathcal{D}^{(1)}$, because the condition for symmetry on a domain, $(\psi_1, P\psi_2) = (P\psi_1,\psi_2)$, for all pairs of vectors ψ_1, ψ_2 from that domain, implies the boundary condition

$$\overline{\psi_1(a)}\psi_2(a) = \overline{\psi_1(0)}\psi_2(0).$$

This leads to the possible domains of symmetry

$$\mathcal{D}^{(1)}_\alpha := \{\psi \in \mathcal{D}^{(1)} \,|\, \psi(a) = e^{i\alpha}\psi(0)\},$$

for each $\alpha \in [0,2\pi)$. The restriction of P to each $\mathcal{D}^{(1)}_\alpha$ gives a selfadjoint operator P_α. One checks that is has a purely discrete spectrum, with eigenvalues

$$p_n^\alpha = \frac{\hbar}{a}(\alpha + 2\pi),$$

and a corresponding orthonormal basis of eigenfunctions

$$\phi_n^\alpha(x) = \frac{1}{\sqrt{a}}e^{\frac{i}{\hbar}p_n^\alpha x},$$

for $n = 0, \pm 1, \pm 2, \ldots$. Note that P defined on the domain consisting of all functions ψ which vanish in $x = 0$ and $x = a$ would be too small. The restriction of P to this domain would be symmetric but *not* selfadjoint. This gives us a simple example of a symmetric operator which is not selfadjoint, but has (an infinite number of) selfadjoint extensions.

For the discussion of the physical interpretation of this situation we consider the possibilities for the energy operator, restrictions of the differential operator $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ to suitable domains. Starting from the P^α we find selfadjoint operators $H_\alpha = \frac{(P_\alpha)^2}{2m}$ defined on the domains $\mathcal{D}^{(2)}_\alpha$ consisting of the functions ψ in $L^2([0,a],dx)$ that have second derivatives which are again in $L^2([0,a],dx)$ and satisfy moreover the boundary conditions $\psi(a) = e^{i\alpha}\psi(0)$ and $\psi^{(1)}(a) = e^{i\alpha}\psi^{(1)}(0)$. They have the same orthonormal systems $\{\phi^\alpha_n\}_n$ of eigenvectors as the P_α. The energy eigenvalues are

$$E^\alpha_n = \frac{(p^\alpha_n)^2}{2m} = \frac{\hbar^2}{2ma^2}(\alpha + 2\pi n)^2,$$

for $n = 0, \pm 1, \pm 2, \ldots$. There is an additional selfadjoint energy operator H^0, n.l. the restriction of $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ to the space $\mathcal{D}^{(2),0}$ of all ψ in $L^2([0,a],dx)$, having second derivative $\psi^{(2)}$ in $L^2([0,a],dx)$, and with boundary condition $\psi(a) = \psi(0) = 0$. H^0 has an orthonormal basis of eigenfunctions

$$\psi^0_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right),$$

with eigenvalues

$$E^0_n = \frac{\hbar^2}{2m}\left(\frac{\pi n}{a}\right)^2,$$

for $n = 1, 2, \ldots$.

Taking H_α for $\alpha = 0$ as energy operator means that when the particle reaches one endpoint of the interval $[0,a]$ it immediately reappears at the other endpoint. The motion is periodic and the points $x = 0$ and $x = a$ can be identified; the particle moves on a circle. For $\alpha \neq 0$ the particle passes a barrier at $x = 0 = a$, at which it picks up a phase, as is usual in the transmission of waves. The case with energy operator H^0 describes a particle moving in box in the ordinary sense; it is reflected at the walls of the box and the sign of its velocity changes instantaneously. Note that in this case no proper selfadjoint momentum operator can be defined. This is because we have in a certain sense a singular limit, even in the classical case, with an infinite force at the wall driving the particle back, a limit of a finite repulsive force over a short interval near the wall. In any case, this quantum mechanical model of a particle in a box illustrates in a simple way the physical meaning of different selfadjoint extensions of a symmetric operator.

8.4. *The tunnel effect*

Consider a 1-dimensional particle moving in a potential $V(x)$ which vanishes for all real x, except in two intervals, $[-(a+d),-a]$ and $[a,a+d]$, on which one has $V(x) = E_0$, with E_0, a and d positive constants and d much smaller than a, i.e. a potential $V(x)$ which consists of two walls of hight E_0 and thickness d. In the classical description a particle with kinetic energy $\frac{p^2}{2m} < E_0$ cannot pass the potential walls. If it is inside the interval $[-a, a]$ it will remain inside, when it is outside it will remain outside. A particle with kinetic energy larger than E_0 can move freely along the real line; it passes over the walls, its velocity only momentarily perturbed by the potential. The quantum situation is different. Suppose that we are certain the particle is at a given time t_1 inside the interval $[-a, a]$. This means that the support of its wavefunction $\psi(x, t_1)$ is contained in $[-a, a]$. One can show that the time evolution is such that the wave function will spread instantaneously; at each later time t_2 it will be nonvanishing at arbitrary points x outside $[-a, a]$, i.e. there is a nonzero probability of finding the particle outside the walls. Conversely, if we know the particle to be outside the walls at an initial time, the chance that we may find it inside at a later time is nonzero. The reason for this is that a strictly localized wave function, i.e. a wave function with compact support, contains all possible energies in its decomposition with respect to the eigenfunctions of the energy operator. A wave function of which the components are cut off below a certain energy, say the energy E_0 of the potential walls, is not localized. The corresponding particle can be found inside as well outside a given interval. This phenomenon that a quantum particle cannot be contained in a region for an indefinite lenght of time and it can always pass through potential walls is called the *tunnel effect*.

9. THE HARMONIC OSCILLATOR

9.1. *Introduction*

The great success of quantum mechanics between the years 1924 and 1927 was its ability to give a qualitatively *and* quantitatively satisfactory description of atomic spectra. By this it established itself as *the* theoretical model for submicroscopic physics. A simple but typical example in this context was the *hydrogen atom*. An even simpler quantum mechanical model is that of the *harmonic oscillator*, which will be treated in this chapter. Like the model for the hydrogen atom it can be explicitly solved by elementary means, i.e. the formulas for its energy levels and energy eigenstates can be found in closed form. The differences between the quantum version and the classical version of the harmonic oscillator are very characteristic for the differences between quantum and classical mechanics in general. This makes it excellent for pedagogical purposes. It is also of great practical use, because it gives a good first approximation to many more complicated and more realistic physical systems.

9.2. *The classical harmonic oscillator*

A well-known system in elementary classical physics is that of a particle attached to one end of a metal spring. As long as the spring is not stretched too much, the particle will be driven back, in the direction of the point where the string is fixed, with a force proportional to distance to this point. This situation is idealized in the mechanical model of a *classical harmonic oscillator*: a point particle of mass m moving in R^1 under the influence of a force $F = -kx$, with k the 'spring constant', implying that Newton's equation $F = ma = m\frac{d^2x}{dt^2}$ is

$$\frac{d^2}{dt^2}x(t) + \frac{k}{m}x(t) = 0.$$

Note that the force on the particle comes from the potential $V(x) = \frac{1}{2}kx^2$. The general solution, for arbitrary initial position $x(0)$ and velocity $\dot{x}(0) = \left(\frac{dx}{dt}\right)_{t=0}$ is easily found to be

$$x(t) = \dot{x}(0)\omega^{-1}\sin\omega t + x(0)\cos\omega t,$$

with ω defined as $\sqrt{k/m}$. The motion is *periodic*; the particle oscillates around the origin $x = 0$ with 'circle frequency' ω, a characteristic constant of the system. Kinetic energy is constantly transformed into potential energy and vice versa, but the total energy remains the same. This energy depends depends on the initial values of the motion or on the maximum amplitude $|x_{max}| = (2E/m\omega)^{1/2}$. The possible energy values of the system form a *continuum*; E can have an arbitrary nonnegative value, with for $E = 0$ the particle at rest in the origin $x = 0$, as a limiting case, the only *stationary* state.

The system can be put in Hamiltonian form, with canonical coordinates p and x, with a Hamiltonian function

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

and Hamiltonian equations

$$\frac{dx}{dt} = \frac{p}{m}, \quad \frac{dp}{dt} = -m\omega^2x,$$

together equivalent to the second order equation

$$\frac{d^2x}{dt^2} + \omega^2x = 0.$$

9.3. *The quantum oscillator*

As was already indicated in the introductory section, many important systems in physics can in first approximation be desribed by a harmonic oscilator or by systems of harmonic oscillators. The basic reason for this is that a general potential $V(x)$ with a minimum in $x = 0$ can be expanded around $x = 0$ as

$$V(x) = V(0) + V'(0)x + \frac{1}{2}V''(0)x^2 + \ldots$$

with V', V'' the first, respectively the second derivative of V. The first term is a constant and does therefore not affect the dynamics, the second term vanishes because V has a minimum in $x = 0$, so the first nonzero term is a term quadratic in x, i.e. a harmonic potential. A similar argument can of course be used when V has a minimum in an arbitrary $x = x_0$. The role of the harmonic oscillator model, as a simple starting point for the description of situations in which particles are bound to each other by strong forces, is even more important in quantum physics than in classical physics. This gives another justification for the detailed discussion of the quantum mechanical 1-dimensional harmonic oscillator in this chapter.

The state space $\mathcal{H}$ for the quantum mechanical oscillator is the Hilbert space $L^2(R^1, dx)$, its Hamiltonian operator

$$H = \frac{1}{2m}P^2 + \frac{1}{2}m\omega^2 Q^2.$$

This operator can be shown to be essentially selfadjoint on a suitable domain of smooth functions, e.g. $\mathcal{S}(R^1)$.

Remark: The 'prescription' by which the quantum Hamiltonian is obtained from the classical Hamiltonian is here still unambiguous, even though P does not commute with Q. There would be a problem if the classical Hamiltonian function would for instance contain a term p^3q^3. The operator P^3Q^3 is not hermitian symmetric, so is not admissable. Classically one has

$$p^3q^3 = \frac{1}{2}\left((pq)^3 + (qp)^3\right) = \frac{1}{2}\left(p^3q^3 + q^3p^3\right).$$

Both the combinations $\frac{1}{2}\left((PQ)^3 + (QP)^3\right)$ and $\frac{1}{2}\left(P^3Q^3 + Q^3P^3\right)$ are hermitian symmetric. They are however not the same, so it is not clear which one should be chosen as quantum observable. It also not immediately obvious whether both operators are essentially selfadjoint.

Studying a quantum system the central task is to find the eigenvalues and eigenvectors, or more rigorously the spectral resolution, of the Hamiltonian – usually the energy operator – of the system. Only in a few cases this problem can be solved exactly. The hydrogen atom is one of these cases; the harmonic oscillator another.

Solving the eigenvalue / eigenvector problem $H\psi = E\psi$ for the harmonic oscillator means solving the differential equation

$$\left(-\frac{\hbar}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\,\omega^2x^2\right)\psi(x) = E\psi(x),$$

for suitable, i.e. square integrable functions ψ. This problem was solved first by a straightforward application of a general method for studying solutions of second order differential equations of a certain type; later a more algebraic method was found which uses in an ingenious way the quantum mechanical commutation relations. The first method will be briefly scketched here; the second will be treated in more detail in the next section.

Choose a new dimensionless variable

$$u = \sqrt{\frac{m\omega}{\hbar}}\, x,$$

use instead of E the dimensionless quantity

$$\varepsilon = \frac{E}{\hbar\omega} - \frac{1}{2},$$

and define

$$f(u) = e^{\frac{m\omega}{2\hbar}x^2}\psi(\sqrt{\frac{\hbar}{m\omega}}\, x).$$

This leads to a differential equation for f as a function of u, which is equivalent to the original equation and which is

$$\frac{d^2 f}{du^2} - 2u\frac{df}{du} + 2\varepsilon f = 0.$$

Expand the function f into a power series $f(u) = a_0 + a_1 u + a_2 u^2 + \ldots$. Substitution of this series in the differential equation gives a simple recursion relation for the coefficients,

$$a_{n+2} = \frac{2(n-\varepsilon)}{(n+1)(n+2)} a_n,$$

for $n = 0, 1, 2, \ldots$. Given a_0, this relation determines the coefficients for even n; given a_1 one obtains those for odd n. The first case gives an even function of the variable u, the second case an odd function. Note that substitution of the power series for ψ in the original equation would not give a useful recursion relation; in fact the nontrivial part of this procedure is to find a transformation to a new equation for which the recursion relation is simple and determines the coefficients. One next studies the asymptotic behaviour of the coefficients a_n for $n \to \infty$ and finds that there are two possibilities. The first is that series of coefficients $\{a_n\}$ is infinite. In that case the function $f(u)$ behaves as ce^{u^2} for $u \to \pm\infty$. This gives for the original function ψ a total exponential factor $e^{\frac{1}{2}u^2}$. Such a solution ψ is not square integrable and is therefore not acceptable as wave function. We are left with the second possibility: the series breaks off and $f(u)$ is a polynomial. This happens precisely for integer values of ε. For $\varepsilon = n_0$ we clearly have that all a_n are nonzero for $n \leq n_0$ and vanish for $n \geq n_0 + 2$. These results together give the solution of the original eigenvalue / eigenvector problem $H\psi = E\psi$ as

$$E_n = \hbar\omega(n + 1/2)$$

for the eigenvalues, and for the eigenfunctions

$$\psi_n(x) = N_n H_n(\sqrt{m\omega/\hbar}\; x)\, e^{-\frac{m\omega}{2\hbar}x^2},$$

for $n = 0, 1, 2, \ldots$. The N_n are normalization constants equal to

$$N_n = \frac{1}{2^{n/2}(n!)^{1/2}}\left(\frac{m\omega}{\hbar\pi}\right)^{1/4}.$$

The $H_n(\cdot)$ are the *Hermite polynomials*, well-known from other areas of applied mathematics. The first five Hermite polynomials are

$$\begin{aligned} H_0(u) &= 1 \\ H_1(u) &= 2u \\ H_2(u) &= -2 + 4u^2 \\ H_3(u) &= -12u + 8u^3 \\ H_4(u) &= 12 - 48u^2 + 16u^4. \end{aligned}$$

One finally shows that this is the complete solution: the spectrum of H is purely discrete and the eigenfunctions ψ_n form an orthonormal basis in the Hilbert space $\mathcal{H}$.

These results should be compared with what we know about the classical situation: A classical oscillator has a *continuum* of possible energy values, the interval $[0, +\infty)$ and a *single* stationary state, the situation in which the particle has energy 0 and is at rest in the origin. The possible energy values of a quantum oscillator are *discrete*, $E_n = \hbar\omega(n + 1/2)$, for $n = 0, 1, \ldots$; there is an *infinite sequence* of stationary states, the corresponding eigenstates ψ_n, in which the 'groundstate' ψ_0, the state with the lowest energy, has a nonzero 'rest energy' $\frac{1}{2}\hbar\omega$.

9.4. *Lowering and raising operators*

The starting point of the second method is a transformation of the operators P and Q into a pair of non-selfadjoint operators A and A^*. Define

$$A = \alpha P + i\beta Q, \qquad A^* = \alpha P - i\beta Q.$$

By choosing the real parameters α and β as

$$\alpha = (2\hbar)^{-\frac{1}{2}}(m\omega)^{-\frac{1}{2}}, \qquad \beta = -(2\hbar)^{-\frac{1}{2}}(m\omega)^{\frac{1}{2}}$$

and using the basic commutation relation

$$[P, Q] = \frac{\hbar}{i}\,1$$

one finds for the new operators the commutation relation

$$[A, A^*] = 1$$

and for the Hamiltonian operator H the expression

$$H = \hbar\omega(A^*A + 1/2).$$

In all this we use $\mathcal{S}(R^1)$ as common invariant domain of definition for the operators. Denote A^*A as N. The operators N and H have the same eigenvectors; eigenvalues ε of N correspond with eigenvalues E of H through the relation

$E = \hbar\omega(\varepsilon + 1/2)$. We therefore study the slightly more convenient eigenvalue / eigenvector problem

$$N\psi = \varepsilon\psi.$$

The solution of this problem is obtained in a procedure consisting of the following steps:

a. From the basic commutation relation $[A, A^*] = 1$ one easily derives the relations

$$[N, A] = -A, \qquad [N, A^*] = A^*.$$

(For example: $[N, A] = A^*AA - AA^*A = -[A, A^*]A = -A$).

b. These commutation relations are used to prove a lemma, which is the principal ingredient of the procedure:

Lemma: If ψ is an eigenvector of N with eigenvalue ε, then either $A\psi = 0$ or the vector $A\psi$ is an eigenvector of N with eigenvalue $\varepsilon - 1$. At the same time either $A^*\psi = 0$ or the vector $A^*\psi$ is an eigenvector of N with eigenvalue $\varepsilon + 1$.

Proof: $N(A\psi) = [N, A]\psi + AN\psi = -A\psi + \varepsilon A\psi = (\varepsilon - 1)(A\psi)$, which states that $A\psi$ is an eigenvector of N, with eigenvalue $\varepsilon - 1$, unless $A\psi = 0$. Similarly one has $N(A^*\psi) = [N, A^*]\psi + A^*N\psi = A^*\psi + \varepsilon A^*\psi = (\varepsilon + 1)(A^*\psi)$.

Remark: Because of these properties A is called a *lowering operator* and A^* a *raising operator*. Systems of such lowering and raising operators $A_1, A_2, \ldots$ and $A_1^*, A_2^*, \ldots$, with commutation relations

$$[A_j, A_k^*] = \delta_{jk}1, \qquad [A_j, A_k] = [A_j^*, A_k^*] = 0,$$

are important in other areas of physics. In elementary particle physics such operators are called *annihilation* and *creation operators*.

c. Eigenvalues of N are necessarily nonnegative. Let ε be an eigenvalue, with ψ the corrresponding eigenvector. One has

$$0 \leq (A\psi, A\psi) = (\psi, A^*A\psi) = (\psi, N\psi) = \varepsilon(\psi, \psi).$$

Because $(\psi, \psi) > 0$, ε must be *nonnegative*.

d. Suppose there is an eigenvector ψ with eigenvalue ε. Repeated action of A on ψ will give a sequence of new eigenvectors $A\psi, A^2\psi, \ldots$ with eigenvalues $\varepsilon - 1, \varepsilon - 2, \ldots$. These eigenvalues cannot become negative, so this sequence has to break off. This means that that there is a vector $\psi_0 = 0$ and a nonegative real number ε_0, such that $N\psi_0 = \varepsilon_0\psi_0$ and $A\psi_0 = 0$. This implies $0 = (A\psi_0, A\psi_0) = (\psi_0, N\psi_0) = \varepsilon_0(\psi_0, \psi_0)$. Because $(\psi_0, \psi_0) > 0$ this gives $\varepsilon_0 = 0$. The result of this is that the existence of an eigenvector ψ with eigenvalue ε entails the existence of an eigenvector ψ_0 with a *lowest* eigenvalue $\varepsilon_0 = 0$. Starting from this ψ_0 we can apply the operator A^*, and obtain a sequence of eigenvectors $A^*\psi_0, (A^*)^2\psi_0, \ldots$, with eigenvalues $1, 2, \ldots$. Suppose that for a given n from $[0, 1, 2, \ldots]$ the vector $(A^*)^{n+1}\psi_0 = 0$, while $(A^*)^n \neq 0$. Then

$$\begin{aligned} &((A^*)^{n+1}\psi_0, (A^*)^{n+1}\psi_0) = ((A^*)^n\psi_0, AA^*(A^*)^n\psi) = \\ &= ((A^*)^n\psi_0, (N+1)(A^*)^n\psi_0) = (n+1)((A^*)^n\psi_0, (A^*)^n\psi_0) \neq 0. \end{aligned}$$

This means that the upward sequence $\psi_0, A^*\psi_0, (A^*)^2\psi_0, \ldots$ does *not* break off. Note that the action of A and A^* leaves this sequence invariant, up to real factors: $A((A^*)^n\psi_0) = (AA^*)((A^*)^{n-1}\psi_0) = (1+N)((A^*)^{n-1}\psi_0) = (n+1)(A^*)^{n-1}\psi_0$ and $A^*((A^*)^n\psi_0) = (A^*)^{n+1}\psi_0$. The vectors $(A^*)^n\psi$ can be normalized by using the above formula. to normalize the. One has

$$||(A^*)^{n+1}\psi_0||^2 = ((A^*)^{n+1}\psi_0, (A^*)^{n+1}\psi_0) = (n+1)((A^*)^n\psi_0, (A^*)^n\psi_0) = \\ = (n+1)\,||(A^*)^n\psi_0||^2 = \ldots = (n+1)!\,||\psi_0||^2.$$

We choose $(\psi_O, \psi_0) = 1$ and obtain then an orthonormal sequence of eigenvectors $\psi_0, \psi_1, \ldots$, with ψ_n defined as

$$\psi_n = \frac{1}{\sqrt{n!}}\,(A^*)^n\psi_0.$$

e. Our result sofar is that the eigenvectors of N, in the domain $\mathcal{S}(R^1)$, occur in infinite orthonormal sequences $\psi_0, \psi_1, \psi_2, \ldots$, with corresponding sequences of eigenvalues $\varepsilon = 0, 1, 2, \ldots$. The number of such sequences depends on the number of (linear independent) 'ground states' ψ_0. To find the possible vectors ψ_0 one must leave the purely algebraic context and return to the the explicit Hilbert space picture. A state ψ_0 with lowest eigenvalue $\varepsilon_0 = 0$ satisfies $A\psi_0 = 0$, i.e. is a solution of the equation $(\alpha P + i\beta)\psi_0 = 0$, or more explicitly,

$$\frac{d}{dx}\psi_0(x) = \frac{\beta}{\alpha\hbar}x\psi_0(x).$$

This is an elementary differential equation, which has the general solution

$$\psi_0(x) = c\,e^{\frac{\beta}{2\alpha\hbar}x^2},$$

with c a constant. Substitution of the expressions for α and β gives

$$\psi_0(x) = c\,e^{-\frac{m\omega}{2\hbar}x^2}.$$

The standard Gaussian integral $\int_{-\infty}^{+\infty} e^{-y^2}dy = \pi^{1/2}$ is used to normalize ψ_0, which gives for the constant c the condition $|c|^2 = (m\omega/\hbar\pi)^{1/2}$. With the obvious choice for c one obtains finally the single 'ground state' eigenfunction

$$\psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}.$$

From this the other eigenfunctions ψ_n are obtained as

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\,((A^*)^n\psi_0)(x).$$

One can show, using explicit Hilbert space properties, that the system $\{\psi_n\}$ forms an orthonormal basis for $\mathcal{H} = L^2(R^1, dx)$. This shows that the ψ_n, with their eigenvalues $\varepsilon = n$, give a complete (discrete) spectral resolution for the operator N and therefore for the operator $H = \hbar\omega(N + 1/2)$, with eigenvalues $E_n = \hbar\omega(n + 1/2)$. One can of course verify that the ψ_n here are the same as the ones found in the preceding section.

9.5. *Time evolution*

The quantum oscillator has an infinite sequence of stationary states, the energy eigenfunctions $\psi_0, \psi_1, \ldots$, for which the predictions of the results of measurements of arbitrary observables are constant in time. (Note however that an *actual* measurement would instantly transform the stationary state into an in general nonstationary state, in the case of a measurement of position with a wave function concentrated around the observed position value). In Section 8.1. we derived equations for the time evolution of the mean values of position and momentum for a general wave packet, which strongly resemble the classical equations. For the harmonic oscillator these *are* the classical equations: because of $\overline{\frac{dV}{dx}} = \overline{\frac{d}{dx}(\frac{1}{2}m\omega^2)x^2} = m\omega^2\overline{x}$ one obtains

$$\begin{aligned} m\frac{d}{dt}\overline{x}(t) &= \overline{p}(t) \\ \frac{d}{dt}\overline{p}(t) &= -\, m\omega^2\overline{x}(t). \end{aligned}$$

This implies that all the stationary states ψ_n have $\overline{x} = 0$ and $\overline{p} = 0$, just like the single stationary state $x = 0$, $p = 0$ for the classical oscillator, but at the same time with $\Delta x \neq 0$ and $\Delta x \neq 0$. The ground state ψ_0 is a *minimal uncertainty state*, as will be shown in the next section. A general state ψ can be expanded as $\psi = \sum_{n=0}^{\infty} c_n\psi$; its time evolution is therefore given by the formula

$$\psi(t) = \sum_{n=0}^{\infty} e^{-i\omega(n+1/2)t} c_n(0)\psi_n.$$

The time evolution is particularly interesting for the so called *coherent states*, a class of minimal uncertainty states which emerge here quite naturally by using the operators A and A^*. This will be discussed in the next section.

9.6. *Coherent states*

The ground state ψ is a solution of the equation $A\psi = 0$, i.e. it is an eigenvector of the operator A with eigenvalue 0; and as such it is unique up to scalar factor. Has A has other eigenvectors? The eigenvalue / eigenvector problem for A is an unusual one, because A is not symmetric or selfadjoint. It has nevertheless a fairly simple solution which is moreover of physical interest. To find this solution one needs the commutation relation $[A, (A^*)^n] = n(A^*)^{n-1}$ which is obtained from the basic relation $[A, A^*] = 1$ by induction. Expansion of the left-hand side of the equation $A\phi_\lambda = \lambda\phi_\lambda$ with respect to the orthonormal basis $\psi_0, \psi_1, \ldots$ gives

$$A\phi_\lambda = A\left(\sum_{n=0}^{\infty} c_n\psi_n\right) = \sum_{n=0}^{\infty} \frac{c_n}{\sqrt{n!}} A(A^*)^n\psi_0 =$$

$$= \sum_{n=0}^{\infty} \frac{c_n}{\sqrt{n!}} \left([A, (A^*)^n] + (A^*)^n A \right) \psi_0 =$$

$$= \sum_{n=0}^{\infty} \frac{c_n \sqrt{n}}{\sqrt{(n-1)!}} (A^*)^{n-1} \psi_0 =$$

$$= \sum_{n=1}^{\infty} c_n \sqrt{n}\, \psi_{n-1} = \sum_{n=0}^{\infty} c_{n+1} \sqrt{n+1}\, \psi_n .$$

Note that this is only well-defined if the coefficients $c_{n+1}\sqrt{n+1}$ are such that

$$\sum_{n=0}^{\infty} |c_n|^2 \frac{|\lambda|^{2n}}{n!} < \infty.$$

Expansion of the right-hand side gives

$$\lambda \phi_\lambda = \sum_{n=0}^{\infty} \lambda c_n \, \psi_n .$$

By comparing the two expansions one obtains the simple recursion relation $c_{n+1}\sqrt{n+1} = \lambda c_n$, which, after choosing $c_0 = 1$, gives $c_n = \lambda^n / \sqrt{n!}$, for $n = 0, 1, \ldots$. The series of coefficients $\lambda^n/\sqrt{n!}$ is l_2-summable, so the vector ϕ_λ is well-defined. One has

$$||\phi_\lambda||^2 = \sum_{n=0}^{\infty} \frac{|\lambda|^{2n}}{n!} = e^{|\lambda|^2},$$

and similarly, for two different complex numbers λ_1 and λ_2,

$$(\phi_{\lambda_1}, \phi_{\lambda_2}) = \sum_{n=0}^{\infty} \frac{(\overline{\lambda_1} \lambda_2)^n}{n!} = e^{\overline{\lambda_1}\lambda_2}.$$

The vector ϕ_λ can be written as

$$\phi_\lambda = \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} \psi_n = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} (A^*)^n \psi_0 = e^{\lambda A^*} \psi_0,$$

a very appealing and convenient expression, although one should realize that this does *not* mean that the operator-valued exponential function $e^{\lambda A^*}$ has in itself a good mathematical meaning, but only that the special sequence of vectors

$$\psi_0 + A^* \psi_0 + \frac{1}{2!} (A^*)^2 \psi_0 + \frac{1}{3!} (A^*)^3 \psi_0 + \ldots$$

is convergent.

In this manner we have found a complete solution of the rather unusual eigenvalue / eigenvector problem $A\phi_\lambda = \lambda \phi_\lambda$: for a each complex number λ there is a vector

$$\phi_\lambda = \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} \psi_n = e^{\lambda A^*} \psi_0 .$$

The vectors ϕ_λ are normalizable, with norm $||\phi_n|| = e^{|\lambda|}$, and inner product $(\phi_{\lambda_1}, \phi_{\lambda_2}) = e^{\overline{\lambda_1}\lambda_2}$. The eigenvalues λ form a continuum, the complex plane, but the eigenvectors are nevertheless normalizable. The uncountable system $\{\phi_\lambda\}_{\lambda \in C}$ is linearly independent in the sense that each finite subset is linearly independent, even though the Hilbert space is separable. It is a basis of the Hilbert space $\mathcal{H}$, not in the usual sense, but in a generalized 'continuous' way. An arbitrary vector ψ in $\mathcal{H}$ can be written as

$$\psi = \frac{1}{2\pi i} \int_C F_\psi(\lambda)\, e^{-|\lambda|^2} d\overline{\lambda} d\lambda,$$

with $\frac{1}{2\pi i} d\overline{\lambda} d\lambda = \frac{1}{\pi} dx dy$, for $\lambda = x + iy$, and with F_ψ a function which is uniquely determined by

$$F_\psi(\lambda) = (\phi_\lambda, \psi).$$

One can show that $F_\psi(\lambda)$ is *anti-holomorphic*, i.e. its complex conjugate $\overline{F_\psi(\lambda)}$ is holomorphic, and that it satisfies the growth condition

$$\int_C |F_\psi(\lambda)|^2 e^{-|\lambda|^2} d\overline{\lambda} d\lambda < \infty.$$

Such functions form a Hilbert space $\widehat{\mathcal{H}}$ with respect to the inner product

$$(F_1, F_2) = \frac{1}{2\pi i} \int_C \overline{F_1(\lambda)} F_2(\lambda)\, e^{-|\lambda|^2} d\overline{\lambda} d\lambda.$$

The relation between the vectors ψ in $\mathcal{H}$ and the anti-holomorphic functions F in $\widehat{\mathcal{H}}$ given above is a unitary transformation between $\mathcal{H}$ and $\widehat{\mathcal{H}}$. The space $\widehat{\mathcal{H}}$ is called the *Bargmann Hilbert space of anti-holomorphic functions* – or holomorphic functions, if one uses a slightly different convention. It has many interesting mathematical properties.

Remark: Note the difference between this notion of a 'continuous base' and the one suggested by the system of nonnormalizable eigenfunctions $\phi_p(x) = c\, e^{\frac{i}{\hbar}px}$ of the momentum operator P.

In this quantum mechanical context the vectors ϕ_λ, or their normalized versions

$$\tilde{\phi}_\lambda = e^{-\frac{1}{2}|\lambda|^2} \phi_\lambda,$$

are called *coherent states*, a term which has its origin in an application in quantum optics, a subject that cannot be discussed here. (Strictly speaking the term 'state' should be reserved for the normalized vectors $\tilde{\phi}_\lambda$, but the ϕ_λ are often more convenient to use and are therefore usually also called states.)

To understand the *physical properties* of (normalized) coherent states, we calculate the expectation values $\overline{p}$, $\overline{x}$ and standard deviations Δp, Δx. The inverse transformation formulas

$$P = \frac{1}{2\alpha}(A + A^*)$$
$$Q = \frac{1}{2i\beta}(A - A^*),$$

with $\alpha = (2m\hbar\omega)^{-1/2}$ and $\beta = -(m\omega/2\hbar)^{1/2}$, allow us to express P and Q in A and A^*. Note that one has

$$(\tilde{\phi}_\lambda, (A^*)^m A^n \tilde{\phi}_\lambda) = (A^m \tilde{\phi}_\lambda, A^n \tilde{\phi}_\lambda) = \overline{\lambda}^m \lambda^n,$$

for all $m, n = 0, 1, \ldots$. An arbitrary algebraic expression in the A and A^* can be written in what is called *normally ordered form* i.e. as a sum of such double monomials, if necessary after a rearrangement using the basic commutation relation $[A, A^*] = 1$. With this one obtains

$$\overline{p} = (\tilde{\phi}_\lambda, P\tilde{\phi}_\lambda) = \frac{1}{2\alpha}(\tilde{\phi}_\lambda, (A + A^*)\tilde{\phi}_\lambda) = \frac{1}{2\alpha}(\lambda + \overline{\lambda}) = \frac{1}{\alpha}\,\mathrm{Re}\,\lambda,$$

and similarly

$$\overline{x} = (\tilde{\phi}_\lambda, Q\tilde{\phi}_\lambda) = \frac{1}{2i\beta}(\lambda - \overline{\lambda}) = \frac{1}{\beta}\,\mathrm{Im}\,\lambda.$$

Together this gives

$$\lambda = \alpha\,\overline{p} + i\beta\,\overline{x}.$$

For the calculation of Δp one needs

$$\begin{aligned}\overline{p^2} &= (\tilde{\phi}_\lambda, P^2\tilde{\phi}_\lambda) = \frac{1}{4\alpha^2}(\tilde{\phi}_\lambda, (A^2 + (A^*)^2 + A^*A + AA^*)\tilde{\phi}_\lambda) = \\ &= \frac{1}{4\alpha^2}(\tilde{\phi}_\lambda, (A^2 + (A^*)^2 + 2A^*A + 1)\tilde{\phi}_\lambda) = \frac{1}{4\alpha^2}(\lambda^2 + \overline{\lambda}^2 + 2|\lambda|^2 + 1).\end{aligned}$$

One finds

$$(\Delta p)^2 = \overline{p^2} - (\overline{p})^2 = \frac{1}{4\alpha^2}(\lambda^2 + \overline{\lambda}^2 + 2|\lambda|^2 + 1) - \frac{1}{4\alpha^2}(\lambda + \overline{\lambda})^2 = \frac{1}{4\alpha^2},$$

and therefore $\Delta p = 1/2\alpha = (m\omega)^{1/2}(\hbar/2)^{1/2}$. Similarly one obtains $(\Delta x)^2 = 1/4\beta^2$ or $\Delta x = -1/2\beta = (m\omega)^{-1/2}(\hbar/2)^{1/2}$. Combining the results on p and x one obtains finally

$$\Delta p\,\Delta x = -\frac{1}{4\alpha\beta} = \frac{1}{2}\hbar,$$

which means that each normalized coherent state $\tilde{\phi}_\lambda$ is a *minimum uncertainty state*.

Conclusion: For each value $\overline{p}$ and $\overline{x}$ there is a minimum uncertainty state, the normalized coherent state $\tilde{\phi}_\lambda$, an eigenvector of A with eigenvalue λ, with

$$\lambda = \alpha\,\overline{p} + i\beta\,\overline{x} = (2m\hbar\omega)^{1/2}\overline{p} + i(m\omega/2\hbar)^{1/2}\overline{x}.$$

All these minimum states have the *same* standard deviations $\Delta p = 1/2\alpha = (m\omega)^{1/2}(\hbar/2)^{1/2}$ and $\Delta x = -1/2\beta = (m\omega)^{-1/2}(\hbar/2)^{1/2}$. The minimum states associated with a quantum harmonic oscillator in this way form a 2-parameter subset of the 3-parameter set of minimum states found in Section 7.4.

9.7. *Time evolution of coherent states*

An interesting physical aspect of the coherent states of an harmonic oscillator is their behaviour under time evolution. For an arbitrary state $\psi = \sum_{n=0}^{\infty} c_n \psi_n$ the time evolution is given by the 1-parameter group of unitary operators $e^{-\frac{i}{\hbar}tH}$, acting as

$$e^{-\frac{i}{\hbar}tH}\psi = \sum_{n=0}^{\infty} e^{-i\omega(n+1/2)t} c_n \psi_n .$$

For a coherent state

$$\phi_\lambda = \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} \psi_n$$

the time evolution becomes

$$e^{-\frac{i}{\hbar}tH}\phi_\lambda = \sum_{n=0}^{\infty} \frac{e^{-i\omega(n+1/2)t}\lambda^n}{\sqrt{n!}} \psi_n = e^{-\frac{i}{2}\omega t} \sum_{n=0}^{\infty} \frac{\lambda(t)^n}{\sqrt{n!}} \psi_n ,$$

with $\lambda(t) = e^{-i\omega t}\lambda$. This means that the coherent state ϕ_λ is transformed – up to the phase factor $e^{-\frac{i}{2}\omega t}$ – into a new coherent state $\phi_{\lambda(t)}$: the set of coherent states is mapped onto itself.

The wave function of a (normalized) coherent state $\tilde{\phi}_\lambda$ moves periodically, up to an irrelevant phase factor. The corresponding probability density $|\tilde{\phi}_\lambda(x)|^2$ is Gaussian. It moves exactly like a 'smeared' classical oscillator with frequency ω. Its width is constant in time and equal to $(m\omega)^{-1/2}(\hbar/2)^{1/2}$. In the classical limit, the limit of a macroscopic situation, this becomes the harmonic motion of a point particle.