Quantum Mechanics

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0.1 Schrödinger equation

0.1.1 Time evolution

In qm time is a parameter and not an observable/operator. H labels a state given at a time. This implies that we may envirage that, if a physical system is represented by $|\alpha\rangle$ at the time t_0, at a later time, the state may differ. The new "evolved" state from t_0 to t can be denoted by

$$|\alpha, t_0; t\rangle, \quad t \geq t_0$$

such that

$$|\alpha, t_0; t_0\rangle = |\alpha\rangle$$

The transition from $|\alpha\rangle$ to $|\alpha, t_0; t\rangle$ is given by the so-called time-evolution operator $\hat{U}(t, t_0)$, such that

$$|\alpha, t_0; t\rangle = \hat{U}(t, t_0)|\alpha\rangle \tag{0.1.1}$$

The time-evolution operator has the following properties:

- Unitarity. Suppose that at t_0 $|\alpha\rangle$ is expanded in terms of the (orthonormal) eigenstates $|a\rangle$ of some observable A

$$|\alpha\rangle = \sum_a |a\rangle\langle a|\alpha, t_0; t\rangle = \sum_a c_a(t_0)|a\rangle \tag{0.1.2}$$

  Thus, at a later time $t\rangle t_0$ we have

$$|\alpha, t_0; t\rangle = \sum_a c_a(t)|a\rangle \tag{0.1.3}$$

  where $c_a(t)$ is the prob. amp. of finding $|\alpha\rangle$ at $|a\rangle$. Although we expect that in general for any particular a, the prob. amplitudes differ,

$$-c_a(t) \neq c_a(t_0)$$

  the sum of all probabilies must be unity at all times, i.e.,

$$\sum_a |c_a(t)|^2 = \sum_a |c_a(t_0)|^2 = 1 \tag{0.1.4}$$

  (as long as the states $|\alpha\rangle$ and $|a\rangle$ are "correctly" normalized). This implies that

$$\langle\alpha|\alpha\rangle = \sum_{a'}\sum_a c^*_{a'}(t_0)\langle a'|a\rangle c_a(t_0) = \sum_a |c_a(t_0)|^2 = 1 \tag{0.1.5}$$

  and consequently

$$\langle\alpha, t_0; t|\alpha, t_0; t\rangle = \sum_a |c_a(t)|^2 = 1 \tag{0.1.6}$$

  That is, the state $|\alpha\rangle$ remain normalized at all times. For terms of (0.1.1), this is satisfied as long as

$$\hat{U}^\dagger(t, t_0)\hat{U}(t, t_0) = 1 \tag{0.1.7}$$

- Time composition:

$$\hat{U}(t_2, t_0) = \hat{U}(t_2, t_1)\hat{U}(t_1, t_0) \qquad t_0\langle t_1\langle t_2 \tag{0.1.8}$$

- Infinitesimal form. We can also propose an infinitesimal form for $\hat{U}(t, t_0)$, such that

$$|\alpha, t_0; t_0 + dt\rangle = \hat{U}(t_0 + dt, t_0)|\alpha\rangle, \qquad \lim_{dt\to 0}\hat{U}(t_0 + dt, t_0) = 1 \tag{0.1.9}$$

  We can note that this together with the previous properties is satisfied if

$$\hat{U}(t_0 + dt, t_0) = 1 - i\hat{\Omega}dt \tag{0.1.10}$$

when $\hat{\Omega}$ is a Hermitian operator. This can be shown as follows. Notice that

$$\begin{aligned}\hat{U}^\dagger(t_0+dt,t_0)\hat{U}(t_0+dt,t_0) &= (1+i\hat{\Omega}dt)(1-i\hat{\Omega}dt)\\ &= 1+i(\hat{\Omega}^\dagger-\hat{\Omega})dt+O(dt^2)\end{aligned}$$

which equals the identity as long as $\hat{\Omega}=\hat{\Omega}^\dagger$ (Hermitian) and dt^2 is negligilble. Furthermore, the time composition is also direct

$$\begin{aligned}\hat{U}(t_0+dt_1+dt_2,t_0+dt_1)\hat{U}(t_0+dt_1,t_0) &= (1-i\hat{\Omega}dt_2)(1-i\hat{\Omega}dt_1)\\ &= 1-i\hat{\Omega}(dt_2+dt_1)+O(dt_1dt_2)\\ &= \hat{U}(t_0+dt_1+dt_2,t_0)\end{aligned}$$

Borrwing from classical mechanics the idea that the Hamiltonian H is the generator of time evolution, we can asser that

$$\hat{\Omega}=\frac{\hat{H}}{\hbar} \tag{0.1.11}$$

which has the righ dimensions of frequency. Therefore, we obtain

$$\hat{U}(t_0+dt,t_0)=1-\frac{i}{\hbar}\hat{H}dt \tag{0.1.12}$$

for (0.1.11) we have used $\hbar$ to get the right dimensions, recalling the Planck radiation $E=\hbar\omega$.

These properties lead to and interesting differential quation. Using the time decomposition property, we see that

$$\hat{U}(t+dt,t_0)=\hat{U}(t+dt,t)\hat{U}(t,t_0)=(1-\frac{i}{\hbar}\hat{H}dt)\hat{U}(t,t_0) \tag{0.1.13}$$

Note now that

$$\hat{U}(t+dt,t_0)-\hat{U}(t,t_0)=-\frac{i}{\hbar}\hat{H}dt\hat{U}(t,t_0) \tag{0.1.14}$$

which implies

$$i\hbar\frac{\hat{U}(t+dt,t_0)-\hat{U}(t,t_0)}{dt}=\hat{H}\hat{U}(t,t_0)$$

that can be written in the differential form

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t_0,t)=\hat{H}\hat{U}(t,t_0) \tag{0.1.15}$$

This is the Schrödinger equation for the time-evolution operator and is the most fundamental equation of quantum mechanics. Multiplying (0.1.15) by the ket $|\alpha\rangle=|\alpha,t_0;t_1\rangle$, we find

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t,0)|\alpha\rangle=\hat{H}\hat{U}(t,t_0)|\alpha\rangle$$

$$i\hbar\frac{\partial}{\partial t}|\alpha,t_0;t\rangle=\hat{H}|\alpha,t_0;t\rangle \tag{0.1.16}$$

which is the Schrödinger eq. for a state.

The Hamiltonian $\hat{H}$ has in principle an arbitrary form (it can be an abstract op., or a differential op., or have matrix form) and be time-dependent or time-independent. We can straightforwardly obtain the form of $\hat{U}(t,t_0)$ for a time-independent Hamiltonian by solving (0.1.15):

$$\hat{U}(t,t_0)=\exp(-\frac{i}{\hbar}H(t-t_0)) \tag{0.1.17}$$

which makes sense in general as the series

$$\hat{U}(t,t_0)=1-\frac{i}{\hbar}\hat{H}(t-t_0)+\frac{1}{2!}\Big(\frac{-i}{\hbar}\hat{H}(t-t_0)\Big)^2 \tag{0.1.18}$$

A time-dependent Hamiltonian is more complicated. We must distinguish two cases:

- when $[\hat{H}(t_1), \hat{H}(t_2)] = 0$, and
- when $[\hat{H}(t_1), \hat{H}(t_2)] \neq 0$

In the former case, the solution of (0.1.15) reads

$$\hat{U}(t, t_0) = \exp\Big(-\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t')\Big) \tag{0.1.19}$$

To solve (0.1.15) when $[\hat{H}(t_1), \hat{H}(t_2)] \neq 0$, we first point out that this differential equation can be restated as

$$\hat{U}(t, t_0)\Big|_{t=t_0}^{t} = -\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t')\hat{U}(t', t_0)$$

recalling that $\hat{U}(t_0, t_0) = 1$ we then have

$$\hat{U}(t, t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t')\hat{U}(t', t_0) \tag{0.1.20}$$

By iteration, we can find the approximate solution

$$\begin{aligned}
\hat{U}(t, t_0) &= 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t')\Big[1 - \frac{i}{\hbar}\int_{t_0}^{t'} dt'\,\hat{H}(t'')\hat{U}(t'', t_0)\Big] \\
&= 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t') + \Big(\frac{-i}{\hbar}\Big)^2\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\,\hat{H}(t')\hat{H}(t'')\hat{U}(t'', t_0) \\
&= 1 + \sum_{n=1}^{\infty}\Big(\frac{-i}{\hbar}\Big)^n\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2\cdots\int_{t_0}^{n-1} dt_n\,\hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n)
\end{aligned} \tag{0.1.21}$$

well-known as the Dyson series.

0.1.2 Time evolution of stationary energy eigenstates

Let us suppose that the Hamiltonian is time-independent. We would like to figure out the evolution of an arbitrary state $|\alpha\rangle$. This is particularly simple if we expand $|\alpha\rangle$ in the basis of eigenstates $|a\rangle$ of an operator $\hat{A}$, such that

$$[\hat{A}, \hat{H}] = 0 \tag{0.1.22}$$

i.e., compatible with $\hat{H}$. It follows that $\{|a\rangle\}$ are energy eigenstates too, whose energy eigenvalues are

$$\hat{H}|a\rangle = E_a|a\rangle \tag{0.1.23}$$

Expanding the time-evolution operator in the states $|a\rangle$, we find

$$\begin{aligned}
\hat{U}(t, 0) = \exp\Big(-\frac{i}{\hbar}\hat{H}t\Big) &= \sum_{a'}|a'\rangle\langle a'|\exp(-i\hat{H}t/\hbar)\sum_{a}|a\rangle\langle a| \\
&= \sum_{a,a'}|a'\rangle\langle a|\langle a'|\exp(-i\hat{H}t/\hbar)|a\rangle \\
&= \sum_{a}\exp(-iE_a t/\hbar)|a\rangle\langle a|
\end{aligned} \tag{0.1.24}$$

Now expanding $|\alpha\rangle$ in the basis of energy eigenstates, we see that

$$\begin{aligned}
|\alpha\rangle &= \sum_a \langle a|\alpha\rangle|a\rangle = \sum_a c_a(t=0)|a\rangle \\
\Rightarrow |\alpha;t\rangle = U(t,0)|\alpha\rangle &= \sum_{a'} \exp\Big(-iE_{a'}t/\hbar\Big)|a'\rangle\langle a'|a\rangle c_a(t=0) \\
&= \sum_a c_a(t=0)\exp(-iE_a t/\hbar)|a\rangle \\
&\equiv \sum_a c_a(t)|a\rangle
\end{aligned}$$

where we realize the time evolution of the expansion coefficients.

Notice that for $|\alpha\rangle = |a\rangle$, we find that

$$|a;t\rangle = \exp(-iE_a t/\hbar)|a\rangle \tag{0.1.25}$$

so that any simultaneous eigenstate of H and A remains so at all time.

0.1.3 Expectation values

We are interested in the expectation value of an observable B in the state

$$|a;t\rangle = \hat{U}(t,0)|a\rangle$$

as given in (0.1.26). The expectation value is computed as

$$\langle\hat{B}\rangle = \langle a|\hat{U}^\dagger(t,0)\hat{B}\hat{U}(t,0)|a\rangle = \langle a|\exp(iE_a t/\hbar)\hat{B}\exp(-iE_a t/\hbar)|a\rangle$$

Since $U(t,0)$ is a numeric phase, the result is

$$\langle\hat{B}\rangle = \langle a;t|\hat{B}|a;t\rangle = \langle a|\hat{B}|a\rangle \tag{0.1.26}$$

i.e., expectation values do not change in time for $|\alpha\rangle = |a\rangle$. This is why these states are called stationary.

The nonstationary states $|\alpha\rangle = \sum_a c_a(0)|a\rangle$ are different. In this case, we have

$$\begin{aligned}
\langle\hat{B}\rangle = \langle\alpha;t|\hat{B}|\alpha;t\rangle &= \langle\alpha|\hat{U}^\dagger(t,0)\hat{B}\hat{U}(t,0)|\alpha\rangle \\
&= \sum_a\sum_{a'} \langle a|c_a^*(0)\exp(iE_a t/\hbar)\hat{B}c_{a'}(0)\exp(-iE_{a'}t/\hbar)|a'\rangle \\
&= \sum_a\sum_{a'} c_a^*(0)c_{a'}(0)\exp(-i(E_{a'}-E_a)t/\hbar)\langle a|\hat{B}|a'\rangle \\
&= \sum_a\sum_{a'} c_a^*(0)c_{a'}(0)\exp(-i\omega_{a'a}t)\langle a|\hat{B}|a'\rangle
\end{aligned} \tag{0.1.27}$$

where the Bohr's frequency $w_{a'a} = \frac{1}{\hbar}(E_{a'} - E_a)$ is the oscillation frequency of the expectation value, and $\langle a|\hat{B}|a'\rangle$ denote the matrix elements of the observable B in the basis of A.

0.1.4 Schrödinger's wave equation

Schrödinger's equation in space representation

Let us define the position states $|\vec{x}\rangle$ as the eigenstates of the position operator $\hat{\vec{x}}$, such that

$$\hat{\vec{x}}|\vec{x}'\rangle = \vec{x}'|\vec{x}'\rangle \tag{0.1.28}$$

Thier orthonormality is given by

$$\langle \vec{x} | \vec{x}' \rangle = \delta^3(\vec{x} - \vec{x}') \tag{0.1.29}$$

Expanded in these terms, an arbitrary physical state $|\alpha\rangle$ is given by

$$|\alpha\rangle = \int d^3x \, |\vec{x}\rangle\langle\vec{x}|\alpha\rangle \equiv \int d^3 \, \psi_\alpha(\vec{x})|\vec{x}\rangle$$

where $\psi_\alpha(\vec{x})$ is usually called the wave function of the state $|\alpha\rangle$ in the representation of positions. Note that the interpretation of $\psi_\alpha(\vec{x})$ is analogous to that of the expansion coefficient $c_a = \langle a|\alpha\rangle$ of our previous discussion, i.e., probability amplitud, such that $|\psi_\alpha(\vec{x})|^2 \, d^3x$ is the probability of finding in a narrow region d^3x around $\vec{x}$.

One may be interested in finding the element $\langle\beta|\hat{A}|\alpha\rangle$ for some states $|\alpha\rangle$, $|\beta\rangle$, in the position basis

$$\begin{aligned} \langle\beta|\hat{A}|\alpha\rangle &= \int d^3x \int d^3x' \, \langle\beta|\vec{x}\rangle\langle\vec{x}|\hat{A}|\vec{x}'\rangle\langle\vec{x}'|\alpha\rangle \\ &= \int d^3x \int d^3x' \, \psi^*_\beta \langle\vec{x}|\hat{A}|\vec{x}'\rangle\psi_\alpha(\vec{x}') \end{aligned} \tag{0.1.30}$$

which depends on the matrix element $\langle\vec{x}|\hat{A}|\vec{x}'\rangle$ of $\hat{A}$. This expression is greatly simplified if $\vec{A}$ is a polynomial of the operator $\vec{x}$, for example, $\hat{A}$ can take the form[1] in one dimension

$$\hat{A} = \frac{1}{2}m\omega^2\vec{x}^2 \tag{0.1.31}$$

In this case, the matrix element in (0.1.30) looks like

$$\begin{aligned} \langle\vec{x}|\hat{A}|\vec{x}'\rangle \mapsto \langle x|\hat{A}|x'\rangle &= \frac{1}{2}m\omega^2\langle x|(\hat{x}^2|x'\rangle) \\ &= \frac{1}{2}m\omega^2\langle x|(|x'\rangle x'^2) = \frac{1}{2}m\omega^2 x'^2\langle x|x'\rangle \\ &= \frac{1}{2}m\omega^2 x'^2\delta(x - x') \end{aligned}$$

where we have used (0.1.28) and (0.1.29) in ther 1D versions. This expresion can be generalized for $\hat{A} = f(\hat{\vec{x}})$ to

$$\langle\vec{x}|f(\hat{\vec{x}})|\vec{x}'\rangle f(\vec{x}')\delta^3(\vec{x} - \vec{x}') \tag{0.1.32}$$

and thus we obtain in this case

$$\langle\beta|\hat{A}|\alpha\rangle = \int d^3x \, \psi^*_\beta f(\vec{x})\psi_\alpha(\vec{x}) \tag{0.1.33}$$

To arrive at the wave equation proposed by Schrödinger, we need further consider the representation of the momentum operator $\hat{\vec{p}}$ in the position basis

$$\begin{aligned} \langle\vec{x}|\hat{\vec{p}}|\alpha\rangle &= \int d^3x' \, \langle\vec{x}|\vec{x}'\rangle\langle\vec{x}'|\hat{\vec{p}}|\alpha\rangle = \int d^3x' \, \delta^3(\vec{x} - \vec{x}') \int d^3x'' \, \langle\vec{x}'|\hat{\vec{p}}|\vec{x}''\rangle\langle\vec{x}''|\alpha\rangle \\ &= \int d^3x'' \, \langle\vec{x}|\hat{\vec{p}}|\vec{x}''\rangle\psi_\alpha(\vec{x}'') \\ &= \int d^3x''\delta^3(\vec{x} - \vec{x}')\big(-i\hbar\vec{\nabla}''\big)\psi_\alpha(\vec{x}'') \\ &= -i\hbar\vec{\nabla}\psi_\alpha(\vec{x}) \end{aligned} \tag{0.1.34}$$

Let us now consider the Schrödinger equaiton, (0.1.16),

$$i\hbar\frac{\partial}{\partial t}|\alpha, t_0; t\rangle = \hat{H}|\alpha, t_0; t\rangle$$

in the position representation, with a Hamiltonian operator given by

$$\hat{H} = \frac{1}{2m}\hat{\vec{p}}^2 + \hat{V}(\hat{\vec{x}}) \tag{0.1.35}$$

[1] As we shall see, this form corresponds to the potential of the harmonic oscillator.

where $\hat{V}(\hat{\vec{x}})$ is a polynomial function of $\hat{\vec{x}}$ and, thus, a Hamiltonian operator. From (0.1.34), we see that

$$\langle\vec{x}|\hat{V}(\hat{\vec{x}})|\vec{x}'\rangle = V(\vec{x}'')\delta^3(\vec{x}-\vec{x}') \tag{0.1.36}$$

Multiplying the Schrödinger equation for states (0.1.16) by the bra $\langle\vec{x}|$ we find

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\langle\vec{x}|\alpha, t_0; t\rangle &= \langle\vec{x}|\frac{1}{2m}\hat{\vec{p}}^2|\alpha, t_0; t\rangle + \langle\vec{x}|\hat{V}(\hat{\vec{x}})|\alpha, t_0; t\rangle \\ &= \frac{1}{2m}(-i\hbar\vec{\nabla})^2\langle\vec{x}|\alpha, t_0; t\rangle + V(\vec{x})\langle\vec{x}|\alpha, t_0; t\rangle \end{aligned} \tag{0.1.37}$$

where we have used (0.1.34) and (0.1.33) with $\langle\beta| = \langle\vec{x}|$. Defining

$$\psi_\alpha(\vec{x}, t) \equiv \langle\vec{x}|\alpha, t_0; t\rangle, \tag{0.1.38}$$

we obtain the time-dependent Schrödinger's wave equation

$$i\hbar\frac{\partial}{\partial t}\psi_\alpha(\vec{x}, t) = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_\alpha(\vec{x}, t) + V(\vec{x})\psi_\alpha(\vec{x}, t) \tag{0.1.39}$$

The stationary wave equation is obtained when $|\alpha\rangle = |a\rangle$ is an energy eigenstate and thus stationary. From (0.1.25) we have that

$$\begin{aligned} \langle\vec{x}|\alpha; t\rangle = \langle\vec{x}|a; t\rangle = \exp(-iE_a t/\hbar)\langle\vec{x}|a\rangle &= \exp(-iE_\alpha t/\hbar)\langle\vec{x}|\alpha\rangle \\ \Leftrightarrow \psi_\alpha(\vec{x}, t) &= \exp(-iE_\alpha t/\hbar)\psi_\alpha(\vec{x}) \end{aligned} \tag{0.1.40}$$

where we have defined $\psi_\alpha(\vec{x}) \equiv \langle\vec{x}|\alpha\rangle$ in analogy with (0.1.38). It then follows that (0.1.39) becomes

$$E_\alpha\psi_\alpha(\vec{x}) = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_\alpha(\vec{x}) + V(\vec{x})\psi_\alpha(\vec{x}) \tag{0.1.41}$$

when the time dependence carried by the time-evolution operator has been factorized and eliminated.

Schrödinger's equation in momentum representation

As in the configuration space, we can now define the eigenstates of the momentum operator $\hat{\vec{p}}$ as

$$\hat{\vec{p}}|\vec{p}'\rangle = \vec{p}'|\vec{p}'\rangle, \tag{0.1.42}$$

satisfying the orthonormality condition

$$\langle\vec{p}|\vec{p}'\rangle = \delta^3(\vec{p}-\vec{p}') \tag{0.1.43}$$

and the completeness relation

$$1 = \int d^3p|\vec{p}\rangle\langle\vec{p}| \tag{0.1.44}$$

An arbitrary state in the basis reads

$$|\alpha\rangle = \int d^3\,p|\vec{p}\rangle\langle\vec{p}|\alpha\rangle = \int d^3|,\phi_{\alpha(\vec{p})}|\vec{p}\rangle \tag{0.1.45}$$

where we have defined the momentum-space wave function

$$\phi_\alpha(\vec{p}) \equiv \langle\vec{p}|\alpha\rangle \tag{0.1.46}$$

normalized as

$$\int d^3p\,|\phi_\alpha(\vec{p})|^2 = \int d^3p\,\langle\alpha|\vec{p}\rangle\langle\vec{p}|\alpha\rangle = \langle\alpha|\alpha\rangle = 1 \tag{0.1.47}$$

if $|\alpha\rangle$ is correctly normalized. The wave function $\phi_\alpha(\vec{p})$ is related to $\psi_\alpha(\vec{x})$ by

$$\phi_\alpha(\vec{p}) = \langle\vec{p}|\alpha\rangle = \int d^3x\,\langle\vec{p}|\vec{x}\rangle\langle\vec{x}|\alpha\rangle = \int d^3x\,\langle\vec{p}|\vec{x}\rangle\psi_\alpha(\vec{x}) \tag{0.1.48}$$

and conversely

$$\psi_\alpha(\vec{x}) = \int d^3x \, \langle \vec{x}|\vec{p}\rangle \phi_\alpha(\vec{p}) \tag{0.1.49}$$

where $\langle \vec{p}|\vec{x}\rangle = \langle \vec{x}|\vec{p}\rangle^*$ is yet unknown. To figure out $\langle \vec{p}|\vec{x}\rangle$, let us compute

$$\begin{aligned}\langle \vec{x}|\hat{\vec{p}}|\vec{p}\rangle &= \int d^3x' \, \langle \vec{x}|\hat{\vec{p}}|\vec{x}'\rangle\langle \vec{x}'|\vec{p}\rangle \\ &= -i\hbar\vec{\nabla}\langle \vec{x}|\vec{p}\rangle \end{aligned}\tag{0.1.50}$$

which, using (0.1.42), implies

$$\vec{p}\langle \vec{x}|\vec{p}\rangle = -i\hbar\vec{\nabla}\langle \vec{x}|\vec{p}\rangle \tag{0.1.51}$$

whose solution reads

$$\langle \vec{x}|\vec{p}\rangle = N \exp(i\vec{p}\cdot\vec{x}/\hbar) \tag{0.1.52}$$

The normalization factor can easily be found by computing

$$\begin{aligned}\langle \vec{x}|\vec{x}'\rangle &= \int d^3p \, \langle \vec{x}|\vec{p}\rangle\langle \vec{p}|\vec{x}'\rangle \\ &= N^2 \int d^3p \, \exp\Big(-i\vec{p}\cdot(\vec{x}-\vec{x}')/\hbar\Big) \\ &= N^2(2\pi\hbar)^3\delta^3(\vec{x}-\vec{x}') \end{aligned}\tag{0.1.53}$$

where the last step is the result of realizing that the integral is just a Fourier transform. Notice that the l.h.s. is actually just $\delta^3(\vec{x}-\vec{x}')$, which finally lead to

$$N^2 = (2\pi\hbar)^{-3} \tag{0.1.54}$$

Replacing into (0.1.52), we find that

$$\langle \vec{x}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \exp(i\vec{p}\cdot\vec{x}/\hbar) \tag{0.1.55}$$

It then follows from (0.1.48) and (0.1.49) that $\phi_\alpha(\vec{p})$ is just the Fourier transform of $\psi_\alpha(\vec{x})$, and vice versa

$${}_\alpha(\vec{x}) = \int d^3x \, \frac{1}{2\pi\hbar}^{3/2} \exp\Big(i\vec{p}\cdot\vec{x}/\hbar\Big)\phi_{\alpha(\vec{p})} \tag{0.1.56a}$$

$$\phi_\alpha(\vec{p}) = \int d^3x \, \frac{1}{2\pi\hbar}^{3/2} \exp\Big(-i\vec{p}\cdot\vec{x}/\hbar\Big)\psi_\alpha(\vec{x}) \tag{0.1.56b}$$

Let us use these results to find the Schrödinger's wave equation in momentum space for the Hamiltonian (0.1.35), defining additionally

$$\phi_\alpha(\vec{p}, t) \equiv \langle \vec{p}|\alpha, t_0; t\rangle \tag{0.1.57}$$

We have

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\langle \vec{p}|\alpha, t_0; t\rangle &= \langle \vec{p}|\frac{1}{2m}\hat{\vec{p}}^2|\alpha, t_0; t\rangle \\ &+ \int d^3p' \, \langle \vec{p}|\hat{V}(\hat{\vec{x}})|\vec{p}'\rangle\langle \vec{p}'|\alpha, t_0; t\rangle \\ &= \frac{1}{2m}\vec{p}^2\phi_\alpha(\vec{p}, t) + \int d^3p' \int d^3x \int d^3x' \, \langle \vec{p}|\vec{x}\rangle\langle \vec{x}|\hat{V}(\hat{\vec{x}})|\vec{x}'\rangle\langle \vec{x}'|\vec{p}'\rangle\phi_\alpha(\vec{p}, t) \\ &= \frac{\vec{p}^2}{2m}\phi_\alpha(\vec{p}, t) \\ &+ \frac{1}{(2\phi\hbar)^3}\int d^3p' \int d^3x \int d^3x' \, \exp(-i\vec{p}\cdot\vec{x}/\hbar)V(\vec{x})\delta^3(\vec{x}-\vec{x}')\exp(i\vec{p}'\cdot\vec{x}'/\hbar)\phi_\alpha(\vec{p}, t) \\ &= \frac{\vec{p}^2}{2m}\phi_\alpha(\vec{p}, t) \\ &+ \frac{1}{(2\pi\hbar)^{3/2}}\int d^3p' \int \frac{d^3x}{(2\pi\hbar)^{3/2}} \exp(-i(\vec{p}-\vec{p}')\cdot\vec{x}/\hbar)V(\vec{x})\phi(\vec{p}, t) \end{aligned}$$

which finally yields

$$i\hbar\frac{\partial}{\partial t}\phi_\alpha(\vec{p},t) = \frac{\vec{p}^2}{2m}\phi_\alpha + \frac{1}{(2\pi\hbar)^{3/2}}\int d^3p'\,V(\vec{p}-\vec{p}')\phi_\alpha(\vec{p},t) \tag{0.1.58}$$

where

$$V(\vec{p}-\vec{p}') \equiv \frac{1}{(2\pi\hbar)^{3/2}}\int \exp(-i(\vec{p}-\vec{p}'')\cdot\vec{x}/\hbar)V(\vec{x})\,d^3x \tag{0.1.59}$$

Continuity equation

If we let the probability density of a system to be defined as

$$\rho \equiv \psi^*_\alpha(\vec{x},t)\psi_\alpha(\vec{x},t) \tag{0.1.60}$$

then one easily finds that (omitting for simplicity the dependence on $\vec{x}$ & t)

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= \psi^*_\alpha\frac{\partial}{\partial t}\psi_\alpha + \frac{\partial}{\partial t}\psi^*_\alpha\psi_\alpha \\ &= \psi^*_\alpha\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_\alpha + V\psi_\alpha\right) - \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi^*_\alpha + V\psi^*_\alpha\right)\psi_\alpha \\ &= \frac{i\hbar}{2m}\left[\psi^*_\alpha\vec{\nabla}^2\psi_\alpha - (\vec{\nabla}^2\psi^*_\alpha)\psi_\alpha\right] \\ &= \frac{i\hbar}{2m}\left[\vec{\nabla}(\psi^*_\alpha\cdot\vec{\nabla}\psi_\alpha) - \vec{\nabla}\psi^*_\alpha\cdot\vec{\nabla}\psi_\alpha - \vec{\nabla}\cdot((\vec{\nabla}\psi^*_\alpha)\psi_\alpha) + \vec{\nabla}\psi^*_\alpha\cdot\vec{\nabla}\psi_\alpha\right] \\ &= \frac{i\hbar}{2m}\vec{\nabla}\cdot\left(\psi^*_\alpha\vec{\nabla}\psi_\alpha - (\vec{\nabla}\psi^*_\alpha)\psi_\alpha\right) \\ &= -\vec{\nabla}\vec{j}\end{aligned} \tag{0.1.61}$$

where

$$\vec{j} \equiv \left(\psi^*_\alpha\vec{\nabla}\psi_\alpha - (\vec{\nabla}\psi^*_\alpha)\psi_\alpha\right)\frac{i\hbar}{2m} \tag{0.1.62}$$

Rewriting (0.1.61) in these terms, we find

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0 \tag{0.1.63}$$

which coincides with the well-known continuity equation for a probability density ρ and a probability current $\vec{j}$, defined respectively by (0.1.60) & (0.1.62) It's interesting to realize that any continuity relation reveals a conserved quantity. In this case, the proability

$$P = \int d^3x\,\rho \tag{0.1.64}$$

is conserved (as expected):

$$\frac{dP}{dt} = \int_V d^3x\,\frac{\partial p}{\partial t} = -\int_{\partial V} d\vec{S}\cdot\vec{j} = 0 \tag{0.1.65}$$

which vanishes on ly if (0.1.62) vanishes at the boundary ∂V located infinitely far away. This condition is satisfied because $\lim_{\vec{x}\to\infty}\psi_\alpha(\vec{x},t) = 0$ is a condition of square integrability, i.e., for P in (0.1.64) to be finite always.

0.1.5 Elementary 1 quantum systems

Harmonic oscillator in operator method

The harmonic oscillator is one of the most important quantum systems because any physical system is some approximation (around its stability point) resembles an harmonic oscillator. The potential of this system is give, as in classical mechanics, by

$$\hat{V}(\hat{x}) = \frac{1}{2}m\omega^2\hat{x}^2 \tag{0.1.66}$$

We would like to find the eigenstates of the Hamiltonian as a time-independent system. To do so, we shall follow the elegant procedure envisages by Heisenberg based on the non-hermitian "ladder operators"

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right) \tag{0.1.67a}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right) \tag{0.1.67b}$$

which let one identify the operators $\hat{x}$ ans $\hat{p}$ as

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) \tag{0.1.68a}$$

$$\hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^\dagger - \hat{a}) \tag{0.1.68b}$$

The ladder operators do not commute:

$$\begin{aligned}[\hat{a}, \hat{a}^\dagger] &= \frac{m\omega}{2\hbar}\left([\hat{x}, -\frac{i\hat{p}}{m\omega}] + [-\frac{i\hat{p}}{m\omega}, \hat{x}]\right) \\ &= \frac{i}{2\hbar}\left(-[\hat{x}, \hat{p}] + [\hat{p}, \hat{x}]\right)\end{aligned} \tag{0.1.69}$$

Defining the so-called "number operator"

$$\hat{N} \equiv \hat{a}\hat{a}^\dagger \tag{0.1.70}$$

it is easy to realize that in terms of $\hat{x}$ and $\hat{p}$

$$\begin{aligned}\hat{N} &= \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\right) + \frac{i}{2\hbar}[\hat{x}, \hat{p}] \\ &= \frac{1}{\hbar\omega}\left(\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right) - \frac{1}{2}\end{aligned} \tag{0.1.71}$$

Therefore, it follows that the Hamiltonian can be expressed in terms of the number operator as

$$\hat{H} = \hbar\omega\left(\hat{N} + 1/2\right) \tag{0.1.72}$$

Note that $\hat{H}$ and $\hat{N}$ are compatible (and hermitian) operators because

$$[\hat{H}, \hat{N}] = 0;$$

they can thus be simultaneously diagonalized, so that the eigenstates of $\hat{N}$ are also energy eigenstates. The eigenstates of $\hat{N}$ are defined by

$$\hat{N}|n\rangle = n|n\rangle \tag{0.1.73}$$

where n i san arbitrary real number at this point. It thn follows that

$$\hat{H}|n\rangle = \hbar\omega(n + 1/2)|n\rangle \tag{0.1.74}$$

Inserting (0.1.74) in the time-independent Schrödinger's equation, we identify

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

as the energy asociated with the energy eigenstate $|n\rangle$. We can determine the values that n can take by exploring the action of the ladder operators on $|n\rangle$. Note first that

$$\begin{aligned}[\hat{N}, \hat{a}^\dagger] &= [\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger \\ [\hat{N}, \hat{a}] &= [\hat{a}^\dagger\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}]\hat{a} = -\hat{a}\end{aligned} \tag{0.1.75}$$

where (0.1.69) has been used. Applying these results, we readily see that

$$\hat{N}(\hat{a}^\dagger|n\rangle) = \Big([\hat{N}, \hat{a}^\dagger] + \hat{a}^\dagger\hat{N}\Big)|n\rangle = (n+1)(\hat{a}^\dagger|n\rangle) \tag{0.1.76a}$$

$$\hat{N}(\hat{a}|n\rangle) = \Big([\hat{N}, \hat{a}] + \hat{a}\hat{N}\Big)|n\rangle = (n-1)(\hat{a}|n\rangle) \tag{0.1.76b}$$

Eq (0.1.76a) implies that $\hat{a}^\dagger|n\rangle$ has the same eigenvalues as the state $|n+1\rangle$ or, in other words, that the action of the operator $\hat{a}^\dagger$ raises a state from $|n\rangle$ to $|n+1\rangle$. Analogously, $\hat{a}$ lowers the state from $|n\rangle$ to $|n-1\rangle$. This is why the ladder operators $\hat{a}$ and $\hat{a}^\dagger$ are known as lowering and rising operators, respectively. It immediatly folows that the following relations must hold

$$\begin{aligned}\hat{a}|n\rangle &= c|n-1\rangle \\ \hat{a}^\dagger|n\rangle &= d|n+1\rangle\end{aligned} \tag{0.1.77}$$

where c and d are numbers that may be determinated by imposing the orthogonality (we shall impose orthonormality) of the eigenstates of the Hermitian operator $\hat{N}$. The norm of $\hat{a}|n\rangle$ is computed as

$$|c|^2\langle n-1|n-1\rangle = \langle n|\hat{a}^\dagger\hat{a}|n\rangle = n\langle n|n\rangle,$$

which implies

$$|c|^2 = n \tag{0.1.78}$$

for $\langle n|m\rangle = \delta_{n,m}$. Note that we can further assume that c (and d) is real because

$$a^\dagger a|n\rangle = a^\dagger c_n|n-1\rangle = c_n d_{n-1}|n\rangle = n|n\rangle$$

and n is real. Further we assume by convention that c (and d) is positive. This yield

$$c = \sqrt{n} \tag{0.1.79}$$

Similarly, normalizing $\hat{a}^\dagger|n\rangle$ we find

$$|d|^2\langle n+1|n+1\rangle = \langle n|\hat{a}\hat{a}^\dagger|n\rangle = \langle n|[\hat{a}, \hat{a}^\dagger] + \hat{a}^\dagger\hat{a}|n\rangle = (n+1)\langle n|n\rangle$$

which yields

$$d = \sqrt{n+1} \tag{0.1.80}$$

We have therefore obtained

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \tag{0.1.81a}$$

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{0.1.81b}$$

with $n \geq 0$ to provide reasonable results. Since the smallest value that n can take is $n = 0$ and all states created by $\hat{a}^\dagger$ differ by a unit of n, n must be integer. Therefore, eq. (0.1.74) can be interpreted as a rule of energy quantization. Notice that the sate of lowert energy satisfies

$$\hat{a}|0\rangle = 0 \tag{0.1.82}$$

i.e., it is anihilated bythe lowering operator $\hat{a}$. Eq. (0.1.82) can be considered a definition of the ground state. Note that the ground state has the non-vanishing energy $\frac{1}{2}\hbar\omega$. We can now obtain an arbitrary state $|n\rangle$ by the repeated action of $\hat{a}^\dagger$ on $|0\rangle$. We see that

$$|1\rangle = \hat{a}^\dagger|0\rangle \tag{0.1.83}$$

and then, from (0.1.81b)

$$|2\rangle = \frac{\hat{a}^\dagger}{\sqrt{2}}|1\rangle = \frac{(\hat{a}^\dagger)^2}{\sqrt{2}}|0\rangle \tag{0.1.84a}$$

$$|3\rangle = \frac{\hat{a}^\dagger}{\sqrt{3}}|2\rangle = \frac{(\hat{a}^\dagger)^3}{\sqrt{3!}}|0\rangle \tag{0.1.84b}$$

and so on. We find the general expression

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle \tag{0.1.85}$$

A useful observation is that the states $\{|n\rangle\}$ are not eigenstates of $\hat{x}$ and $\hat{p}$, as expected, because $[\hat{H}, \hat{x}]$ and $[\hat{H}, \hat{p}]$ do not vanish, in general.

We can explicitly show that neither $\hat{x}$ nor $\hat{p}$ are diagonal in the basis of energy eigenstates:

$$\begin{aligned}
\langle m|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle m|\hat{a} + \hat{a}^\dagger|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\langle m|n-1\rangle + \sqrt{n+1}\langle m|n+1\rangle\right] \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right]
\end{aligned} \tag{0.1.86a}$$

$$\langle m|\hat{p}|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\langle m|\hat{a}^\dagger - \hat{a}|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\left[\sqrt{n+1}\delta_{m,n+1} - \sqrt{n}\delta_{m,n-1}\right] \tag{0.1.86b}$$

where the expresions (0.1.67) have been used. With this formalism, we can compute the energy wavefunctions in the position representation. Let us start by obtaining $\psi_0 \equiv \langle x|0\rangle$. To do so, recall that the ground state is anihilated by $\hat{a}$, so that

$$\langle x|\hat{a}|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\langle x|\hat{x} + \frac{i\hat{p}}{m\omega}|0\rangle = 0 \tag{0.1.87}$$

Inserting a unity, we have

$$\int dx'\,\langle x|\hat{x} + \frac{i\hat{p}}{m\omega}|x'\rangle\langle x'|0\rangle = \int dx'\,\delta(x-x')\Big(x + \frac{i}{m\omega}(-i\hbar\frac{d}{dx})\Big)\psi_0 = 0 \tag{0.1.88}$$

which, after integration and rearranging the terms, yields

$$\frac{d\psi_0(x)}{dx} = -\frac{m\omega}{\hbar}x\psi_0(x) \tag{0.1.89}$$

From (0.1.89), we realize that

$$\psi_0(x) = A_0\exp(-\frac{1}{2}\frac{m\omega}{\hbar}x^2)$$

or in terms of the dimensionless coordinate $\tilde{x} = \sqrt{\frac{m\omega}{\hbar}}x$

$$\psi_0(\tilde{x}) = A_0\exp(-\frac{1}{2}\tilde{x}^2) \tag{0.1.90}$$

A_0 can be found by normalizing

$$\int dx\,\psi_0(\tilde{x})\psi_0(\tilde{x}) = A_0\sqrt{\frac{\hbar}{m\omega}}\int d\tilde{x}\,\exp(-\tilde{x}^2) = A_0^2\sqrt{\frac{\hbar\pi}{m\omega}} = 1, \tag{0.1.91}$$

which leads finally to

$$\psi_0(\tilde{x}) = \left(\frac{\hbar\pi}{m\omega}\right)^{-1/4}\exp(-\frac{1}{2}\tilde{x}^2) \tag{0.1.92}$$

$\psi_n(\tilde{x})$ can be obtained from inspecting $\langle x|n\rangle$:

$$\begin{aligned}
\langle x|1\rangle &= \langle x|\hat{a}^\dagger|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\langle x|\hat{x} - \frac{i\hat{p}}{m\omega}|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}(x - \frac{\hbar}{m\omega}\frac{d}{dx})\psi_0(x)\\
\langle x|2\rangle &= \langle x|\frac{(\hat{a})^2}{\sqrt{2}}|0\rangle = \frac{1}{\sqrt{2}}\big(\sqrt{m\omega 2\hbar}\big)^2(x - \frac{\hbar}{m\omega})^2\psi_0(x)\\
&\vdots\\
\langle x|n\rangle &= \langle x|\frac{(\hat{a})^n}{\sqrt{n!}}|0\rangle = \frac{1}{\sqrt{n!2^n}}\frac{1}{\left(\frac{\hbar}{m\omega}\right)^n}\Big(x - \frac{\hbar}{m\omega}\frac{d}{dx}\Big)^n\psi_0(x)
\end{aligned} \tag{0.1.93}$$

The latter can be rewritten in terms of $\tilde{x}$ as

$$\psi_0(\tilde{x}) = \frac{1}{\sqrt{n!2^n}}\frac{1}{\left(\frac{\hbar}{m\omega}\right)^n}\bigg(\sqrt{\frac{\hbar}{m\omega}}\tilde{x} - \frac{\hbar}{m\omega}\bigg)^n\psi_0(\tilde{x}) \tag{0.1.94}$$

that is,

$$\psi_n(\tilde{x}) = \frac{1}{\sqrt{n!2^n}}(\frac{\hbar\pi}{m\omega})^{-1/4}(\tilde{x} - \frac{d}{d\tilde{x}})^n\exp(-\frac{1}{2}\tilde{x}^2) \tag{0.1.95}$$

Interestingly, the Rodrigues' formula for the Hermite polynomials reads[2]

$$H_n(\tilde{x}) = \exp\Big(\frac{1}{2}\tilde{x}^2\Big)\Big(\tilde{x} - \frac{d}{d\tilde{x}}\Big)^n\exp\Big(-\frac{1}{2}\tilde{x}^2\Big) \tag{0.1.96}$$

Therefore, (0.1.95) can be rewritten as

$$\psi_n(\tilde{x}) = \frac{1}{\sqrt{n!2^n}}\Big(\frac{\hbar\pi}{m\omega}\Big)^{-1/4}\exp\Big(-\frac{1}{2}\tilde{x}^2\Big)H_n(\tilde{x}) \tag{0.1.97}$$

A few observations are in order. Firstly, as depected, the wavefunctions are eigher symmetric or antisymmetric, but the probability densities $|\psi_n|^2$ are always symmetric on $\tilde{x}$ (or x). It then immediately follows that $\langle\hat{x}\rangle = 0$. This result can be easily verified in the operator formalism, following our result (0.1.86a)

$$\langle\hat{x}\rangle = \langle n|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\Big(\sqrt{n}\delta_{n,n-1} + \sqrt{n+1}\delta_{n,n+1}\Big) = 0 \tag{0.1.98}$$

Similarly, from (0.1.86b), we find that

$$\langle\hat{p}\rangle = p \tag{0.1.99}$$

Furthermore, we can compute the expectation values of $\hat{x}^2$ & $\hat{p}^2$ as follows

$$\begin{aligned}
\langle\hat{x}^2\rangle = \frac{\hbar}{2m\omega}\langle n|\big(\hat{a} + \hat{a}^\dagger\big)|n\rangle &= \frac{\hbar}{2m\omega}\langle n|\big(\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2}\big)|n\rangle\\
&= \frac{\hbar}{2m\omega}\langle n|(1 + 2\hat{a}\hat{a}^\dagger)|n\rangle = \frac{\hbar}{2m\omega}(1+2n)
\end{aligned} \tag{0.1.100a}$$

where we used that $\langle n|\hat{a}^2|n\rangle = \langle n|(\hat{a}^\dagger)^2|n\rangle = 0$ and (0.1.69). Similarly,

$$\langle\hat{p}^2\rangle = -\frac{m\hbar\omega}{2}\langle n|(\hat{a}^\dagger - \hat{a})^2|n\rangle = -\frac{m\hbar\omega}{2}\langle n|(-\hat{a}\hat{a}^\dagger - \hat{a}\hat{a}^\dagger)|n\rangle = \frac{m\hbar\omega}{2}(1+2n) \tag{0.1.101}$$

Noticing now that $\langle(\Delta\hat{x})^2\rangle = \langle\hat{x}^2\rangle$ because of (0.1.98), and $\langle(\Delta\hat{p})^2\rangle = \langle\hat{p}^2\rangle$ because of (0.1.99), we find the uncertainty relation

$$\langle(\Delta\hat{x})^2\rangle\langle(\Delta\hat{p})^2\rangle = \frac{\hbar^2}{4}(1+2n)^2, \tag{0.1.102}$$

which satisfies the uncertainty principle. We notice that the state of minimal uncertainty is precisely the ground state, which, as given by (0.1.92), has a Gaussian profile that are typically considered maximally coherent. A second

[2] See e.g. Arfken 1985, p.270

observation regards the natural question of how these states evolve in time. In section (2.1), we learned that stationary states, such as $|n\rangle$ evolve trivially as

$$|n,t\rangle = \exp\Big(-\frac{i}{\hbar}\hat{H}t\Big)|n\rangle = \exp(-i\omega(n+1/2)t)|n\rangle \tag{0.1.103}$$

For these states, one can easely verify that

$$\langle n;t|\hat{x}|n;t\rangle = \langle n|\hat{a}|n\rangle = 0 = \langle n|\hat{p}|n\rangle = \langle n;t|\hat{p}|n;t\rangle \tag{0.1.104}$$

and, thus, the uncertainty relation (0.1.102) holds still. A natural puzzle is that $\langle\hat{x}\rangle = 0$ even through the system we analize is a harmonic oscillator. From classical mechanics, one may have expected on oscillatory behavior. How come that this fails quantum-mechanically? The answer is trivial: we have considered only stationary states, which may not capture all features of the system. Non-stationary states fo the form

$$|\alpha\rangle = \sum_n c_n|n\rangle \tag{0.1.105}$$

as discussed around (0.1.27), have a non-trivial evolution even if the Hamiltonian is time-independent. We shall shortly see that these is a special kind of non-stationary states that keep the nature of the classical harmonic oscillator, the so-called coherent states. A second observation conserns the method we have used to determine the features of the quantum harmonic oscillator. The method consists in defining the ladder operators subject to a fundamental quantum request: that the operators $\hat{\vec{x}}$ and $\hat{\vec{p}}$ (int the dimensionality of the problem) comply with $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$. This procedure is usually called canonical quantization and is applied to a great variety of non-relativistic quantum systems, (almost) all quantum field theories (or relativistic quantum systems) and even more complex theories, such as string theory. Finally, we must mention on an interpreattion of this canonical quantization in terms of the ladder operators called the second quantizaton. As we have seen, the energy of the harmonic oscillator is quantized as

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

which is (almost) identical to Plank's proposed quantization of the electromagnetic radiation $\hbar\omega n$, except for the conditional energy shift $\frac{1}{2}\hbar\omega$. In Einstein's original resolution to the photoelectric effect, the energy shift does not apper and the value of n counts the number of electromagnetic-radiation quanta or photons. Later, Einstein himself realized that an energy shift proportional to $\frac{1}{2}\hbar\omega$ was needed to understand e.g., the puzzle of black-body radiation. This energy shift can be interpreted as the vacuum energy. Thus, in Heisenberg's formulation, $|0\rangle$ corresponds to the vaccum state, while the states $|1\rangle$,$|2\rangle$, $|3\rangle$, $\ldots$ may correspond to a physical system with one, two, three, $\ldots$ photons or particles, in general. Notice that in this interpreation $\hat{a}^\dagger$ and $\hat{a}$ operate as creation and annihilation operators

$$\hat{a}^\dagger|n\rangle \mapsto |n+1\rangle$$
$$\hat{a}|n\rangle \mapsto |n-1\rangle$$

creating and annihilating particles. This interpretation finds an appropiate environment particularly in quantum field theories, where such processes occur naturally. It is important to mention though that, as long as one considers the non-relativistic Schrödinger wave equation with a Mermitian potential $\hat{V} = \hat{V}^\dagger$, we shall be interested only in elastic processes, where the number of particles do not change.

Coherent states

We would like to identify non-stationary states of the harmonic oscillator that behave as much as possible like classical systems. Schrödinger identified this kind of states in 1926, searching for solutions of his wave equation compatible with the correspondence principle (i.e., that in a limit behave as classical systems). One condition on these states is then that they do not lose their structure as they evolve in time, i.e., that their dispersion keeps a minimal value. A clear example of such a state is the ground state $|0\rangle$, which in the position space is given by the Gaussian profile (0.1.90)

$$\psi_0(\tilde{x}) = A_0 \exp(-\frac{1}{2}\tilde{x}^2)$$

Note that, according to (0.1.102), this state has minimal uncertainty

$$\langle(\Delta\hat{x}^2)\rangle\langle(\Delta\hat{p})^2\rangle = \frac{\hbar^2}{4}$$

For these reasons, coherent states are frequently called Gaussian states, minimal uncertainty states, and also canonical coherent states, as there are many other types of coherent states. It is possible to show that these canonical coherent states can be defined as the eigenstates of the annihilation operator $\hat{a}$

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \alpha \in \mathbb{C} \tag{0.1.106}$$

The explicit expression of $|\alpha\rangle$ can be found from comparing

$$\langle n|a|\alpha\rangle = (\langle n|a)|\alpha\rangle = \sqrt{n+1}\langle n+1|\alpha\rangle, \tag{0.1.107a}$$
$$\text{and}\langle n|a|\alpha\rangle = \langle n|(a|\alpha\rangle) = \alpha\langle n|\alpha\rangle, \tag{0.1.107b}$$

where (0.1.81b) has been used. Recalling the form of $|\alpha\rangle$ (0.1.105), we then find that

$$c_{n+1} = \frac{\alpha}{\sqrt{n+1}}c_n \tag{0.1.108}$$

where, furthermore, from (0.1.79),

$$c_n \equiv \langle n|\alpha\rangle = \langle 0|\frac{(\hat{a})^n}{\sqrt{n!}}|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}}\langle 0|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}}c_0 \tag{0.1.109}$$

It then follows that

$$|\alpha\rangle = \sum_n c_n|n\rangle = \sum_n \frac{\alpha^n}{\sqrt{n!}}c_0\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle = c_0\exp(\alpha\hat{a}^\dagger)|0\rangle \tag{0.1.110}$$

(Notice that (0.1.108) is just a consistency check of (0.1.109).) The constant c_0 can be found by normalizing the state as follows

$$\begin{aligned} 1 = \langle\alpha|\alpha\rangle &= |c_0|^2\langle 0|\exp(\alpha^*\hat{a})\exp(\alpha\hat{a}^\dagger)|0\rangle \\ &= |c_0|^2\langle 0|\Big(1+\alpha^*\hat{a}+\frac{\alpha*\hat{a}^2}{2}+\ldots\Big)\Big(1+\alpha^*\hat{a}^\dagger+\frac{\alpha*(\hat{a}^\dagger)^2}{2}+\ldots\Big)|0\rangle \\ &= |c_0|^2\langle 0|\Big(1+|\alpha|^2\hat{a}\hat{a}^\dagger+\frac{(|\alpha|^2)^2}{2}\hat{a}^2(\hat{a}^\dagger)^2+\ldots\Big)|0\rangle \\ &= |c_0|^2\Big(1+|\alpha|^2+\frac{1}{2}(|\alpha|^2)^2+\ldots\Big) = |c_0|^2\exp(|\alpha|^2) \end{aligned} \tag{0.1.111}$$

where in the third row we used that $\langle 0|\hat{a}^n(\hat{a}^\dagger)^m|0\rangle = 0$ for $n \neq m$, and in the fourth row that $(\hat{a}\hat{a}^\dagger)^n = (1+\hat{a}^\dagger\hat{a})^n$ and $\langle 0|\hat{a}^\dagger\hat{a}|0\rangle = 0$. Thus, eq. (0.1.110) becomes

$$|\alpha\rangle = \exp(-|\alpha|^2/2)\exp(\alpha\hat{a}^\dagger)|0\rangle \tag{0.1.112}$$

We may also viwe the coherent states as the ground state of a new set of annihilation and creation operators defined as

$$\hat{b} = \hat{a} - \alpha \quad \text{and} \quad \hat{b}^\dagger = \hat{a}^\dagger - \alpha^* \tag{0.1.113}$$

which implies

$$\hat{b}|\alpha\rangle = 0 \tag{0.1.114}$$

We further observe that in configuration space, the coherent states are just given by a shifted harmonic-oscillator ground state

$$\psi_\alpha(x) = \Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4}\exp\Big(-\frac{m\omega}{2\hbar}(x-x_0)^2\Big) \tag{0.1.115}$$

because

$$\begin{aligned} \langle x|\hat{a}|\alpha\rangle &= \int dx'\,\langle x|\sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x}+\frac{i\hat{p}}{m\omega}\Big)|x'\rangle\langle x'|\alpha\rangle \\ &= \sqrt{\frac{m\omega}{2\hbar}}\Big(x+\frac{\hbar}{m\omega}\frac{d}{dx}\Big)\psi_{alpha}(x) \\ &= \sqrt{\frac{m\omega}{2\hbar}}\Big(x-(x-x_0)\Big)\psi_\alpha(x) \\ &= x_0\sqrt{\frac{m\omega}{2\hbar}}\psi_\alpha(x) \end{aligned} \tag{0.1.116}$$

while, on the left-hand side we also have

$$\langle x|\hat{a}|\alpha\rangle = \alpha\langle x|\alpha\rangle = \alpha\psi_\alpha(x) \tag{0.1.117}$$

yielding

$$x_0 = \alpha\sqrt{\frac{2\hbar}{m\omega}} \tag{0.1.118}$$

It is left as an exercise tot he curious reader the explicit computation of $\langle x|\alpha\rangle$, which may be quite illustrative of the kind of computations one frequently finds in Heisenberg's formalism. Notice now that, as expected, the average value of $\hat{x}$ in $\alpha\rangle$ is shifted:

$$\begin{aligned}\langle\alpha|\hat{x}|\alpha\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\langle\alpha|\hat{a}+\hat{a}^\dagger|\alpha\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}}(\alpha+\alpha^*) = \sqrt{\frac{\hbar}{2m\omega}}2\Re\alpha \\ &= \sqrt{\frac{\hbar}{2m\omega}}2x_0\sqrt{\frac{m\omega}{2\hbar}} = x_0,\end{aligned} \tag{0.1.119}$$

where we have used (0.1.118)

Harmonic oscillator in configuration space

In the configuration space, the stationary Schrödinger wave eq. is given by (0.1.41):

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

Choosing, as before, the dimensionless coordinate

$$\tilde{x} = \sqrt{\frac{m\omega}{\hbar}}x, \tag{0.1.120}$$

one obtains

$$-\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\frac{d^2\psi}{d\tilde{x}^2} + \frac{1}{2}m\omega^2\frac{\hbar}{m\omega}\tilde{x}^2\psi = E\psi$$

which implifies to

$$\psi''(\tilde{x}) - \tilde{x}^2\psi(\tilde{x}) = -\frac{2E}{\hbar\omega}\psi(\tilde{x}) \tag{0.1.121}$$

Motivated by the fact that the homogeneous analog of (0.1.121) has the solution $\psi_{\text{homog}} = \exp\Big(-\frac{1}{2}\tilde{x}^2\Big)$, we propose the ansatz

$$\psi(\tilde{x}) = A\exp(-\frac{1}{2}\tilde{x}^2)u(\tilde{x}) \tag{0.1.122}$$

Inserting (0.1.122) in (0.1.121), we find

$$A\exp\Big(-\frac{1}{2}\tilde{x}^2\Big)\Big(u'' - 2\tilde{x}u' - u + \tilde{x}u - \tilde{x}u + \frac{2E}{\hbar\omega}u\Big) = 0, \tag{0.1.123}$$

wich can be rewritten simply as

$$u'' - 2\tilde{x}u' + (\lambda-1)u = 0 \quad \text{with} \quad \lambda = \frac{2E}{\hbar\omega} \tag{0.1.124}$$

A very similar differential equation was found by Hermite:

$$u'' - 2\tilde{x}u' + 2nu = 0, \tag{0.1.125}$$

who also demonstrated that $n \in \mathbb{Z}$ for (0.1.126) to have solutions[3]. This implies that

$$\lambda_n - 1 = 2n \Leftrightarrow \frac{2E_n}{\hbar\omega} = 2n+1, \quad n \in \mathbb{Z} \tag{0.1.126}$$

[3]See §13 of Arfken, Math. Meth. for Physicists. 1985; app A2 of De la Peña, Introducción a la Mecánica Cuántica

which coincides with the result we obtained before in terms of the number operator. The solution of (0.1.126) correspond to the Hermite polynomials, given by (0.1.96) or equivalently by

$$u(\tilde{x}) = H_n(\tilde{x}) = (-1)^n \exp(\tilde{x}^2)\frac{d^n}{d\tilde{x}^n}\exp(-\tilde{x}^2), \qquad n \in \mathbb{Z} \tag{0.1.127}$$

From our ansatsz (0.1.122), we obtain

$$\psi_n(\tilde{x}) = A_n \exp(-\frac{1}{2}\tilde{x}^2)H_n(\tilde{x}) \tag{0.1.128}$$

The normalization constants A_n can be computed by applying the orthogonality relation of Hermite polynomials

$$\int_{-\infty}^{\infty} d\tilde{x}\ \exp(-\tilde{x}^2)H_n(\tilde{x})H_m(\tilde{x}) = 2^n n!\sqrt{\pi}\delta_{n,m}, \tag{0.1.129}$$

as follows

$$1 = \int_{-\infty}^{\infty} \psi_n^*(x)\psi_{n'}(x) = \sqrt{\frac{\hbar}{m\omega}}\int_{-\infty}^{\infty} d\tilde{x}\,|A_n|^2 \exp(-\tilde{x}^2)H_n^2(\tilde{x}) = |A_n|^2\sqrt{\frac{\hbar}{m\omega}}2^n n!\sqrt{n}$$

Thus, we have

$$A_n = \left(\sqrt{\frac{\hbar\pi}{m\omega}}2^n n!\right)^{-1/2} \tag{0.1.130}$$

up to an unphysical phase[4]. Note that eqs. (0.1.130) and (0.1.128) yield our previous result, (0.1.95). Besided the contact of this formalism with some common mathematical tool, it is hard to identify a reason to prefer this method before Heisenberg's method with Dirac's ladder operators.

Free particle in one dimension

In contrast to the harmonic oscillator, a free particle has no potential bo bind it. Thus, it cannot be confined and can therefore have arbitrary energy. This is the simplest quantum system, but it is useful to make a couple of remarks. The Schrödinger's wave eq. is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \tag{0.1.131}$$

We can define the wave number

$$k^2 = \frac{2mE}{\hbar^2}\rangle 0, \tag{0.1.132}$$

which simplifies (0.1.131) to

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \tag{0.1.133}$$

whose solution is

$$\psi(x) = A\exp(ikx) + B\exp(-ikx) \tag{0.1.134}$$

From (0.1.40), we can easily obtain the time dependence of the wave-function as

$$\psi(x,t) = \exp(-i\omega t)\psi(x) = A\exp\Big(i(kx-\omega t)\Big) + B\exp\Big(-i(kx+\omega t)\Big) \tag{0.1.135}$$

where we defined $\omega = E/\hbar$ in agreement with Plack's hypothesis. We realize that the first term is right-moving "plane"-wave with phase velocity ω/k whereas the second term corresponds to a left-moving "plane"-wave. Clearly, left and right waves can be treated independently, reason why many authors disregard one of both waves. Let us now compute the momentum associated with $\psi(x)$ in (0.1.134). In the configuration space, we have

$$-i\hbar\frac{d}{dx}\psi(x) = -i\hbar(ik)\Big(A\exp(ikx) - B\exp(-ikx)\Big) \tag{0.1.136}$$

where, as expected, we see that the momentum of the first term is opposite to the one of the second term, and we identify the relation

$$p = \pm\hbar k \pm \sqrt{2mE} \tag{0.1.137}$$

[4]In QM, a physical state is not represented by a specific normalized vector on Hilber space, but by a ray, i.e., a class of all vectors differeing only a phase factors. So, these phases are not measurable and thus unphysical.

where the sign depends on the motion of the wave. Clearly, the normalization of the solution (0.1.134) cannot be done in a traditional from by simply setting

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)\, dx = 1$$

Dirac suggested to normalize by using a sort of orthonormality realtion. For simplicity, let us consider only a right-moving wave rewritten as

$$\psi_p(x) = A \exp\Big(\frac{i}{\hbar}px\Big) \tag{0.1.138}$$

where the index p labels the solution with momentum p. Let us compute

$$\int_{-\infty}^{\infty} \psi_p^*(x)\psi_{p'}(x)\, dx = |A|^2 \int_{-\infty}^{\infty} \exp\Big(\frac{i}{\hbar}x(p'-p)\Big)\, dx = |A|^2(2\pi\hbar)\delta(p'-p) \tag{0.1.139}$$

If we wish this eq. to be an orthonormality relation, the result should be $\delta(p'-p)$. Therefore, we identify

$$A = \frac{1}{\sqrt{2\pi\hbar}} \tag{0.1.140}$$

up to an unphysical phase. A similar discussion can be done for the left-moving part of $\psi(x)$. We obtain then

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\Big[\exp\big(i(kx-\omega t)\big) + \exp\big(-i(kx+\omega t)\big)\Big] \tag{0.1.141}$$

It is interesting to solve the problem in the momentum space. Recalling that (or simply using (0.1.58))

$$\langle p|\frac{\hat{p}^2}{2m}|\alpha\rangle = \frac{p^2}{2m}\langle p|\alpha\rangle = \frac{p^2}{2m}\phi_\alpha(p) \tag{0.1.142}$$

we find that the Schrödinger's wave equation to consider reads

$$\Big(\frac{p^2}{2m} - E\Big)\phi(p) = 0 \tag{0.1.143}$$

It is clear then that $\phi(p) = 0$ for all p, excepting when $p = \pm\sqrt{2mE} = \pm\hbar k$, coinciding with (0.1.137). That is,

$$\phi(p) = a\delta(p-\hbar k) + b\delta(p+k\hbar) \tag{0.1.144}$$

Notice that this result can equally be obtained by applying (0.1.56b) to (0.1.134) with the normalizatio constant (0.1.140)

$$\phi(p) = \int dx \frac{1}{\sqrt{2\pi\hbar}} \exp(-ipx/\hbar) \frac{1}{\sqrt{2\pi\hbar}}\Big[\exp(ikx) + \exp(-ikx)\Big] \tag{0.1.145}$$

$$= \frac{1}{2\pi\hbar}\int dx \Big[\exp\Big(-\frac{i}{\hbar}(p-k\hbar)x\Big) + \exp\Big(-\frac{i}{\hbar}(p+k\hbar)x\Big)\Big] \tag{0.1.146}$$

$$= \delta(p-k\hbar) + \delta(p+k\hbar) \tag{0.1.147}$$

and thus in the momentum representation, the wave function is

$$\phi(p,t) = \exp(-i\omega t)\Big[\delta(p-k\hbar) + \delta(p+k\hbar)\Big] \tag{0.1.148}$$

A final remark on the one-dimensional free particle concerns the equivalence of different potentials. It is evident that in the configuration space a constant shift in the energy by $V(x) = V_0 \in \mathbb{R}$ yields the same physics. According to (0.1.59), in the momentum space, although $V(x) = 0$ corresponds to $V(p) = 0$, $V(x) = V_0$ corresponds to

$$V(p-p') = \frac{1}{\sqrt{2\phi\hbar}}\int dx\, \exp\big(-i(p-p')x/\hbar\big)V_0 = V_0\delta(p-p') \tag{0.1.149}$$

which yields the wave equation

$$\frac{p^2}{2m}\phi(p) + \int dp'\, \frac{1}{\sqrt{2\pi\hbar}} V_0\delta(p-p')\phi(p') = E\phi(p),$$

that simplifies to

$$\frac{p^2}{2m}\phi(p) + V_0\phi(p) = E\phi(p) \tag{0.1.150}$$

Remark that (0.1.150) is very close to the analogous equation in the configuration space:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V_0\psi(x) = E\psi(x) \tag{0.1.151}$$

Linear potential

Let us study now a potential, whose solution will be useful whe dealing with approximative methods, such as the WKB approximation that we shall study latter. The linear potential is given by

$$V(x) = k|x| \tag{0.1.152}$$

and is depicted in the figure This potential is symmetric, i.e., invariant under space invsersion

$$x \to -x$$

which can be written in terms of the unitary parity operator $\hat{P}$ such that, in terms of operators,

$$\hat{P}^{-1}\hat{x}\hat{P} = -\hat{x} \tag{0.1.153}$$

and clearly satisfies

$$\hat{P}^2 = \not{1} \qquad \Rightarrow \qquad \hat{P}^{-1} = \hat{P} \tag{0.1.154}$$

An operator $\hat{A}$, such that

$$\hat{P}\hat{A}\hat{P} = -\hat{A} \tag{0.1.155}$$

is said to be odd under parity. If $\hat{A}$ is left invariant under the action of $\hat{P}$, then $\hat{A}$ is even. The position operator is odd. One can further conceive the eigenstates of $\hat{P}$ as

$$\hat{P}|\pm|\rangle = \pm 1|\pm|\rangle \tag{0.1.156}$$

where, an analogy with the operators, or state $|-1\rangle$ ($|+1\rangle$) is said to be odd (even) under parity. In the special situation when the Hamiltonian is parity invariant

$$\hat{P}\hat{H}\hat{P} = \hat{H} \qquad \Rightarrow \qquad [\hat{P}, \hat{H}] = 0, \tag{0.1.157}$$

that is, the (even or odd) eigenstates of $\hat{P}$ are also energy eigenstates. Furthermore, as we shall se in the next session, $[\hat{P}, \hat{P}] = 0$ implies thath parity is conserved. It then follows that stationary states of an even parity/parity-invariant Hamiltonian are eiger even or odd. For the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(|\hat{x}|),$$

we can see that (0.1.155) is satisfied independently of the parity of $\hat{p}$. However, as we shall also see in the next section, for a large class of models

$$\hat{p} = \frac{im}{\hbar}[\hat{H}, \hat{x}] \tag{0.1.158}$$

from which we observe that

$$\hat{P}\hat{p}\hat{P} = \frac{im}{\hbar}\hat{P}[\hat{H}, \hat{x}]\hat{P} = \frac{im}{\hbar}[\hat{H}, \hat{P}\hat{x}\hat{P}] = -\hat{p} \tag{0.1.159}$$

Turning back to our problem, with the potential (0.1.152), we can focus separately in even and odd solution $\psi(x)$ of

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + k|x|\psi(x) = E\psi(x) \tag{0.1.160}$$

Besides demanding that $\psi(x \to \infty) = 0$, we impose for odd solutions that

$$\psi(0) = 0 \qquad \text{because} \quad \psi(0) = -\psi(-0) \tag{0.1.161a}$$

and for even solutions that

$$\psi'(x=0) = 0 \qquad \text{because} \quad \psi'(0) = \lim_{\varepsilon \to 0} \frac{\psi(\varepsilon) - \psi(-\varepsilon)}{\varepsilon} = 0 \tag{0.1.161b}$$

for an infinitesimally small ε. We can rewrite (0.1.160) in terms of the dimensionless coordinate and energy

$$\tilde{x} = \left(\frac{\hbar^2}{mk}\right)^{-1/3} x, \quad \tilde{E} = \left(\frac{\hbar^2 k^2}{m}\right)^{-1/3} E, \tag{0.1.162}$$

as

$$-\frac{\hbar^2}{2m}\left(\frac{\hbar^2}{mk}\right)^{-2/3}\frac{d^2\psi}{d\tilde{x}^2}+\left(\frac{\hbar^2}{mk}\right)^{1/3}k|\tilde{x}|\psi=\left(\frac{\hbar^2k^2}{m}\right)^{1/3}\tilde{E}\psi$$

which is simplified to

$$\psi''-2(|\tilde{x}|-\tilde{E})\psi=0 \tag{0.1.163}$$

At the special point

$$|\tilde{x}|=\tilde{E}\Leftrightarrow E=k|x|, \tag{0.1.164}$$

$\psi(x)$ behaves linearly Classically, this point is a turning point, beyond which a particle with energy E cannot move. As we are about to see, in quantum mechanics, there is a tunneling effect which resides a non vanishing probability for the particle to appear beyond this point, that drops very fast. This behaviour can be easily realized by alowing the change of variable

$$y=2^{1/3}(\tilde{x}-\tilde{E}) \tag{0.1.165}$$

in eq. (0.1.163)

$$\frac{d^2\psi}{dy^2}-|y|\psi=0 \tag{0.1.166}$$

Eq. (0.1.166) is known as the Airy eq., whose solution is the Airy function

$$\psi(y)=\mathrm{Ai}(y) \tag{0.1.167}$$

depicted in the figure. The point $y=0$ corresonds to the classical turning point (0.1.164). The solution obtained here satisfies our expectation about linearity and tunneling effect. Since the potential (0.1.152) is bounded, there are bound states with quantized energies. The energy quantization arises, as frequently, from the boundary condition (0.1.161). For the odd solutions, we must impose that $\psi(x=0)=0$, which implies

$$\mathrm{Ai}(y_n=-2^{1/3}\tilde{E}_n)=0 \tag{0.1.168}$$

i.e., we must identify the zeroes y_n of Ai in order to compute the quantized energies E_n. For the even solutions, we impose $\psi'(x=0)=0$, that amount to demanding

$$\mathrm{Ai}'(y_n=-2^{1/3}\tilde{E}_n)=0, \tag{0.1.169}$$

i.e., we need now the zeroes of the derivative of the Airy function. Some zeroes of $\mathrm{Ai}(y)$ and $\mathrm{Ai}'(y)$ are given in the table. We realize that the lowest energy of the solutions, that is, the energy of the ground state is obtained for the even-parity state with $n=$

$$\begin{aligned}y_1=-1.02=-2^{1/3}\tilde{E}_1&=-2^{1/3}\left(\frac{\hbar^2k^2}{m}\right)^{-1/3}E_1\\ \Leftrightarrow E_1&=\left(\frac{\hbar^2k^2}{m}\right)^{1/3}1.02\end{aligned} \tag{0.1.170}$$

This apparently weird potential has found application especally in the study of a bound system composed of a quark and an antiquark, called quarkonian, where x is interpreted as the distance between these fundamental particles.

0.1.6 Heisenberg and Schrödinger pictures

Unitary operators and symmetry transformations

A symmetry principle is the statement that when we change our point of view in certain ways, the laws of nature do not change. Since states do not characterize any law of nature as they are not observed quantities, they can change. A state, under the action of a symmetry operator $\hat{U}$, is transformed as

$$|\alpha\rangle\mapsto\hat{U}|\alpha\rangle \tag{0.1.171}$$

Since physical laws must not change, in particular transition amplitudes and probability densities must remain invariante:

$$\langle\beta|\alpha\rangle\to\left(\langle\beta|\hat{U}\right)\left(\hat{U}|\alpha\rangle\right)=\langle\beta|\hat{U}^\dagger\hat{U}|\alpha\rangle=\langle\beta|\alpha\rangle \tag{0.1.172}$$

The invariance condition requires then that

$$\hat{U}^\dagger \hat{U} = 1, \tag{0.1.173}$$

i.e., that $\hat{U}$ be unitary. We already know three of this kind of ops.

$$\hat{U} = \exp(-i\hat{\vec{p}} \cdot \vec{x}/\hbar), \qquad \text{translation operator}, \tag{0.1.174a}$$

$$\hat{U} = \hat{U}(t, t_0) = \exp(-i\hat{H}t/\hbar), \qquad \text{time-evolution}, \tag{0.1.174b}$$

$$\hat{U} = \hat{P}, \qquad \text{parity operator}, \tag{0.1.174c}$$

Under the symmetry transformation (0.1.171), the expectation value of the operator $\hat{A}$ is subject to the transformation

$$\langle \hat{A} \rangle \mapsto \langle \alpha | \hat{U}^\dagger \hat{A} \hat{U} | \alpha \rangle \tag{0.1.175}$$

Note that this expression allows for two interpretations: either

- the state is transformed as (0.1.171) prescribes while the operator $\hat{A}$ is unchanged; or
- the state $|\alpha\rangle$ remains invariant while the op. $\hat{A}$ transforms as

$$\hat{A} \mapsto \hat{U}^\dagger \hat{A} \hat{U} \tag{0.1.176}$$

The transformation (0.1.176) is called a similarity transformation (or conjugation) and preserves algebraic relations, such as

$$\left(\hat{U}^\dagger \hat{A} \hat{U}\right)\left(\hat{U}^\dagger \hat{B} \hat{U}\right) = \hat{U}^\dagger \left(\right) \hat{U}, \tag{0.1.177a}$$

$$\hat{U}^\dagger \hat{A} \hat{U} + \hat{U}^\dagger \hat{B} \hat{U} = \hat{U}^\dagger \left(\hat{A} + \hat{B}\right) \hat{U}, \tag{0.1.177b}$$

Note that the second approach in which the operators change rather than the state is closer to our classical understanding of physics, where even the concept of state does not exist. As we shall see, the observation is true in more than one sense in the so-called Heisenberg picture.

Schrödinger vs Heisenberg picture

Let us now consider the time-evolution operator as $\hat{U}$:

$$\hat{U} = \hat{U}(t, t_0) = \exp\bigl(-i\hat{H}(t - t_0)/\hbar\bigr) \tag{0.1.178}$$

where the last equality is valid only for time-independent Hamiltonians. The interpretations of (0.1.175) lead to two equivalent schemes of the dynamics of a quantum system called pictures. The Schrödinger picture associates the dynamics of a system to the state, as described by (0.1.1)

$$|\alpha, t_0; t\rangle = \hat{U}(t, t_0)|\alpha\rangle,$$

i.e., it's the frame we have used so far. In the Schrödinger picture, the operators associated to observables do not evolve in time. The second scheme is called the Heisenberg picture. In this picture, the states $|\alpha\rangle$ remain unchanged whereas observables evolve as prescribed by (0.1.176), which allows one to relate both pictures:

$$\hat{A}_H(t) = \hat{U}^\dagger(t, 0)\hat{A}_S \hat{U}(t, 0), \tag{0.1.179}$$

valid also for time-dependent Hamiltonians. Here $\hat{A}_S$ denotes an arbitrary observable operator in the Schrödinger picture or at time $t_0 = 0$ in the Heisenberg picutre, whereas $\hat{A}_H(t)$ denotes the evolving observable operator at time t in the Heisenberg picture. In this picture, the states $|\alpha\rangle$ do not change,

$$|\alpha; t\rangle_H = |\alpha\rangle, \qquad \forall t, \tag{0.1.180}$$

where $|\alpha\rangle$ is the state at $t_0 = 0$ in the Schrödinger picture. Interestingly, the expectation values coincide in both pictures:

$$_S\langle\alpha; t|\hat{A}_S|\alpha; t\rangle_S = {}_S\langle\alpha|\hat{U}^\dagger(t,0)\hat{A}_S\hat{U}(t,0)|\alpha\rangle_S = {}_H\langle\alpha, t|\hat{A}_H(t)|\alpha, t\rangle_H$$

This is an important observation related to the fact that both pictures are equivalent, i.e., lead to the same physical observations.

Another important remark concerns the time-dependence of the operator $\hat{A}_S$. So far, our discussion seems to imply that $\hat{A}_S$ does not depend on time. However, a counterexample is simply to consider a time-dependent Hamiltonian (as in a time-changing magnetic field affecting an acelerated particle) in the Schrödinger picture. This time-dependence shall be independent of the time-evolution operator $\hat{U}(t,0)$ and is therefore additional to the time evolution of the operator $\hat{A}_H$ in the Heisenberg picture.

In the Heisenberg picture, the dynamics of the system are no longer generated by the Schrödinger equation, but by a differential equation containing the dynamics of the operators $\hat{A}_H$. To arrive at this eq., recall first that the Schrödinger equation for the time evolution operator reads:

$$i\hbar\frac{\partial\hat{U}}{\partial t} = \hat{H}\hat{U}, \tag{0.1.181}$$

Let us compute the derivative of $\hat{A}_H$

$$\begin{aligned}\frac{d}{dt}\hat{A}_H = \frac{d}{dt}\left(\hat{U}^\dagger\hat{A}_S\hat{U}\right) &= \left(\frac{\partial\hat{U}^\dagger}{\partial t}\right)\hat{A}_S + \hat{U}^\dagger\hat{A}_S\left(\frac{\partial\hat{U}}{\partial t}\right) + \hat{U}^\dagger\frac{\partial\hat{A}_S}{\partial t}\hat{U} \\ &= -\frac{1}{i\hbar}\hat{U}^\dagger\hat{H}\hat{A}_S\hat{U} + \frac{1}{i\hbar}\hat{U}^\dagger\hat{A}_S\hat{H}\hat{U} + \hat{U}^\dagger\frac{\partial\hat{A}_S}{\partial t}\hat{U},\end{aligned} \tag{0.1.182}$$

where we have used (0.1.181) and its conjugate. Since $\hat{U}$ is unitary,

$$\hat{U}^\dagger\hat{H}\hat{A}_S\hat{U} = \hat{U}^\dagger\hat{H}\hat{U}\hat{U}^\dagger\hat{A}_S\hat{U} = \hat{U}^\dagger\hat{H}\hat{U}\hat{A}_H(t) = \hat{H}\hat{A}_H(t) \tag{0.1.183}$$

wgere we have used the fact that $\hat{U}(t, t_0)$ commutes with $\hat{H}$. Repeating those steps for the second term in (0.1.182), we obtain

$$\frac{d}{dt}\hat{A}_H = \frac{1}{i\hbar}\left[\hat{A}_H(t), \hat{H}\right] + \hat{U}^\dagger\frac{\partial\hat{A}_S}{\partial t}\hat{U} \tag{0.1.184}$$

This is the celebrated Heisenberg equation of motion, which governs the time-evolution of a quantum system in the Heisenberg picture.

In the most common text-book cases, $\hat{A}_S$ does not depend on time. Thus, the Heisenberg equation reduces to

$$i\hbar\frac{d}{dt}\hat{A}_H = \left[\hat{A}_H, \hat{H}\right] \tag{0.1.185}$$

Note the enormous similarity with the classical Hamilton's equation

$$\frac{d}{dt}\hat{A}(p,q,t) = \left\{A(p,q,t), H\right\} + \frac{\partial A}{\partial t} \tag{0.1.186}$$

in terms of the Poisson bracket

$$\left\{A, H\right\} = \frac{\partial A}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial H}{\partial q} \tag{0.1.187}$$

for $A = A(p,q,t)$ an arbitrary function of the canonical coordinates (p,q) and time, and the classical Hamiltonian H. For some applications, it turns out to be useful that in comparing (0.1.184) and (0.1.186), it seems that they can be related to each other by replacing the Poisson bracket by the commutator, up to a factor $i\hbar$:

$$\underset{\text{classical}}{\left\{,\right\}} \leftrightarrow \underset{\text{quantum}}{\tfrac{1}{i\hbar}\left[,\right]} \tag{0.1.188}$$

It can easily be tested by noticing that $\{x, p\} = 1$ while $[\hat{x}, \hat{p}] = i\hbar$.

The Ehrenfest theorem

Let us consider again the simplest time-independent Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{x})$$

The position operator $\hat{x}$ commutes with $\hat{V}(\hat{x})$, but does not commute with $\hat{p}^2$. Thus, the commutator of $\hat{x}$ with $\hat{H}$ reads

$$\left[\hat{x}, \hat{H}\right] = \frac{1}{2m}\left[\hat{x}, \hat{p}\right] = \frac{1}{2m}\Big(\left[\hat{x}, \hat{p}\right]\hat{p} + \hat{p}\left[\hat{x}, \hat{p}\right]\Big) = \frac{i\hbar}{m}\hat{p} \tag{0.1.189}$$

Hence, the equation of motion for $\hat{x}$ in the Heisenberg picture is given by

$$m\frac{d\hat{x}_H}{dt} = \hat{p}_H, \tag{0.1.190}$$

which resembles the clasical relation. Further, we can determine the Heisenberg equation for $\hat{p}$ by realizing e.g. in the configuration space that

$$\left[\hat{p}, f(\hat{x})\right] = -i\hbar f'(\hat{x}) \tag{0.1.191}$$

Therefore, we have

$$\left[\hat{p}, \hat{H}\right] = \left[\hat{p}, \hat{V}(\hat{x})\right] = -i\hbar\hat{V}', \tag{0.1.192}$$

whence

$$\frac{d\hat{p}_H}{dt} = -\hat{V}', \tag{0.1.193}$$

where the prime denotes the derivative w.r.t. $\hat{x}$. Putting together (0.1.190) and (0.1.193) we find a well-known relation

$$m\frac{d^2\hat{x}_H}{dt^2} = -\hat{V}', \tag{0.1.194}$$

which represents the quantum analogous of Newton's second law.

We can generalize (0.1.194) in 3D to yeld

$$m\frac{d\hat{\vec{x}}_H}{dt^2} = -\bar{\nabla}\hat{V}(\hat{\vec{x}}). \tag{0.1.195}$$

This relation is valid in the Heisenberg picture. To obtain a more general equation, let us take the expectation values in a general state $|\alpha\rangle$ in the Heisenberg picture. Note first that

$$\langle\alpha|m\frac{d^2\hat{\vec{x}}}{dt^2}|\alpha\rangle = m\frac{d^2}{dt^2}\langle\alpha|\hat{\vec{x}}|\alpha\rangle = m\frac{d^2\langle\hat{x}\rangle}{dt^2}, \tag{0.1.196}$$

and thus

$$m\frac{d^2\langle\hat{x}\rangle}{dt^2} = -\big\langle\vec{\nabla}V\big(\hat{\vec{x}}\big)\big\rangle. \tag{0.1.197}$$

Eq. (0.1.197) is know as the Ehrenfest theorem. Since expectation values coincide in Schrödinger and Heisenberg pictures, the Ehrenfest theorem is valid in general, despite the fact that we deduced it in a specific picture. Note that a similarly general result can be achieved by averaging Heisenberg equation (0.1.185)

$$i\hbar\frac{d}{dt}\langle\hat{A}\rangle = \Big\langle\left[\hat{A}, \hat{H}\right]\Big\rangle. \tag{0.1.198}$$

Time evolution of the harmonic oscillator in 1D

By applying the Heisenberg equation with the potential (0.1.66)

$$\hat{V}(\hat{x}) = \frac{1}{2}m\omega^2\hat{x}^2,$$

we find

$$\frac{d\hat{p}}{dt} = -\frac{d\hat{V}}{d\hat{x}} = -m\omega^2\hat{x}. \tag{0.1.199}$$

The Heisenberg equation for $\hat{x}$ is still given by (0.1.190)

$$m\frac{d}{dt}\hat{x} = \hat{p}, \tag{0.1.200}$$

Solving (0.1.199) and (0.1.200) simplifies greatly by using once again the formalism of Dirac's operators (0.1.67). From the definition of the annihilation operator

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x} + \frac{i\hat{p}}{m\omega}\Big),$$

we see in the Heisenberg picture that

$$\begin{aligned}\frac{d\hat{a}}{dt} &= \sqrt{\frac{m\omega}{2\hbar}}\Big(\frac{d\hat{x}}{dt} + \frac{i}{m\omega}\frac{d\hat{p}}{dt} = \sqrt{\frac{m\omega}{2\hbar}}\Big(\frac{\hat{p}}{m} - \frac{i}{m\omega}m\omega^2\hat{x}\Big)\\ &= \sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{p}m - i\omega\hat{x}\Big) = -i\omega\hat{a}\Big),\end{aligned} \tag{0.1.201}$$

from which trivially follows

$$\frac{d\hat{a}^\dagger}{dt} = i\omega\hat{a}^\dagger. \tag{0.1.202}$$

We have now a system of decoupled differential equations, whose solutions are

$$\hat{a}(t) = \hat{a}(0)\exp(-i\omega t), \qquad \hat{a}^\dagger(0) = \hat{a}^\dagger(0)\exp(i\omega t) \tag{0.1.203}$$

Notice that the number operator

$$\hat{N}(t) = \hat{a}^\dagger(t)\hat{a}(t) = \hat{a}^\dagger(0)\hat{a}(t)$$

is time-independent, as expected because the Hamiltonian does not depend on time. (Recall that $\hat{H} = \hbar\omega(\hat{N} + 1/2)$.)

Writing $\hat{x}(t)$ in terms of $\hat{a}(t)$ and $\hat{a}^\dagger(t)$, we obtain

$$\begin{aligned}\hat{x}(t) &= \sqrt{\frac{\hbar}{2m\omega}}\Big[\hat{a}(t) + \hat{a}^\dagger(t)\Big] = \sqrt{\frac{\hbar}{2m\omega}}\Big[\hat{a}(0)\exp(-i\omega t) + \hat{a}^\dagger(0)\exp(i\omega t)\Big]\\ &= \sqrt{\frac{\hbar}{2m\omega}}\Big[\big(\hat{a}(0) + \hat{a}^\dagger(0)\big)\cos\omega t + i\big(\hat{a}^\dagger(0) - \hat{a}(0)\big)\sin\omega t\Big]\\ &= \sqrt{\frac{\hbar}{2m\omega}}\Big[\sqrt{\frac{2m\omega}{\hbar}}\hat{x}(0)\cos\omega t + \sqrt{\frac{2}{m\hbar\omega}}\hat{p}(0)\sin\omega t\Big].\end{aligned}$$

which is simplified to

$$\hat{x}(t) = \hat{x}(0)\cos\omega t + \frac{\hat{p}(0)}{m\omega}\sin\omega t. \tag{0.1.204}$$

Analogously, one can verify that

$$\hat{p}(t) = \hat{p}(0)\cos\omega t - m\omega\hat{x}(0)\sin\omega t. \tag{0.1.205}$$

Let us now figure out the time evolution of canonical coherent states. Recall that from their definition (0.1.106), they are eigenstates of the annihilation operator, satisfying at $t_0 = 0$

$$\hat{a}(0)|\alpha\rangle = \alpha|\alpha\rangle \tag{0.1.206}$$

It then follows thath the expected value of $\hat{x}(t)$ is

$$\begin{aligned}\langle\hat{x}(t)\rangle_\alpha = \langle\alpha|\hat{x}(t)|\alpha\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\langle\alpha|\hat{a}(0)\exp(-i\omega t) + \hat{a}^\dagger(0)\exp(i\omega t)|\alpha\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}}\Big(\alpha\exp(-i\omega t) + \alpha^*\exp(i\omega t)\Big) \\ &= \sqrt{\frac{\hbar}{2m\omega}}2\Re\alpha\cos\omega t \\ &= x_0\cos\omega t,\end{aligned} \tag{0.1.207}$$

where we have adopted the result obtained in

$$\alpha = x_0\sqrt{\frac{m\omega}{2\hbar}} \in \mathbb{R}. \tag{0.1.208}$$

Note that the oscillating behavior $\langle\hat{x}(t)\rangle_\alpha$ mathces the classical result, displaying again the characteristic features of coherent states.

We are now in position to compute the wave function of canonical coherent states including their time evolution. Notice first that (0.1.206) can be rewritten as

$$\hat{a}(0)|\alpha\rangle = \hat{a}(t)\exp(i\omega t)|\alpha\rangle = \sqrt{\frac{m\omega}{2\hbar}}x_0|\alpha\rangle, \tag{0.1.209}$$

where we have used (0.1.208).

In the configuration space, (0.1.209) yields

$$\exp(i\omega t)\langle x|a(t)|\alpha\rangle = x_0\sqrt{\frac{m\omega}{2\hbar}}\langle x|\alpha\rangle. \tag{0.1.210}$$

The left-hand side of (0.1.210) multiplied by $\omega\exp(-i\omega t)$ leads to

$$\begin{aligned}\omega\langle x|\sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x}(t) + \frac{i\hat{p}(t)}{m\omega}|\alpha\rangle &= \omega\int dx'\,\langle x|\Big(\hat{x} + \frac{i\hat{p}}{m\omega}\Big)|x'\rangle\langle x'|\alpha\rangle\sqrt{\frac{m\omega}{1\hbar}} \\ &= \omega\Big(x + \frac{\hbar}{m\omega}\frac{d}{dt}\Big)\langle x|\alpha\rangle\sqrt{\frac{m\omega}{2\hbar}}\Big)\end{aligned} \tag{0.1.211}$$

where we omit the time dependence of $\hat{x}$ and $\hat{p}$ to simplify the notation.

Defining $\psi_\alpha(x,t) \equiv \langle x|\alpha\rangle$ and multiplying by $\omega\exp(-i\omega t)$ also the right hand side of (0.1.210), we obtain

$$\omega\Big(x + \frac{\hbar}{m\omega}\frac{d}{dx}\Big)\psi_\alpha(x,t) = \omega x_0\exp(-i\omega t)\psi_\alpha(x,t), \tag{0.1.212}$$

which, rewritten in the form

$$\frac{d}{dx}\psi_\alpha(x,t) = -\frac{m\omega}{\hbar}(x - x_0\exp(-i\omega t))\psi_\alpha(x,t) \tag{0.1.213}$$

has the direct solution

$$\psi_\alpha = A(t)\exp^{-\frac{m\omega}{2\hbar}(x - x_0\exp(-i\omega t))^2} \tag{0.1.214}$$

Note that (0.1.214) is very similar to the time-independent solution (0.1.115). The difference is now that the shift of the Gaussian is time-dependent.

This is easily explained considering that the expected value of $\hat{x}$ in the state described by (0.1.115) is $\langle\hat{x}\rangle = x_0$ (c.f. (0.1.119)), whereas in the time-dependent solution (0.1.214) it is $\langle\hat{x}(t)\rangle = x_0\cos\omega t$, (0.1.207). However, (0.1.214) is shifted by more than only $\langle\hat{x}\rangle$; it contains one additional shift by $ix_0\sin\omega t$. Rewritting the exponent in (0.1.214) in terms of the expected values (0.1.207) and

$$\langle\hat{p}(t)\rangle_\alpha = -m\omega x_0\sin\omega t, \tag{0.1.215}$$