Quantum Mechanics

Saúl Ramos-Sánchez

12 de septiembre de 2015

1. Schrödinger equation

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 $|\alpha>$ 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

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

such that

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

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

$$|\alpha, t_0; t>= \hat{U}(t, t_0)|\alpha> \tag{1.1}$$

The time-evolution operator has the following properties:

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

  $$|\alpha>= \sum_a |a>< a|\alpha, t_0; t>= \sum_a c_a(t_0)|a> \tag{1.2}$$

  Thus, at a later time $t > t_0$ we have

  $$|\alpha, t_0; t>= \sum_a c_a(t)|a> \tag{1.3}$$

  where $c_a(t)$ is the prob. amp. of finding $|\alpha>$ at $|a>$. 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.,

  $$\sum_a |c_a(t)|^2 = \sum_a |c_a(t_0)|^2 = 1 \tag{1.4}$$

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

$$< \alpha|\alpha >= \sum_{a'}\sum_{a} c^*_{a'}(t_0) < a'|a > c_a(t_0) = \sum_{a} |c_a(t_0)|^2 = 1 \tag{1.5}$$

and consequently

$$< \alpha, t_0; t|\alpha, t_0; t >= \sum_{a} |c_a(t)|^2 = 1 \tag{1.6}$$

That is, the state $|\alpha>$ remain normalized at all times. For terms of 1.1, this is satisfied as long as

$$\hat{U}^\dagger(t, t_0)\hat{U}(t, t_0) = 1 \tag{1.7}$$

- Time composition:

$$\hat{U}(t_2, t_0) = \hat{U}(t_2, t_1)\hat{U}(t_1, t_0) \qquad t_0 < t_1 < t_2 \tag{1.8}$$

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

$$|\alpha, t_0; t_0 + dt >= \hat{U}(t_0 + dt, t_0)|\alpha >, \qquad \lim_{dt\to 0} \hat{U}(t_0 + dt, t_0) = 1 \tag{1.9}$$

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

$$\hat{U}(t_0 + dt, t_0) = 1 - i\Omega\hat{)}dt \tag{1.10}$$

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

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

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

$$\hat{\Omega} = \frac{\hat{H}}{\hbar} \tag{1.11}$$

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

$$\hat{U}(t_0 + dt, t_0) = 1 - \frac{i}{\hbar}\hat{H}dt \tag{1.12}$$

for (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

$$\hat{U}(t + dt, t_0) = \hat{U}(t + dt, t)\hat{U}(t, t_0) = (1 - \frac{i}{\hbar}\hat{H}dt)\hat{U}(t, t_0) \tag{1.13}$$

Note now that

$$\hat{U}(t+dt,t_0)-\hat{U}(t,t_0)=-\frac{i}{\hbar}\hat{H}dt\hat{U}(t,t_0) \tag{1.14}$$

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

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t_0,t)=\hat{H}\hat{U}(t,t_0) \tag{1.15}$$

This is the Schrödinger equation for the time-evolution operator and is the most fundamental equation of quantum mechanics. Multiplying (1.15) by the ket $|\alpha>=|\alpha,t_0;t_1>$, we find

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

$$i\hbar\frac{\partial}{\partial t}|\alpha,t_0;t>=\hat{H}|\alpha,t_0;t> \tag{1.16}$$

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 (1.15):

$$\hat{U}(t,t_0)=\exp(-\frac{i}{\hbar}H(t-t_0)) \tag{1.17}$$

which makes sense in general as the series

$$\hat{U}(t,t_0)=1-\frac{i}{\hbar}\hat{H}(t-t_0)+\frac{1}{2!}\Big(\frac{-i}{\hbar}\hat{H}(t-t_0)\Big)^2 \tag{1.18}$$

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 (1.15) reads

$$\hat{U}(t,t_0)=\exp\Big(-\frac{i}{\hbar}\int_{t_0}^{t}dt'\,\hat{H}(t')\Big) \tag{1.19}$$

To solve (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

$$\hat{U}(t,t_0)=1-\frac{i}{\hbar}\int_{t_0}^{t}dt'\,\hat{H}(t')\hat{U}(t',t_0) \tag{1.20}$$

By iteration, we can find the approximate solution

$$\begin{aligned}
\hat{U}(t,t_0) &= 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t')\Big[1 - \frac{i}{\hbar}\int_{t_0}^{t'} dt'\,\hat{H}(t'')\hat{U}(t'',t_0)\Big] \\
&= 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t') + \Big(\frac{-i}{\hbar}\Big)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t')\hat{H}(t'')\hat{U}(t'',t_0) \\
&= 1 + \sum_{n=1}^{\infty}\Big(\frac{-i}{\hbar}\Big)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{n-1} dt_n\,\hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n)
\end{aligned} \tag{1.21}$$

well-known as the Dyson series.

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 $|\alpha>$. This is particularly simple if we expand $|\alpha>$ in the basis of eigenstates $|a>$ of an operator $\hat{A}$, such that

$$[\hat{A},\hat{H}] = 0 \tag{1.22}$$

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

$$\hat{H}|a>= E_a|a> \tag{1.23}$$

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

$$\begin{aligned}
\hat{U}(t,0) = \exp\Big(-\frac{i}{\hbar}\hat{H}t\Big) &= \sum_{a'}|a'><a'|\exp(-i\hat{H}t/\hbar)\sum_{a}|a><a| \\
&= \sum_{a,a'}|a'><a|<a'|\exp(-i\hat{H}t/\hbar)|a> \\
&= \sum_{a}\exp(-iE_a t/\hbar)|a><a|
\end{aligned} \tag{1.24}$$

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

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

where we realize the time evolution of the expansion coefficients.

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

$$|a;t>= \exp(-iE_a t/\hbar)|a> \tag{1.25}$$

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

1.3. Expectation values

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

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

as given in (1.26). The expectation value is computed as

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

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

$$< \hat{B} >=< a; t|\hat{B}|a; t >=< a|\hat{B}|a > \tag{1.26}$$

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

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

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

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

1.4. Schrödinger's wave equation

1.4.1. Schrödinger's equation in space representation

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

$$\hat{\vec{x}}|\vec{x}' >= \vec{x}'|\vec{x}' > \tag{1.27}$$

Thier orthonormality is given by

$$< \vec{x}|\vec{x}' >= \delta^3(\vec{x} - \vec{x}') \tag{1.28}$$

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

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

where $\psi_\alpha(\vec{x})$ is usually called the wave function of the state $|\alpha >$ in the representation of positions. Note that the interpretation of $\psi_\alpha(\vec{x})$ is analogous to that of the expansion coefficient $c_a =< a|\alpha >$ 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 $<\beta|\hat{A}|\alpha>$ for some states $|\alpha>$, $|\beta>$, in the position basis

$$
\begin{aligned}
<\beta|\hat{A}|\alpha> &= \int d^3x \int d^3x' \; <\beta|\vec{x}><\vec{x}|\hat{A}|\vec{x}'><\vec{x}'|\alpha> \\
&= \int d^3x \int d^3x' \, \psi^*_\beta <\vec{x}|\hat{A}|\vec{x}'> \psi_\alpha(\vec{x}') \qquad (1.29)
\end{aligned}
$$

which depends on the matrix element $<\vec{x}|\hat{A}|\vec{x}'>$ 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

$$
\hat{A} = \frac{1}{2} m\omega^2 \vec{x}^2 \qquad (1.30)
$$

In this case, the matrix element in (1.29) looks like

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

where we have used (1.27) and (1.28) in ther 1D versions. This expresion can be generalized for $\hat{A} = f(\hat{\vec{x}})$ to

$$
<\vec{x}|f(\hat{\vec{x}})|\vec{x}'> f(\vec{x}')\delta^3(\vec{x} - \vec{x}') \qquad (1.31)
$$

and thus we obtain in this case

$$
<\beta|\hat{A}|\alpha> = \int d^3x \, \psi^*_\beta f(\vec{x}) \psi_\alpha(\vec{x}) \qquad (1.32)
$$

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

$$
\begin{aligned}
<\vec{x}|\hat{\vec{p}}|\alpha> &= \int d^3x' \; <\vec{x}|\vec{x}'><\vec{x}'|\hat{\vec{p}}|\alpha> = \int d^3x' \, \delta^3(\vec{x} - \vec{x}') \int d^3x'' \; <\vec{x}'|\hat{\vec{p}}|\vec{x}''><\vec{x}''|\alpha> \\
&= \int d^3x'' \; <\vec{x}|\hat{\vec{p}}|\vec{x}''> \psi_\alpha(\vec{x}'') \\
&= \int d^3x'' \delta^3(\vec{x} - \vec{x}')\big(-i\hbar\vec{\nabla}''\big)\psi_\alpha(\vec{x}'') \\
&= -i\hbar\vec{\nabla}\psi_\alpha(\vec{x}) \qquad (1.33)
\end{aligned}
$$

Let us now consider the Schrödinger equaiton, (1.16),

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

in the position representation, with a Hamiltonian operator given by

$$
\hat{H} = \frac{1}{2m}\hat{\vec{p}}^2 + \hat{V}(\hat{\vec{x}}) \qquad (1.34)
$$

where $\hat{V}(\hat{\vec{x}})$ is a polynomial function of $\hat{\vec{x}}$ and, thush, a Hamiltonian operator. From (1.33), we see that

$$
<\vec{x}|\hat{V}(\hat{\vec{x}})|\vec{x}'> = V(\vec{x}'')\delta^3(\vec{x} - \vec{x}') \qquad (1.35)
$$

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

Multiplying the Schrödinger equation for states (1.16) by the bra $<\vec{x}|$ we find

$$i\hbar\frac{\partial}{\partial t} <\vec{x}|\alpha, t_0; t> = <\vec{x}|\frac{1}{2m}\hat{\vec{p}}^2|\alpha, t_0; t> + <\vec{x}|\hat{V}(\hat{\vec{x}})|\alpha, t_0; t>$$
$$= \frac{1}{2m}(-i\hbar\vec{\nabla})^2 <\vec{x}|\alpha, t_0; t> + V(\vec{x}) <\vec{x}|\alpha, t_0; t> \quad (1.36)$$

where we have used (1.33) and (1.32) with $<\beta| = <\vec{x}|$. Defining

$$\psi_\alpha(\vec{x}, t) \equiv <\vec{x}|\alpha, t_0; t>, \quad (1.37)$$

we obtain the time-dependent Schrödinger's wave equation

$$i\hbar\frac{\partial}{\partial t}\psi_\alpha(\vec{x}, t) = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_\alpha(\vec{x}, t) + V(\vec{x})\psi_\alpha(\vec{x}, t) \quad (1.38)$$

The stationary wave equation is obtained when $|\alpha> = |a>$ is an energy eigenstate and thus stationary. From (1.25) we have that

$$<\vec{x}|\alpha; t> = <\vec{x}|a; t> = \exp(-iE_a t/\hbar) <\vec{x}|a> = \exp(-iE_\alpha t/\hbar) <\vec{x}|\alpha>$$
$$\Leftrightarrow \psi_\alpha(\vec{x}, t) = \exp(-iE_\alpha t/\hbar)\psi_\alpha(\vec{x}) \quad (1.39)$$

where we have defined $\psi_\alpha(\vec{x}) \equiv <\vec{x}|\alpha>$ in analogy with (1.37). It then follows that (1.38) becomes

$$E_\alpha\psi_\alpha(\vec{x}) = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_\alpha(\vec{x}) + V(\vec{x})\psi_\alpha(\vec{x}) \quad (1.40)$$

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

1.4.2. 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

$$\hat{\vec{p}}|\vec{p}\,'> = \vec{p}\,'|\vec{p}\,'>, \quad (1.41)$$

satisfying the orthonormality condition

$$<\vec{p}|\vec{p}\,'> = \delta^3(\vec{p} - \vec{p}\,') \quad (1.42)$$

and the completeness relation

$$1 = \int d^3p|\vec{p}><\vec{p}| \quad (1.43)$$

An arbitrary state in the basis reads

$$|\alpha> = \int d^3\,p|\vec{p}><\vec{p}|\alpha> = \int d^3|, \phi_{\alpha(\vec{p})}|\vec{p}> \quad (1.44)$$

where we have defined the momentum-space wave function

$$\phi_\alpha(\vec{p}) \equiv <\vec{p}|\alpha> \quad (1.45)$$

normalized as

$$\int d^3p\,|\phi_\alpha(\vec{p})|^2 = \int d^3p\ <\alpha|\vec{p}><\vec{p}|\alpha> = <\alpha|\alpha> = 1 \quad (1.46)$$

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

$$\phi_\alpha(\vec{p}) =< \vec{p}|\alpha >= \int d^3x \ < \vec{p}|\vec{x} >< \vec{x}|\alpha >= \int d^3x \ < \vec{p}|\vec{x} > \psi_\alpha(\vec{x}) \tag{1.47}$$

and conversely

$$\psi_\alpha(\vec{x}) = \int d^3x \ < \vec{x}|\vec{p} > \phi_\alpha(\vec{p}) \tag{1.48}$$

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

$$\begin{aligned} < \vec{x}|\hat{\vec{p}}|\vec{p} > &= \int d^3x' \ < \vec{x}|\hat{\vec{p}}|\vec{x}' >< \vec{x}'|\vec{p} > \\ &= -i\hbar\vec{\nabla} < \vec{x}|\vec{p} > \end{aligned} \tag{1.49}$$

which, using (1.41), implies

$$\vec{p} < \vec{x}|\vec{p} >= -i\hbar\vec{\nabla} < \vec{x}|\vec{p} > \tag{1.50}$$

whose solution reads

$$< \vec{x}|\vec{p} >= N \exp(i\vec{p}\cdot\vec{x}/\hbar) \tag{1.51}$$

The normalization factor can easily be found by computing

$$\begin{aligned} < \vec{x}|\vec{x}' > &= \int d^3p \ < \vec{x}|\vec{p} >< \vec{p}|\vec{x}' > \\ &= N^2 \int d^3p \exp\Big(-i\vec{p}\cdot(\vec{x}-\vec{x}')/\hbar\Big) \\ &= N^2(2\pi\hbar)^3\delta^3(\vec{x}-\vec{x}') \end{aligned} \tag{1.52}$$

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

$$N^2 = (2\pi\hbar)^{-3} \tag{1.53}$$

Replacing into (1.51), we find that

$$< \vec{x}|\vec{p} >= \frac{1}{(2\pi\hbar)^{3/2}} \exp(i\vec{p}\cdot\vec{x}/\hbar) \tag{1.54}$$

It then follows from (1.47) and (1.48) that $\phi_\alpha(\vec{p})$ is just the Fourier transform of $\psi_\alpha(\vec{x})$, and vice versa

$$\psi_\alpha(\vec{x}) = \int d^3x \, \frac{1}{2\pi\hbar}^{3/2} \exp\Big(i\vec{p}\cdot\vec{x}/\hbar\Big)\phi_{\alpha(\vec{p})} \tag{1.55}$$

$$\phi_\alpha(\vec{p}) = \int d^3x \, \frac{1}{2\pi\hbar}^{3/2} \exp\Big(-i\vec{p}\cdot\vec{x}/\hbar\Big)\psi_\alpha(\vec{x}) \tag{1.56}$$

Let us use these results to find the Schrödinger's wave equation in momentum space for the Hamiltonian (1.34), defining additionally

$$\phi_\alpha(\vec{p}, t) \equiv< \vec{p}|\alpha, t_0; t > \tag{1.57}$$

We have

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

which finally yields

$$
i\hbar\frac{\partial}{\partial t}\phi_\alpha(\vec{p},t) = \frac{\vec{p}^2}{2m}\phi_\alpha + \frac{1}{(2\pi\hbar)^{3/2}}\int d^3p' \, V(\vec{p}-\vec{p}')\phi_\alpha(\vec{p},t) \tag{1.58}
$$

where

$$
V(\vec{p}-\vec{p}') \equiv \frac{1}{(2\pi\hbar)^{3/2}}\int \exp(-i(\vec{p}-\vec{p}'')\cdot\vec{x}/\hbar)V(\vec{x})\, d^3x \tag{1.59}
$$

1.4.3. Continuity equation

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

$$
\rho \equiv \psi_\alpha^*(\vec{x},t)\psi_\alpha(\vec{x},t) \tag{1.60}
$$

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

$$
\begin{aligned}
\frac{\partial\rho}{\partial t} &= \psi_\alpha^*\frac{\partial}{\partial t}\psi_\alpha + \frac{\partial}{\partial t}\psi_\alpha^*\psi_\alpha \\
&= \psi_\alpha^*\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_\alpha + V\psi_\alpha\right) - \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_\alpha^* + V\psi_\alpha^*\right)\psi_\alpha \\
&= \frac{i\hbar}{2m}\left[\psi_\alpha^*\vec{\nabla}^2\psi_\alpha - (\vec{\nabla}^2\psi_\alpha^*)\psi_\alpha\right] \\
&= \frac{i\hbar}{2m}\left[\vec{\nabla}\big(\psi_\alpha^*\cdot\vec{\nabla}\psi_\alpha\big) - \vec{\nabla}\psi_\alpha^*\cdot\vec{\nabla}\psi_\alpha - \vec{\nabla}\cdot\big((\vec{\nabla}\psi_\alpha^*)\psi_\alpha\big) + \vec{\nabla}\psi_\alpha^*\cdot\vec{\nabla}\psi_\alpha\right] \\
&= \frac{i\hbar}{2m}\vec{\nabla}\cdot\left(\psi_\alpha^*\vec{\nabla}\psi_\alpha - (\vec{\nabla}\psi_\alpha^*)\psi_\alpha\right) \\
&= -\vec{\nabla}\vec{j}
\end{aligned} \tag{1.61}
$$

where

$$\vec{j} \equiv \left(\psi_\alpha^* \vec{\nabla}\psi_\alpha - (\vec{\nabla}\psi_\alpha^*)\psi_\alpha\right)\frac{i\hbar}{2m} \tag{1.62}$$

Rewriting (1.61) in these terms, we find

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0 \tag{1.63}$$

which coincides with the well-known continuity equation for a probability density ρ and a probability current $\vec{j}$, defined respectively by (1.60) & (1.62) It's interesting to realize that any continuity relation reveals a conserved quantity. In this case, the proability

$$P = \int d^3x\, \rho \tag{1.64}$$

is conserved (as expected):

$$\frac{dP}{dt} = \int_V d^3x\, \frac{\partial p}{\partial t} = -\int_{\partial V} d\vec{S}\cdot\vec{j} = 0 \tag{1.65}$$

which vanishes on ly if (1.62) vanishes at the boundary ∂V located infinitely far away. This condition is satisfied because $\lim\limits_{\vec{x}\to\infty} \psi_\alpha(\vec{x},t) = 0$ is a condition of square integrability, i.e., for P in (1.64) to be finite always.

1.5. Elementary 1 quantum systems

1.5.1. 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

$$\hat{V}(\hat{x}) = \frac{1}{2}m\omega^2\hat{x}^2 \tag{1.66}$$

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"

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right) \tag{1.67a}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right) \tag{1.67b}$$

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

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) \tag{1.68a}$$

$$\hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^\dagger - i\hat{a}) \tag{1.68b}$$

The ladder operators do not commute:

$$\begin{aligned}
[\hat{a},\hat{a}^\dagger] &= \frac{m\omega}{2\hbar}\left([\hat{x}, -\frac{i\hat{p}}{m\omega}] + [-\frac{i\hat{p}}{m\omega}, \hat{x}]\right) \\
&= \frac{i}{2\hbar}\left(-[\hat{x},\hat{p}] + [\hat{p},\hat{x}]\right)
\end{aligned} \tag{1.69}$$

Defining the so-called "number operator"

$$\hat{N} \equiv \hat{a}\hat{a}^\dagger \tag{1.70}$$

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

$$\begin{aligned}\hat{N} &= \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\right) + \frac{i}{2\hbar}[\hat{x}, \hat{p}] \\ &= \frac{1}{\hbar\omega}\left(\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right) - \frac{1}{2}\end{aligned} \tag{1.71}$$

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

$$\hat{H} = \hbar\omega\left(\hat{N} + 1/2\right) \tag{1.72}$$

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

$$\hat{N}|n >= n|n > \tag{1.73}$$

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

$$\hat{H}|n >= \hbar\omega(n + 1/2)|n > \tag{1.74}$$

Inserting (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 $|n >$. We can determine the values that n can take by exploring the action of the ladder operators on $|n >$. Note first that

$$\begin{aligned}[\hat{N}, \hat{a}^\dagger] &= [\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger \\ [\hat{N}, \hat{a}] &= [\hat{a}^\dagger\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}]\hat{a} = -\hat{a}\end{aligned} \tag{1.75}$$

where (1.69) has been used. Applying these results, we readily see that

$$\hat{N}(\hat{a}^\dagger|n >) = \left([\hat{N}, \hat{a}^\dagger] + \hat{a}^\dagger\hat{N}\right)|n >= (n+1)(\hat{a}^\dagger|n >) \tag{1.76a}$$

$$\hat{N}(\hat{a}|n >) = \left([\hat{N}, \hat{a}] + \hat{a}\hat{N}\right)|n >= (n-1)(\hat{a}|n >) \tag{1.76b}$$

Eq (1.76a) implies that $\hat{a}^\dagger|n >$ has the same eigenvalues as the state $|n+1 >$ or, in other words, that the action of the operator $\hat{a}^\dagger$ raises a state from $|n >$ to $|n+1 >$. Analogously, $\hat{a}$ lowers the state from $|n >$ to $|n-1 >$. 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

$$\begin{aligned}\hat{a}|n > &= c|n-1 > \\ \hat{a}^\dagger|n > &= d|n+1 >\end{aligned} \tag{1.77}$$

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 $\hat{a}|n >$ is computed as

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

which implies

$$|c|^2 = n \tag{1.78}$$

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

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

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

$$c = \sqrt{n} \tag{1.79}$$

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

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

which yields

$$d = \sqrt{n+1} \tag{1.80}$$

We have therefore obtained

$$\hat{a}|n > = \sqrt{n}|n-1 > \tag{1.81a}$$

$$\hat{a}^\dagger|n > = \sqrt{n+1}|n+1 > \tag{1.81b}$$

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. (1.74) can be interpreted as a rule of energy quantization. Notice that the sate of lowert energy satisfies

$$\hat{a}|0 >= 0 \tag{1.82}$$

i.e., it is anihilated bythe lowering operator $\hat{a}$. Eq. (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 $|n >$ by the repeated action of $\hat{a}^\dagger$ on $|0 >$. We see that

$$|1 >= \hat{a}^\dagger|0 > \tag{1.83}$$

and then, from (1.81b)

$$|2 > = \frac{\hat{a}^\dagger}{\sqrt{2}}|1 > = \frac{(\hat{a}^\dagger)^2}{\sqrt{2}}|0 > \tag{1.84a}$$

$$|3 > = \frac{\hat{a}^\dagger}{\sqrt{3}}|2 > = \frac{(\hat{a}^\dagger)^3}{\sqrt{3!}}|0 > \tag{1.84b}$$

and so on. We find the general expression

$$|n >= \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0 > \tag{1.85}$$

A useful observation is that the states $\{|n >\}$ 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:

$$
\begin{aligned}
< m|\hat{x}|n > = \sqrt{\frac{\hbar}{2m\omega}} < m|\hat{a}+\hat{a}^{\dagger}|n > &= \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n} < m|n-1> + \sqrt{n+1} < m|n+1>\right] \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right] \qquad (1.86a)
\end{aligned}
$$

$$
< m|\hat{p}|n > = i\sqrt{\frac{m\hbar\omega}{2}} < m|\hat{a}^{\dagger}-\hat{a}|n > = i\sqrt{\frac{m\hbar\omega}{2}}\left[\sqrt{n+1}\delta_{m,n+1} - \sqrt{n}\delta_{m,n-1}\right] \qquad (1.86b)
$$

where the expresions (1.67) have been used. With this formalism, we can compute the energy wavefunctions in the position representation. Let us start by obtaining $\psi_0 \equiv < x|0 >$. To do so, recall that the ground state is anihilated by $\hat{a}$, so that

$$
< x|\hat{a}|0 > = \sqrt{\frac{m\omega}{2\hbar}} < x|\hat{x} + \frac{i\hat{p}}{m\omega}|0 > = 0 \qquad (1.87)
$$

Inserting a unity, we have

$$
\int dx' \; < x|\hat{x} + \frac{i\hat{p}}{m\omega}|x' >< x'|0 > = \int dx' \, \delta(x-x')\Big(x + \frac{i}{m\omega}(-i\hbar\frac{d}{dx})\Big)\psi_0 = 0 \qquad (1.88)
$$

which, after integration and rearranging the terms, yields

$$
\frac{d\psi_0(x)}{dx} = -\frac{m\omega}{\hbar}x\psi_0(x) \qquad (1.89)
$$

From (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 $\tilde{x} = \sqrt{\frac{m\omega}{\hbar}}x$

$$
\psi_0(\tilde{x}) = A_0 \exp(-\frac{1}{2}\tilde{x}^2) \qquad (1.90)
$$

A_0 can be found by normalizing

$$
\int dx \, \psi_0(\tilde{x})\psi_0(\tilde{x}) = A_0\sqrt{\frac{\hbar}{m\omega}}\int d\tilde{x} \, \exp(-\tilde{x}^2) = A_0^2\sqrt{\frac{\hbar\pi}{m\omega}} = 1, \qquad (1.91)
$$

which leads finally to

$$
\psi_0(\tilde{x}) = (\frac{\hbar\pi}{m\omega})^{-1/4}\exp(-\frac{1}{2}\tilde{x}^2) \qquad (1.92)
$$

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

$$
\begin{aligned}
< x|1 > = < x|\hat{a}^{\dagger}|0 > \quad &= \sqrt{\frac{m\omega}{2\hbar}} < x|\hat{x} - \frac{i\hat{p}}{m\omega}|0 > \qquad = \sqrt{\frac{m\omega}{2\hbar}}(x - \frac{\hbar}{m\omega}\frac{d}{dx})\psi_0(x) \\
< x|2 > = < x|\frac{(\hat{a})^2}{\sqrt{2}}|0 > &= \frac{1}{\sqrt{2}}\big(\sqrt{m\omega 2\hbar}\big)^2\big(x - \frac{\hbar}{m\omega}\big)^2\psi_0(x) \\
&\vdots \\
< x|n > = < x|\frac{(\hat{a})^n}{\sqrt{n!}}|0 > &= \frac{1}{\sqrt{n!2^n}}\frac{1}{\big(\frac{\hbar}{m\omega}\big)^n}(x - \frac{\hbar}{m\omega}\frac{d}{dx})^n\psi_0(x) \qquad (1.93a)
\end{aligned}
$$

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

$$
\psi_0(\tilde{x}) = \frac{1}{\sqrt{n!2^n}}\frac{1}{\big(\frac{\hbar}{m\omega}\big)^n}\Big(\sqrt{\frac{\hbar}{m\omega}\tilde{x} - \frac{\hbar}{m\omega}}\Big)^n\psi_0(\tilde{x}) \qquad (1.94)
$$

that is,

$$\psi_n(\tilde{x}) = \frac{1}{\sqrt{n!2^n}}\big(\frac{\hbar\pi}{m\omega}\big)^{-1/4}\big(\tilde{x} - \frac{d}{d\tilde{x}}\big)^n \exp(-\frac{1}{2}\tilde{x}^2) \tag{1.95}$$

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

$$H_n(\tilde{x}) = \exp\Big(\frac{1}{2}\tilde{x}^2\Big)\Big(\tilde{x} - \frac{d}{d\tilde{x}}\Big)^n \exp\Big(-\frac{1}{2}\tilde{x}^2\Big) \tag{1.96}$$

Therefore, (1.95) can be rewritten as

$$\psi_n(\tilde{x}) = \frac{1}{\sqrt{n!2^n}}\Big(\frac{\hbar\pi}{m\omega}\Big)^{-1/4} \exp(-\frac{1}{2}\tilde{x}^2)H_n(\tilde{x}) \tag{1.97}$$

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 $<\hat{x}>= 0$. This result can be easily verified in the operator formalism, following our result (1.86a)

$$<\hat{x}>=<n|\hat{x}|n>= \sqrt{\frac{\hbar}{2m\omega}}\Big(\sqrt{n}\delta_{n,n-1} + \sqrt{n+1}\delta_{n,n+1}\Big) = 0 \tag{1.98}$$

Similarly, from (1.86b), we find that

$$<\hat{p}>= p \tag{1.99}$$

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

$$\begin{aligned}<\hat{x}^2> = \frac{\hbar}{2m\omega} <n|\big(\hat{a}+\hat{a}^\dagger\big)|n> &= \frac{\hbar}{2m\omega} <n|\big(\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2}\big)|n> \\ &= \frac{\hbar}{2m\omega} <n|(1+2\hat{a}\hat{a}^\dagger)|n>= \frac{\hbar}{2m\omega}(1+2n)\end{aligned} \tag{1.100a}$$

where we used that $<n|\hat{a}^2|n>=<n|(\hat{a}^\dagger)^2|n>= 0$ and (1.69). Similarly,

$$<\hat{p}^2>= -\frac{m\hbar\omega}{2} <n|(\hat{a}^\dagger - \hat{a})^2|n>= -\frac{m\hbar\omega}{2} <n|(-\hat{a}\hat{a}^\dagger - \hat{a}\hat{a}^\dagger)|n>= \frac{m\hbar\omega}{2}(1+2n) \tag{1.101}$$

Noticing now that $<(\Delta\hat{x})^2>=<\hat{x}^2>$ because of (1.98), and $<(\Delta\hat{p})^2>=<\hat{p}^2>$ because of (1.99), we find the uncertainty relation

$$<(\Delta\hat{x})^2><(\Delta\hat{p})^2>= \frac{\hbar^2}{4}(1+2n)^2, \tag{1.102}$$

which satisfies the uncertainty principle. We notice that the state of minimal uncertainty is precisely the ground state, which, as given by (1.92), has a Gaussian profile that are typically considered maximally coherent. A second observation regards the natural question of how these states evolve in time. In section (2.1), we learned that stationary states, such as $|n>$ evolve trivially as

$$|n,t>= \exp(-\frac{i}{\hbar}\hat{H}t)|n>= \exp(-i\omega(n+1/2)t)|n> \tag{1.103}$$

For these states, one can easely verify that

$$<n;t|\hat{x}|n;t>=<n|\hat{a}|n>= 0 =<n|\hat{p}|n>=<n;t|\hat{p}|n;t> \tag{1.104}$$

and, thus, the uncertainty relation (1.102) holds still. A natural puzzle is that $<\hat{x}>= 0$ even through the system we analize is a harmonic oscillator. From classical mechanics, one may have expected on oscillatory

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

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

$$|\alpha >= \sum_n c_n |n > \tag{1.105}$$

as discussed around (**??**), 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, $|0>$ corresponds to the vaccum state, while the states $|1>$,$|2>$, $|3>$, ... may correspond to a physical system with one, two, three, ... photons or particles, in general. Notice that in this interpreation $\hat{a}^\dagger$ and $\hat{a}$ operate as creation and annihilation operators

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

creating and annihilating particles. This interpretation finds an appropiate environment particularly in quantum field theories, where such processes