QUANTUM MECHANICS
Lecture 8

The quantum harmonic oscillator

Enrico Iacopini

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D. J. Griffiths: paragraph 2.3

The harmonic oscillator

Quantum Harmonic Oscillator

1. Let us start from the **classical equation** of the harmonic oscillator.
2. As it is well known, its equation of motion reads

$$m\ddot{x} = F(x) = -k\,x$$

and this equation rules many physical systems, such as the **pendulum**, a mass attached to a **spring**, the **small oscillations** around a stable equilibrium position, etc ...

3. The restoring force admits a potential which is given by $V(x) = \frac{1}{2}k\,x^2$ $\left(\Rightarrow F(x) = -\frac{dV}{dx}\right)$.

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The harmonic oscillator

If we define

$$\omega \equiv \sqrt{\frac{k}{m}}$$

the solutions of the harmonic oscillator equation are

$$x(t) = A\,sin\,\omega t + B\,cos\,\omega t$$

where A and B are integration constants, to be determined from the initial conditions.

The QM harmonic oscillator

1. The hamiltonian of the harmonic oscillator is

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

   and, therefore, the $time - independent$ Schrödinger equation is the following

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

2. There are **two ways** to solve it:
3. **the algebraic method**
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The algebraic method

Let us start with the **algebraic method**.

1. The equation to be solved is

$$\hat{H}\,\psi \equiv \left[\frac{\hat{p}^2}{2m} + \frac{1}{2}\,m\,\omega^2\hat{x}^2\right]\psi = E\,\psi$$

where $\hat{H}$, $\hat{p}$ and $\hat{x}$ are the hamiltonian, the momentum and the position operators.

2. Let us start by rewriting the hamiltonian $\hat{H}$ as follows

$$\hat{H} = \frac{1}{2m}\left[\hat{p}^2 + (m\omega\hat{x})^2\right] = \hbar\omega\left\{\frac{1}{2m\,\hbar\omega}\left[\hat{p}^2 + (m\omega\hat{x})^2\right]\right\}$$

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The algebraic method

The quadratic structure of $\hat{H}$ suggests to write the adimensional term in brackets as follows

$$\frac{1}{2m\hbar\omega}\left[\hat{p}^2 + (m\omega\hat{x})^2\right] =$$

$$= \left[\frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} - i\,\hat{p})\right]\left[\frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} + i\,\hat{p})\right] \equiv$$

$$\equiv \mathbf{a}_+ \cdot \mathbf{a}_-$$

where we have defined the two operators $\mathbf{a}_\pm$ as follows

$$\mathbf{a}_\pm \equiv \frac{\mathbf{1}}{\sqrt{\mathbf{2m}\hbar\omega}}(\mathbf{m}\omega\hat{\mathbf{x}} \mp \mathbf{i}\,\hat{\mathbf{p}})$$

The algebraic method

1. **But, is it correct ?**
   Let us see ...
2. We have

$$a_+ \cdot a_- = (m\omega\hat{x} - i\,\hat{p})\,(m\omega\hat{x} + i\,\hat{p}) =$$
$$= (m\omega\hat{x})^2 + im\omega\,\hat{x}\hat{p} - im\omega\,\hat{p}\hat{x} + (\hat{p})^2$$

   but $\quad im\omega\,\hat{x}\hat{p} - im\omega\,\hat{p}\hat{x} = im\omega(\hat{x}\hat{p} - \hat{p}\hat{x})$
   is equal to zero or not ?
3. In case of numerical quantities, the answer, of course, would be **yes**, but for operators ?
4. Here, in fact, we have to do with the **commutator** of the two operators $\hat{x}$ and $\hat{p}$:

$$\hat{x}\hat{p} - \hat{p}\hat{x} \equiv [\hat{x}, \hat{p}]$$

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The algebraic method

To verify if the commutator is null or not, we have to see which is the result of its application to a generic function $f(x)$. We have

$$\begin{aligned}
[\hat{x}, \hat{p}]\, f &= (\hat{x}\hat{p} - \hat{p}\hat{x}) f = \hat{x}\hat{p} f - \hat{p}\hat{x} f = \\
&= \hat{x}\left(-i\hbar \frac{\partial f}{\partial x}\right) - \hat{p}(x f) = \\
&= -i\hbar\, x\, \frac{\partial f}{\partial x} + i\hbar \frac{\partial}{\partial x}(x\, f) = \\
&= -i\hbar\, x\, \frac{\partial f}{\partial x} + i\hbar f + i\hbar\, x\, \frac{\partial f}{\partial x} = i\hbar f \Rightarrow \\
&\Rightarrow \; [\hat{\mathbf{x}}, \hat{\mathbf{p}}] = \mathbf{i}\hbar
\end{aligned}$$

The algebraic method

1. This means that

$$a_-a_+ = \frac{1}{2m\hbar\omega}\left\{(m\omega\hat{x})^2 + (\hat{p})^2 - im\omega[\hat{x},\hat{p}]\right\} =$$

$$= \frac{1}{2m\hbar\omega}\left\{(m\omega\hat{x})^2 + (\hat{p})^2 + m\hbar\omega\right\} \Rightarrow$$

$$\Rightarrow \hbar\omega\, a_-a_+ = \frac{1}{2m}\left\{(m\omega\hat{x})^2 + (\hat{p})^2\right\} + \frac{\hbar\omega}{2}$$

2. and therefore

$$\hat{H} = \hbar\omega\left(a_-a_+ - \frac{1}{2}\right)$$

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The algebraic method

1. The non-null commutator between $\hat{x}$ and $\hat{p}$ implies that also the two operators $\mathbf{a}_+$ and $\mathbf{a}_-$ **do not commute**.

2. In fact it turns out that

$$\mathbf{a}_+ \, \mathbf{a}_- = \frac{1}{2m\hbar\omega} \left\{ (m\omega\,\hat{x})^2 + (\hat{p})^2 - m\hbar\omega \right\}$$

whereas we have already seen that

$$\mathbf{a}_- \, \mathbf{a}_+ = \frac{1}{2m\hbar\omega} \left\{ (m\omega\,\hat{x})^2 + (\hat{p})^2 + m\hbar\omega \right\}$$

and therefore

$$[\mathbf{a}_-, \mathbf{a}_+] = \mathbf{1}$$

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and therefore

$$[\mathbf{a}_-, \mathbf{a}_+] = \mathbf{1}$$

The algebraic method

1. Let us apply these results to our problem: **the solution of the time-independent** Schrödinger equation

$$\hat{H}\,\psi = E\,\psi$$

2. Let us start by observing that, from what we have seen, the hamiltonian operator $\hat{H}$ can be written in both the following ways

$$\hat{H} = \hbar\omega\left(a_- a_+ - \frac{1}{2}\right)$$

$$\hat{H} = \hbar\omega\left(a_+ a_- + \frac{1}{2}\right)$$

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The algebraic method

Let ψ be a solution of the time-independent Schrödinger equation, corresponding to the energy E, and let us define the new function $a_+\psi$. We have

$$
\begin{aligned}
\widehat{H}\,a_+\psi &= \hbar\omega\left(a_+a_- + \frac{1}{2}\right)a_+\psi = \\
&= \hbar\omega\left(a_+a_-a_+ + \frac{1}{2}a_+\right)\psi = \\
&= \hbar\omega\left\{a_+\left(a_-a_+ - \frac{1}{2}\right) + a_+\right\}\psi = \\
&= \left\{a_+\hbar\omega\left(a_-a_+ - \frac{1}{2}\right) + \hbar\omega\,a_+\right\}\psi = \\
&= a_+\,\widehat{H}\psi + \hbar\omega\,a_+\psi = (E + \hbar\omega)a_+\psi
\end{aligned}
$$

The algebraic method

1. This means that the function $a_+\psi$ solves the Schrödinger equation for the energy $E + \hbar\omega$.
2. In the same way, we can show that

$$\hat{H}\, a_-\psi = (E - \hbar\omega)\, a_-\psi$$

3. Therefore, starting from a solution for the energy E, we can apparently build an ***infinite chain*** of solutions, corresponding to the energies $E \pm n\,\hbar\omega$.
4. **But is the chain really infinite on both sides ?**

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Let us observe that

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

and the expectation values of $\hat{p}^2$ and $\hat{x}^2$ can only be positive quantities, in fact, no matter what Ψ is, we have

$$< \hat{p}^2 > = \int dx\, \Psi^*(\hat{p}^2\, \Psi) = \int dx\, (\hat{p}\Psi)^*(\hat{p}\Psi) > 0$$
$$< \hat{x}^2 > = \int dx\, \Psi^*(\hat{x}^2\, \Psi) = \int dx\, (\hat{x}\Psi)^*(\hat{x}\Psi) > 0$$

Therefore, also $< \hat{H} >$ must be strictly positive and, as a consequence, **no stationary state can exist corresponding to negative energies.**

The algebraic method

1. Let us reconsider, then, the way in which we have established in general that

$$\hat{H}\, a_- \psi = (E - \hbar\omega)\, a_- \psi$$

2. In drawing this conclusion, we have implicitly assumed that the function **$a_- \psi$ is not the null function !**
3. In fact, **if $a_- \psi = 0$ the *chain* stops at** E and the wave function ψ_0 for which $a_- \psi_0 = 0$ represents the state with the **lowest possible energy.**
4. On this state, we have

$$\hat{H}\psi_0 = \hbar\omega \left(a_+ a_- + \frac{1}{2} \right) \psi_0 = \frac{\hbar\omega}{2} \psi_0 \Rightarrow$$

$$\Rightarrow \quad E_0 = \frac{1}{2}\hbar\omega$$

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3. In fact, **if $\mathbf{a_{-}\psi = 0}$ the *chain* stops at** E and the wave function $\psi_{\mathbf{0}}$ for which $a_{-}\psi_{0} = 0$ represents the state with the **lowest possible energy.**
4. On this state, we have

$$\widehat{H}\psi_0 \;=\; \hbar\omega\left(a_{+}a_{-} + \frac{1}{2}\right)\psi_0 = \frac{\hbar\omega}{2}\psi_0 \;\Rightarrow$$
$$\Rightarrow \quad E_0 = \frac{1}{2}\hbar\omega$$

The algebraic method

Let us determine the function ψ_0 corresponding to the **ground state** of the harmonic oscillator: we have

$$a_- \psi_0 = 0 \Rightarrow$$

$$\Rightarrow \frac{1}{\sqrt{2m\hbar\omega}} (m\omega\hat{x} + i\hat{p})\, \psi_0 = 0 \Rightarrow$$

$$\Rightarrow 0 = m\omega x\, \psi_0 + \hbar \frac{d\psi_0}{dx} \quad \Rightarrow \frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar}\, x\, \psi_0$$

$$\Rightarrow \boldsymbol{\psi_0(x) = A_0\, e^{-\frac{m\omega}{2\hbar}x^2} = A_0\, e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2} = A_0\, e^{-\frac{1}{2}\xi^2}}$$

where we have defined

$$x_0 \equiv \sqrt{\frac{\hbar}{m\omega}} \quad and \quad \xi \equiv \frac{x}{x_0}$$

The algebraic method

Concerning the ψ_0 normalization, it is easy to verify that we must have

$$A_0 = \frac{1}{\sqrt{x_0\sqrt{\pi}}} = \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{\frac{1}{4}} \Rightarrow$$

$$\psi_0(x) = \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2} = \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\xi^2}$$

In fact

$$1 = \int dx\,|\psi_0(x)|^2 = \int x_0\,d\xi\,|A_0|^2\,e^{-\xi^2} =$$

$$= x_0\,|A_0|^2\sqrt{\pi} \Rightarrow A_0 = \frac{1}{\sqrt{x_0\sqrt{\pi}}}$$