QUANTUM MECHANICS
Lecture 10

Still about the quantum harmonic oscillator

Enrico Iacopini

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D. J. Griffiths: paragraph 2.3

The analitic method

In the previous lecture we have seen that, if we define

$$x_0 = \sqrt{\frac{\hbar}{m\omega}}; \quad \xi = \frac{x}{x_0}; \quad E = k\,\hbar\omega$$

the time-independent Schrödinger equation for the harmonic oscillator

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

becomes

$$\frac{d^2\psi(\xi)}{d\xi^2} - \xi^2\psi(\xi) + 2k\,\psi(\xi) = 0$$

and, given its asymptotic behaviour, **it may be appropriate** to look for solutions of the type

$$\psi(\xi) = e^{-\frac{1}{2}\xi^2}\,\chi(\xi)$$

The analytic method

We have

$$\frac{d\psi}{d\xi} = -\xi\, e^{-\frac{1}{2}\xi^2}\chi + e^{-\frac{1}{2}\xi^2}\,\frac{d\chi}{d\xi}$$

$$\begin{aligned}\frac{d^2\psi}{d\xi^2} &= -e^{-\frac{1}{2}\xi^2}\chi + \xi^2\, e^{-\frac{1}{2}\xi^2}\chi - \xi\, e^{-\frac{1}{2}\xi^2}\,\frac{d\chi}{d\xi} - \\ &- \xi\, e^{-\frac{1}{2}\xi^2}\,\frac{d\chi}{d\xi} + e^{-\frac{1}{2}\xi^2}\,\frac{d^2\chi}{d\xi^2} \\ &= e^{-\frac{1}{2}\xi^2}(\xi^2-1)\,\chi - 2\,\xi\, e^{-\frac{1}{2}\xi^2}\,\frac{d\chi}{d\xi} + \\ &+ e^{-\frac{1}{2}\xi^2}\,\frac{d^2\chi}{d\xi^2}\end{aligned}$$

The analytic method

1. Therefore, the Schrödinger equation

$$\frac{d^2\psi(\xi)}{d\xi^2} - \xi^2\,\psi(\xi) + 2\kappa\psi(\xi) = 0$$

becomes

$$\left[e^{-\frac{1}{2}\xi^2}(\xi^2 - 1)\chi - 2\xi e^{-\frac{1}{2}\xi^2}\frac{d\chi}{d\xi} + e^{-\frac{1}{2}\xi^2}\frac{d^2\chi}{d\xi^2}\right] -$$
$$-\xi^2 e^{-\frac{1}{2}\xi^2}\chi + 2\kappa e^{-\frac{1}{2}\xi^2}\chi = 0$$

2. and, after multiplying by $e^{\frac{1}{2}\xi^2}$, we finally obtain

$$\frac{d^2\chi}{d\xi^2} - 2\xi\frac{d\chi}{d\xi} + (2\kappa - 1)\chi = 0$$

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$$\frac{d^2\chi}{d\xi^2} - 2\xi\frac{d\chi}{d\xi} + (2\kappa - 1)\chi = 0$$

is the **Hermite differential equation.**

2. To obtain functions

$$\psi(\xi) = \chi(\xi)\, e^{-\frac{1}{2}\xi^2}$$

that can be normalized, we need that $(2\kappa - 1) = 2n$ with $n = 0, 1, 2, 3, \ldots$ and, in this case, the solutions of the above equation are the Hermite polynomials $\chi(\xi) = H_n(\xi)$.

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The analytic method

1. Since we have defined $E = \kappa\,\hbar\omega$ and
   $\mathbf{2\kappa - 1 = 2n \quad \Rightarrow \quad \kappa = n + \frac{1}{2}}$
   we conclude, once again, that the only possible energy values for the stationary states of a quantum oscillator are
   $\mathbf{E_n = (n + \frac{1}{2})}\hbar\omega$.

2. The corresponding w.f. ψ_n are
   $$\psi_n \;=\; A_n\, e^{-\frac{1}{2}\xi^2}\, H_n\,(\xi)$$
   or, more explicitly
   $$\psi_n(x) \;=\; A_n\, e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2}\, H_n\left(\frac{x}{x_0}\right)$$
   in agreement with the result already obtained with the algebraic method.

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Conclusion

The normalization constant A_n can be determined in the usual way

$$1 = |A_n|^2 \int dx\, H_n^2\left(\frac{x}{x_0}\right) e^{-\left(\frac{x}{x_0}\right)^2}$$

and we obtain again $\left(x_0 = \sqrt{\frac{\hbar}{m\omega}}\right)$

$$\psi_n(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n\, n!}} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}\; H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)$$

for the energies $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$.

Completeness

Similarly to what we have seen for the infinite potential well, also for the harmonic oscillator it turns out that **the set of the ψ_n solving the time independent Schrödinger equation is complete.**

This means that **every square integrable and differentiable function $f(x)$ can be written as**

$$f(x) = \sum_n c_n \, \psi_n(x), \;\; with \;\; c_n = \int dx \; \psi_n^*(x) \, f(x)$$

A remark

1. Let us start by considering the stationary state of the harmonic oscillator described by the w.f. Ψ_n. We know that

$$< H >= E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

2. But, what about the expectation values of the kinetic and potential energy $< T >$ and $< V >$.
3. In Classical Mechanics, their average values over a full time period are equal.
4. **What happens in *Q.M.* ?**

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A remark

1. Let us start by evaluating $< T >= \frac{1}{2m} < \hat{p}^2 >$.
2. We can calculate $< \hat{p}^2 >$ using the definition, but there is a more elegant way to do it, using the raising/lowering operators !
3. Let us remember that

$$a_\pm = \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega\hat{x} \mp i\hat{p}\right)$$

$$\Rightarrow \quad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}\left(a_+ - a_-\right)$$

$$\Rightarrow \quad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(a_+ + a_-\right)$$

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1. Therefore, we have

$$\hat{p}^2 = -\frac{m\hbar\omega}{2}\Big(a_+ - a_-\Big)\Big(a_+ - a_-\Big) =$$
$$= -\frac{m\hbar\omega}{2}\Big(a_+a_+ - a_+a_- - a_-a_+ + a_-a_-\Big)$$

2. But, clearly, for any given stationary state ψ_n

$$< a_+a_+ >=< a_-a_- >= 0$$

and therefore

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But we have already shown that $a_+ a_- \psi_n = n\, \psi_n$ and $a_- a_+ \psi_n = (n+1)\psi_n$, therefore, being ψ_n normalized, we have

$$< \hat{p}^2 > = \frac{m\hbar\omega}{2}(n + n + 1) = (2n+1)\frac{m\hbar\omega}{2}$$

$$\Rightarrow < T > = \frac{1}{2m} < \hat{p}^2 > = \frac{\hbar\omega}{4}(2n+1) =$$

$$= \frac{1}{2}(n + \frac{1}{2})\hbar\omega = \frac{1}{2}\, E_n$$

A remark

1. Since $< V >=< H > - < T >$, clearly also for $< V >$ we have

$$< V >= \frac{1}{2} E_n =< T >$$

in agreement with Classical Mechanics.

2. This result holds for stationary states: in general, as shown in Appendix 1, we have

$$\begin{aligned} < T > &= \frac{1}{2} < H > + A\, cos(2\omega t + \phi) \\ < V > &= \frac{1}{2} < H > - A\, cos(2\omega t + \phi) \end{aligned}$$

where A and ϕ are suitable real quantities.

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A further remark

1. We have seen both in the case of the infinite square well and of the harmonic oscillator that **the ground stationary state possesses an energy higher than zero** :
   - for the infinite square well we have seen that

$$E_{min} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 = \frac{1}{2m}\left(\frac{\hbar}{a}\right)^2 \pi^2$$

   - for the harmonic oscillator, we have got

$$E_{min} = \frac{1}{2}\hbar\omega$$

2. But in Classical Mechanics these energies can be as small as we want and **also null**. **Why it is not so also in *Q.M.* ?**

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A further remark

1. The reason is in the **uncertainty principle**.
2. Let us start by considering the harmonic oscillator: the energy expectaction value reads

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$$
$$\Rightarrow \quad E \equiv < \hat{H} > = \frac{1}{2m} < \hat{p}^2 > + \frac{1}{2} m\omega^2 < \hat{x}^2 >$$

3. If we consider any stationary state, $< \hat{x} > = < \hat{p} > = 0$ and this clearly holds also for the state of minimal energy, therefore

$$E = \frac{1}{2m}\sigma_p^2 + \frac{1}{2} m\omega^2 \sigma_x^2$$

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$$\sigma_x \sigma_p \geq \frac{\hbar}{2} \Rightarrow \sigma_p \geq \frac{\hbar}{2}\frac{1}{\sigma_x}$$

therefore

$$E \geq \frac{1}{2m}\left(\frac{\hbar}{2}\right)^2 \frac{1}{\sigma_x^2} + \frac{1}{2} m\omega^2 \sigma_x^2 \equiv F(\sigma_x)$$

2. The function $F(\sigma_x)$ has a minimum when $\frac{dF}{d\sigma_x} = 0$. The σ_x corresponding to the minimum is the solution of the equation

$$\frac{dF}{d\sigma_x} = \frac{1}{2m}\left(\frac{\hbar}{2}\right)^2 \frac{-2}{\sigma_x^3} + \frac{1}{2} m\omega^2\, 2\sigma_x = 0 \Rightarrow$$

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A further remark

1. In other words, the minimum of $F(\sigma_x)$ is reached when

$$m\omega^2\tilde{\sigma}_x = \frac{1}{m}\left(\frac{\hbar}{2}\right)^2 \frac{1}{\tilde{\sigma}_x^3} \Rightarrow$$

$$\Rightarrow \tilde{\sigma}_x^4 = \left(\frac{\hbar}{2}\right)^2 \frac{1}{m^2\omega^2} = \left(\frac{\hbar}{2m\omega}\right)^2 \Rightarrow$$

$$\Rightarrow \tilde{\sigma}_x^2 = \frac{\hbar}{2m\omega}$$

2. For this value of $\tilde{\sigma}_x$ we have

$$F(\tilde{\sigma}_x) = F_{min} = \frac{1}{2m}\left(\frac{\hbar}{2}\right)^2 \frac{2m\omega}{\hbar} + \frac{1}{2}m\omega^2 \frac{\hbar}{2m\omega} =$$

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A further remark

In conclusion, for the harmonic oscillator,
because of the uncertainty principle,
the expectation value of the energy on any state must be such that

$$E = < \hat{H} > \geq F(\sigma_x) \geq F(\tilde{\sigma}_x) \equiv F_{min} = \frac{\hbar\omega}{2}$$

A further remark

1. In the case of the infinite square well, since the particle must stay between 0 and a, the worst case (highest value) corresponds to $\sigma_x^2 = \frac{a^2}{4}$, when the particle is found for half the cases immediately near 0 and for half the cases immediately near a.

2. Therefore, because of the uncertainty principle, we will always have that

$$\sigma_p \geq \frac{\hbar}{2}\frac{1}{\sigma_x} \geq \frac{\hbar}{2}\frac{2}{a} = \frac{\hbar}{a}$$

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1. But the particle energy is constituted only by the kinetic term, and, since on every stationary state $< p >= 0$, we will have

$$E \equiv < \hat{H} >= \frac{< \hat{p}^2}{2m} = \frac{\sigma_p^2}{2m} \geq \frac{1}{2m}\left(\frac{\hbar}{a}\right)^2 \quad (1)$$

which states that the uncertainty principle forbids again the possibility of $E = 0$,

2. The energy of the infinite square well ground state was found to be

$$E_1 = \frac{1}{2m}\left(\frac{\pi\hbar}{a}\right)^2$$

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Exercise

A harmonic oscillator is described, at $t = 0$, by the w.f. $\Psi(x,0) = A\left(4\psi_0(x) + 3i\,\psi_1(x)\right)$

a) find the normalization constant A;

b) determine the p.d.f $|\psi(x,t)|^2$;

c) find $< x >$, $< p >$ and $< E >$ as functions of time.