QUANTUM MECHANICS
Lecture 9

The quantum harmonic oscillator

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D. J. Griffiths: paragraph 2.3

Still about the algebraic method

In the previous lecture, we concluded that the normalized wave function ψ_0 of the harmonic oscillator ground state is

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

where $\xi \equiv \frac{x}{x_0}$, $x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$ and the energy corresponding to ψ_0 is $E_0 = \frac{1}{2}\hbar\omega$.
We have also seen that

- ψ_0 is defined by the equation $\;\; a_-\,\psi_0 = 0$;
- the w.f. ψ_n of the excited states, corresponding to the energies $E_n = (n+\frac{1}{2})\hbar\omega$ are $\;\propto (a_+)^n\,\psi_0$, where $a_\pm \equiv \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega\hat{x} \mp i\hat{p}\right)$.

Still about the algebraic method

Before considering the problem of the normalization of the ψ_n, let us point out an interesting property of these functions: since

$$\begin{aligned} \hat{H}\psi_n &\equiv \hbar\omega\left(a_+a_- + \frac{1}{2}\right)\psi_n \equiv \\ &\equiv \hbar\omega\left(a_-a_+ - \frac{1}{2}\right)\psi_n = \\ &= \hbar\omega\left(n + \frac{1}{2}\right)\,\psi_n \end{aligned}$$

then we must have

$$a_+a_-\,\psi_n = n\,\psi_n; \qquad a_-a_+\,\psi_n = (n+1)\,\psi_n$$

Still about the algebraic method

Concerning now the ψ_n normalization, let us start by assuming that ψ_n is normalized and let us consider the problem of the normalization of the function $a_+\psi_n \propto \psi_{n+1}$. We have

$$\int dx (a_+\psi_n)^* \cdot (a_+\psi_n) =$$

$$= \frac{1}{\sqrt{2m\hbar\omega}} \int dx \left\{(m\omega\hat{x} - i\hat{p})\,\psi_n\right\}^* \cdot (a_+\psi_n) =$$

$$= \frac{1}{\sqrt{2m\hbar\omega}} \int dx\, \psi_n^* \cdot \left\{(m\omega\hat{x} + i\hat{p}) \cdot (a_+\psi_n)\right\} =$$

$$= \int dx\, \psi_n^*(a_-a_+\psi_n) = (n+1)\int dx\, \psi_n^*\psi_n = n+1$$

which implies that the normalization condition requires that $\psi_{n+1} = \frac{1}{\sqrt{n+1}}\, a_+\psi_n$.

Still about the algebraic method

and this result can be generalized as follows

$$\begin{aligned}\psi_n &= \frac{1}{\sqrt{n!}}\,(a_+)^n\,\psi_0 = \\ &= \frac{1}{\sqrt{n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}(a_+)^n\,e^{-\frac{1}{2}\xi^2}\end{aligned}$$

Still about the algebraic method

To determine **the esplicit form** of the ψ_n, let us start by observing that, using the definitions already established for $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ and $\xi = \frac{x}{x_0}$, we have

$$
\begin{aligned}
a_+ &= \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega\, x_0\, \xi - \frac{\hbar}{x_0}\frac{d}{d\xi}\right) = \\
&= \frac{1}{\sqrt{2m\hbar\omega}}\frac{\hbar}{x_0}\left(\frac{m\omega}{\hbar}x_0^2\,\xi - \frac{d}{d\xi}\right) = \\
&= \frac{1}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega}}\,\frac{1}{x_0}\left(\frac{m\omega}{\hbar}x_0^2\,\xi - \frac{d}{d\xi}\right) = \\
&= \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)
\end{aligned}
$$

Still about the algebraic method

But $\left(\xi - \frac{d}{d\xi}\right)^n e^{-\frac{1}{2}\xi^2}$ will be, clearly, the product of a suitable polynomial $P_n(\xi)$ of degree n, times the exponential $e^{-\frac{1}{2}\xi^2}$:

$$\left(\xi - \frac{d}{d\xi}\right)^n e^{-\frac{1}{2}\xi^2} = P_n(\xi)\, e^{-\frac{1}{2}\xi^2}$$

with $P_0 = 1$.

Still about the algebraic method

We have

$$P_{n+1}(\xi)e^{-\frac{1}{2}\xi^2} \equiv \left(\xi - \frac{d}{d\xi}\right)^{n+1} e^{-\frac{1}{2}\xi^2} =$$

$$= \left(\xi - \frac{d}{d\xi}\right)\left[\left(\xi - \frac{d}{d\xi}\right)^{n} e^{-\frac{1}{2}\xi^2}\right] = \left(\xi - \frac{d}{d\xi}\right)\left[P_n(\xi)e^{-\frac{1}{2}\xi^2}\right] =$$

$$= \xi\, P_n(\xi)e^{-\frac{1}{2}\xi^2} - \frac{dP_n}{d\xi}e^{-\frac{1}{2}\xi^2} + \xi\, P_n(\xi)e^{-\frac{1}{2}\xi^2} =$$

$$= \left(2\xi\, P_n(\xi) - \frac{dP_n}{d\xi}\right)e^{-\frac{1}{2}\xi^2} \Rightarrow$$

$$\Rightarrow P_{n+1}(\xi) = 2\xi\, P_n(\xi) - \frac{dP_n}{d\xi}$$

The above recursion formula, with the initial condition $P_0 = 1$, defines the so-called **Hermite polynomials** $H_n(\xi) \equiv P_n(\xi)$.

Still about the algebraic method

We can, therefore, conclude that the w.f. of the stationary states of the harmonic oscillator are given by

$$\begin{aligned}\psi_n(\xi) &= \frac{1}{\sqrt{n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\left(a_+\right)^n e^{-\frac{1}{2}\xi^2} = \\ &= \frac{1}{\sqrt{n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\left[\frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)\right]^n e^{-\frac{1}{2}\xi^2} = \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^n\, n!}}\, H_n(\xi)\, e^{-\frac{1}{2}\xi^2}\end{aligned}$$

where $\xi \equiv \frac{x}{x_0}$, $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ and $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$.

Properties of the Hermite polynomials

Concerning the Hermite polynomials, they are such that they satisfy

- the recursion relation

$$H_{n+1}(\xi) = 2\xi\, H_n(\xi) - \frac{d}{d\xi} H_n(\xi)$$

- the second-order linear differential equation

$$\frac{d^2 H_n}{d\xi^2} - 2\xi\, \frac{dH_n}{d\xi} + 2n\, H_n = 0$$

- the equations

$$\frac{d}{d\xi} H_n(\xi) = 2n\, H_{n-1}(\xi)$$

$$H_n(-\xi) = (-1)^n\, H_n(\xi)$$

$$\int d\xi\, H_n(\xi)\, H_m(\xi)\, e^{-\xi^2} = \sqrt{\pi}\, 2^n\, n!\, \delta_{nm}$$

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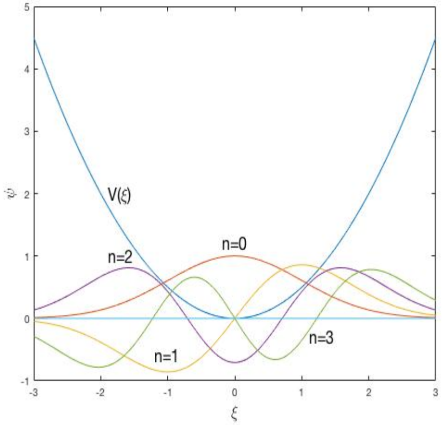
The Hermite polynomials

The first seven Hermite polynomials H_n are the following

$$\begin{aligned}
H_0 &= 1; \\
H_1 &= 2\xi; \\
H_2 &= 4\xi^2 - 2; \\
H_3 &= 8\xi^3 - 12\xi; \\
H_4 &= 16\xi^4 - 48\xi^2 + 12; \\
H_5 &= 32\xi^5 - 160\xi^3 + 120\xi; \\
H_6 &= 64\xi^6 - 480\xi^4 + 720\xi^2 - 120; \\
&\dots
\end{aligned}$$

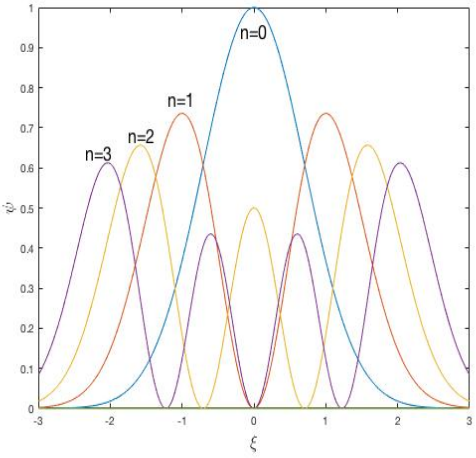
Some wave-function shapes...



Shape of the potential energy V and w.f. for the stationary states with $n = 0, 1, 2, 3$.

P.d.f concerning the first four states

Probability densities for the states with $n = 0, 1, 2, 3$.



The analitic method

Let us see, now, how it works the **analitic method** to solve the time-independent Schrödinger equation for the harmonic oscillator.

1. We have to solve the equation

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

2. If we make use of the already given definition $x_0 \equiv \sqrt{\frac{\hbar}{m\,\omega}}$ and we put $E = \kappa\,\hbar\omega$, we obtain

$$\frac{d^2\psi(x)}{dx^2} - \frac{1}{x_0^2}\left(\frac{x}{x_0}\right)^2\psi(x) = -\frac{2\kappa}{x_0^2}\psi(x) \quad (1)$$

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The analitic method

and in terms of the previously defined adimensional variable $\xi \equiv \frac{x}{x_0}$, since

$$\frac{d}{dx} = \frac{1}{x_0}\frac{d}{d\xi} \quad \Rightarrow \quad \frac{d^2}{dx^2} = \frac{1}{x_0^2}\frac{d^2}{d\xi^2}$$

the differential equation (1)

$$\frac{d^2\psi(x)}{dx^2} - \frac{1}{x_0^2}\left(\frac{x}{x_0}\right)^2 \psi(x) = -\frac{2\kappa}{x_0^2}\psi(x)$$

multiplied by x_0^2, becomes

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

The analitic method

1. In the asymptotic region ($\xi \to \pm\infty$), the term $2\kappa\psi(\xi)$ will be negligible compared with $-\xi^2\psi(\xi)$; therefore, in this region the equation can be approximated with

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

2. Let us consider, now, the functions $\psi = e^{\pm\frac{1}{2}\xi^2}$. They are such that

$$\frac{d\psi}{d\xi} = \pm\xi e^{\pm\frac{1}{2}\xi^2} \Rightarrow$$

$$\frac{d^2\psi}{d\xi^2} = \pm e^{\pm\frac{1}{2}\xi^2} + \xi^2 e^{\pm\frac{1}{2}\xi^2}$$

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The analitic method

1. However, since we are looking for square integrable functions, we can accept only $e^{-\frac{1}{2}\xi^2}$, which is an **approximate solution** of the **asymptotic approximation** of the $time-independent$ Schrödinger equation.
2. It is **not** a solution of our problem, **but it gives the idea** of looking for solutions in which this function enters as a factor, to explain the asymptotic trend. For this reason, we define

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

3. Since $e^{-\frac{1}{2}\xi^2}$ is non-zero everywhere, the above definition **does not introduce any limitation** in the solution set.

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