# Some PSTricks macros for the study of quantum mechanics

***Energy levels of a harmonic potential***

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# 1 Energy levels of a harmonic potential

The harmonic potential is given as

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2 \qquad \omega = \sqrt{\frac{k}{m}}.$$

The depending SCHRÖDINGER equation in one dimension is

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} = (E - V(x))\Psi(x) \tag{1}$$

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} + \frac{1}{2}kx^2\Psi(x) = E\Psi(x).$$

Using

$$a^2 = \frac{\hbar}{\sqrt{mk}} \quad \Rightarrow \quad \hbar^2 = a^4 mk$$

we get

$$\begin{aligned}
\frac{-a^4 mk}{2m}\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} + \frac{1}{2}kx^2\Psi(x) &= E\Psi(x) \\
\frac{-a^4 k}{2}\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} + \frac{1}{2}kx^2\Psi(x) &= E\Psi(x) \quad \Big| \cdot \frac{2}{k} \\
-a^4\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} + x^2\Psi(x) &= \frac{2E}{k}\Psi(x) \quad \big| : (-a^2) \\
a^2\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} - \frac{x^2}{a^2}\Psi(x) &= -\frac{2E}{a^2 k}\Psi(x).
\end{aligned}$$

Using

$$\frac{2E}{a^2 k} = \frac{2E}{\frac{\hbar}{\sqrt{mk}}k} = \frac{2E}{\hbar\omega} = E^*$$

we get

$$a^2\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} - \frac{x^2}{a^2}\Psi(x) = -E^*\Psi(x). \tag{2}$$

Transformation of the variable

$$\xi = \frac{x}{a}.$$

The derivatives are

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\xi} &= a\frac{\mathrm{d}}{\mathrm{d}x} \\
\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} &= a^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}.
\end{aligned}$$

This finally leads to

$$\frac{\mathrm{d}^2\Psi(\xi)}{\mathrm{d}\xi^2} - \xi^2\Psi(\xi) = -E^*\Psi(\xi)$$

or

$$\frac{\mathrm{d}^2\Psi(\xi)}{\mathrm{d}\xi^2} + (E^* - \xi^2)\Psi(\xi) = 0. \tag{3}$$

For large $\xi^2$ we can ignore $E^*$ and get the *asymptotic equation*

$$\frac{\mathrm{d}^2\Psi(\xi)}{\mathrm{d}\xi^2} = \xi^2\Psi(\xi). \tag{4}$$

And since it is a second order differential equation, a possible solution is easy to see as

$$\Psi(\xi) = A\mathrm{e}^{-\frac{\xi^2}{2}} + B\mathrm{e}^{\frac{\xi^2}{2}}.$$

To not diverge however into $\infty$, we force $B = 0$, so the *asymptotic solution* to equation 4 is

$$\Psi(\xi) = A\mathrm{e}^{-\frac{\xi^2}{2}}.$$

With *variation of the constant* we write $\Psi(\xi) = H(\xi)\mathrm{e}^{-\frac{\xi^2}{2}}$ and solve the equation for $H(\xi)$. The two derivatives of $\Psi(\xi)$ are (using the product rule)

$$\begin{aligned}
\Psi(\xi) &= H(\xi)\mathrm{e}^{-\frac{\xi^2}{2}} \\
\frac{\mathrm{d}\Psi(\xi)}{\mathrm{d}\xi} &= \left(\frac{\mathrm{d}H(\xi)}{\mathrm{d}\xi} - \xi H(\xi)\right)\mathrm{e}^{-\frac{\xi^2}{2}} \\
\frac{\mathrm{d}^2\Psi(\xi)}{\mathrm{d}\xi^2} &= \left(\frac{\mathrm{d}^2H(\xi)}{\mathrm{d}\xi^2} - H(\xi) - \xi\frac{\mathrm{d}H(\xi)}{\mathrm{d}\xi} - \xi\left(\frac{\mathrm{d}H(\xi)}{\mathrm{d}\xi} - \xi H(\xi)\right)\right)\mathrm{e}^{-\frac{\xi^2}{2}} \\
&= \left(\frac{\mathrm{d}^2H(\xi)}{\mathrm{d}\xi^2} - 2\xi\frac{\mathrm{d}H(\xi)}{\mathrm{d}\xi} + (\xi^2 - 1)H(\xi)\right)\mathrm{e}^{-\frac{\xi^2}{2}}.
\end{aligned}$$

Inserting it into equation 3 we get

$$\begin{aligned}
\left(\frac{\mathrm{d}^2H(\xi)}{\mathrm{d}\xi^2} - 2\xi\frac{\mathrm{d}H(\xi)}{\mathrm{d}\xi} + (\xi^2 - 1)H(\xi)\right)\mathrm{e}^{-\frac{\xi^2}{2}} + (E^* - \xi^2)H(\xi)\mathrm{e}^{-\frac{\xi^2}{2}} = 0 \quad | \cdot \mathrm{e}^{\frac{\xi^2}{2}} \\
\frac{\mathrm{d}^2H(\xi)}{\mathrm{d}\xi^2} - 2\xi\frac{\mathrm{d}H(\xi)}{\mathrm{d}\xi} + (E^* - 1)H(\xi) = 0.
\end{aligned}$$

To solve the second order differential equation in $H(\xi)$ we develop a power series:

$$\begin{aligned}
(E^* - 1)H(\xi) &= (E^* - 1)\sum_{n=0}^{\infty} a_n\xi^n = \sum_{n=0}^{\infty}(E^* - 1)a_n\xi^n \\
-2\xi\frac{\mathrm{d}H(\xi)}{\mathrm{d}\xi} &= -2\xi\sum_{n=1}^{\infty} a_n n\xi^{n-1} = \sum_{n=0}^{\infty} -2a_n n\xi^n \\
\frac{\mathrm{d}^2H(\xi)}{\mathrm{d}\xi^2} &= \sum_{n=2}^{\infty} a_n n(n-1)\xi^{n-2} = \sum_{n=0}^{\infty} a_{n+2}(n+1)(n+2)\xi^n
\end{aligned}$$

Inserting it into equation 3

$$\sum_{n=0}^{\infty} a_{n+2}(n+1)(n+2)\xi^n + \sum_{n=0}^{\infty} -2a_n n\xi^n + \sum_{n=0}^{\infty} (E^* - 1)a_n\xi^n = 0$$

$$\sum_{n=0}^{\infty} \left(a_{n+2}(n+1)(n+2) + a_n(E^* - 1 - 2n)\right)\xi^n = 0.$$

This only can be zero for all $\xi$ if

$$a_{n+2}(n+1)(n+2) + a_n(E^* - 1 - 2n) = 0.$$

Written as a fraction

$$\frac{a_{n+2}}{a_n} = \frac{2n + 1 - E^*}{(n+1)(n+2)}.$$

This however diverges for $n \to \infty$, so the power series must stop at a value $n^*$, where all following coefficients $n > n^*$ are zero. Thus

$$2n^* + 1 - E^* = 0 \quad \Rightarrow \quad E^* = 2n^* + 1 \quad \text{for} \quad n^* = 0, 1, 2, \ldots$$

We now see that the energy is quantized!

Resubstituting $E^*$

$$E^* = \frac{2E}{\hbar\omega}$$

and solving for $E$ gives

$$\frac{2E}{\hbar\omega} = 2n^* + 1$$
$$E = \left(n^* + \frac{1}{2}\right)\hbar\omega = E_{n^*}.$$

The lowest possible energy we get for $n^* = 0$

$$E_0^* = \frac{1}{2}\hbar\omega,$$

and see this lowest energy is non-zero.

The energy difference $\Delta E$ between two adjacent energy levels is

$$\Delta E = E_{n^*+1} - E_{n^*} = \left(n^* + 1 + \frac{1}{2}\right)\hbar\omega - \left(n^* + \frac{1}{2}\right)\hbar\omega = \hbar\omega.$$

Now what are the polynomials $H(\xi)$? These are the well-known as the Hermite-polynoms. Thus the Eigenfunctions are determined as

$$\Psi_{n^*}(\xi) = N_{n^*}H_{n^*}(\xi)\mathrm{e}^{-\frac{\xi^2}{2}},$$

where $N_{n^*}$ (respectively $a_0$, $a_1$) is determined by normalization (to be read in some further literature):

$$N_{n^*} = \frac{1}{\sqrt{2^{n^*}n^*!\sqrt{\pi}}}$$

thus

$$\Psi_{n^*}(\xi) = \frac{1}{\sqrt{2^{n^*} n^*! \sqrt{\pi}}} H_{n^*}(\xi) \mathrm{e}^{-\frac{\xi^2}{2}}.$$

The HERMITE-polynomes are generated with the following formula:

$$H_{n^*}(\xi) = (-1)^{n^*} \mathrm{e}^{\xi^2} \frac{\mathrm{d}^{n^*}}{\mathrm{d}x^{n^*}} \mathrm{e}^{-\xi^2} \quad n^* = 0, 1, 2, \ldots$$

Explicitly we get:

$$\begin{aligned}
H_0(\xi) &= (-1)^0 \mathrm{e}^{\xi^2} \mathrm{e}^{-\xi^2} = 1 \\
H_1(\xi) &= (-1)^1 \mathrm{e}^{\xi^2} \frac{\mathrm{d}}{\mathrm{d}\xi} \mathrm{e}^{-\xi^2} = -\mathrm{e}^{\xi^2} \mathrm{e}^{-\xi^2} \cdot (-2\xi) = 2\xi \\
H_2(\xi) &= (-1)^2 \mathrm{e}^{\xi^2} \frac{\mathrm{d}^2}{\mathrm{d}\xi^2} \mathrm{e}^{-\xi^2} = \mathrm{e}^{\xi^2} \mathrm{e}^{-\xi^2} \cdot (4\xi^2 - 2) = 4\xi^2 - 2 \\
H_3(\xi) &= (-1)^3 \mathrm{e}^{\xi^2} \frac{\mathrm{d}^3}{\mathrm{d}\xi^3} \mathrm{e}^{-\xi^2} = -\mathrm{e}^{\xi^2} \mathrm{e}^{-\xi^2} \cdot (-8\xi^3 + 12\xi) = 8\xi^3 - 12\xi \\
H_4(\xi) &= \ldots = 16\xi^4 - 48\xi^2 + 12 \\
H_5(\xi) &= \ldots = 32\xi^5 - 160\xi^3 + 120\xi \\
H_6(\xi) &= \ldots = 64\xi^6 - 480\xi^4 + 720\xi^2 - 120 \\
H_7(\xi) &= \ldots = 128\xi^7 - 1344\xi^5 + 3360\xi^3 - 1680\xi \\
H_8(\xi) &= \ldots = 256\xi^8 - 3584\xi^6 + 13440\xi^4 - 13440\xi^2 + 1680 \\
H_9(\xi) &= \ldots = 512\xi^9 - 9216\xi^7 + 48384\xi^5 - 80640\xi^3 + 30240\xi \\
H_{10}(\xi) &= \ldots = 1024\xi^{10} - 23040\xi^8 + 161280\xi^6 - 403200\xi^4 + 302400\xi^2 - 30240
\end{aligned}$$