HW3 – Stationary solutions of the 1D Schrödinger equation

Enrique Gómez Cruz
Facultad de Ciencias, Universidad Nacional Autónoma de México.

The quantum harmonic oscillator is

$$\left(-\frac{\hbar}{2m}\frac{d^2}{dz^2}+\frac{1}{2}m\omega z^2\right)\psi(z)=E\psi(z)$$

This equation is perfectly suited to be solved with the Numerov algorithm since it is of the form

$$f''+k(x)f=0$$

By introducing a change of variable and scaling the energy with the following definitions

$$E\equiv\epsilon\hbar\omega \qquad z\equiv\sqrt{\frac{\hbar}{m\omega}}x$$

We get a dimensionless form of the quantum harmonic oscillator

$$\psi''+(2\epsilon-x^2)\psi=0 \tag{1}$$

Where the dimensionless energy is ϵ and the scaled potential is $v(x)=x^2/2$

To see if a given energy was an eigenenergy we applied Numerov to equation 1 to get a discrete form of the wave function ψ. If we have an eigenenergy then the tail of the wavefunction must oblige to the border conditions $\psi(x_0)=0$ and $\psi(x_N)=0$, where x_0 and x_N define the borders where the wave function must vanish.

By construction, our implementation of the Numerov algorithm assures that the border condition $\psi(x_0)=0$ is always true. But the other border condition must be checked by testing if the tail of the wavefunction doesn't diverge.

The program *schrodingerEquation1D-Numerov.cpp* shows the energies for which the border conditions are true. If you run the program you can see that this are of the form

$$\epsilon=n+\frac{1}{2},\, n\in\mathbb{N}$$

The next figures show some of the eigenfunctions found.

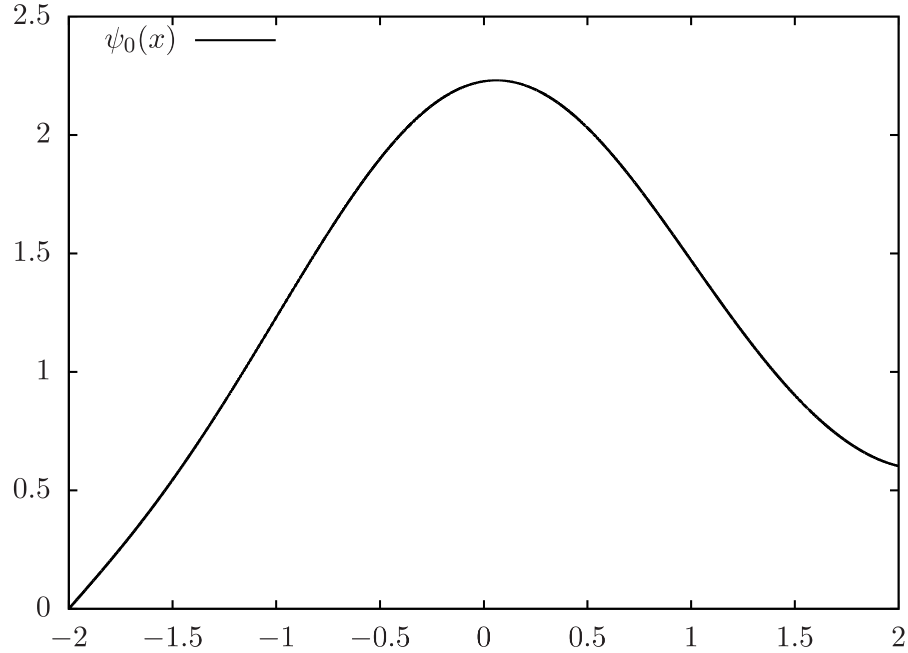

Figure 1: Ground state eigenfunction.

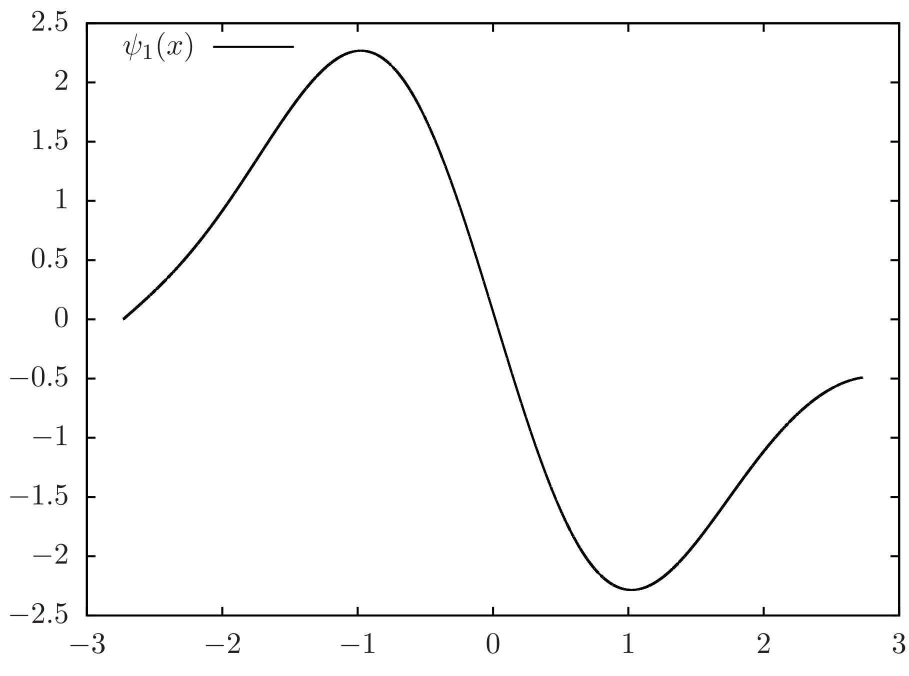

Figure 2: Wave function for $n = 1$

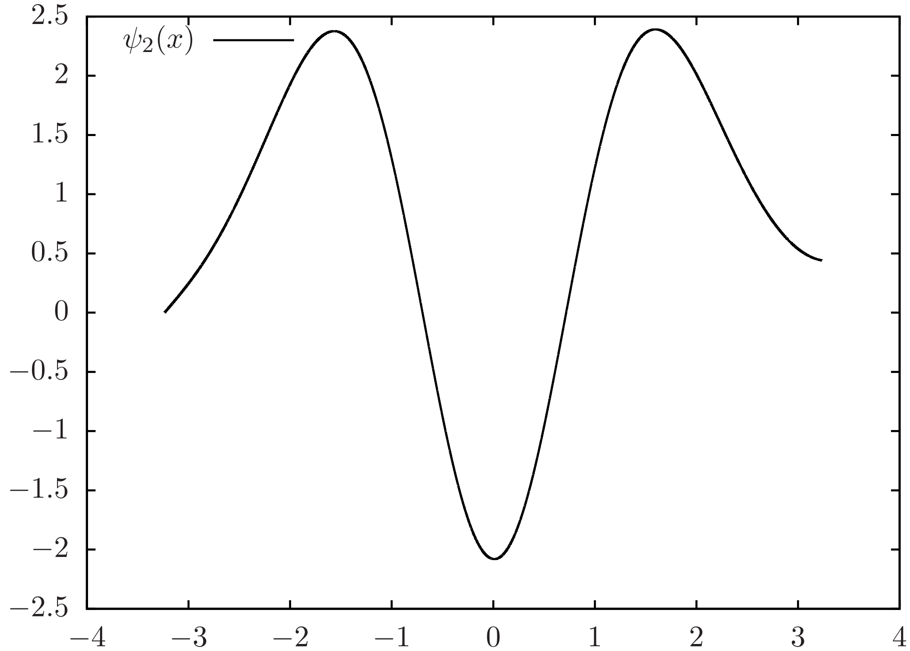

Figure 3: Wave function for $n = 2$

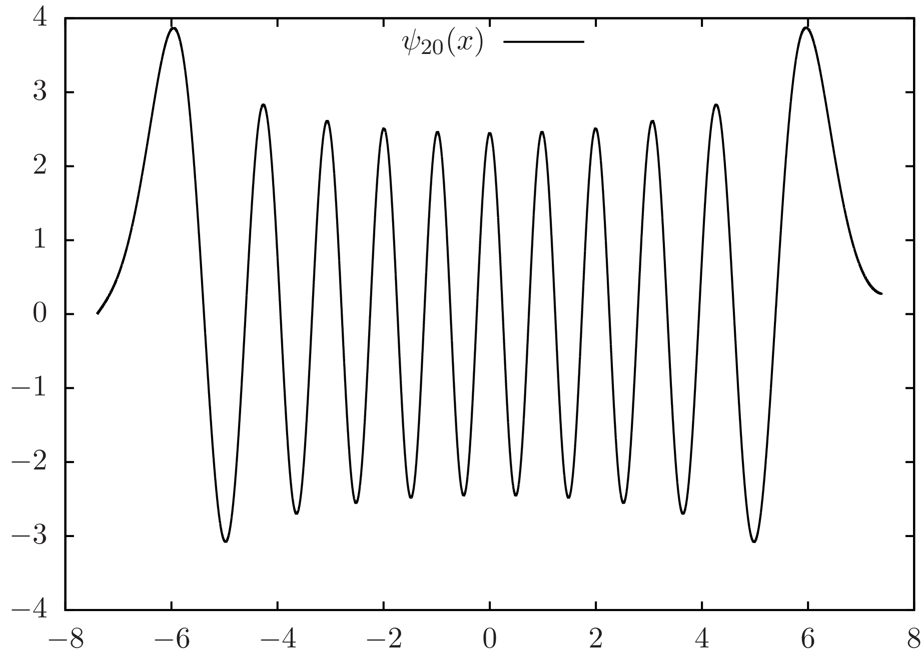

Figure 4: Wave function for $n = 20$

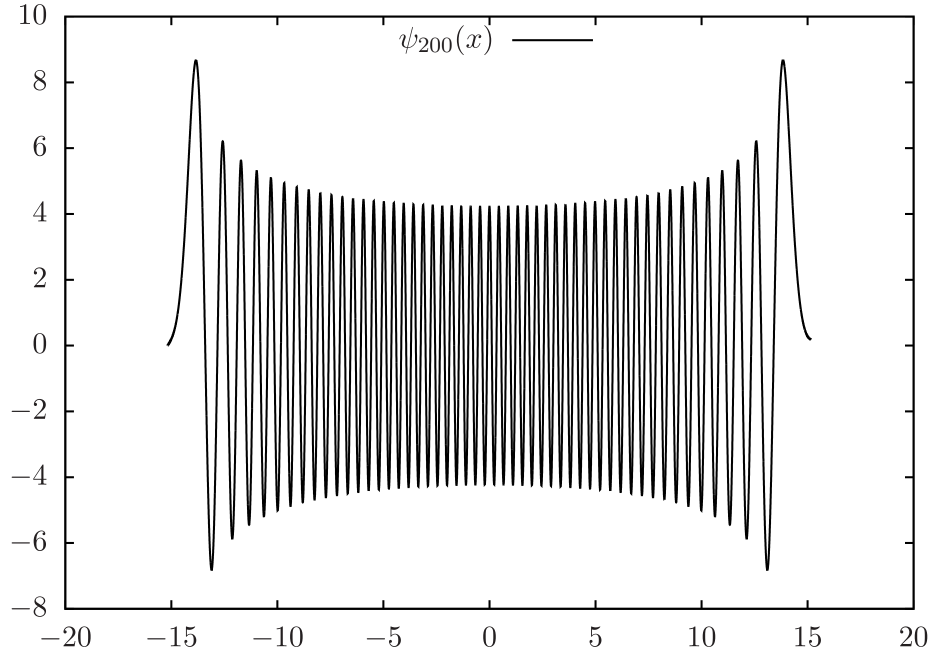

Figure 5: Wave function for $n = 200$

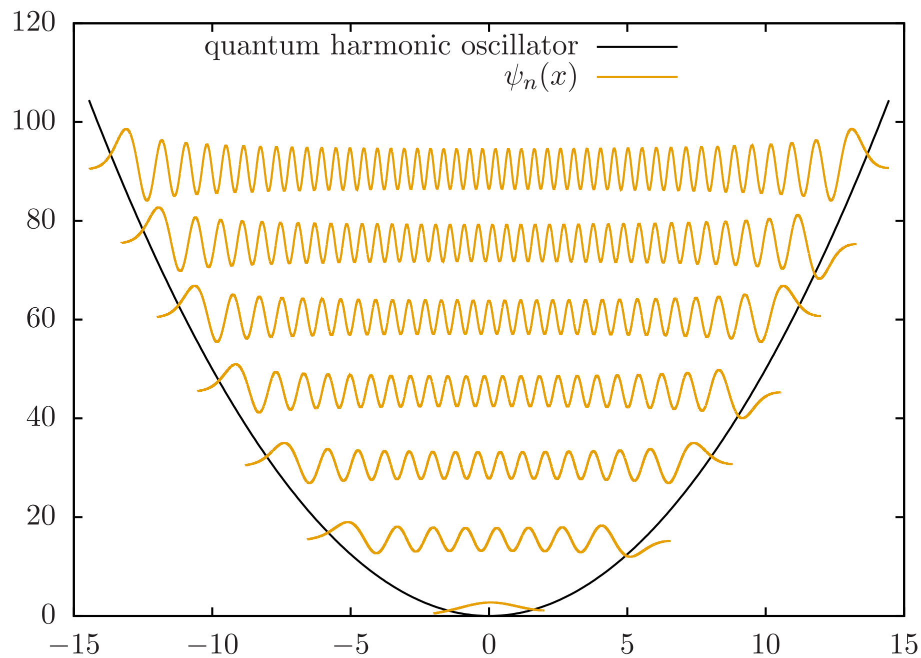

Figure 6: Scaled potential for the quantum harmonic oscillator and some eigenfuncions