Computational Physics

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In quantum mechanics, the motion of an electron in a parabolic potential well (quantistic harmonic oscillator) is described by the equation:

$$\frac{d^2\psi(x)}{dx^2} = (x^2 - 2n - 1)\psi(x)$$

with $x \in [-\infty, +\infty]$ and boundary conditions: $\psi(x) = 0$ for $x \to \pm\infty$.

This equation has an analytic solution in the form:

$$\psi(x) = \psi_n(x) = H_n(x)e^{-\frac{x^2}{2}}$$

where the functions $H_n(x)$ are the so-called *Hermite polynomials*, which are polynomials of degree n for $x \in [-\infty, +\infty]$.

The first seven Hermite polynomials are (for $n = 0, \ldots, 6$):

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

Solve numerically the equation for the quantistic harmonic oscillator for the values of n given above, in a suitable interval $x \in [0, a]$ (see the suggestion below about how to find an appropriate value of a), with boundary conditions:

$$\begin{cases} \psi(x=0) = (-1)^{n/2}\frac{n!}{(n/2)!} & \text{for even } n \\ \psi'(x=0) = (-1)^{(n-1)/2}\frac{(n+1)!}{[(n+1)/2]!} & \text{for odd } n \end{cases}$$

and compare the results with the analytic solution given above.

Suggestion: the equation should be solved in an infinite interval, that is of course not possible numerically. However, due to the presence of the term $e^{-\frac{x^2}{2}}$, the solution becomes quickly very close to zero, even for relatively small values of x. Therefore, one can integrate the equation in an interval $x \in [0, +a]$ such that the solution is larger or equal than the machine precision ($\epsilon \sim 2.2 \cdot 10^{-16}$ for the type "`double`"). In order to find the value of a, (since the functional form for $H_n(x)$ is not known *a-priori*), one can notice that the dominant term (for large values of x) for $H_n(x)$ is $H_n(x) \sim h(x, n) = 2^n x^n$. Therefore, one can estimate the value of a as the maximum value for which $h(x, n)$ is (approximately) larger or equal than the machine precision ϵ.