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Computational Physics I

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3.1 Hermite polynominals
The quantum mechanical wave functions of an harmonic oscillator are given by

$$\psi_n(x) = \frac{1}{\sqrt{c_n}} H_n(x) e^{-x^2/2} \tag{1}$$

with normalization constant $c_n = \sqrt{\pi} 2^n n!$, when x is measured in units of the characteristic length $a = \sqrt{\hbar/(m\omega)}$.
Using the recursion relation $H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$ for the Hermite polynominals, derive a recursion relation for ψ_n and plot the probability densities $|\psi_n(x)|^2$ for the first 20 states.

3.2 Specific heats
The contribution of rotational degrees of freedom to the specific heat of diatomic molecules follows from the partition function

$$Z(T) = \sum_{J=0}^{\infty} (2J+1) e^{-J(J+1)\Theta/T} \tag{2}$$

where $\Theta = \hbar^2/(2Ik_B)$ with I the moment of inertia sets the temperature.
Note that the partition function and the inner energy are related by

$$U(T) = kT^2 \frac{\partial}{\partial T} \ln Z(T) \tag{3}$$

and inner energy and the specific heat by

$$C_R(T) = \frac{\partial U(T)}{\partial T}\,. \tag{4}$$

Tabulate $Z(T)$ over a sufficient range of temperatures well below and above Θ and calculate and plot $U(T)$ and $C(T)$.

3.3 Complex Newton method and Julia sets
Consider the Newton method in the complex plane for a generic polynomial of cubic order,

$$p(z) = z^3 + (a-1)z - a \tag{5}$$

Put $a = 0$ and determine the points z_0 which iterate towards the root at $z = 1$. Display the number of iterates needed to reach a disk of radius 10^{-2} near $z = 1$. The boundary of this set is the Julia set for this mapping. You may zoom into the Julia set and magnify parts of it to reveal its intricate structure.

Now take $a = 0.32 + i1.64$ and map out the points where the Newton method does not converge to any root. In addition to the thin set of the previous case there is now a set of full measure where the Newton method does not converge to a root. What does it do instead?
Hint: In Python, complex numbers are implemented as `z = x + 1j * y`. Their real and imaginary parts are accessed via `z.real` and `z.imag`, respectively.

3.4 Vibrating beams

The vibrations of a thin beam are described by a fourth order differential equation for the displacement A,

$$\frac{d^4A}{dx^4} = \kappa^4 A \tag{6}$$

with $\kappa^4 = \omega^2\rho S/(EI_y)$. Here, ρ = density, S = cross sectional area, E = Youngs modulus, I_y = moment of inertia. The boundary conditions for a clamped beam are $A = 0$ and $A' = 0$ at both ends.

The general solution has the form

$$A = a\cos\kappa x + b\sin\kappa x + c\cosh\kappa x + d\sinh\kappa x \tag{7}$$

and can be specialized for a clamped beam of length l to

$$A = (\sin\kappa l - \sinh\kappa l)(\cos\kappa x - \cosh\kappa x) - (\cos\kappa l - \cosh\kappa l)(\sin\kappa x - \sinh\kappa x) \tag{8}$$

The condition for the eigenvalues becomes

$$\cos\kappa l\cosh\kappa l = 1 \tag{9}$$

Verify the above expressions and determine κl for the lowest 5 modes and plot the corresponding eigenmodes $A(x)$.