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Computational Physics II

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7.1. Random Hamiltonians

Define a matrix A_{ij} with normal distributed random elements, and turn it into a symmetric matrix $H_{ij} = (A_{ij} + A_{ji})/\sqrt{8}$. Compute the eigenvalues h_i of H and normalize them by $x_i = h_i/\sqrt{N}$ where N is the dimension of the matrix.
Show that the density of eigenvalues is given by the Wigner semicircle law,
$\rho(x) = (2/\pi)\sqrt{1-x^2}$.
To this end, focus on the integrated density of states,

$$I(\phi) = \frac{\phi}{\pi} + \frac{1}{2} + \frac{1}{2\pi}\sin(2\phi) \tag{1}$$

with $\phi(x) = \operatorname{asin} x$ (values of x that are outside $|x| \leq 1$ can be omitted: this then reduces the actual number of eigenvalues.). The integrated density for the numerical eigenvalues is a function that is flat between eigenvalues and increases by $1/N$ at every eigenvalue.

When the (normalized) eigenvalues are substituted in the integrated density of states, the new sequence has the property that the mean spacing between eigenvalues is $1/N$. To get a mean spacing of 1, put $z_i = NI(\phi(x_i))$ and determine $s_i = z_{i+1} - z_i$.
Verify that the mean spacing $\langle s_i \rangle = 1$.
Determine the distribution of spacings and compare the histogram to Wigners approximate formula for the density of spacings

$$P(s) = \frac{\pi}{2} s\, e^{-\frac{\pi}{4}s^2} \tag{2}$$

7.2. Verlet integration

The position space Verlet algorithm updates integrates Newtons law $\ddot{x} = a(t)$ with acceleration $a(t)$ according to the rule

$$x(t+\delta t) = 2x(t) - x(t-\delta t) + a(t)(\delta t)^2 \,. \tag{3}$$

To start it, one needs two previous time-steps. Assuming that the integration starts with velocity zero, one may use $x(t+\delta t) = x(t) + a(t)(\delta t)^2/2$ (with an obvious extension if the velocity is not zero).
Use the position space Verlet algorithm to integrate a 1-d harmonic oscillator $\ddot{x} = -x$ over one period and compare the numerical and exact positions as function of the step size.
Similarly, use the Verlet algorithm to integrate the 2d Coulomb problem

$$H = (p_x^2 + p_y^2)/2 - 1/r \,. \tag{4}$$

Starting from the initial conditions $(x, y, p_x, p_y) = \left(r_0, 0, 0, \sqrt{(2-r_0)/r_0}\right)$ the exact trajectory is an ellipsoid that returns after a time 2π. For $r_0 = 1$, the trajectory is a circle.
Increase r_0 towards $r_0 = 2$ (so that the starting point corresponds to the aphel of the trajectory), and study how the accuracy (for fixed step size) deteriorates as $r_0 \to 2$.
Try this also for different step sizes.