

Exercise Week XII

Numerov's algorithm

Using the simplest version of the implementation of the Numerov's algorithm (see `harmonic0.f90`) perform the following computational experiments:

1. Calculate and plot eigenfunctions for various values of n (number of nodes of the eigenfunction), from $n=0, 1, 2, \dots$. Let the code find the correct energy value (choosing "0" when the code asks for an energy value). It may be useful to plot, together with eigenfunctions or eigenfunctions squared, the classical probability density, contained in the fourth column of the output file. It will clearly show the classical inversion points. See `harmonic0.gp1` on Moodle as an example of a macro for `gnuplot`.
2. Specify an energy value not corresponding to an eigenvalue. Look at the resulting wavefunctions.
3. Specify an energy value close to but not exactly corresponding to an eigenvalue. Look at the resulting wavefunctions.
4. Examine the effects of the parameters `xmax`, `mesh`. For a given Δx , how large can be the number of nodes?
5. Verify how close you go to the exact results (remember that there is a convergence threshold on the energy hardwired in the code). What are the factors that affect the accuracy of the results?
6. (*optional*) Repeat the numerical experiments with the improved `harmonic1.f90` code.