<u>**PHYS580 Lab 13, November 21, 2018**</u>

Assignment: in today's lab exercise you will compute solutions to the time-independent Schroedinger equation in one dimensions.

1. Use the starter programs *shoot.m* and *potential.m* (or your own equivalent routines) to study one-dimensional quantum mechanics with square-well potentials. First, obtain the first few even and odd parity solutions for a single square well of depth $V = 10^5$. Automate the iteration process so that your program automatically zooms in to the solutions without your having to direct by hand the iteration direction and step size at each step. Then, repeat the calculation with a secondary barrier of height $V = 100$ added at the center of the well, spanning $[-a, a]$ in x. Compare the resulting states and energies to the exact results for infinite barriers given in Eqs. (10.6) – (10.8) in the textbook, and explain the differences.

2. Next, use the programs *matchlj.m / lj.m* and *var3.m / calc_energy_var.m / normalize.m* (or your own equivalent codes) to obtain the first few energy levels (both energies and wave functions) for a Lennard-Jones potential of dimensionless energy scale $\varepsilon = 10$ and length scale $\sigma = 1$. Do you get essentially identical ground states with the two methods?

   For the variational approach, it can be important to employ good strategy to speed up convergence by varying the magnitude of wave function updates (variable fr), and possibly having nonzero "temperature" T along the way (even though you are only trying for the ground state). The strategy of using $T > 0$ in the variational approach is the idea behind *simulated annealing*.

   [OPTIONAL] Try to find an excited bound state with the matching method. To support multiple bound states, you will need to make the LJ well much deeper, e.g., $\varepsilon = 30$. Note that the larger the energy, the more nodes the wave function has.