

## Using the Variational method to get accurate energies

The number of basis functions  $N$  (40 in the program) and starting and ending positions of the box (" $x_i$ " and " $x_f$ " in the program) were chosen so that the energies shown are accurate to 0.1% or better. If you want to use the program to calculate energies for your own potential (and I encourage you to try this !) you need to :

- make sure that  $x_i$  is small enough and  $x_f$  is large enough that the wavefunction is zero before it reaches the end of the box. Since you're using a particle in a box basis set, the basis functions (and hence the wavefunctions you calculate) are zero outside the box. If you make the box too small, you will artificially compress the wavefunction and will increase its energy.

- make sure that you use enough basis functions (using more basis functions gives more accurate results, but makes the program slower - the execution time is approximately proportional to  $N^2$ .)

The variational method always gives energies that are above the real energies, so try each of the steps above and check to see if the energies you're interested in change significantly (lower energy = better). If they don't, then you're done !