Spring, 2008

Physics 780.20: Assignment #3

These exercises are follow-ups to class and background-note discussion of Richardson extrapolation (session 4), eigensystems (session 5), and adaptive numerical routines (the last one is a bonus problem). These involve modifications to the `derivative_test.cpp` code and the `eigen_basis.cpp` code. Please ask questions! It is due at the end of the day (midnight) on Thursday, May 1.

To "hand in" the assignment, upload to Carmen a zip archive of your program files (with the answers to any questions in the comments) and a postscript file of the log-log plot. Use C++ and any plotting program you want (gnuplot is recommended). *Check the 780.20 webpage for suggestions and hints.* Please give feedback early and often.

1. It's time to start thinking about a 780.20 project. Please send email to furnstahl.1@osu.edu with a (brief!) description of your ideas for a project. They can be very vague at this point; we will refine them as the quarter progresses! See the 780 webpage for some past project descriptions.

2. Add a subroutine to take the Richardson extrapolation used in the "`extrap_diff`" subroutine one step further. That is, `extrap_diff` calls `central_diff` with two different values of h and then combines them to extrapolate to smaller h (leading to an error proportional to h^4). Now write a new routine (called `extrap_diff2`) that calls `extrap_diff` with two different values of h and combines them appropriately to get a still steeper dependence of the error on h. Verify the result by making an error plot (you may want to increase the starting value of h to 0.5). [A new version of `derivative_test.cpp` with `extrap_diff` explicitly written with `central_diff` is available from the 780 homepage.]

3. Modify `eigen_basis.cpp` so that you can print out (to a file is best!) the approximate wave function corresponding to a given state (e.g., the ground state or the first excited state). Plot the exact ground state wave function and the approximate wave function (as a function of r) for one of the potentials (your choice; I like the Coulomb best!) with a fixed b (your choice) for basis sizes of 1, 5, 10, and 20. Comment on the nature of the convergence and speculate about choosing b based on your plots. Make sure that the wave functions are normalized.

4. (BONUS) Make the calculation using the central difference method *adaptive*. That is, you specify the function but don't specify the value of h. Instead, your program determines (or,

more precisely, estimates) the optimal value of h automagically and uses that. Compare the h chosen by your program for the function described above to the value you would select based on the error plot.

5. (BONUS) Devise a measure of how close the approximate wave function is to the exact wave function and determine how this measure scales with the basis size D.