Computational Physics Project 8

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1 Bound States by Diagonalization

1.1 Harmonic Oscillator

The only change made to the base program `diag-box-demo.f90` to achieve solutions to the harmonic oscillator program was to the potential at the start of the program. The potential at point i is $v_i = (r_i - (N/2)\delta x)^2$, where r_i is the distance from the origin, δx is the change in time, and N is the total number of points. Note that the potential is centered around the center of the box. Solutions are plotted with various box sizes. The total number of points is either 1,000 (for box sizes of 20 and 2,000) or 2,000 (for a box size of 200).

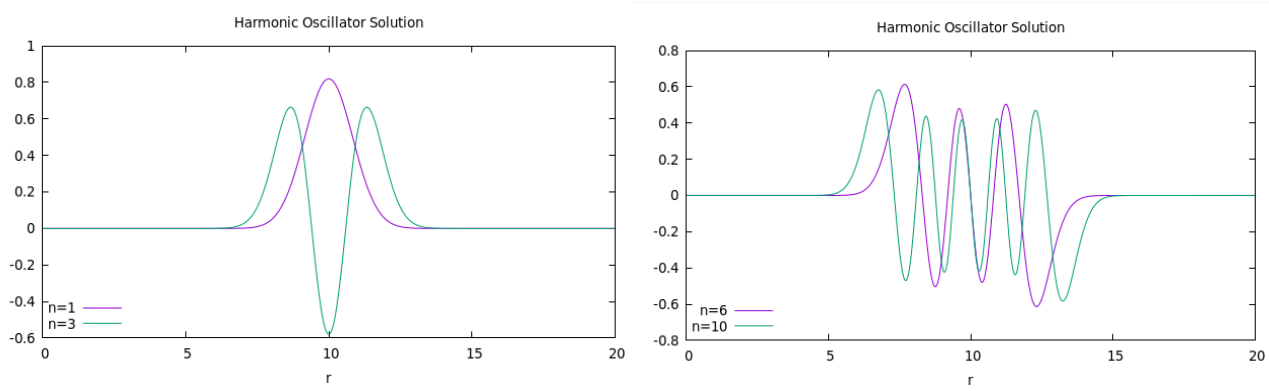

Figure 1: Harmonic Oscillator solution with a box size of 20 units.

```
energies for l =   0:

  7.070818E-01  2.121195E+00  3.535209E+00  4.949122E+00  6.362936E+00  7.776649E+00  9.190263E+00
```

Figure 2: Energy eigenvalues for a box size of 20 units

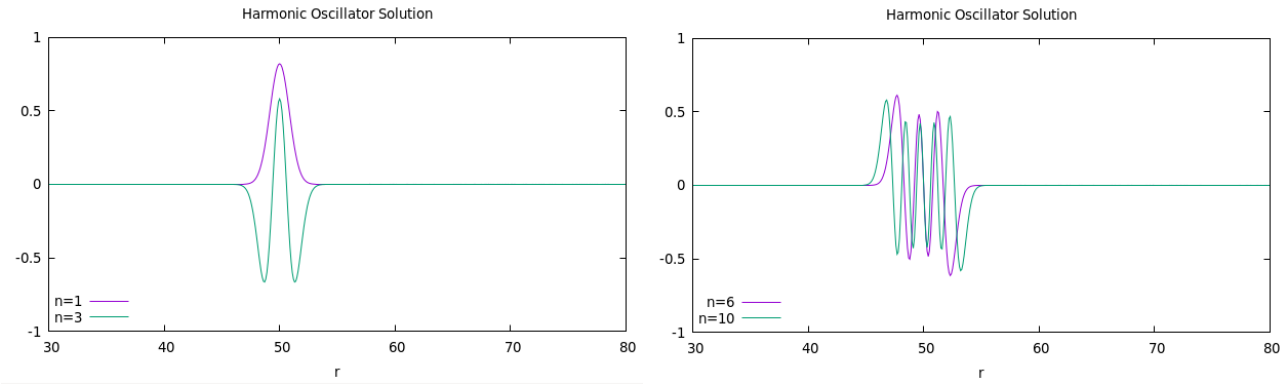

Figure 3: Harmonic Oscillator solution with a box size of 100 units.

```
energies for l =   0:

  7.064812E-01  2.118190E+00  3.527389E+00  4.934072E+00  6.338231E+00  7.739859E+00  9.138950E+00
```

Figure 4: Energy eigenvalues for a box size of 100 units

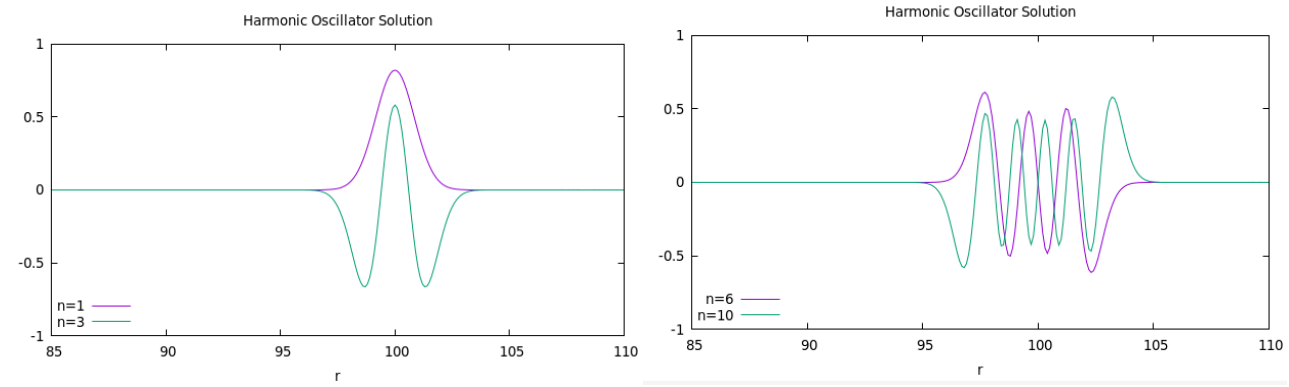

Figure 5: Harmonic Oscillator solution with a box size of 200 units.

```
energies for l =   0:

  7.064812E-01  2.118190E+00  3.527389E+00  4.934072E+00  6.338231E+00  7.739859E+00  9.138950E+00
```

Figure 6: Energy eigenvalues for a box size of 200 units

1.2 Coulomb Potential

With an attractive Coulomb potential of $V(r) = -\frac{1}{r}$, solutions are plotted with various box sizes. The total number of points is either 1,000 (for box sizes of 20 and 100) or 2,000 (for a box size of 200).

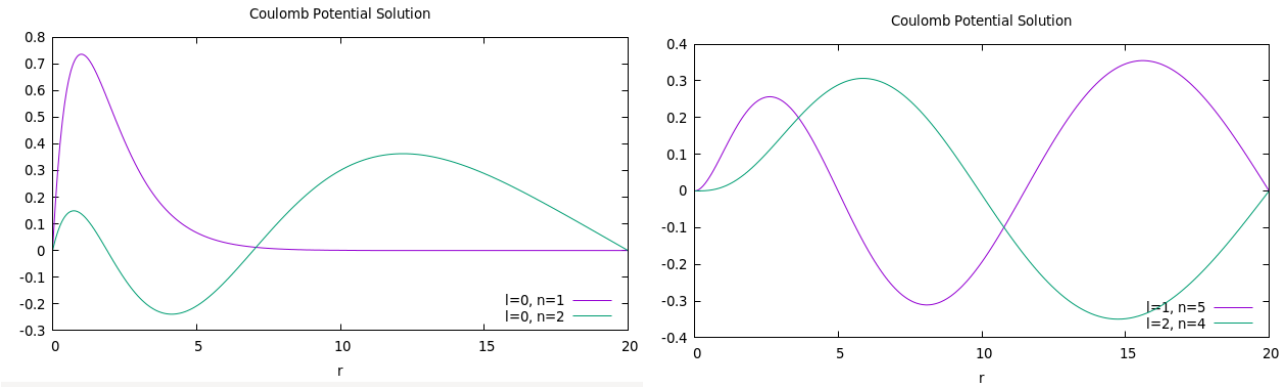

Figure 7: Coulomb solution with a box size of 20 units.

For $l = 0$, $n = 1$, the energy eigenvalue is -0.500. For $l = 0$, $n = 2$ the energy eigenvalue is -0.1249.

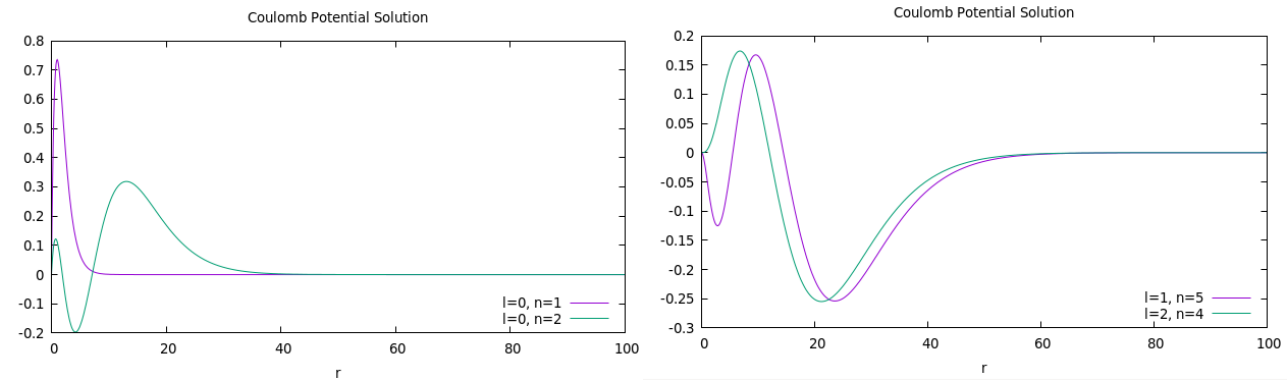

Figure 8: Coulomb solution with a box size of 100 units.

For $l = 0$, $n = 1$, the energy eigenvalue is -0.4988. For $l = 0$, $n = 2$ the energy eigenvalue is -0.1249.

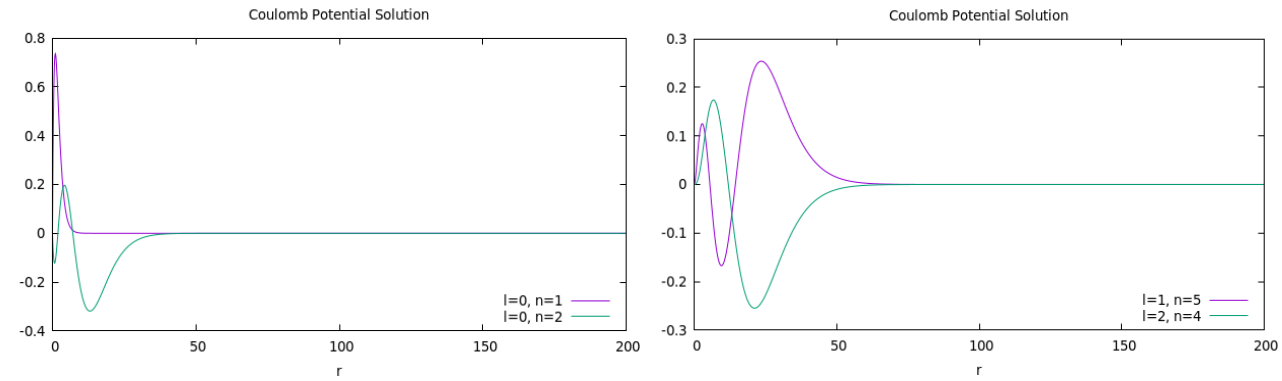

Figure 9: Coulomb solution with a box size of 200 units.

For $l = 0$, $n = 1$, the energy eigenvalue is -0.4988. For $l = 0$, $n = 2$ the energy eigenvalue is -0.1249. These values

match that of the 100-unit-sized box.

1.3 Rydberg Orbitals

Numerous adjustments to the `diag-box-demo.f90` program to plot the Rydberg orbitals for high n. Both `hint1.f90` and `hint2.f90` were used, with adjustments made to the bounds of many arrays to be compatible with the hints' computation methods. 2,000 points were used to exhibit proper boundary conditions for $n = 8$.

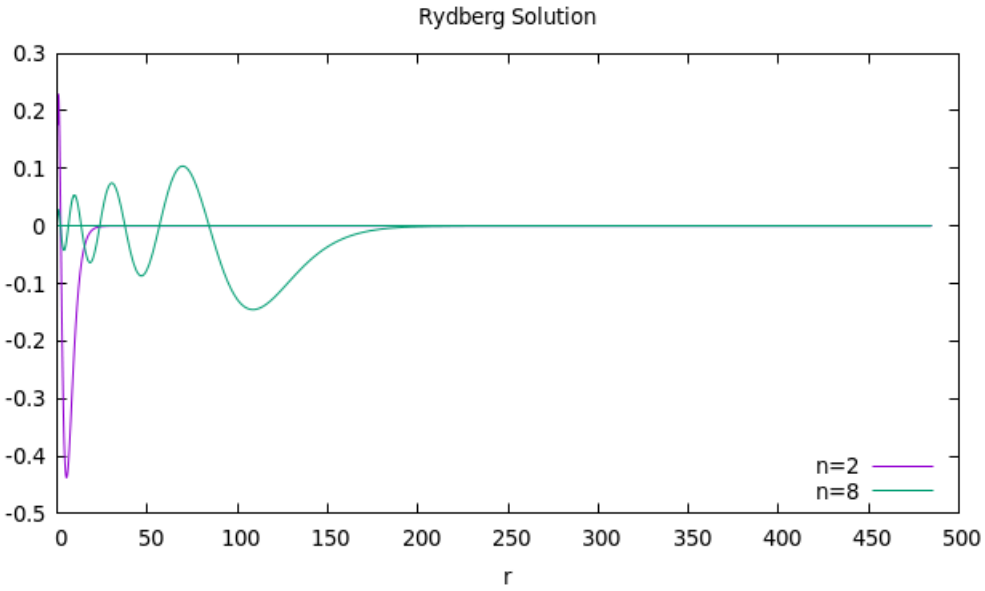

Figure 10: Rydberg orbital for $n = 1$ and $n = 8$

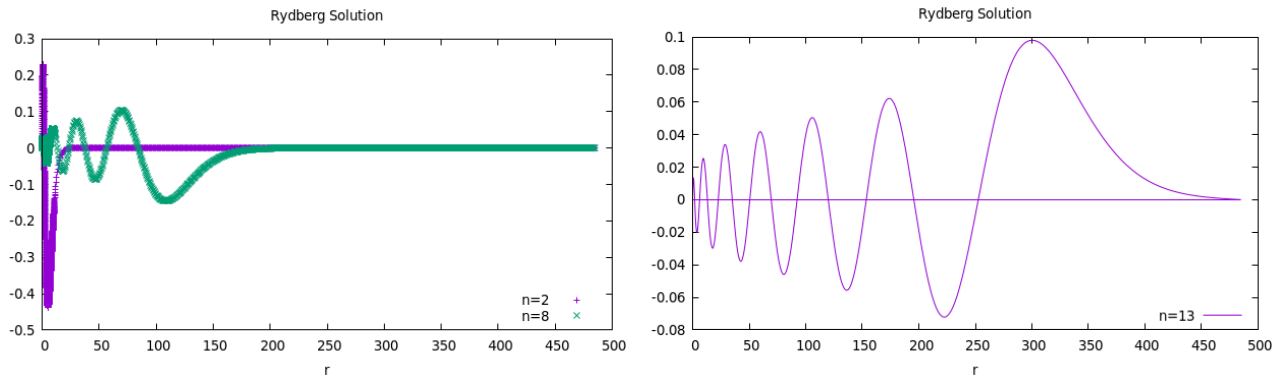

Figure 11: Rydberg orbital for $n = 1$ and $n = 8$ (left, with points) and $n = 13$ (right)

1.4 Conclusion

Varying the box size for the harmonic oscillator and Coulomb potential problems caused small, yet noticeable changes in energy eigenvalues. Proper boundary conditions for the wave functions of the harmonic oscillator were observed in all box sizes. Proper boundary conditions for the Coulomb potential were only observed in larger box sizes.

Obtaining the Rydberg orbitals for high n in the Coulomb problem took a larger number of points to obtain. Using 2,000 points allowed us to calculate the wave function of $n = 13$ with proper boundary conditions. Calculating higher orbital states will take more points, requiring a higher computational complexity.