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CHEG 827
Progress Report

Achieved Up to Date

- Draft of introduction and methods sections of report.
- Can generate the plane wave basis set with a given energy cutoff.
- Can generate the secular Hamiltonian matrix for an arbitrary potential.
- Can solve for the top eigenvalues and eigenvectors of the secular Hamiltonian matrix.

Next steps

- Find realistic scaling for a nonzero potential.
- Find a faster integration procedure. Perhaps decompose the potential into Fourier components.
- Find a numerically well-behaved way to treat another simple system such as the hydrogen atom.

Problems

- The integration (used for evaluating each element of the matrix A) is slow. It is limiting over finding the eigenvalues. This will limit the number of basis functions that can be used.
- Trying to figure out a way to deal with divergent potentials. Ex: v(r) = -1/r for a hydrogen atom.
- High dimensionality makes the problem very intensive. Integrating over 3-D spaces takes many more points than in 2-D or 1-D.

Test Problem: Periodic box with 0 potential. In this case the solutions will be single plane waves. The energy will be the kinetic potential of each plane wave. Here eigenvectors with the same eigenvalue are being added.

Ham =

19.7392	0	0	0	0	0	0	0
0	39.4784	0	0	0	0	0	0
0	0	59.2176	0	0	0	0	0
0	0	0	39.4784	0	0	0	0
0	0	0	0	98.6960	0	0	0
0	0	0	0	0	118.4353	0	0
0	0	0	0	0	0	98.6960	0
0	0	0	0	0	0	0	78.9568

V =

0.0000	-0.0000	0	0	0.0000	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.4244
-0.0000	-0.0000	0.0000	-0.0000	-1.0000	-0.0000
-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.9055
-0.0000	0.9152	0.4031	-0.0000	-0.0000	0.0000
-1.0000	0	-0.0000	0.0000	0	-0.0000
0.0000	0.4031	-0.9152	0.0000	-0.0000	-0.0000
-0.0000	0.0000	0.0000	1.0000	-0.0000	0

```
ans =

  118.4353
   98.6960
   98.6960
   78.9568
   59.2176
   39.4784

Elapsed time is 6.972058 seconds.
```