Computational Methods: Homework 4: Lanczos

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Homework is due in three weeks.

In class we have discussed the Lanczos method and how to obtain information on $F(z) = \langle \phi_0 \mid \mathcal{O}^\dagger (z - H)^{-1} \mathcal{O} \mid \phi_0 \rangle$, where z is a complex variable. Here is a simple homework that will illustrate the method of moments for the kinetic energy operator in in the morse potential.

- The first thing to do is obtain the lowest eigenvalue of the Morse potential (recall we looked at morse-pot.f90 earlier in the year) using the Lanczos routine. This requires you to combine programs somehow ;-).
- Make a plot of the convergence with iteration number of the lowest eigenvalue coming from your Lanczos routine.
- You can actually investigate the wave function that is obtained from Lanczos as we have discussed in class. How does the lowest eigenvalue wavefunction for the Lanzcos algorithm compare to the lowest eigenvalue wavefunction from the original Morse solver?
- Using the kinetic energy matrix as your operator $\mathcal{O}$, make a plot of $F(z)$ as a function of z. Since z is complex, you may want to do a contour plot of $\mid F(z) \mid$ as a function of $Re(z)$ and $Im(z)$. What can you say about the convergence of the continued fraction method? Does it converge as quickly as the eigenvalue problem?