# Ground State Calculator: Ideas

Adam J. Robinson

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# 1 General Ideas

## 1.1 A Method for Determining Excited State Energies

All stationary states are orthogonal. Addtionally, the first excited state is the state that is both orthogonal to the ground state and minimizes the expectation value of the Hamiltonian. It may be possible to find excited states by taking a Fourier Transform of the ground state, into frequency space. This would make it easy to determine trial wavefunctions which are orthogonal to the ground state. If the expectation value of the Hamiltonian for sine and cosine states can be determined, this can be used to find the orthogonal state that minimizes the expectation value of the Hamiltonian. Further analysis will be neccesary to determine whether or not this process will actually be practical.

## 1.2 Monte Carlo Optimization

Perform Monte Carlo based determination of the ground state energy. The process can be made faster by determining a rate at which to decrease the size of the terms added to the wavefunction. This rate would have to be determined through experimentation (probably not analyticlly, but maybe). The mean and standard deviation of the change in energy expected from each step could then be estimated. These values can be used to adjust the accuracy of the Monte Carlo integration techniques being used. Early in the process, low accuracy integration can be used, so long as the error is an order of magnitude less than the expected change in the energy with each step.

## 1.3 Quantum Dynamics

Derive and expression for the change in the expectation value of the Hamiltonian with respect to the change in the nuclear coordinates. This should be possible to do analytically. Use this expression to calculate the force at each point in time and perform velocity-verlet integration, much like a traditional molecular dynamics simulation.

## 1.4 Solid State Approximation

Determine a means of making the wavefunctions and Hamiltonian contains a perdiodic boundary condition. In theory, this would make the system capable of finding energies for bulk crystal structures. If this was to work exceptionally well, it might be a competitor to DFT for certain systems.

# 2 Optimization Ideas