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Applying the Conjugate Gradient Method in an Infinite Dimensional Hilbert Space

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The ground state wave function and energy of a quantum system with a given Hamiltonian may be approximated using perturbation theory or the variational method. Both methods have limitations, the former requiring the Hamiltonian perturbation be small enough for the series to converge while the latter being only as good as the choice of functions used in the expansion, ultimately providing only an approximate ground state whose mean energy is an upper bound to the ground state energy.

The iterative method of Gradient Descent (GD) applied to the energy expectation functional of the wave function can overcome the limitations of the aforementioned methods. Applying GD in an infinite-dimensional space is achievable by careful bookkeeping of only the non-zero components of the state vector in the chosen basis of expansion and those matrix elements of the Hamiltonian in that basis required to calculate the next iteration. For a Hamiltonian with a sufficiently sparse matrix representation in the chosen basis, the calculation is numerically tractable. Unsurprisingly, however, the GD method applied in infinite dimensions suffers from the same convergence problems that it suffers from in finite-dimensional space.

In finite dimensional problems the Conjugate Gradient (CG) method overcomes the GD convergence limitations using improved search directions. CG will be formulated in infinite dimensions for a quantum system with a time-independent Hamiltonian. Polak-Ribière and Fletcher-Reeves versions of CG will be implemented. The method will be used to find energy eigenstates and eigenvalues using three functionals of the wave function, one based on energy expectation, one on its variance, and a third utilizing a Lagrange multiplier. Several simple quantum systems will illustrate the method.

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