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Implementing the Gradient Descent Method in an Infinite Dimensional Hilbert Space

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Approximation of the ground state wave function and energy of a quantum system is often achieved using perturbation theory or the variational method. The former approach suffers from the requirement that the Hamiltonian perturbation be small enough for the series to converge while the variational method is only as good as the choice of functions used in the expansion, providing only an approximate ground state whose mean energy is an upper bound to the ground state energy. The method of gradient descent, typically used for optimizing functions over finite dimensions, may be generalized to the infinite-dimensional Hilbert space of a quantum mechanical system to avoid both previous limitations. One may find the ground state of a quantum system by minimizing the energy functional of the wave function of the system via iterative calculation of better approximations using the gradient of the functional. This can be achieved in an infinite-dimensional setting 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 iterative approximation via gradient descent. The sparse nature of the Hamiltonian matrix elements in a chosen basis for many quantum systems ensures that subsequent iterations of the state vector have only a finite number of non-zero components, thereby making the method computationally tractable.

The gradient descent method will be formulated for a quantum system with a time-independent Hamiltonian. The algorithm will be illustrated with a simple quantum system. The impact of symmetry in the choice of initial state vector will be discussed. Limitations of the method and potential improvements (e.g. conjugate gradient) will be considered.

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