CHAPTER OVERVIEW

2: Approximation Methods

Approximation methods can be used when exact solutions to the Schrödinger equation cannot be found. In applying quantum mechanics to 'real' chemical problems, one is usually faced with a Schrödinger differential equation for which, to date, no one has found an analytical solution. This is equally true for electronic and nuclear-motion problems. It has therefore proven essential to develop and efficiently implement mathematical methods which can provide approximate solutions to such eigenvalue equations. Two methods are widely used in this context- the variational method and perturbation theory. These tools, whose use permeates virtually all areas of theoretical chemistry, are briefly outlined here, and the details of perturbation theory are amplified in Appendix D
