

Abstract

Hedin's *GW* approximation for the self-energy operator has become the primary theoretical tool for computing band structures over the past 20 years. During this time the method has matured from an approximation applied only to the most simple model systems to a fully *ab initio* technique.

This thesis presents a study of the applicability of the *GW* approximation to excitation spectra of finite and extended systems. During the course of investigation, we have demonstrated that the accurate excitation energies may be obtained in an *ab initio* approach within the pseudopotential approximation. We also study the applicability of the method to metallic systems, with a particular emphasis on bulk sodium.

Ground state total energies are explored as a relatively new application of the approximation. We compute energies for model finite systems and isolated atoms, and present the first analysis of the affects of including self-consistency within the *GW* approximation for inhomogeneous systems.