On Thomas-Fermi Theory and Extensions

Of concern to quantum chemists and solid state physicists is the approximate numerical computation of the ground state wave function, and the ground state energy and density for molecular and other quantum mechanical systems. Since the number of molecules in bulk matter is of the order of 10^{26}, direct computation is too cumbersome or impossible in many situations. In 1927, L. Thomas and E. Fermi proposed replacing the ground state wave function by the ground state density, which is a function of only three variables. Independently, each found an approximate expansion for the energy associated with a density. (The wave function uniquely determines the density, but not conversely.)

A computationally better approximate expansion was found in the 1960's by W. Kohn and his collaborators; for this work Kohn got the Nobel Prize in Chemistry in 1998. A successful attempt to put Thomas-Fermi theory into a rigorous mathematical framework was begun in the 1970's by E. Lieb and B. Simon and was continued and expanded by Ph. Benilan, H. Brezis and others. Very little rigorous mathematics supporting Kohn density functional theory is known. In this talk I will present a survey of rigorous Thomas-Fermi theory, including recent developments and open problems (in the calculus of variations and semi linear elliptic systems).