THE CALCULATION OF ENERGY FOR ATOMS, MOLECULES AND CRYSTALS

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Introduction

The ground state energy will determine the equilibrium properties of any system. In principle, if the ground state energy is known, all the relevant parameters can be derived accordingly. All the systems of interests such as crystals, multilayers systems, alloys and magnetics systems are composed of atoms and molecules of different arrangements. Therefore the best starting point to compute the energies of the complex systems of interest is to compute the energy of simple systems first, namely the energy of atoms and molecules. The energy can be computed if the wave function of the systems is known i.e. if the Shroedinger equations for the systems can solved. Even for the relatively simple multi-electrons systems or molecules, there is no analytical solution. Hence numerical techniques are employed. In using this approach, various sampling assumptions were made so that the problems are tractable. Even then it still involved some heavy computing.

Materials and Methods

There are two major approaches to the numerical energy computation. First and the straight forward way is to solve Shroedinger equation for the systems. The well-known example of this approach is the Hartree-Fock technique. This technique has become the benchmark for energy computation in the quantum physical chemistry. The approach involves the solution of many-electrons Shroedinger equation by assuming that the electron moves in the average potential due to the nucleus and other electrons. Hence the potential is composed of two main components, the single electron potential and the electron-electron potential. The computation of electron-electron potential is very demanding, but it can be reduced considerably by using Slater's $X\forall$ potential. The second technique approach involves using the electron density as the defining quantities. It is vigorously shown that the ground state of the electrons system is determined by the electrons density functionals (Kohn and Sham, 1965). The technique is known as density funtionals theory. The simplest example of this technique is the Fermi-Thomas model of the atom. This is the main technique used in energy band calculations of crystal.

Results and Discussion

While the Hartree-Fock technique is more straight forward, (hence the interpretations and causes for errors are also straight forward), the amount of computations is more demanding, hence only simple molecules can be computed using this technique. In Hartree-Fock technique, the solutions are obtained by solving the Shroedinger equations iteratively. Two main techniques used in solving the equations are Green function technique and basis function technique, (where the non-linear Fock equation are linearised and normal matrix algebra are utilised). Both techniques are being employed. The Green function technique is employed to compute the ground state energy of atoms. The results obtained are quite close to those reported in the literature but did not obtain the expected accuracy of the technique. Currently the basis function technique being developed will be applied both to atoms and simple molecules. Both $X\forall$ and the vectors model of multielectrons atoms are being computed for the electron-electron interaction. Their results are within reasonable agreements with each other hence the more computationally efficient $X\forall$ techniques will be used. For the density functional theory, the total energy for the Fermi-Thomas was computed and the answer obtained was comparable to the ones quoted in the literature (Parr and Yang, 1989). Three mains variants of the model were solved, namely the Fermi-Thomas, Fermi-Thomas-Dirac and Fermi-Thomas-Dirac – Weisteker models. The technique employed the intial value problem, which was solved using second order Runge-Kutta. The continuation of jobs will involve using Linear Muffin-Tin orbitals to solve the many atoms- molecules and crystals.

Conclusions

The results obtained from the computations that have been carried out were quite encouraging. It is comparable to the quoted values from the literature.

References

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