Physics 489 S 04 Lecture 17
Density Functional Theory
Notes on WWW pages as a pdf file; also related to A & M Chpt. 17

1. The many-body electron problem
2. Hohenberg-Kohn Theorems
   (a) The ground state density $n(\mathbf{r})$ determines *all* properties of the many-body system of electrons
   (b) There exists (in principle!) a functional $F[n(\mathbf{r})]$ which when minimized determines the exact ground state energy and density
3. Kohn-Sham Ansatz
   (a) Replace the interacting electron problem with a non-interacting problem *with the same density* $n(\mathbf{r})$
   (b) Can use independent particle methods to solve for $n(\mathbf{r})$
   (c) Solution of Schrödinger Eq. for *independent* electrons moving in a potential $V_{eff}(\mathbf{r})$, which is a functional of $n(\mathbf{r})$
   (d) Same approach as the "Hartree" methods, A & M Chpt. 17
4. Functionals for Exchange and Correlation
   (a) Must be derived from some many-body calculation
   (b) LDA - Local Density Approximation
      i. Widely used assumption - that the exchange and correlation energy at a point $\mathbf{r}$ is *the same as in a homogeneous electron gas of density* $n(\mathbf{r})$
      ii. Best calculations are those of Ceperley and Alder using Quantum Monte Carlo Methods
      iii. With that assumption, one can solve the independent particle Kohn-Sham equations to essentially arbitrary accuracy!
   (c) GGA - Generalized Gradient Approximations
   The success of these approximations has led to the wide spread use of DFT in chemistry
5. Solution of the Kohn-Sham "Schrödinger-like" Equations
   (a) Results: H, He, H_2
   (b) Results: Atomic examples
   (c) Results: Solids
   (d) Results: Molecules: GGA
   (e) Failures!