Lecture 17: Density functional theory

The Kohn-Sham formulation of the density functional theory is explained. We contrast the Thomas-Fermi approximation and the Kohn-Sham treatment of the kinetic energy. The local density functional theory is explained as a practical method to treat exchange and correlation in a self-consistent band calculation. The limitations of the local density functional approximation is discussed, starting with the Heitler London approximation for hydrogen molecules. The notion of the Mott insulator is introduced.

Reading: Marder 9.3.1, 9.3.2