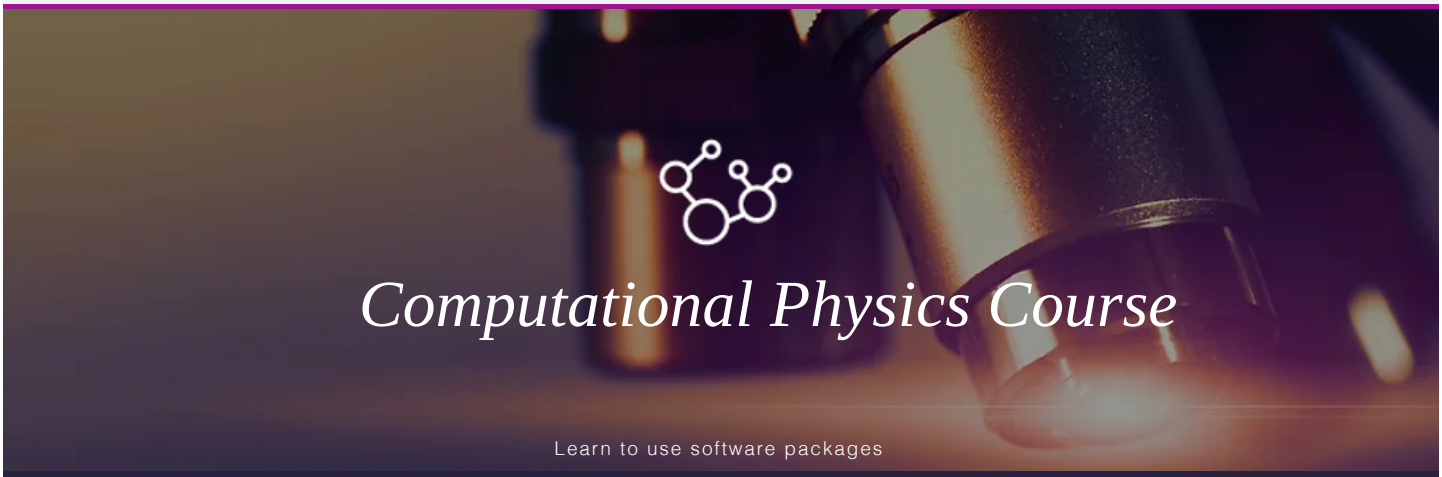

Density functional theory (DFT)

Principle of DFT is in the one-to-one correspondence between the particle density ρ(r) and the ground-state wave function Ψ(r1 ,r2,...rN).

That is, different density corresponds to different wave function. You might think it strange because the functional space is apparently larger for the wave function, but it is not the case. This is what Hohenberg and Kohn showed in 1964. The functional space of the antisymmetric function of degree 3N is huge, but the space spanned by the solution of the Schrodinger equation is not so large because the ground state is determined by the external potential V(r), which is a function of degree 3.

Hohenberg, Pierre; Walter Kohn (1964). "Inhomogeneous electron gas". Physical Review. 136 (3B): B864–B871.

Having learned DFT, let us move to learning program packages. We begin by learning Quantum Espresso

The University of Tokyo