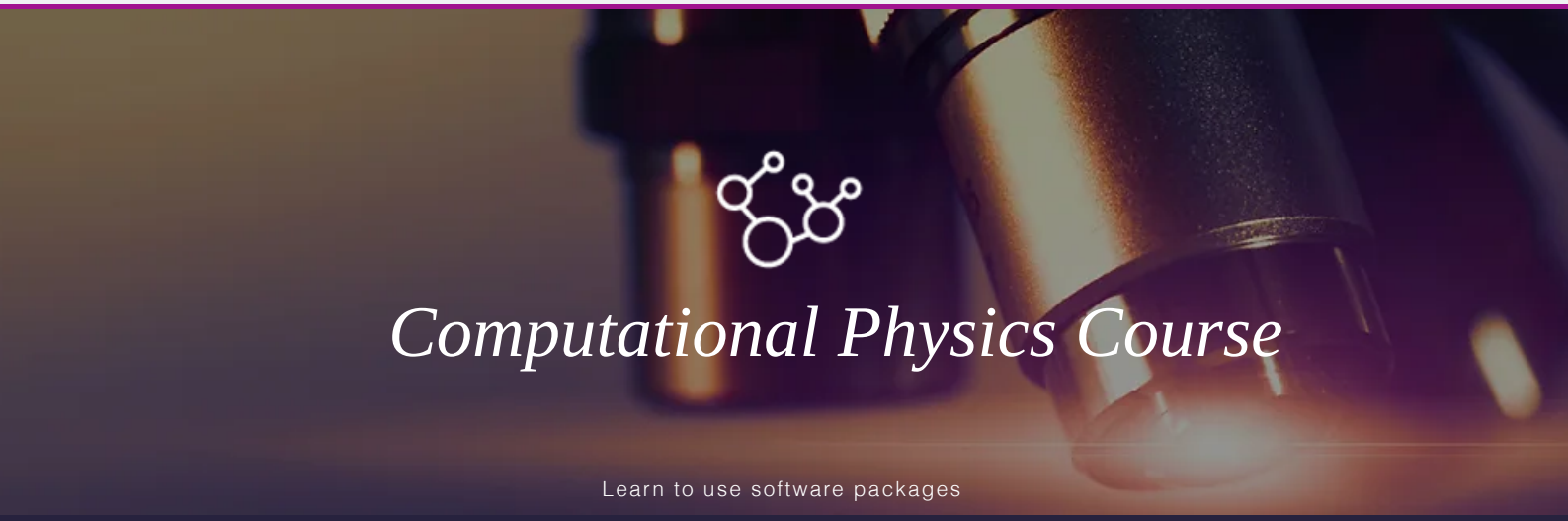
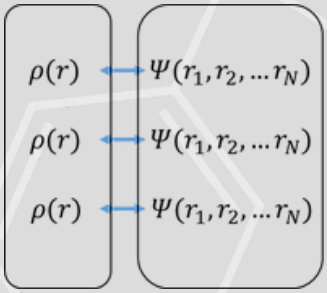


Density functional theory (DFT)

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 and vice versa. 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.

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

Why is the Hohenberg-Kohn theorem so important?

The theorem tells us that we need only the density to characterize the ground-state; the wave function is not essentially important. It also tells us that we need only three parameters x,y, and z for a 3D system instead of 3*N* parameters required to characterize the wave function, where *N* is the number of particles, which in this course are mostly electrons.

If we know the density ρ, we can uniquely determine the external potential *v* applied to the system [HK theorem] and thus determine the wave function by solving the Sroedinger equation; here the external potential is originated from the Coulomb potential from nuclei and/or the electromagnetic field. This way, physical quantities such as the kinetic energy and the potential energy are, in general, functional of the density. This is the reason why this theory is called the density functional theory (DFT).

In particular, the total energy takes a minimal value for the ground state density ρ0. So, by minimizing the total energy with respect to the density, we can obtain the ground state density, and then characterize the ground state.

Unfortunately, however, there is no guiding principle to determine the functional. Researchers took trials and errors to develop an approximate functional, and owing to the effort, DFT can be practically and reliably applied to large number of materials.

DFT1.pdf DFT2.pdf DFT3.pdf

lecture. Let us use this excellent slide to learn DFT. The slide, separated into three PDF files, contains basics appearing in many DFT textbooks:

1. Hartree-Fock theory
2. Thomas Fermi theory
3. Hohenberg-Kohn Theorem
4. Kohn-Sham method
5. Local density approximation and its extension
6. Application to molecular conductance (For later use)

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Here I would like to give a summary of the density functional theory, which I hope will supplement the lecture given be Bahramy-sensei.

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