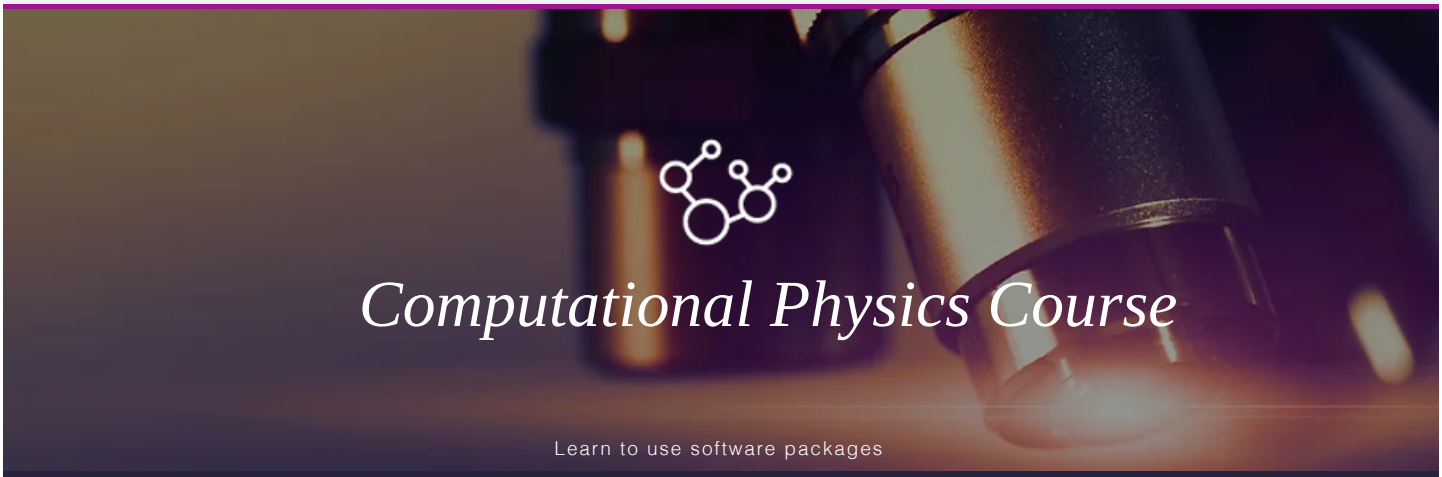


1. What is Hartree-Fock?
First, let us remind what was HF?

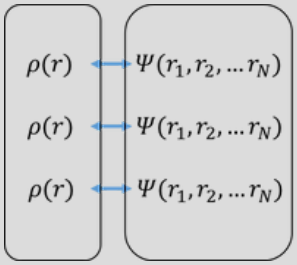
PDF

Next, consider the HF exchange in more detail as a preparation to learn DFT.

PDF

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?

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.

Having leaned the exchange hole of HF approximation and the exchange-correlation hole of exact wave function, let us consider how the exchange-correlation may be obtained. According to DFT, it can be given as a functional of the density. Once the functional form has been obtained, one can solve the many-body problem exactly. Is that possible? The answer is no, but people have found approximate forms, which are improving year by year. In the end, one can expect almost perfect form will be found although I do not know if that can be handled feasibly or not: It might be possible that quantum Monte Carlo simulation is more feasible.

2. More about density functional theory?
I present you modern density functional theory.

Here I provide additional comment on the response function

Also, I provide implication of the ACFDT

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

The University of Tokyo