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Why is the Hohenberg-Kohn theorem so important?

This theorem tells us that we need only 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 $3N$ 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 Schrodinger 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 ρ_0 . 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 this effort, DFT can be practically and reliably applied to large number of materials.



The University of Tokyo

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