Orbital-free density functional theory: functional derivative of the kinetic energy for spherically symmetric systems

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According to the Hohenberg-Kohn theorem the density can be obtained from the Euler equation. As the kinetic energy functional is unknown, density functional calculations are mainly based on the Kohn-Sham scheme. Recently, there is a growing interest in orbital-free methods. It is a huge simplification as only one equation (the Euler equation) has to be solved instead of several Kohn-Sham equations.

The talk will present an ensemble extension of the problem. This generalization allows us to solve the original Euler equation [1, 2, 3]. Ensemble non-interacting kinetic energy functional is constructed for spherically symmetric systems and the differential virial theorem is derived for the ensemble. Then a first-order differential equation is derived for the functional derivative of the ensemble non-interacting kinetic energy. A special case of the solution provides the solution of the original orbital-free problem for spherically symmetric systems.

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