Potential Functionals: Solution to the v-representability Problem and Theoretical Foundation for the Optimized Effective Potential in Density Functional Theory

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We have constructed a functional of external potentials and its variational principle for the ground-state energy. This potential functional formulation is dual to the density functional approach and provides a solution to the v -representability problem in the original Hohenberg-Kohn theory. A second potential functional for Kohn-Sham non-interacting systems establishes the theoretical foundation for the optimized effective potential (OEP) approach and results in efficient approaches for ensemble Kohn-Sham calculations.

We have developed efficient methods for OEP calculations, based on direct optimization in the potential functional space. Calculations with exact exchange and with exact exchange plus correlation will be presented.

Time permitted, I will present a direct optimization method for the computation of the Kohn-Sham kinetic energy functional, the exchange-correlation potential and other density functionals including the exchange-correlation energy from a given electron density. The method is based on the construction of variational functionals of the one-electron potential.

References

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