The Adiabatic-Connection Dissipation-Fluctuation Theorem as Route to a New Generation of Density-Functional Methods

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The adiabatic-connection dissipation-fluctuation theorem provides a rigorous basis for constructing correlation functionals for density-functional methods within the Kohn-Sham formalism [1]. In the simplest case, the correlation energy within the direct random phase approximation is obtained. By considering besides the Coulomb kernel also the exact frequency-dependent Kohn-Sham exchange kernel in the construction of the correlation functional, methods with a wide applicability and an unprecedented accuracy are obtained [1–4]. Systems that are problematic or not accessible for standard density-functional methods can be handled. For example, electronic structures characterized by static correlation can be treated [2] as well as Van-der-Waals interactions [3]. On the other hand, challenges like higher computational effort or questions of numerical stability come along with these new approaches. The current status and the perspectives of approaches based on the adiabatic-connection dissipation-fluctuation theorem are discussed.


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