A Moreau–Yosida-Based Kohn–Sham Inversion Scheme

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Abstract

Density-functional theory (DFT) is central to efficient calculations in chemistry, materials science, and solid-state physics. While formally exact, the universal density functional is, in general, unknown and must therefore be approximated. Most applications use the Kohn–Sham formulation of DFT to compute ground-state densities, but the inverse Kohn–Sham problem – recovering the non-interacting potential from a given density – is equally fundamental. Kohn–Sham inversion has been proposed as a route to obtaining accurate exchange-correlation potentials and improving functional approximations. In this talk, I will present a rigorous inversion scheme based on a Moreau–Yosida-regularised formulation of DFT, which enables the extraction of the exchange-correlation potential as a strict mathematical limit. This regularisation not only stabilises the inversion but also provides a framework for deriving error bounds, thereby bridging theory and computation [1]. Using periodic homogeneous Sobolev spaces, the theoretical framework harmonises with the physics of periodic systems, and the structure of the inversion scheme allows it to be implemented in existing electronic structure codes, such as DFTK. This enables the inversion to be performed on realistic systems, such as bulk silicon, gallium arsenide, potassium chloride, and sodium chloride. I will in particular highlight the study of error propagation from the input density to the resulting potential and the consequences of various choices for the guiding functional [2].

References

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2. Bakkestuen, V. H., Penz, M., Falmår, V., Herbst, M. & Laestadius, A. Moreau–Yosida-Based Kohn–Sham Inversion for Periodic Systems. In preparation (2026).