One-body Reduced Density-matrix Functional Theory for the Canonical Ensemble

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One-body reduced density-matrix functional theory was recently presented for the grand canonical ensemble with a finite basis set [1]. We want to study 1RDMFT in the same setting but with fixed number of particles. Unlike in classical thermodynamics this can not be reached through a Legendre transformation due to different underlying spaces.

In this work we require elevated temperature. This guarantees that the 1RDMs generated by potentials do not lie on the boundary of the set of all 1RDMs. This is crucial to show differentiability of the universal functional which can be achieved by using results from convex analysis and invertibility of the potential-to-1RDM map [2]. Finally this allows us to characterize the set of all v-representable 1RDMs in this setting.

References

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[2] Thomas L. Gilbert. "Hohenberg-Kohn theorem for nonlocal external potentials". In: *Physical Review B* 12.6 (1975), p. 2111. DOI: 10.1103/PhysRevB.12.2111.