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Density functional theory and optimal transportation with Coulomb cost. (English)

The present work links the density functional theory (DFT) with the optimal transportation theory (OTT), the goal of which is to transport a “mass” in such a way that the “cost” \( c(y, x) \) for transport from \( x \) to \( y \) is minimized. Thus, one has to minimize the cost functional \( \int c(x, y) \, d\gamma(x, y) \) over a set of joint measures \( \gamma \). The minimizers are called optimal transportation plans. The mathematical novelty of the here considered optimal transportation problem is that in case of Coulomb forces, the cost decreases with the distance of the correlated particles and it has a singularity at zero distance.

The authors briefly review the DFT from a mathematical perspective. They introduce the one-particle and two-particle spatial probability densities of electrons for a molecule with \( N \) electrons. Then the universal Hohenberg-Kohn functional and exchange-correlation functionals are presented. The fundamental problem of DFT, the approximation of the two-particle electron density \( \rho_2 \) by the one-particle density \( \rho \) for the description of the ground state energy of the molecular system is explained. Examples of statistical independence, mean-field theory and local density approximation are discussed.

Having introduced the OTT, it is proven that for any \( \rho \), the optimal transportation problem with Coulomb cost possesses a unique minimizer of a special form for an optimal transport map \( T \) associated with \( \rho \). Some general properties of \( T \) are established, e.g. its existence and uniqueness for any number of electrons and each \( \rho \). The geometrical characterisation as well as the uniqueness of the optimal measure, and some general properties of the optimal cost for equal marginals are considered. In case of equal, radially symmetric marginals, an explicit formula for \( T \) is given. The optimal transportation cost is compared with the Hohenberg-Kohn functional, and it is shown that it is its semiclassical limit in the case of two electrons, as well as a lower bound for any number of electrons.

Reviewer: Claudia-Veronika Meister (Darmstadt)

MSC:
82C70 Transport processes in time-dependent statistical mechanics
49K99 Optimality conditions
28C05 Integration theory via linear functionals (Radon measures, Daniell integrals, etc.), representing set functions and measures
49J40 Variational inequalities

Keywords:
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References:


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