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Dissociating limit in density functional theory with Coulomb optimal transport cost

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Abstract. In the framework of Density Functional Theory with Strongly Correlated Electrons we consider the so-called bond dissociating limit for the energy of an aggregate of atoms. We show that the multi-marginals optimal transport cost with Coulombian electron-electron repulsion describes a dissociation effect. The variational limit is completely calculated in the case of $N = 2$ electrons. The theme of fractional number of electrons appears naturally and brings into play the question of optimal partial transport cost. A plan is outlined to complete the analysis which involves the study of the relaxation of optimal transport cost with respect to the weak* convergence of measures.

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