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Dispersion Interactions in the Strictly Correlated Electron Limit of DFT via Multi-Marginal Optimal Transp

Multi-marginal optimal transport (MMOT) is the general problem of aligning a finite collection of probability measures to minimize some notion of overall cost. Due to its own substantial group of applications MMOT has attracted a great deal of attention. In particular, this problem with the well-known Coulomb cost has allowed the development of a mathematical framework to the strongly correlated systems in Density Functional Theory (DFT). In this talk, I will briefly introduce the mathematical settings for both MMOT and strongly correlated systems in DFT, and connect them with the dissociation limit in DFT.

This is joint work with Augusto Gerolin and Mircea Petrache.