DENSITY FUNCTIONAL THEORY AND OPTIMAL TRANSPORT WITH COULOMB COST

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In this talk I explain a promising and previously unnoticed link between electronic structure of molecules and optimal transportation (OT), and I give some first results. The 'exact' mathematical model for electronic structure, the many-electron Schroedinger equation, becomes computationally unfeasible for more than a dozen or so electrons. For larger systems, the standard model underlying a huge literature in computational physics/chemistry/materials science is density functional theory (DFT). In DFT, one only computes the single-particle density instead of the full many-particle wave function. In order to obtain a closed equation, one needs a closure assumption which expresses the pair density in terms of the single-particle density rho.

We show that in the semiclassical Hohenberg-Kohn limit, there holds an exact closure relation, namely the pair density is the solution to a optimal transport problem with Coulomb cost. We prove that for the case with $N = 2$ electrons this problem has a unique solution given by an optimal map; moreover we derive an explicit formula for the optimal map in the case when ρ is radially symmetric (note: atomic ground state densities are radially symmetric for many atoms such as He, Li, N, Ne, Na, Mg, Cu).

In my talk I focus on how to deal with its main mathematical novelties (cost decreases with distance; cost has a singularity on the diagonal). I also discus the derivation of the Coulombic OT problem from the many-electron Schroedinger equation for the case with $N \geq 3$ electrons, and give some results and explicit solutions for the many-marginals OT problem.

Joint works with Gero Friesecke (TU Munich) and Claudia Klueppelberg (TU Munich).