PIMS / AMI Seminar

Friday, September 21, 2012
3:00 p.m.
CAB 657

"DENSITY FUNCTIONAL THEORY AND OPTIMAL TRANSPORT WITH COULOMB COST"

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Abstract

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 give an explicit characterization of the optimal transport problem for systems with 2 electrons and for systems with infinite numbers of electrons.

Based on joint works with Gero Friesecke (TU Munich), Claudia Klueppelberg (TU Munich), Christian Mendl (TU Munich) and Brendan Pass (UAlberta).

Refreshments will be served in CAB 649 at 2:30 p.m.