MEAN-FIELD MODELS FOR DISORDERED CRYSTALS

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In this talk, I will present a functional setting for mean-field electronic structure models of Hartree-Fock or Kohn-Sham types for disordered crystals.

In these models, electrons are quantum particles whose state is described by a one-particle density matrix, while nuclei are considered as classical particles whose positions and charges are random. The existence of a minimizer of the energy per unit volume and the uniqueness of the ground state density of such disordered crystals, can be proved for the reduced Hartree-Fock model (rHF). Both (short-range) Yukawa and (long-range) Coulomb interactions will be considered. In the former case, we can prove in addition that the rHF ground state density matrix satisfies a self-consistent equation, and that our model for disordered crystals is the thermodynamic limit of the supercell model.

Keywords: random Schrödinger operators, disordered crystals, electronic structure, Hartree-Fock theory, mean-field models, density functional theory, thermodynamic limit

[1] E. Cancès, S. Lahbabi and M. Lewin, *Mean-field models for disordered crystals*, arXiv:1203.0402