End of Term PhD Report:
Mathematical foundations of Density Functional Theory

Simon Bignold

(Advisor: Stefan Adams; 2nd Advisor: Christoph Ortner)

During this term I have undertaken work to start my PhD. I have chosen to undertake research in density functional theory (DFT), specifically in the quantum mechanical case, with the aim of formulating the theory in a more mathematical framework. As initial research I looked at two novel approaches of understanding DFT; optimal transport and effective field theory. To understand DFT using effective field theory, I looked at the paper [Fur]. I researched DFT using optimal transport by reading the paper [CFK12] and investigated the idea of formulating the ideas espoused there in the case of bosons (as opposed to the fermions currently considered) and separately in the case of d-dimensions. I believe that the optimal transport approach will prove easily applicable to the case of bosons, however I believe that the semi-classical limit used to show asymptotic exactness of the method in three dimensions will not be applicable in d-dimensions due to the embeddings required in this method which are dimension dependent.

I then tried to use the Gross-Pitaevskii metholodgy to find an easy example of a limiting case of the free energy that can be formulated using DFT formalism. To research the Gross-Pitaevskii method I looked at Chapter 6 of [LSSY05] and the proof of the statements used there in the paper [LSY00]. Having looked into this method I believe it should be relatively easy to formulate the Gross-Pitaevskii energy in a DFT regime in the case of a real wavefunction. The case of a complex wavefunction which is physically more realistic is harder to approach.

References

[LSY00] E. Lieb, R. Seiringer and J. Yngvason Bosons in a trap: A rigorous derivation of the Gross-Pitaevskii energy functional, Physical Review A, 61, 043602, (2000) .

[CFK12] C. Cotar, G. Friesecke, and C. Klüppelberg, Density functional theory and optimal transport with Coulomb cost, to appear in Communications on Pure and Applied Mathematics, (2012).

[Fur] R.J. Furnstahl, EFT for DFT, Lecture Notes in Physics, Springer, preprint (2007).

[LSSY05] E. Lieb, R. Seiringer, J, Solovej and J. Yngvason, The Mathematics of the Bose Gas and its Condensation, Birkhäuser Verlag, (2005).