Fat solutions of the strongly correlated limit of the exact density functional
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Abstract

Understanding the electronic structure and behavior of materials dates back several decades and remains an active area of scientific research today. One of the most commonly used methods, density functional theory (DFT) typically employs the Kohn-Sham formalism and has led to breakthroughs in a wide range of fields, including solid state physics, condensed matter physics, quantum chemistry and biophysics. Despite its successes, this technique suffers from numerous shortcomings, including an inability to accurately describe strongly correlated materials. The strong interaction limit (SIL) of DFT has been suggested as a way to capture more information on the relevant physics for strongly correlated systems [1, 2]. Within this limit, the strictly correlated electron (SCE) distribution has been proposed as the minimizing distribution for electrons interacting via the Coulomb potential [3]. Furthermore, the connection discovered between the SIL of DFT and optimal transportation theory has provided an avenue with which the validity of the proposed SCE minimizer can be analyzed [3].

Preliminary studies have demonstrated the existence of cases in which the SCE distribution is not the correct minimizer [4]. The optimal minimizers in these cases are diffuse distributions and are commonly called "fat" solutions. This thesis explores the fundamental nature of these fat solutions and identifies key features that can be used to predict whether the minimizing distribution is fat or of SCE-type. Additionally, this thesis examines how the convexity of the interaction potential impacts solutions in one dimension and constructs a preliminary study into the convexity of the interaction potential for three electrons in three dimensions. Furthermore, the results from optimal transport calculations are used to inspect the validity of the SCE distribution in cases of screened interactions.