Water-like density anomaly in spin 1/2 fermions

by

Marco A. Habitzreuter

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ABSTRACT

Water is a substance fundamental to life, in part because some of its properties like the high heat capacity and the negative thermal expansion coefficient for some values of pressure and temperature. More than 70 of these so called water anomalies are known, most of which are subject of intense research, both in search of fundamental explanations and also in terms of technological applications. Some of these anomalous behavior can be qualitatively explained by classical models with competing interactions at different length scales. These length scales are associated with liquid phases of different densities and a possible liquid-liquid critical point.

Other substances can also display a negative thermal expansion coefficient. Interestingly, some of these are inherently quantum in nature, such as ^{3}He and ^{4}He, which are fermions and bosons, respectively. Moreover, electronic correlations in solids are also associated with with unusual thermal expansion properties of some materials.

The most widely used model to study these electronic correlations is the Hubbard model. It is a prototypical Hamiltonian, describing fermions on a lattice with a competition between a local interaction and the lattice tunneling. Although it has been the focus of intense research in the last few decades, recent years have seen a renewed interest due to Quantum Simulators: they allow the creation of this model in the lab, with a great degree of control over the model parameters. This technique allows the understanding of fundamental mechanisms which arise from the model, hence it has been widely used to understand properties of solids.

In this thesis, we study the Hubbard model as a fluid system, showing the existence of water-like anomalies. In particular, we analyze the extended Hubbard model in one and two dimensions for a wide range of model parameters with analytical and numerical techniques, focusing on the parameters which generate a density anomaly. We show that ground state degeneracies generate a residual entropy from which the density anomaly arises, in line with other water models already studied in the literature. Hence, the concept of an anomaly based on competition, which originated in classical systems, holds for the fermionic case. Moreover, the results of this study show that quantum simulations could be used as a proxy to probe fundamental ideas of liquids such as the liquid-liquid critical point.

Thesis supervisor: Marcia C. B. Barbosa
Title: Full Professor of Physics

Secondary supervisor: Eduardo O. Rizzatti