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Observation of antiferromagnetic correlations in the Fermi-Hubbad model

by

Pedro M Duarte

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APPROVED, THESIS COMMITTEE:

Randall G. Hulet, *Chair*
Fayez Sarofim Professor of Physics and Astronomy

Thomas. C. Killian
Professor of Physics and Astronomy

Somebody Else
Professor of Physics and Astronomy

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Abstract

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Many body physics with ultracold atoms

1.1 Motivation: Strongly correlated materials

Our experiences in the physical world can, for the most part, be explained by considering the description of the collections of positively charged nuclei and negatively charged electrons that make up ordinary matter. From high to low energy this includes neutral plasmas, the formation of atoms and molecules in gaseous phase, the condensation of these atoms and molecules into liquid or glassy phases and their susequent crystallization to form solids. At lower energies more exotic phenomena take place, starting with magnetism and going further to superfluidity, superconductivity and the novel examples of modern condensed matter physics such as the fractional quantum Hall effect, heavy electrons, high-temperature superconductors and topological insulators.

In principle, the correct description of all the above phenomena is contained in the Schrödinger equation for the interacting system of electerons and nuclei, where the interaction is given by the Coulomb potential. In practice, we know that even though stating the equation is easy, there is not sufficient computing power available in the world to solve it for systems of more than just a few particles. In the introduction to his book [1], Xiao-Gang Wen points out that back in the 80s a computer with 32 MB of RAM could solve a sytem of 11 interacting electrons. In the 2000s, while computing power has increased more than 100 times, this allows for the addition of only two more electrons to the system.

Despite the above, the use of the Schrödinger equation and perturbation theory for the description of systems of electrons and nuclei has been very succesful over the past century. The most prominent example of this success is our understanding of semiconductors, which are at the root of the electronic devices that permeate all aspects of our lives. The remarkable success of this approach can be traced back to the principle of adiabatic coninuity [2], which states that the quasiparticle low-energy excitations of an interacting system can be closely related to the particles that form the interacting system.

The practical consequence of adiabatic continuity is that interactions seemingly do not play an important role in the low-energy description of the system. For this reason, the free electron model of Drude and Sommerfeld [3] was relatively succesful in explaining electrical and thermal conductivity in metals and the Hall effect. Later on, in 1957, Landau formulated the thery of the Fermi-Liquid [4] and gave a solid basis to the notion of adiabatically connected quasiparticles. To this day, the Fermi-Liquid theory is the starting point for the study of Fermi systems such as conventional metals, ^{3}He and ultracold atomic Fermi gases.

Just as Fermi-Liquid theory is celebrated for its success it is also known for the phenomena that it fails to explain. Starting in the mid 70s and going through the 80s, the discoveries of heavy electron superconductivity [5, 6], the fractional quantum hall effect [7, 8], and high-temperature superconductors [9] sparked a revolution in condensed matter physics [10]. These materials in which the electron behavior cannot be described effectively in terms of non-interacting electron-like quasiparticles came to be known as *strongly correlated materials*. Strongly correlated materials and the concept of emergence, introduced by P.W. Anderson in his famous essay “More is Different” [11], are at the center of modern condensed matter physics.

The behavior of strongly correlated materials is emergent because the low-energy excitations of the system bear no resemblance to its constituent particles. This concept should not be so surprising, after all we are familiar with this definition of emergence whenever a system undergoes a phase transition. For example when a liquid transitions to a crystalline solid, translational symmetry is broken and the low-energy excitations of the system are the quasiparticles known as phonons, which bear no resemblance to the constituent ions and electrons that form the solid.

Strongly correlated materials are are examples of emergent phenomena in which the origin and properties of the low-energy excitations are not as straightforward as those of phonons in a crystalline solid. The fractional quantum Hall state, in which the quasiparticles carry a rational fraction of the charge of an electron serves to illustrate this point. The strong interactions between the electrons in the quantum Hall system (electrons confined in a plane under a very high magnetic field) make the problem intractable from the perturbative point of view and thus the connection between the microscopic degrees of freedom and the collective low-energy excitations is very difficult to establish; certainly not as easy as the connection between the small motion of ions about their equillibrium positions in a crystal and their collective phonon modes. It was Laughlin's insight that led him to postulate the correct wavefunction for the quantum Hall state [8], but the microscopic origin of the state is still under debate.

The challenge posed by strongly correlated materials has led to great discoveries in condensed matter physiccs, such as the concepts of topological order [12] and quantum criticality [13, 14], but also many questions remain unanswered. Furthermore, the problem of strongly correlated materials is only scratching the surface of what is possible and what remains to be discovered. New materials are being synthesized constantly, and among the myriad of possible materials and compunds that can be explored by materials scientists, one can only expect that there will be new states of matter to be found and ones with technological implications that will revolutionize life on earth.

1.2 Quantum simulations with ultracold atoms

We have seen that even though the Schrödinger equation in principle contains a full description of a solid, the solution is practically impossible to compute using a classical computer due to large memory required to represent many-body quantum state. The approach in condensed matter theory, rather than directly aim to solve the Schrödinger equation, is to introduce simplified effective models, which should capture the essential features of the system under study. The solution of the effective model leads to an understanding of the low-energy excitations of the system and gives clues to their microscopic origin.

The Hubbard model is a model that contains only the essential ingredients to describe

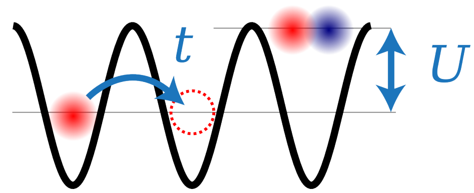

Figure 1.1: Illustration of the Hubbard model

the behavior of strongly interacting electrons in a crystalline solid. The model describes electrons that can hop between sites in a lattice, and which acquire an interaction energy when two electrons are on the same site, see Figure 1.1. In the next chapter I will explian why this is a plausible model to describe some strongly correlated materials; for know I will point out that even though this model is the simplest possible model for strong correlations its solution in more than one dimension has evaded theorists for more than four decades.

It is at this point that ultracold atoms enter the picture. It turns out that a system of ultracold atoms in an optical lattice is a faithful realization of the Hubbard model [15], and so the properties exhibited by the atoms are in fact the solutions of the model. The idea of studying the solutions of a quantum mechanical model using an analogous quantum mechanical system was first proposed by Richard Feynman in 1982 [16] and has been made possible in the last decade due to the advances in production and control of ultracold atomic gases.

Interactions are contact.

Lattice depth can tune U/t (bosons)

Feshbach resonances, can tune interacions (cesium, fermions)

Challenges, temperature: both cooling and thermometry

Approaches: compensation, spin sensitive (this thesis)

In this section I present the model in its original context, as a simplification of the description of valence electrons in crystalline solids. I include some historical background to motivate the reader.

Models for electrons existed which explained conduction phenomena in a succesful manner. Also, models existed which dealt with magnetic phenomena. This section touches on the necessity to formulate a model that could incorporate both transport and magnetic properties of a material. This need arises due to the existence of materials that are at neither end of the spectrum. That is, metals or insulators for which magnetic effects played an imporant role. The simple example being MnO, on which antiferromagnetism was first observed, and the big challenge being high-temperature superconductors.

1.3 Motivation: Quantum magnetism with ultracold atoms

An overview of the literature for observation of quantum magnetism in ultracold atoms

The Fermi-Hubbard model

2.1 The Hubbard model in ultacold atomic gases

This section starts by considering the description of cold atoms in an optical lattice potential. It then considers interactions on the description of the system. The main point of this section is to make the reader aware of what are the approximations that are made whene one says the system of interacting atoms in an optical lattice is described by the single band Hubbard model.

2.1.1 Motion of atoms in an optical lattice potential

2.1.2 Interactions between the atoms

2.2 Simplified treatements

This section explains our understanding of the Fermi-Hubbard model. It starts by building some insight by using the results of exactly solvable models. The results of exct diagonalization in systems of 2-sites and 4-sites are shown. This are going to motivate the antiferromagnetic character of the ground state, while showing that there is always a bit of an admixture of double occupancy in the exact ground state.

The 4-site solution can be used to help understand why the Fermi-Hubbard is relevant to high-Tc superconductors. In this case one can make connections to the d-wave character of ground states upon doping the system.

The exact diagonalization solutions are at zero temperature, so they give most insight to the exact ground states of the system.

2.2.1 Exact diagonalization

2 site exact diagonalization

4 site plaquete an relevance to high-Tc superconductors

2.2.2 Limiting cases

This section deals with the limiting cases of the Fermi-Hubbard parameters. The solutions that are obtained give insights to the workings of the model. The high temperature series expansion is introduced, which is very relevant for calculating thermodynamic quantitites in the temperature regime of a few times T_{Neel}.

U=0 limit, t=0 limit

High temperature series expansion, band and Mott insulating states

small t, the t-J model and antiferromagnetic ground state

2.2.3 Modern approaches

This small section aims to explain the most recente advances in our understanding the Fermi-Hubbard model. This includes QMC, DMFT, etc. The aim of this section is not to provide an introduction to these techniques but mainly to point out the main results and serve as a bibliographic reference.

Enlarging and cooling towards the Neel state in a compensated optical lattice potential

3.1 Compensated optical lattice

3.2 Thermodynamic quantitites in the local density approximation

Experimental diagnostic tools

This chapter aims to describe in detail the different observables that are accesible to the experimetnalist.

4.1 Absorption imaging

4.2 Polarization phase-contrast imaging

4.3 Thermometry of a Fermi gas trapped in a harmonic potential

4.4 Double occupancy measurement in an optical lattice

4.5 Bragg Scattering of light

4.5.1 Non-spin sensitive: crystal structure factor

4.5.2 Spin sensitive: spin-structure factor

Experimental setup and procedures

5.1 Production of a deeply degenerate ^{6}Li spin mixture in a dimple potential

5.2 Compensated optical lattice potential

Studies in a three dimensional optical lattice

Conclusion

BIBLIOGRAPHY

[1] X. Wen, *Quantum Field Theory of Many-Body Systems: From the Origin of Sound to an Origin of Light and Electrons*, *Oxford Graduate Texts* (OUP Oxford, 2004).

[2] A. Altland and B. Simons, *Condensed Matter Field Theory* (Cambridge University Press, 2010).

[3] N. Ashcroft and N. Mermin, *Solid state physics*, *Science: Physics* (Saunders College, 1976).

[4] L. Landau, *Collected papers of L. D. Landau* (Gordon and Breach, 1965).

[5] K. Andres, J. E. Graebner, and H. R. Ott, “¡span class=”aps-inline-formula”¿¡math¿¡mn¿4¡/mn¿¡mi¿f¡/mi¿¡/math¿¡/span¿-Virtual-Bound-State Formation in Ce¡span class=”aps-inline-formula”¿¡math¿¡mrow¿¡msub¿¡mrow¿¡mi mathvariant=”normal”¿Al¡/mi¿¡/mrow¿¡mrow¿¡mn¿3¡/mn¿¡/mrow¿¡/msub¿¡/mrow¿¡/math¿¡/span¿ at Low Temperatures,” Phys. Rev. Lett. **35,** 1779–1782 (1975).

[6] F. Steglich, J. Aarts, C. D. Bredl, W. Lieke, D. Meschede, W. Franz, and H. Schäfer, “Superconductivity in the Presence of Strong Pauli Paramagnetism: Ce¡span class=”aps-inline-formula”¿¡math¿¡mrow¿¡msub¿¡mrow¿¡mi mathvariant=”normal”¿Cu¡/mi¿¡/mrow¿¡mrow¿¡mn¿2¡/mn¿¡/mrow¿¡/msub¿¡/mrow¿¡/math¿¡/span¿¡span class=”aps-inline-formula”¿¡math¿¡mrow¿¡msub¿¡mrow¿¡mi mathvariant=”normal”¿Si¡/mi¿¡/mrow¿¡mrow¿¡mn¿2¡/mn¿¡/mrow¿¡/msub¿¡/mrow¿¡/math¿¡/span¿,” Phys. Rev. Lett. **43,** 1892–1896 (1979).

[7] D. C. Tsui, H. L. Stormer, and A. C. Gossard, “Two-Dimensional Magnetotransport in the Extreme Quantum Limit,” Phys. Rev. Lett. **48,** 1559–1562 (1982).

[8] R. B. Laughlin, "Anomalous Quantum Hall Effect: An Incompressible Quantum Fluid with Fractionally Charged Excitations," Phys. Rev. Lett. **50,** 1395–1398 (1983).

[9] J. Bednorz and K. MÃijller, "Possible highT c superconductivity in the BaâĹŠLaâĹŠCuâĹŠO system," Zeitschrift fÃijr Physik B Condensed Matter **64,** 189–193 (1986).

[10] P. Coleman, "Many Body Physics: Unfinished Revolution," in *International Conference on Theoretical Physics*, D. Iagolnitzer, V. Rivasseau, and J. Zinn-Justin, eds., (BirkhÃďuser Basel, 2004), pp. 559–580.

[11] P. W. Anderson, "More Is Different," Science **177,** 393–396 (1972).

[12] X. G. WEN, "TOPOLOGICAL ORDERS IN RIGID STATES," International Journal of Modern Physics B **04,** 239–271 (1990).

[13] J. A. Hertz, "Quantum critical phenomena," Phys. Rev. B **14,** 1165–1184 (1976).

[14] S. Sachdev, *Quantum Phase Transitions*, *Quantum Phase Transitions* (Cambridge University Press, 2011).

[15] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, "Cold Bosonic Atoms in Optical Lattices," Phys. Rev. Lett. **81,** 3108–3111 (1998).

[16] R. P. Feynman, "Simulating physics with computers," International journal of theoretical physics **21,** 467–488 (1982).