Long-Range Order in the Hubbard Model

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Abstract

This paper begins by analyzing the Fermi-Hubbard Hamiltonian, a hopping model for Fermions on a lattice, and the pathology of the model's extreme cases is discussed. Finally, the usefulness of experiments with ultracold atoms for studying order in these systems is presented.

1 Introduction

The Hubbard model is a minimal quantum mechanical description for particles hopping on a lattice. It is an extension of the tight binding model with an additional term to account for interactions of particles localized on the same lattice site. Depending on the particle statistics involved, the relevant equation is called the Fermi-Hubbard or the Bose-Hubbard model, though the "Fermi" in Fermi-Hubbard is often dropped by convention. These models are characterized by parameters "t" and "U" which are energy scales for hopping between adjacent lattice sites and the energy required to add an additional particle to a site, respectively.[1]

This text centers around the Fermi-Hubbard model, but for pedagogical reasons I will draw on its Bosonic analog at several points. To start, the Bose-Hubbard model is the simpler of the two; Equation 1 shows its form in terms of the Bosonic annihilation and creation operators, $\hat{a}$ and $\hat{a^{\dagger}}$.[2] There first term in the Hamiltonian is the summation all possible nearest neighbor hops taking a particle from R$'$ and moving it to R, just as in the tight binding model. The second is the interaction term that accounts for the energy of placing additional atoms on already occupied sites. The third term is included to account for any external confining potential that may be present in the lattice system; this is especially relevant to atomic lattice systems which will be discussed later.

$$\hat{H} = -t \sum_{\langle R,R' \rangle} \hat{a}^{\dagger}_{R} \hat{a}_{R'} + \frac{U}{2} \sum_{R} \hat{n}_R \left(\hat{n}_R - 1 \right) + \sum_{R} \epsilon_R \hat{n}_R \tag{1}$$

In the Fermi statistics case the model has to be rewritten both to keep track of particle spin and to obey the Pauli exclusion principle. It is more complicated visually, but obeys the same basic ideas as the Bosonic model. The $\hat{a}$'s and $\hat{a^{\dagger}}$'s are replaced with the Fermion operators, $\hat{c}$'s and $\hat{c}^{\dagger}$, and the on-site interaction term enforces that only one of each spin species can exist at each site. Again, an arbitrary confining potential term is included for completeness.

$$\hat{H} = -t \sum_{\langle R,R' \rangle, \sigma} \left(\hat{c}^{\dagger}_{R\sigma} \hat{c}_{R'\sigma} + \hat{c}^{\dagger}_{R'\sigma} \hat{c}_{R\sigma} \right) + U \sum_{R} \hat{n}_{R\uparrow} \hat{n}_{R\downarrow} + \sum_{R} \epsilon_R \hat{n}_R \tag{2}$$

The Hubbard models seems minimal to the point one should not expect it to fully explain a true solid state system, but as it is also general, the hope is that anything gained from the model will also be general. As written, "t" and "U" are mean field quantities but this is not a requirement–the models can easily be made richer by allowing each of these parameters to vary with position such that $t \rightarrow t_{R,R'}$ and $U \rightarrow$

[1] Depending on what side of the condensed matter/ atomic physics fence one sits, the hopping energy can be called either "t" or "J."

[2] The notation used in Reference [1] is recycled throughout this paper for consistency and adherence to a standard notation.

U_R. This extension is useful for studies of disordered lattices and heterostructures or even more complicated potentials. Next-nearest neighbor and farther hopping terms can also be included in the model and often introduce order where it would not have existed otherwise.

2 Lack of Order in Low Dimensional Systems

For now let's consider the mean field Hubbard model without an external potential and examine the two limiting cases. With the hopping parameter "t" set to zero, all that remains to govern the ground state configuration is the on-site energy. Nothing unusual can happen in this case as the Hamiltonian is completely diagonal and there is no interplay between different sites. To fill the lattice one places spins randomly into the system until the chemical potential is reached and no correlation exists among the spin states, long-range or otherwise.

In the opposite case, "U" is set to zero and the model reduces to the well known tight binding model. Using periodic boundary conditions, the single particle ground state wave functions will be of the form $\psi = \frac{1}{\sqrt{N}} e^{ikx}$ with a dispersion relations of form $E(k) = -2t\cos(ka)$, where a is the lattice spacing. In filling the lowest band, one adds spins alternating up and down in a mechanical fashion, and again there is no correlation between spins that exist on different lattice sites.

At both extremes of the Hubbard model, the ground states are paramagnetic and posses no long-range order. But, these two extremes are of very different flavors, and the gray area between them contains all of the interesting physics. Exact results can be found for the ordering of low dimensional and infinite dimensional systems, and a few results are discussed below.

The Lieb-Mattis theorem considers a 1D Hubbard model with finite hopping and interaction terms using open boundary conditions. It compares the energies of fixed particle number ground states as a function of their total spin, and it predicts that the spin zero state is preferred over all others as shown in the inequality in Equation 3. This necessarily rules out the possibility for ferromagnetic ordering in one dimension as it is not spin zero but leaves open the possibility for other kinds of long-range order.[2]

$$E_{\min}(S) < E_{\min}(S+1) \tag{3}$$

The Koma-Tasaki condition considers finite hopping, 1D and 2D Hubbard models and places upper bounds on the spin-spin correlation functions as listed in Equation 4; $\alpha, \beta,$ andγ are constants of the model and $f(\beta)$ is a monotonically decreasing function. In one dimension correlations decay exponentially while adding a second dimensions produces a scale invariant power law decay. The standard interpretation of this result is that there is no long-range order in one or two dimensions and as such, no superconducting states are allowed.[2]

$$|\langle S_R \cdot S_{R'} \rangle| \leq \begin{cases} e^{-\gamma f(\beta)|R-R'|} & \text{for } d=1 \\ |R-R'|^{-\alpha f(\beta)} & \text{for } d=2 \end{cases} \tag{4}$$

The results of the Lieb-Mattis theorem are not robust against changes in boundary conditions or the hopping coordination number, and these failing provide insight into how order emerges in the Hubbard model. For example, if next nearest neighbor hopping is introduced, ferromagnetism can emerge from the model, and use of periodic boundary conditions completely destroys the relations in Equation 3.[2] One can gain some intuition by considering how information is shared through the lattice. If a single site in a one dimensional lattice were sufficiently pathological as to prevent all transmission through it, one site could effectively divide the system into two independent systems. In two dimensions the situation is different as there would have to be continuous line of pathological sites to fragment the lattice; this informs the need to have different functional forms for the correlation functions in one and two dimensions. The failure of the Lieb-Mattis results with periodic conditions or next neighbor hopping can also be interpreted in this light as there are always multiple ways around any pathological site. The moral of the story is "higher coordination number enable more long-range order." To this end, much theoretical work is done in infinite dimensional systems. [3]

3 Optical Lattice Experiments

At first viewing, the Hubbard model seems to be a great tool for understanding basic electronic properties of solid state systems. Pedagogically, it is a wonderful tool, but to apply it to real-world problems, one needs a way to calculate the hopping and on site energy parameters. While the ordering of the system might be approachable from a number of angles, the lack of hard values for "t" and "U" introduce challenges when making comparisons to theory. At best one can compare phase diagrams and observe that the same transitions happen in both theory and in practice. To some degree it is a Catch 22 for solid state systems: one would need a level of understanding more advanced than the Hubbard model to calculate the "t" and "U" in the Hubbard Model. This would make the model necessarily pedagogical, but it is not without application. In the last decade, atomic physics techniques have been used to load Bose and Fermi degenerate clouds into optical lattices where the hopping and interaction energies are not only known, but they can also be easily modified!

Optical lattices create a periodic potential by interfering counter-propagating laser beams, usually along three mutually perpendicular axes. The result is a lattice with well defined depths and on-site interactions. The force on the atoms is proportional to the gradient in the square of the electric field due to the AC Stark shift and is easily calculated. The depth of the lattice is varied with the laser power, and the dimensionality of the lattice produced can be altered by changing the relative

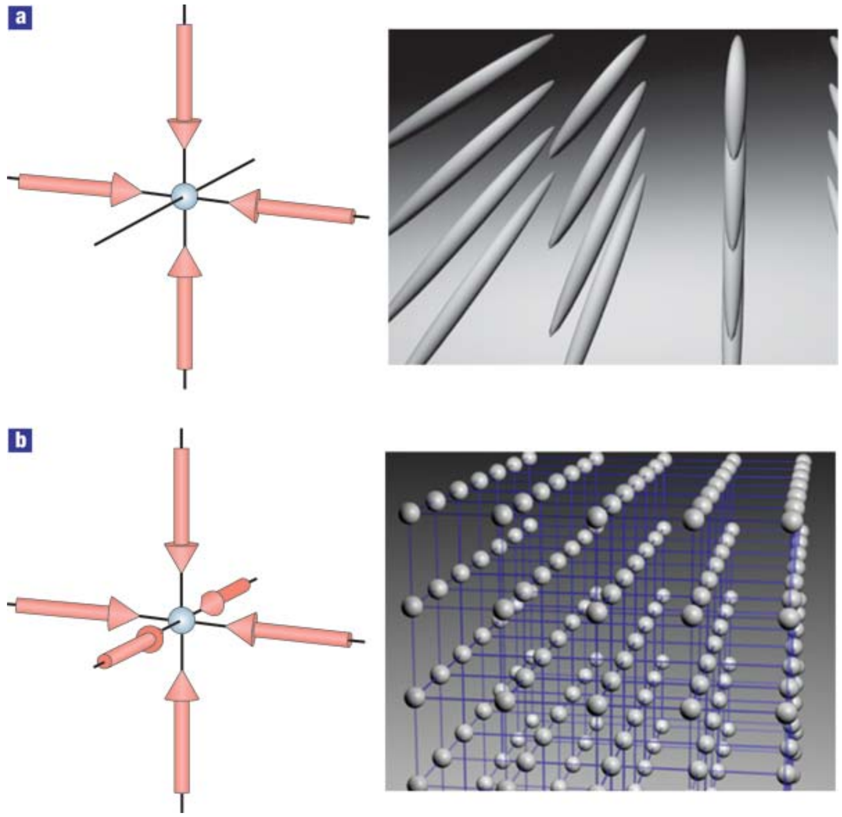


Figure 1: Optical lattices of different dimensions can be created by changing the relative strengths of the lattice beams. [1]

strengths of the lattice beams. For example, if two of the beams have much more power than the third, a series of cigar-shaped one dimensional periodic potentials will be created as in Figure 3a, whereas if all the beams have similar strengths, a standard three dimensional lattice will be produced.

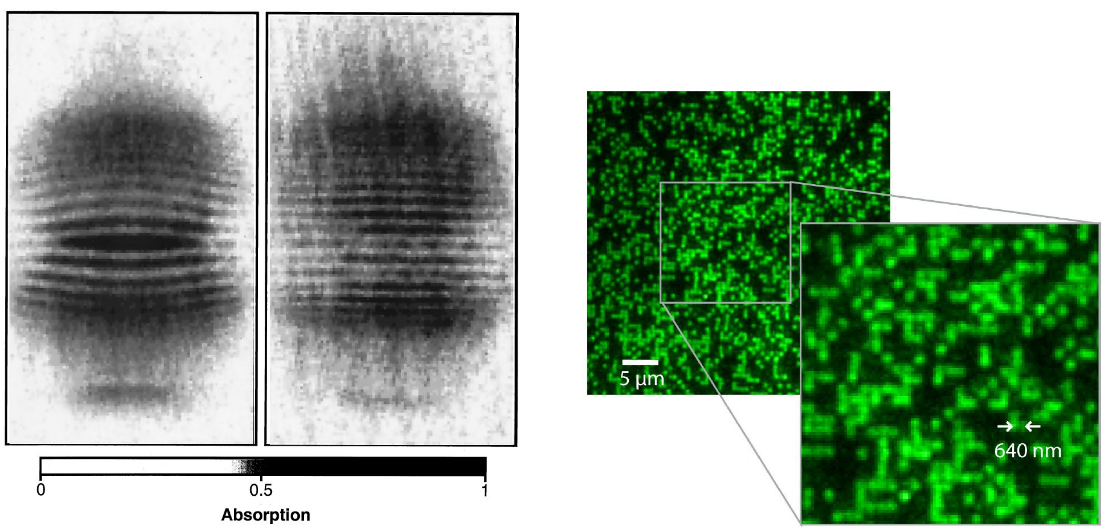
The interaction energy between atoms on the same site is governed by the atomic species chosen; the strength and sign of this interaction can be modified across large ranges with Feshbach resonances. For probing the phase space of the Hubbard model, the ratio of "t" to "U" and the dimensionality of the gas are the relevant quantities, so the technical complication of using Feshbach resonances can often be avoided.[3] The total potential experienced by the atoms in any atomic experiment will be a combination of the lattice beams with whatever confining potential is used to keep

[3]Feshbach resonances are scattering resonances that occur when a bound state channel's energy is close to an open channel, non-bound state between two atomic species. They allow for an inter- or intra-species interaction to be changed from positive to negative scattering lengths. On resonance they completely remove the interaction of the two species. These resonance may also be used during ballistic expansion to remove all interactions between atoms during this stage. [1]

the atoms in the lattice, often a combination of optical and magnetic fields. Because of the confining potentials, these systems have position dependent chemical potentials; this necessitates the presence of the third term we included in Equations 1 and 2.

3.1 Matter Waves and Single Site Imaging

Many methods exist for observing correlations in ultracold atomic systems. The most visibly striking is the observation of interference patterns in overlapped Bose-Einstein condensates as shown in Figure 2a.[4] The two clouds in Figure 2a were produced by evaporatively cooling two separate thermal clouds of sodium atoms in a double well potential.[4] The clouds were sufficiently isolated from each other as they became degenerate that their spontaneously chosen order parameters had a random relative phase such that if they exhibited long range phase coherence, an interference pattern would necessarily be formed. The image was created by shining a sheet of resonant light onto the clouds after a period of free expansion. This technique, though beautiful, cannot be used in Fermi degenerate gases as there is no macroscopically occupied state to interfere. It may have some promise in Bosonic, spin-dependent lattice experiments with a spectator atoms species, but this is an area of research that is just beginning.[5]



(a) Itnerference pattern of two Bose condensates viewed through absorption imaging [4].

(b) In-situ imaging of ^{87}Rb atoms in an optical lattice [6]

Figure 2: Techniques for detecting order in ultracold, atomic gases.

The most direct method for observing order in an optical lattices it to image individual atoms. With direct access to the population map of the spin states across the

[4] The buzz words associated with these experiments are "matter wave" interferometry and the "atom laser," both of which should be considered acceptable physics cocktail party fodder.

lattice, one could make convincing statements about any ordering one is interested in, but this is a new technology and has its share of difficulties. The most formidable problems are creating an imaging system capable of resolving individual lattice sites and placing this imaging system close enough to the atoms to collect enough light for good signal to noise. The site spacing in a standing wave lattice is half of the wavelength of the beams used to create it which for a typical lattices results in a spacing of 400 to 500 nm. This adds additional complication as one has to find an atom with a transition in the 400nm regime[5] as it is difficult to image something smaller than the wavelength of light being used. Single site imaging has been demonstrated with Bose gases in Marcus Greiner's lab as shown in figure 2b. A project to develop in-situ imaging of ultracold Fermionic potassium is currently underway in the Thyweissen's group at Toronto [7] and there are rumors of a similar experiment in Munich.

3.2 Momentum Distribution Fluctuations

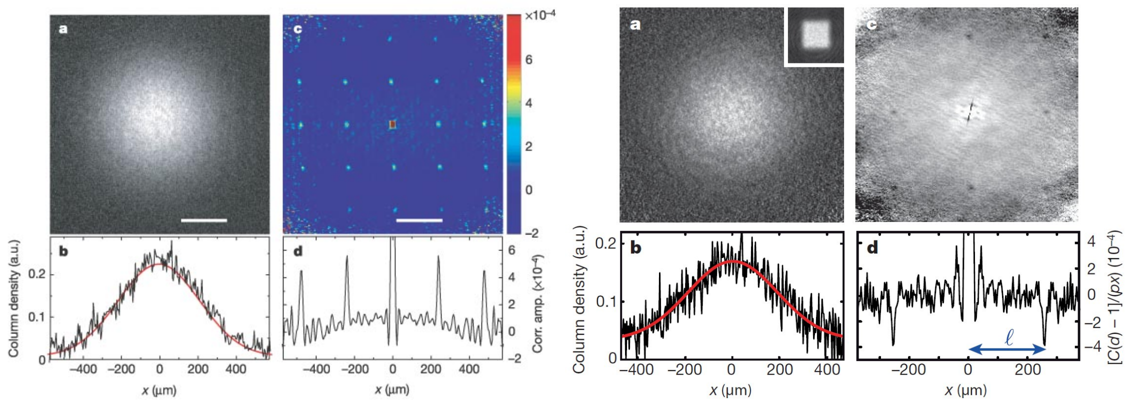
The workhorse for detecting correlations in atomic gases is observations of the fluctuations in the momentum distribution of the cloud. As mentioned with single-site imaging, measuring individual atom positions is technically challenging as the separation of atoms is of the same order as the light used to image them. The momentum distribution on the other hand, is delightfully easy to measure via Time-Of-Flight imaging. By quickly removing the confining potentials for the atoms and allowing the cloud to ballistically expand a direct image of the in trap momentum distribution is produced.[6] The major assumptions in this process are that the in-trap size of the atoms is smaller than any resolvable effect in the image and that interactions during this period of expansion are negligible such that the initial momentum distribution is preserved. This relation is expressed in second quantization notation in Equation 5.[1]

$$\langle \hat{n}_{3D}(x) \rangle_{TOF} = \langle \hat{n}_{3D}(k) \rangle_{trap} \tag{5}$$

In order to gain access to the structure present in the momentum distribution of the cloud, the spatial density-density correlation after Time-Of-Flight imaging is calculated and then related to the in-trap momentum distribution using Equation

[5]Historically, ^{87}Rb has been a great atom to use for ultracold atom experiments as cheap laser diodes existed near 780nm, the wavelength used in the first compact disk drives. Driven by the masses ever increasing need to store data, the new Blu-ray optical drives use a much shorter wavelength to increase storage density. Luckily for fans of ^{40}K, they chose 405nm which sits right next door to the $^4S_{\frac{1}{2}} \rightarrow {}^5P_{\frac{3}{2}}$ transition at 404.5nm.

[6]Depending on what kind of measurement is involved, one can quickly snap off the lattice potential or slowly ramp it down. Snapping off the lattice reduces interactions during ballistic expansion and shows the lattice's diffraction peaks in momentum space. Turning the potential down slowly preserves the lattice momentum states for mapping of the band structure. The resulting images of filling of the Brillouin zone are incredible and more details can be found in Greiner et al. Phys. Rev. Lett. 87 160405 (2001).



(a) Bosonic ^{87}Rb atoms [8]

(b) Fermionic ^{40}K atoms [9]

Figure 3: (a) Absorption image of atomic clouds after Time-Of-Flight. (b) Statistical correlation of several absorption images. (c) 2-D density-density correlation function for momentum distribution. (d) Cross section of correlation function showing bunching and anti-bunching effects.

5. The results of this process and are shown in Equation 6 as well as the reduction and simplification after normal ordering of the operators. Figures 3a and 3b tell the complete story of how the order in the momentum distribution is extracted from the images. Unsurprisingly, the Bosonic example exhibits positive correlations and the Fermionic example exhibits negative correlations. The correlations are on the order of four parts in ten thousand yet are still well above the background. The deviation from the expected unity correlation and anti-correlation are due to the finite resolution of the optical systems.[1]

$$\langle \hat{n}_{3D}(x)\hat{n}_{3D}(x')\rangle_{\mathrm{TOF}} \approx \langle \hat{a}^\dagger(k)\hat{a}(k)\hat{a}^\dagger(k')\hat{a}(k')\rangle_{\mathrm{trap}} \tag{6}$$

$$= \langle \hat{a}^\dagger(k)\hat{a}^\dagger(k')\hat{a}(k')\hat{a}(k)\rangle_{\mathrm{trap}} + \delta_{kk'}\langle \hat{a}^\dagger(k)\hat{a}(k)\rangle_{\mathrm{trap}} \tag{7}$$

Both absorption images in Figure 3 were taken at half filling where the correlation functions would be maximally observable. At this point the Bosonic system is a Mott insulator and the Fermionic system a band insulator. At lower filling fractions, the signal to noise would be worse, and at higher filling atoms are forced into more completely filled bands where smaller fluctuations are allowed.

4 Conclusions

The Hubbard model offers a intuitive description of Fermions moving on a lattice. Much work has been done to understand the consequences of this model both from theory and experiment. Ultracold atoms in optical lattice provided the most direct "real world" simulations of the Hubbard model, and there are many experiments currently underway to map out the Hubbard phase diagram using a variety of techniques to measure any long-range order present in these systems.

On an amusing historical note, the original success of the Hubbard model was its prediction of both metallic and insulating states. Its legacy, other than the huge interest in theory, simulations, and experiments centered around recreating its conditions and understanding its consequences, is in making Green's functions techniques standard tools in the condensed matter toolbox. Hubbard made extensive use of them in his work, and it would be rare to have any discussion of order without this tool. [10]

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