Numerical Studies of Spin-Polarized Fermionic Systems

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My project focused on exploring a spin-polarized system of fermions. By running numerical simulations of this system, I was able to explore interesting new physics and obtain experimentally observable results. My project required a knowledge of the background physics, experimental setup, and theoretical model of the system in order to fully use the numerical analysis technique.

Background Physics

In the Bardeen Cooper Schrieffer (BCS) theory of superconductivity, when the temperature is sufficiently low, a phase transition occurs in which electrons of opposite momentum and opposite spin (for instance, spin-up and spin-down) bind together into Cooper pairs. The origin of the binding is an attraction between electrons which is mediated by interactions with the vibrations of the crystal lattice (phonons). BCS theory is one of the most successful analytic calculations in condensed matter physics. However, in simple systems, the Cooper pairing mechanism only works if the number of spin-up fermions is equal to the number of spin-down fermions. A question then arises as to how pairing proceeds if the fermion populations are imbalanced in what is known as a "spin-polarized" system. My project this summer was to explore this question through numerical simulations.

There have been various possibilities suggested to answer this question. One such possibility was proposed in the 1960's by Fulde and Ferell and independently Larkin and Ovchinnikov and is termed FFLO pairing. In FFLO pairing, imbalanced spin populations form non-zero momentum pairs, with the non-zero momentum arising from the difference in the Fermi wave vectors of the two spin species. Other possibilities distinct from FFLO have also been proposed, such as phase separation between a spin balanced superfluid and a completely spin polarized gas which contains only the excess species. Understanding which of these situations arises has been a focus of experimental studies, as well as many theoretical calculations.

Experimental Studies

Recent experimental studies of imbalanced spin populations have generated a lot of excitement over this topic. Groups at both Rice University and MIT have studied imbalanced fermionic systems in ultra-cold atomic experiments using optical lattices. An optical lattice is composed of standing waves, created by pairs of opposing laser light beams. The atoms are forced to reside in the wells of the wave, which creates a lattice-like configuration. In addition to the optical lattice, there is a magnetic trap imposed on the system so that the atoms are confined to the center of the lattice. If the atoms placed into this system are sufficiently cooled (which is accomplished primarily by laser cooling techniques), they can exhibit quantum mechanical properties such as superfluidity. The experiments placed imbalanced spin populations of $^6\mathrm{Li}$ atoms, which are

fermions, into these optical lattices, and then observed how pairing took place. The main result from these experiments was that the atoms exhibited phase separation. It was found that in the center of the trap there was a perfect superfluid of Cooper pairs, with the densities of the spin-up and spin-down fermions equal. The excess spin-up fermions that did not find partners were expelled to the outsides of this trap, resulting in a phase separation between the superfluid core and the excess non-paired atoms. This was one of the signatures I looked for in my numerical studies.

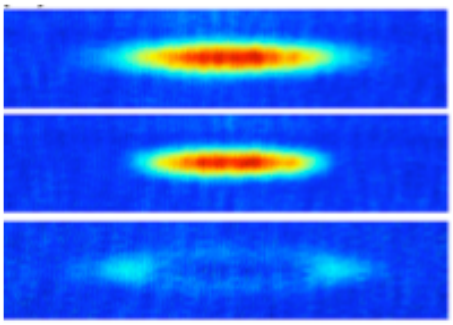


Figure 1: The top panel shows the density in space of the majority component (spin-up particles), the middle panel shows the density of the minority component (spin-down particles), and the bottom panel displays the subtraction of the second from the first. As can be seen, the densities are equal in the center of the trap.

Theoretical Model

My numerical studies used the Hubbard model to represent the above experimental setup. The model was developed in the 1960's as a way to represent anti-ferromagnetic condensed matter systems with repulsive interactions (+U), but its application to optical lattice systems with attractive interactions (-U) is very straightforward. The attractive Hubbard Hamiltonian is

$$H_{Hub} = -t\sum_{i,\sigma}\left(c^{+}_{i,\sigma}c_{i+1,\sigma} + c^{+}_{i+1,\sigma}c_{i,\sigma}\right) - |U|\sum_{i} n_{i\uparrow}n_{i\downarrow} + a\sum_{i} i^{2}\left(n_{i\uparrow} + n_{i\downarrow}\right)$$

It looks a little complicated, but when broken down, the Hamiltonian is very basic. The model takes into account three types of energies in the system: trap energy (which determines where or how fermions fill up the lattice), interaction energy (the energy two fermions, of different spin, have when they occupy the same site), and kinetic energy (which causes the fermions to "hop" from site to site). (See Figure 2.) Looking at each of the corresponding terms in the Hamiltonian:

$$\hat{H}_{trap} = a\sum_{i} i^{2}\left(n_{i\uparrow} + n_{i\downarrow}\right)$$

is the trap energy. Here i is the index of the sites on the optical lattice, and $n_{i\uparrow}$ and $n_{i\downarrow}$ signify the number of spin-up and number of spin-down fermions on site i. This term then simply adds a parabolic trap to the lattice, and the strength of this trap is moderated by the parameter a. Next:

$$\hat{H}_{\text{int}} = -|U|\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

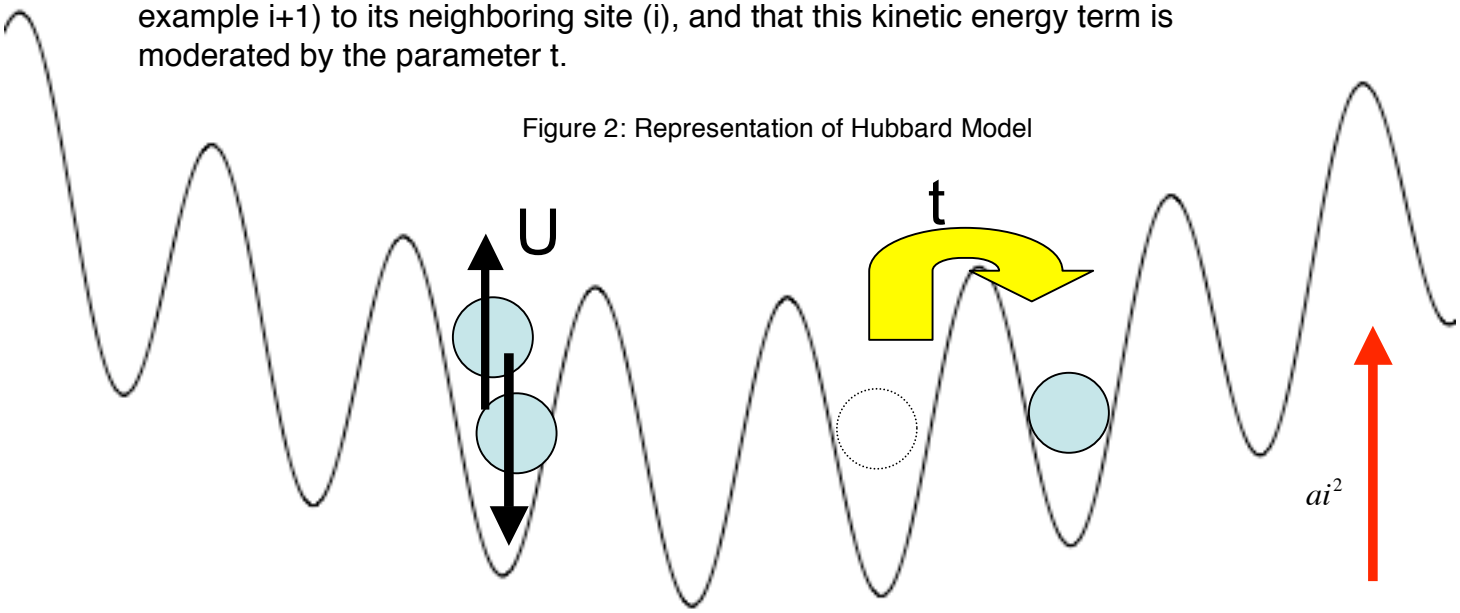
This term provides the interaction energy. For every site where there is both a spin and a spin-down fermion, the interaction energy is -|U|.

Finally,

$$\hat{H}_{kin} = -t\sum_{i,\sigma}\left(c^{+}_{i,\sigma}c_{i+1,\sigma} + c^{+}_{i+1,\sigma}c_{i,\sigma}\right)$$

is the kinetic energy term. The sum is over all sites i and is done separately for the two spins, denoted by σ. $c^{+}_{i,\sigma}$ is a creation operator, creating a fermion of spin σ on site i, while $c_{i+1,\sigma}$ is a destruction operator, destroying a fermion of spin σ on site i+1. Thus we see that this term moves a fermion from one site (for example i+1) to its neighboring site (i), and that this kinetic energy term is moderated by the parameter t.

Figure 2: Representation of Hubbard Model



Methods and Results

There are many *approximate* analytic approaches to the Hubbard Hamiltonian, for example mean field calculations and perturbation ("Feynman diagram") theories. However, the two main routes which treat the Hubbard model exactly are exact diagonalization and numerical simulation. Both methods have their weaknesses and strengths. Diagonalization of the Hamiltonian is useful because it is an exact method, which means that there are no error bars in the solutions. On the other hand, there is a limit to how useful this method can be; as the number of sites is increased, the Hilbert space becomes exceedingly large. Just one site in the Hubbard model has a Hilbert space of size 4: the site can either have no fermions $|0\rangle$, 1 up fermion $|\uparrow\rangle$, 1 down fermion $|\downarrow\rangle$, or both one up and one down fermion $|\uparrow\downarrow\rangle$. Trying to analyze the full Hubbard model with, for example, 10 sites, requires a Hilbert space of over one million! For this reason, when analyzing more complicated systems, numerical simulation must be used. Numerical simulation, which I performed with Quantum Monte Carlo algorithms, can in general analyze an order of magnitude more sites than can the diagonalization method. The QMC algorithm, like diagonalization, treats the

Hubbard model exactly, with no approximations. However, it is a numerical simulation and therefore does have statistical errors which need to be taken into account.

While my project mostly focused on numerical simulations using Quantum Monte Carlo, a small part of my work did involve performing diagonalizations. One of the most straightforward diagonalizations that I performed was for the case of U=0, or for non-interacting species. After numerically calculating the eigenenergies and eigenstates of the diagonalized Hamilotonian, I was able to find the average energy of the system and the average density in space. One interesting result is shown in figure 3, which illustrates the effect of increasing the parameter a, or the trap strength, on the particle density. The figure shows the average density for 13 particles located on a 64 site lattice, at zero temperature. As expected, the particles tend towards the center of the trap, and the peak at the center of the trap becomes more and more sharp as the trap strength increases. A rather non-intuitive result shown in this figure is the non-smooth nature of the density; the particles exhibit oscillations in real space. Note: this diagonalization was only possible for such a large lattice because the interaction between fermions was turned off, so the system was much simplified.

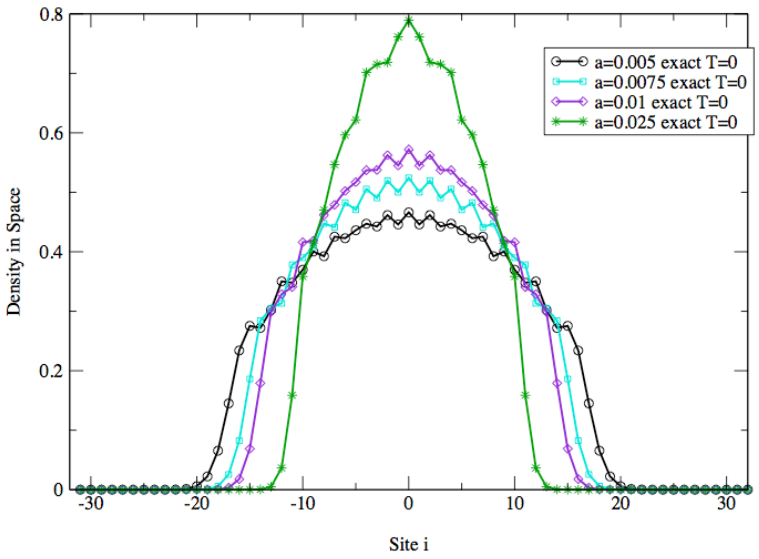


Figure 3: Density in space of 13 particles on a 64 lattice site at zero temperature, for different values of trap energy a.

Quantum Monte Carlo (QMC) simulations formed the main component of my project. The basic idea of QMC is to find the thermodynamically favorable state of a system by allowing the system to evolve over time. Put simply, the algorithm works as follows: First, the particles are placed in a random configuration on the lattice. Next, a change to the system is proposed, which involves moving a small number of the particles to different sites. If the energy (determined by the Hubbard model) of the new state is less than the energy of the current state, the change is accepted. If the energy of the new state is higher than the current

energy, the change is accepted with the Boltzmann probability of $\frac{1}{z}e^{-\hat{H}\beta}$, where Z is the partition function, β is the inverse temperature, and $\hat{H}$ is the Hubbard Hamiltonian. The system is now in a possibly new configuration of particles on the lattice, and the process of proposing changes and updating the system is performed iteratively. Eventually the system settles into its thermodynamically favored state. Using QMC, one can obtain extraordinarily useful information, such as density distributions in real space and in k-space, as well the momentum density distribution of pairs of fermions.

One major goal of my project was to look at the density profiles of the fermions in space in order to understand how pairing was taking place. In figure 4 (a) I show one result of how changing the interaction strength U affected the density profiles. At U=-3, the particle densities have a parabolic shape, as is expected due to the presence of the trap. However, as the interaction energy is increased, the particles attract each other to the center of the trap, and the profiles become much more peaked.

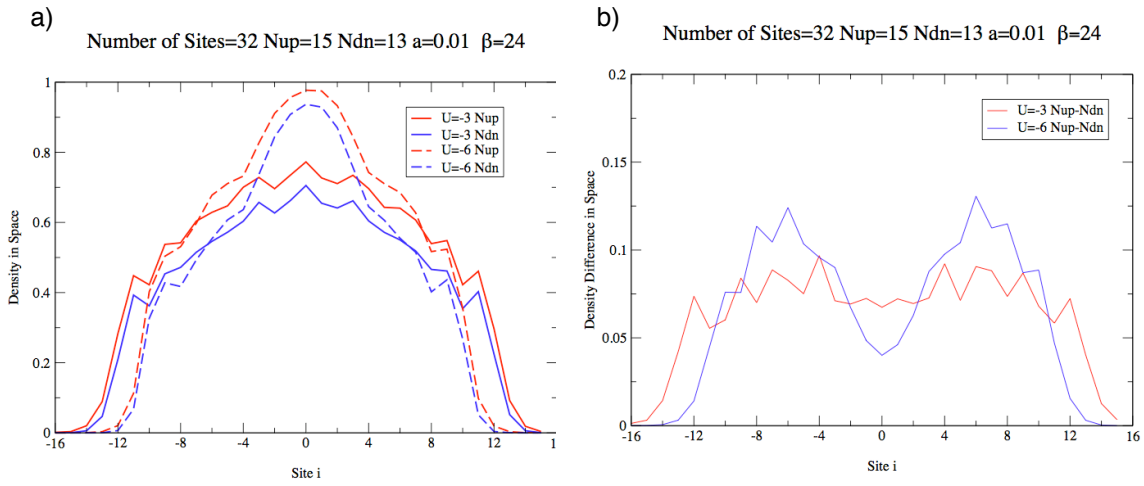


Figure 4. (a) Densities of majority (up) and minority (down) particles in space. (b) Density difference of majority and minority.

I was hoping to see signatures of phase separation as was observed in experiments. In order for there to be phase separation, the densities of the two species must be equal at the center of trap, as this would indicate a pure superfluid core. In figure 3 (b) I show a graph of the difference in the density profiles of the spin-up and spin-down species. For the higher value of |U|, the density difference does decrease in the center of the trap, but it does not reach zero. Although I searched over a large area of parameter space, I was not able to find a case where the density difference did go to zero, or in other words where phase separation took place. We believe that is because we were working

with a 1-D model, whereas the experiments were performed on a 3-D lattice. In general it is much more difficult for systems to exhibit phase separation in 1-D than in higher dimensions.

One of the most important results obtained from QMC was signatures of an exotic superfluid alternative to Cooper pairing. As mentioned above, FFLO is an exotic state of superfluidity which can be used to explain how pairing takes place in systems with imbalanced spin populations. When the populations of the two different fermionic species are unequal, the two Fermi surfaces are no longer aligned, as the majority species fermions take up more momentum values. In FFLO pairing, a majority species atom from the positive (negative) spin-up fermi surface pairs with a minority species atom at the negative (positive) spin-down fermi surface. Since their momenta are not equal and opposite, the pair has a resulting momentum which corresponds to the difference between the two fermi surfaces (see figure 5 (a)). Thus the more imbalanced the two species, the further apart their Fermi surfaces, and therefore the higher a momentum the resulting pair will have. The momentum of the pairs for differing polarizations is shown in figure 4 (b). As predicted by FFLO, the non-zero momentum peak of the pairs lies exactly at the difference between the two fermi surfaces (which is equal to half of the polarization).

a) b)

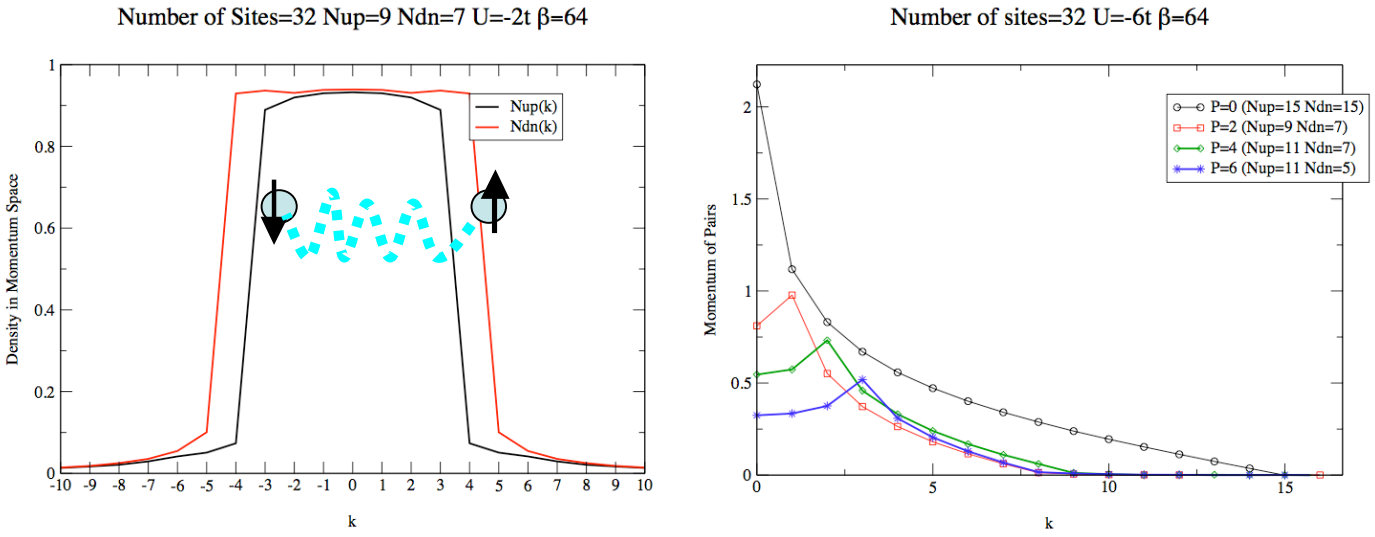


Figure 5. (a) A spin-up particle from the majority species' Fermi surface pairs with a spin-down from the minority species' Fermi surface, resulting in a pair with a total non-zero momentum. (b) Momentum of pairs for differing polarization values. The momentum peak is always at P/2, where P is the polarization Nup-Ndn. This is indicative of FFLO, as P/2 is the difference between the two Fermi surfaces.

This result is important because, as of yet, FFLO has never been seen in ultra-cold atomic systems (though it has been observed recently in condensed matter systems). While FFLO is predicted to take place over a very small portion of

phase space in 3-D, we have found that in 1-D this phase is quite prevalent. Therefore, by making a 1-D optical lattice (something which has been done before), it should be possible to experimentally confirm these results and find signatures of FFLO in a cold atom system.

Conclusion

To fully complete the above studies, there are two main tasks which should be accomplished. First, in order to thoroughly understand the FFLO state that we observed in simulations, it is necessary to obtain a phase diagram that illustrates how different factors, such as the polarization and interaction energy, affect the pairing. Second, further research should focus on performing similar simulations with a 2-D QMC code, as the higher dimensionality may provide results more similar to the experimental results, such as phase separation. However, though more work should be done to complete this study, this summer's project has still been very useful in understanding spin-polarized fermionic systems. The two most important results have been ruling out phase separation in 1-D over a large area of parameter space, as well as uncovering and studying the FFLO phase.