

A Systematic Study of the Mean Field Approximation for the Hubbard Model

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Abstract

We performed systematic investigations of mean field ground states of interacting two dimensional (2D) lattice models. Specifically, we address the effect of supercell ("cluster") size in the types of solutions that arise, treating doping levels that are either commensurate with, or incommensurate with, the supercell size, for interaction strengths ranging from the perturbative range to the strong interactions regime. We consider the basic Hubbard model on a 2D square lattice, with hopping amplitude $-t$, providing the kinetic energy and the on-site repulsion U (Hubbard U) providing the energy of interaction. The mean field solutions allow us to assess global characteristics such as charge and spin order, tendencies toward phase separation, and distribution of single particle eigenvalues (density of states [DOS]). The degree of localization of individual eigenstates, as provided by the inverse participation ratio, provides a new and innovating window into the character of the system.

I. INTRODUCTION

Model Hamiltonian approaches have provided the core of research on correlated electron systems, displaying the basic phenomena and providing understanding of the fundamental processes that are involved. In the absence of exact solutions except for some very particular cases, approximations are required to enable progress. The earliest approach was "Hartree-Fock" (HF) - a mean field approach that approximates electron-electron interactions, which are the hangup, with interaction with an average potential (the mean field) that is determined self-consistently to minimize the energy, or at finite temperature the thermodynamic potential. The HF method has provided invaluable guidance in interacting systems.

In spite of all of the increasing sophistication and elegance of state of the art methods, the mean field approach remains of great importance and may be experiencing a resurgence. With simultaneous treatment of all of the charge, spin, orbital, and lattice degrees of freedom as well as variable electron den-

sity, there are many variables (parameters) to manipulate, and mean field enables investigations that are not viable with more realistic but much more time consuming methods. Mean field studies remain an essential tool in the theorist's arsenal.

II. THEORY BACKGROUND

The tight-binding model is an approach to the calculation of electronic band structure using an approximate set of eigenfunctions based upon superposition of orbitals for isolated atoms located at each atomic site. The tight binding approximation deals with the case in which the overlap of the wave functions is enough to require corrections to the picture of isolated atoms, but not so much as to render the atomic description completely irrelevant. This model is incomplete for our needs. It uses only kinetic energy and no potential energy. Therefore we need a more specific model. Since I have used the name of electronic band structure in defining the TB model here is some information about it.

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The electronic band structure of a solid describes the ranges of energy that an electron in the solid might or might not have. The ranges of energy in a solid where no electron states can exist is called a band gap or an energy gap. In insulators and semiconductors an important band gap is situated between the valence band and the conduction band. The valence band is situated below the band gap, if it is present. The electrons here are bound to the atom, they cannot move freely within the atomic lattice. They are present at absolute zero temperature. The valence band is the highest range of electron energies. The conduction band sits on top of the band gap (if there is one). The electron is no longer bound to the atom and is therefore free to move as it pleases within the atomic lattice. In insulators and conductors the levels are respected, while in metals, the bands cross each other.

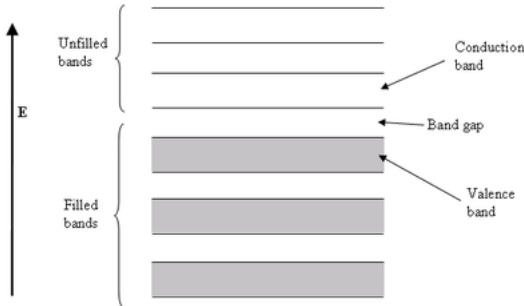


Figure 1: The electronic band structure of a solid

There are many models used in physics, but for our purpose, the Hubbard Model seemed to be a suitable choice. The Hubbard model is an approximate model used to describe the transition between conduction and insulating systems. It is the simplest model of interacting particles in a lattice, with only two terms in the Hamiltonian: a kinetic term allowing for tunneling (hopping) of particles between sites of the lattice and a potential term consisting of an on-site interaction. In our case, the Hubbard Model adds an important element, which is the potential energy of interaction.

But when talking about these models we really need to explain something about the Mean Field Theory. MFT is studying the behavior of large and complex stochastic (a system whose

state is non-deterministic, random) models by simplifying them to a simple system. When talking about these random systems we are referring to the electrons inside the periodic lattice which are free to hop randomly inside the atomic lattice.

A many body system is very hard to understand and solve exactly because there are too many interactions happening. That is why all these interactions are approximated by an average, which becomes the external field. The problem goes now from an n -body system to a one body system, a problem that can be solved. That doesn't mean that the problem is simple. There is still a part that is a little problematic. When summing over all states, the interaction terms in the Hamiltonian give some combinatorics (study of finite discrete structures) problems, which are a little difficult to solve.

Since there are no exact solutions (with a few exceptions) we need to use approximation methods to help in our study. The HF method is one of these methods and has provided invaluable guidance in interacting systems. The Hartree-Fock method is an approximation method used in the determination of the wave function and the energy of a quantum many-body system in a stationary state (state with a single definite energy). The Hartree equation is the approximate solution of the Schrodinger equation given that after computing the final field from the charge distribution, this field must be self-consistent with the initial field.

III. SETTING UP THE PROBLEM

When using the Hubbard Model we have to make sure that some assumptions are met. The atoms are arranged in periodic patterns over long distances and are stable for a long time. We have used lattices that are periodic, the 8×8 , 16×16 , 24×24 , 32×32 and even some 64×64 lattices. We assumed that atoms have a simple energy level the electrons can occupy, the electrons are interacting through the on-site Coulomb interaction, the kinetic energy is characterized by hopping of electrons between

atomic sites and since the atomic orbitals die off exponentially, the electrons are allowed to hop only to the nearest neighbor.

We set up a Hamiltonian starting from random initial density. The Hubbard Hamiltonian for fermions is written as:

$$H = -t \sum_{\langle \alpha, \beta \rangle \sigma} \hat{c}_{\alpha, \sigma}^\dagger \hat{c}_{\beta, \sigma} + U \sum_{\alpha} \hat{n}_{\alpha \uparrow} \hat{n}_{\alpha \downarrow} \quad (1)$$

where $\hat{c}_{\beta \sigma}$ destroys the electron with spin σ at site β , and $\hat{c}_{\alpha \sigma}^\dagger$ creates an electron with the same spin.

Since there can be up to 2 electrons per site the total number of electrons in the system can be $2N$ (where N is the number of sites). We set up the system, initially, to have only one electron per site, which is called half filling.

The hopping parameter is set to -1, which allows the electrons to hop to neighboring sites. For the half-filling case we are looking at there is 1 atom for cell and 1 orbital.

IV. RESULTS

During our research we looked at a few different things. We checked to see what the lowest energy (ground state energy) looks like in different lattices. We studied the dependence on supercell (cluster) size, compared commensurate vs incommensurate states (#of electrons/spin \leftrightarrow # of atomic sites), we assessed global characteristics like the distribution of single particle eigenvalues (density of states), and in the end we looked at the inverse participation ratio (IPR) vs the energy of the state, which may not have been done previously.

The amix is set to 0.3 or 0.1, with a few exceptions for $u=2$, where both the 24×24 lattice and the 32×32 were not converging in 2500 iterations. The amix represents the percentage of the output of the previous solution that is mixed into the input for the new one. What we observed was that the larger the lattice the harder it was to find a percentage that would allow for convergence. Therefore for some cases we had to use an amix of 0.6, 0.7 and even 0.8.

If for the previous lattices, 30 percent of the solutions were diverging (with the best amix for that case), when we went for a higher lattice, 40×40 , we noticed that most of the solutions were diverging. It is true that we tried only a few cases, because due to the size of the matrix (1600×1600) it was taking too long to get solutions. For example, it took three days to get 10 solutions for parameters, $u=2$, polarization=1/8. This case is also the most difficult one. When the fraction p , of number of spins up minus number of spins down over the total number of spins is 1/8, it is very hard to get results. It is a transition region from strong to weak onsite interactions, which caused problems for us but also gave the most interesting results. For the 24×24 and 32×32 lattices the interval with problems was for polarization between 1/4 and 1/16, and it was getting much larger for 40×40 lattices. For the small numbers of runs done for 64×64 lattices, it became a real problem to get convergent solutions.

A. Varying the interaction strength

Looking at the ground state total energy (Figure 2, first graph) it becomes clear very quickly that for $u=1$, the ground state energy stays almost the same with changes after the fourth decimal. The behaviour is the same for all lattice sizes. What is interesting is that for polarizations closing on 0, there are some changes at the third and fourth decimal for the 16×16 lattice and the same changes happen in the 32×32 lattice for larger polarizations. The 24×24 and 32×32 lattices have the same ground state energy, while when closing on polarization 1, the 16×16 and 24×24 lattices have the same solution. For $u=4$ (Figure 2, last graph), due to the strong regime of the on-site energy the interactions are localized, therefore we don't get a global organized picture. We do not necessarily find the ground state energy, unless we look at the case with only spins up, where no matter what size of lattice we look at the energy stays the same. For any other case the differences in energy, in the same lattice, are varying from 0.02 to 0.06 and this fluctuation happens for

all lattices. But when taking an average of the energy, for all lattices the energy tends to converge towards the same value. The $u=2$ case (Figure 2, second graph) seems to be on the transition line between the higher on-site interactions that are localized and the lower ones that are global. Therefore the solutions for the ground state energy are different for different lattice sizes, especially the 8×8 lattice. The 8×8 lattice doesn't allow us to see the big picture. The differences go up to the first decimal. It seems that the larger the lattice becomes the smaller the difference gets, where that happens only after the fourth decimal. As in the case for $u=4$, when there are only spins up, the energy is identical for all 4 lattices.

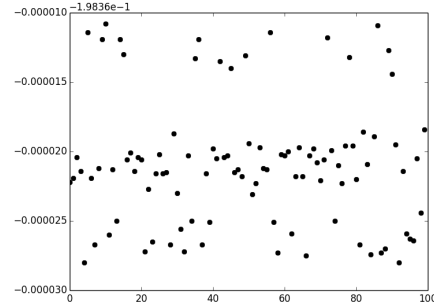


Figure 2c: 32×32 lattices with $p=1/2$ and $u=3$; the x -axis represents the run number while the Y -axis represents the total energy of that specific run

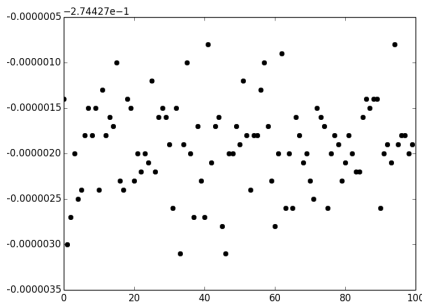


Figure 2a: 32×32 lattices with $p=1/2$ and $u=1$; the x -axis represents the run number while the Y -axis represents the total energy of that specific run

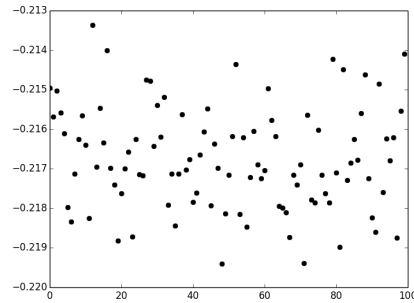


Figure 2d: 32×32 lattices with $p=1/2$ and $u=4$; the x -axis represents the run number while the Y -axis represents the total energy of that specific run

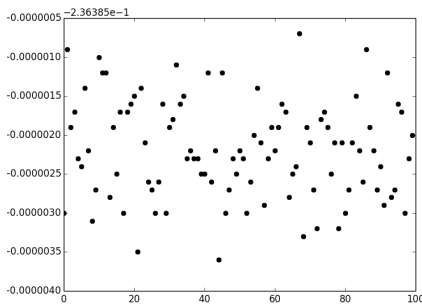


Figure 2b: 32×32 lattices with $p=1/2$ and $u=2$; the x -axis represents the run number while the Y -axis represents the total energy of that specific run

B. Varying the lattice size

A different way to look at the results is by analyzing the cluster size. Due to the strong local on-site interactions happening for $u=4$, there isn't much to see in the solution (Figure 3). There is little correlation from site to site, the global interactions are very weak leaving the magnetization to look just disorganized. We get the same type of solution for any lattice size and any combination of spins up and spins down.

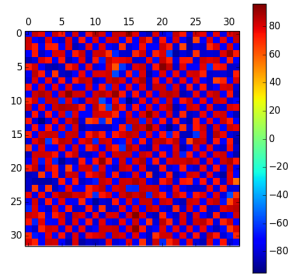


Figure 3: 32x32 lattice, $u=4$, $p=1/2$; each little square represents a site and the colors go from spin up-dark red to spin down-dark blue

Due to the strong local interactions the solution for the ground state gives either the anti-ferromagnetic (the spins of the electrons align in a regular pattern with the neighboring site - one up, one down) solution or some type of a cluster or stripes solution. For small polarizations (up to $p=1/16$) the solution seems to be a variation of stripes, while for larger polarization we get clusters. (Figure 4)

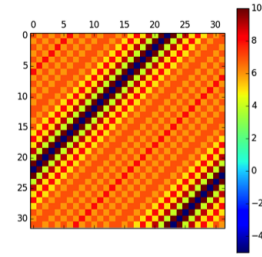


Figure 4c: Stripped solution for small polarizations and $u=1$

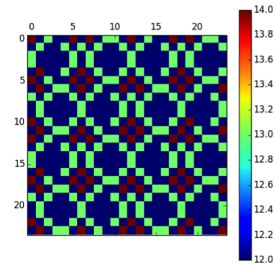


Figure 4d: Cluster solution for larger polarizations and $u=1$

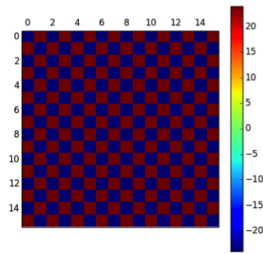


Figure 4a: The anti-ferromagnetic solution for $u=1$

There is an interesting result for $p=1/9$ which is incommensurate with the chosen lattice sizes. See Fig.5. The 16x16 lattice has a striped solution while the 24x24 and 32x32 lattices have cluster solutions. Otherwise, all solution are consistent.

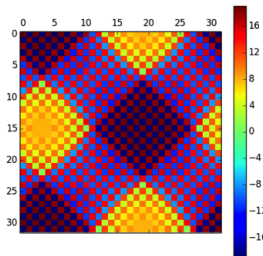


Figure 4b: Stripped solution for small polarizations and $u=1$

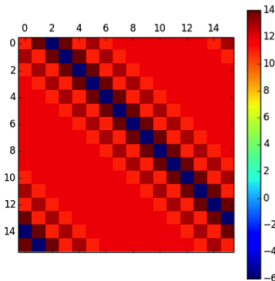


Figure 5a: For $u=1$; $p=1/9$; lattice size 16x16

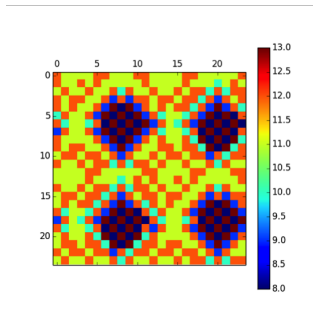


Figure 5b: For $u=1$; $p=1/9$; lattice size 24×24

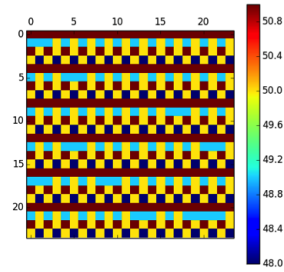


Figure 6b: Polarization $1/2$, $u=1$, 24×24 lattice

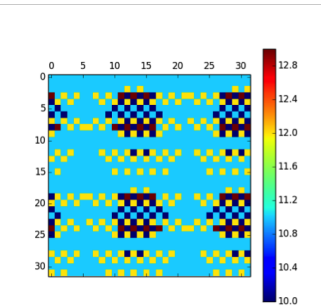


Figure 5c: For $u=1$; $p=1/9$; lattice size 32×32

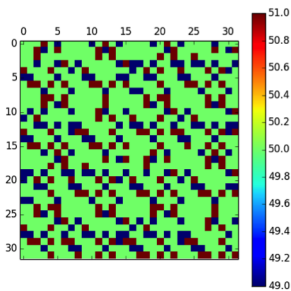


Figure 6c: Polarization $1/2$, $u=1$, 32×32 lattices

Another interesting result happens for $p=1/2$, where the bigger the lattice gets, the more disorganized the solution appears. (Figure 6) There is a strong dependence on lattice size.

But the most interesting and diverse solutions are seen in the transition case which is for onsite interaction $u=2$. The only constant results are that from the 8×8 lattice you can't conclude much, and the larger lattices tend to give the same type of solution, whatever that solution might be. But here it ends because, the solutions are everything from stripes or clusters to discs, rings, waves and other shapes and forms with no names. A few examples of phase separation can be seen in Figure 7

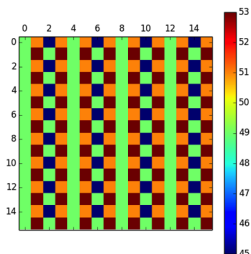


Figure 6a: Polarization $1/2$, $u=1$, 16×16 lattice

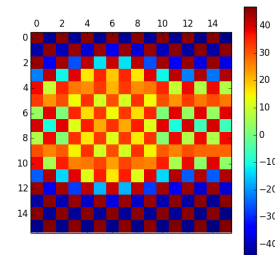


Figure 7a: Solution for $u=2$, lattice size 16×16

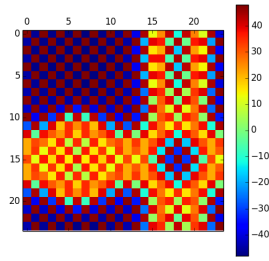


Figure 7b: Solution for $u=2$, lattice size 24×24

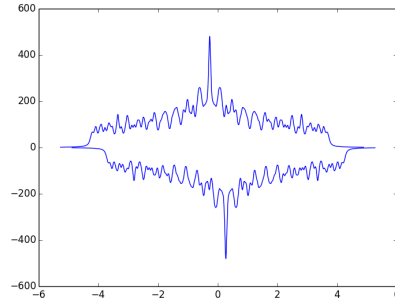


Figure 8: DOS for $u=1$ with shifted peaks due to the difference in spins

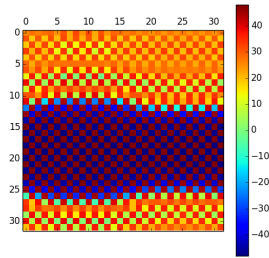


Figure 7c: Solution for $u=2$, lattice size 32×32

The HF solutions allow us to assess global characteristics like the distribution of single particle eigenvalues. So, another way to look at the results is by analyzing the density of states. DOS describes the number of states per interval of energy at each energy level that are available to be occupied by electrons. A high DOS at a specific energy level means that there are many states available for occupation. Plots of the DOS can be seen on Figure 8. On the top image, the interactions between electrons are not strong when the onsite energy is 1 giving this perfect solution with the peak right in the middle and a shift between the spin up and down, due to imposed spin polarization. In the right picture, due to the strong regime of the onsite energy ($u=4$), the number of states per interval of energy are organized in a symmetrical picture, with a flip of the spin. The up spin goes down on the other side of the band gap and the down spin goes up. There can also be seen the peaks where the density of states is at its highest.

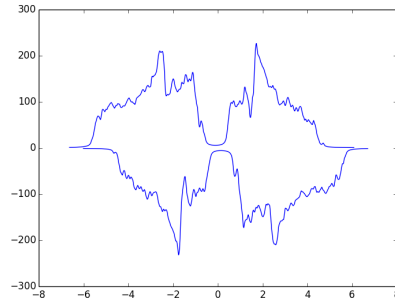


Figure 8: DOS for $u=4$ with peaks for the highest density and gaps

C. A new type of characterization

A different way to look at the results is by analyzing the solutions of the inverse participation ratio versus the energy of states. The IPR provides a measure of the extension over sites of the eigenstates. We did a set of runs only on 24×24 and 32×32 lattices, for onsite repulsion u of 1, 2, and 4 and polarization $1/16$, $2/16$, and $3/16$. It can be seen how much the interactions affect the results. Weak interactions form a straight line ($u=1$), while strong interaction ($u=4$) give a visible gap. The solutions for $u=1$, give an expected result. The values of eigenenergies for every spin are close together, the majority forming a line. When looking at different polarizations the values form a distinctive line for bigger polarization and get a little spread for smaller polarization. It can also be easily seen that number of spins up

and spins down play a role in the forming of a gap around the point of 0 eigenenergy.

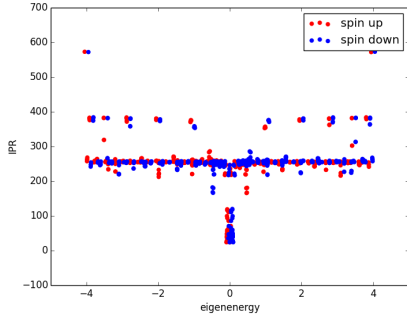


Figure 9: IPR vs energy for $u=1, p=1/16$

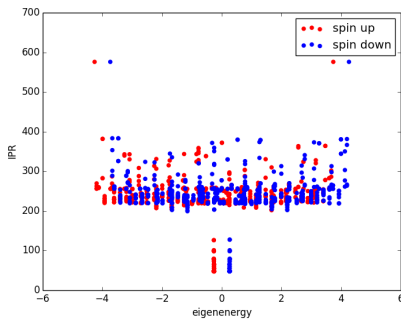


Figure 9: IPR vs energy for $u=1, p=2/16$

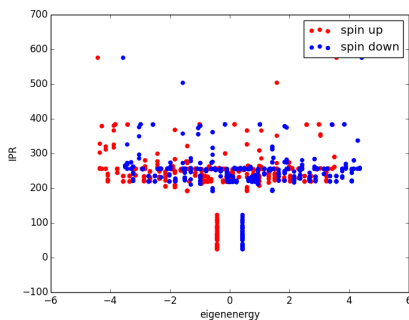


Figure 9: IPR vs energy for $u=1, p=3/16$

The tendency for $u=2$ of the values of spins up and down is to converge towards the point of 0 IPR near 0 eigenenergy. The graph shows a sharper slope for higher polarization.

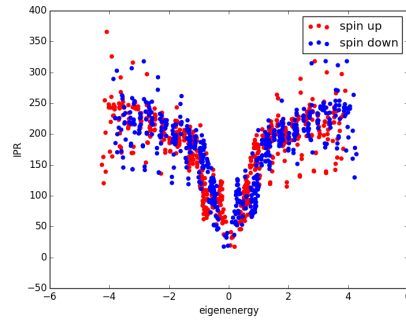


Figure 10a: IPR vs energy for $u=2, p=1/16$

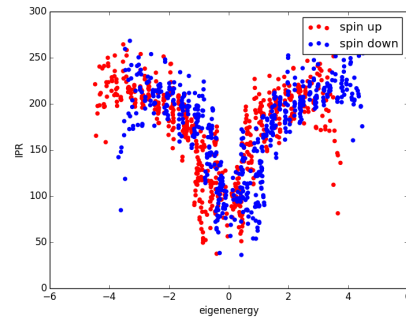


Figure 10b: IPR vs energy for $u=2, p=2/16$

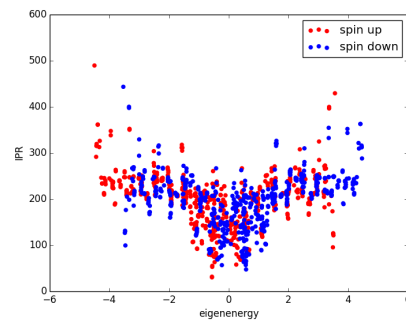


Figure 10c: IPR vs energy for $u=2, p=3/16$

Stronger interactions of the electrons of the onsite energy $u=4$, give a totally different picture when compared to the solution of a strong interaction. We don't even get the curvy solution of the $u=2$. Here, in either side of the 0 eigenenergy forms an arrow head with a quite a big gap in between either side, as seen in Figure 11.

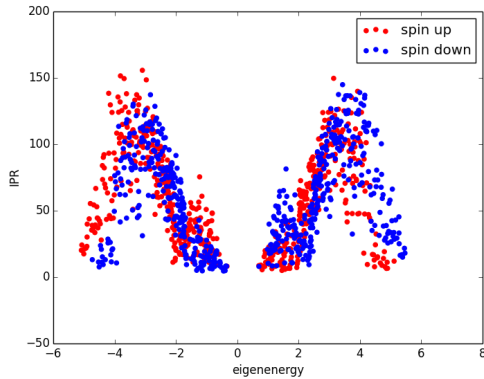


Figure 11a: IPR vs energy for $u=4, p=1/16$

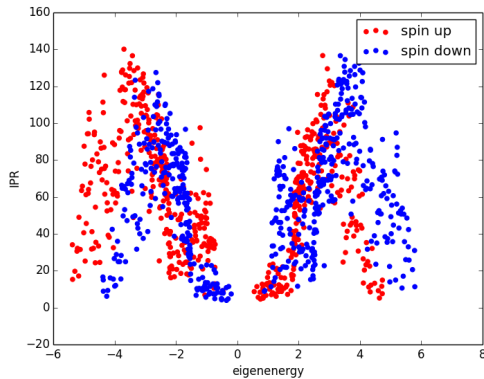


Figure 11b: IPR vs energy for $u=4, p=2/16$

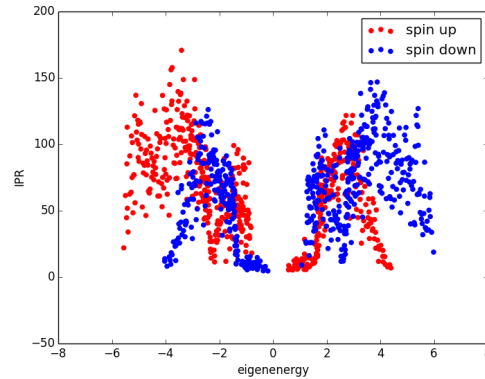


Figure 11c: IPR vs energy for $u=4, p=3/16$

V. CONCLUSION

We have studied Mean Field Theory on a 2D lattice to obtain some insight into how correlated electron systems behave. The MFT helped us analyze the results and assess global characteristics of the system. Even though they are not very complicated or the most realistic methods, for many properties what makes them so valuable is the amount of variables that we can work with and manipulate. Work like this, has been done before, but usually only on 8×8 lattices. Since we have worked with much larger lattices (the largest being 64×64), we have been able to see how the system changes and what are the tendencies of those changes when working at a bigger scale. One direction would be to work on even larger lattices, but for now we are unable to do so, due to computational problems. Computers are not fast enough to give results in real time. We hope that our results, while giving some answers that theoretical physicist have been looking for, will make them investigate further and revisit simple methods that can still give insight into the world of correlated electron systems.

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