Second Semester Report

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Ph.D. Thesis topic:

Electronic and magnetic properties of exotic nanomaterials

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Introduction:

Using the Hubbard model on an interacting electron system would result in quantitive predictions of some of the system properties. Although the meanfield approximation is not a silver bullet, it is a useful tool to explore certain aspects of the Hubbard model, such as the nature of electonic exitations and the magnetic phase diagram. Thus, working with it will give us a tool to describe those systems.

The mean-field approximation transforms many-body Hubbard model into a non-interacting problem. But it comes with a cost, the problem should be solved selfconsistently. The meanfiled approximation also makes it possible to sove the problem in reciprocal space, further simplifying the computational task. From the meanfield solution the magnetic phase diagram can be constructed. This can be done by the following:

1) Mean filed solution is used for calculating the free energy. Comparing the free energy of different phases phase diagram is constructed.

2) Competition of Coulomb and kinetic energy gives rise to 3 phases.

During this semester my focus was on working on this model. I started by applying it to a simple square lattice, which will in the future be generalized to a more complex system.

Description of research work carried out in the current semester:

I managed to map the parameter space spanned by the occupation number and Coulomb energy, thus obtaining a phase diagram. In Fig.1 I depict the Free energy in terms of Coulomb repulsion at fixed occupation number for the three investigated magnetic patterns. Fig 1 and Fig 2 below shows the free energy Vs coulomb repulsion. in figure 1 we can see where the system exchange (at $t/U = 0.13$) from one configuration to another based on its free energy behavior. Figure 2 shows the phase diagram, the boundaries between the phases were obtained from the crossing point in figure 1.Those configurations were considered for a square lattice. I used the square lattice as the first step for different systems, as a next stem I'm planning on the use the same procedure for zig-zag graphene nanoribbons which host particular edge states with zero kinetic energy making them an ideal venue for localizing magnetic degrees of freedom. We suspect that we might find some interesting magnetic behavior at the edges of these ribbons, as the kinetic energy of the electrons at such site is almost zero comparing to the bulk electrons. Due to the corona pandemic, our work was limited to what resources we had.

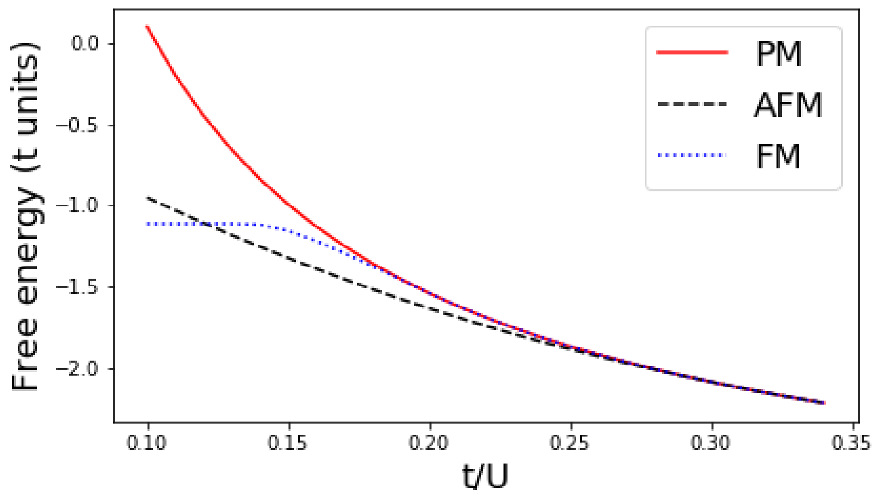

Figure 1. A phase transition occurs where magnetic-energy curves cross each other. For n=0.8 the system becomes ferromagnetic below t/U = 0.13.

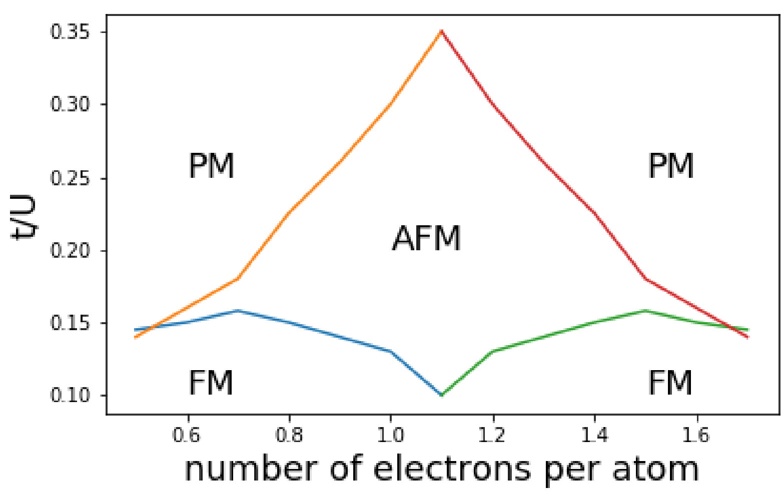

Figure 2. Ground-state phase diagram of the Hubbard model on a square lattice as a function of the ratio t/U and of the electron filling.

Studies in the current semester:

During this semester I enrolled in two courses:

1. Deep learning and machine learning in natural sciences: During this class, we have been introduced to what machine learning is. We walked through any concepts that are essential for such a study. Such as neural networks, classifiers, activations functions, convolutional layers. The main work during this course was focused on image classification techniques. We had two projects where we were asked to classify objects into classes. The first one was to estimate the redshifts of outer galaxies using their photometric data. The second one was more challenging due to the complexity of the data we had. The requirement was to distinguish a picture of whether it was tiger mosquito or not from many different types of mosquitos. In both projects I used python and google Tensor Flow pakge to do the projects. I'm planning to use the skills that I have acquired in this course in my future research.

2. Carbon Nanostructures: The main scope of this course as the title suggest is to introduce us to what carbon atoms structure can have. First e we discussed the history of how these structures were discovered. The first structure was fullerene, we went through how it was discovered, how to produce it, what is its electronic structure. We saw what kind of techniques we can use to determine wither we had fullerene or other kind of carbon structure. Such as mass spectroscopy, NMR, or X-Ray diffraction. We went through what type of pyramidalization it has and how this would lead us to its electronic structure. As a further step a Symmetry analysis were conducted, and the main focus was on Icosahedral group.

Workshops and seminars in the current semester:

Dues to the corona pandemic we were limited to our group meetings, they were conducted online on Microsoft teams. During these meetings I had a presentation where I summarized my work during the semester, and I presented my results of the Hubbard model.

References:

Claveau, Yann & Arnaud, Brice & Matteo, Sergio. (2014). Mean-field solution of the Hubbard model: The magnetic phase diagram. European Journal of Physics. 35. 035023. 10.1088/0143-0807/35/3/035023.