Forth Semester Report

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Ph.D. Thesis topic:

Electronic and magnetic properties of exotic nanomaterials

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Introduction:

Solid-state physics and materials science physics is at the forefront of today's emerging technologies. New exotic materials, such as graphene and topological materials, have ushered in a significant development in technological areas, from molecular sensors to nanoscaled energy harvesters, from ultra-dense and ultra-fast classical computer memories to architectural elements in a future quantum computer. The constituent electronic and magnetic degrees of freedom in these materials give rise to emergent quantum states with interesting properties, making them ideal candidates for a variety of novel applications. During my PhD research, I will attempt to build new theoretical tools in order to better comprehend the outcomes of experiments with unusual materials. The research will be based on the following tree pillars: 1. First-principles modeling of exotic nanomaterials, 2. Development of simple analytic toy models and effective theories, 3. Calculation of experimentally relevant electronic and magnetic properties.

Summary of research work carried out in the previous three semesters:

When applied to an interacting electron system, the Hubbard model yields qualitative predictions of some of the system's properties. Although the mean-field approximation is not a perfect solution, it is a useful tool for investigating certain aspects of the Hubbard model, such as the nature of electronic excitations and the magnetic phase diagram. Working with it will thus provide us with a tool for describing those systems. The many-body Hubbard model is transformed into a non-interacting problem using the mean-field approximation. However, it has a cost and the problem should be resolved selfconsistently. The meanfiled approximation also allows you to solve the problem in reciprocal space, which makes the computational effort more easier. The magnetic phase diagram can be built from the mean-field solution.

Hubbard model was the center point of my work. The reason for choosing the Hubbard model is that it is an excellent tool to understand the realistic magnetic interactions. I reproduced the results from [1], Which is shown in Fig 1. I was able to create a phase diagram by mapping the parameter space spanned by the occupation number and interaction strength U, the boundaries of the phasese (ferromagnetic,antiferromagnetic and paramagnetic) can be concluded from the crossing points in Fig 2. While in Fig 2. the three magnetic patterns investigated, I represent the free energy in terms of Coulomb repulsion for a fixed occupation number, we can see where the system flip (at t/U = 0.13) from ferromagnetic configuration at large U to antiferromagnetic at small U based on its free energy behavior.

Flat bands occur in topological system's that are of interest. As in 2D graphene and 3D nodal line semimetals (ABC graphite is a simple example). An experimental physics team at Wigner Research Institute (Péter Nemes-Incze's group) ,the group conducts experiments on the surface state of ABC graphite. They looked for possible surface magnetism signatures. Splitting of the surface flat band was observed in some samples.

For approaching this problem, we used the SIESTA code to create a self-consistent Hamiltonian based on DFT calculations. Then, extracting Heisenberg model parameters from ab initio calculations. Despite the fact that the Heisenberg model stated that the magnetic configuration in question is the true ground state, the calculated critical temperature was much lower than the

experimentally observed one. In order to performe this calculations I used a code provided by my supervisor[2] and made appropriate changes.

We've done more DFT calculations at this stage, which indicate that a simple Heisenberg model might not be able to explain the structure. At this point, we're looking for a model that will work well in our situation. Fig. 2 shows the this is the spatial dependence of the exchange coupling.

I applied the knowledge I gained from studying the Hubbard model on a square lattice to graphene nanoribbons as well. To investigate the exchange interactions, we first constructed the Hamiltonian for graphene nanoribbons. Graphene nanoribbons host specific edge states with zero kinetic energy as well, making them an ideal venue for localizing magnetic degrees of freedom. Since the kinetic energy of the electrons at such sites is almost zero compared to the bulk electrons, it is expected the interaction will alter these states leading possibly to form some magnetic behavior . The ultimate goal is to investigate how Heisenberg model parameters that describe a mapping to classical spins describe edge magnetism in these topological systems [3].

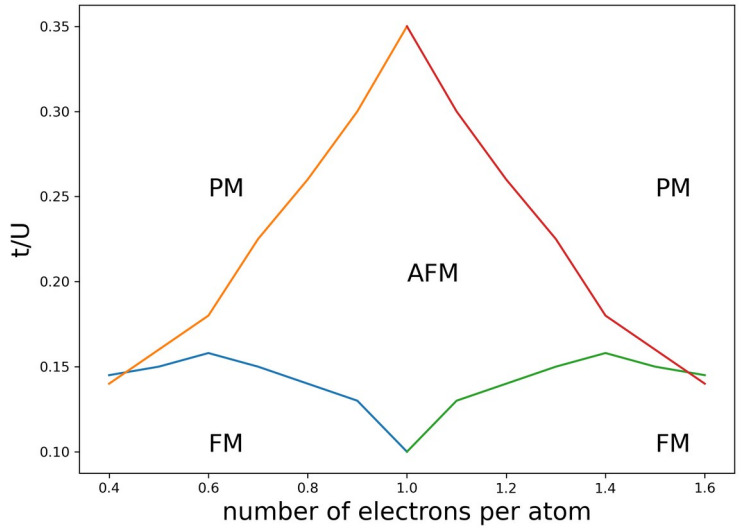

Figure 1: Ground-state phase diagram of the Hubbard model on a square lattice as a function of the ratio t/U and of the electron filling (where t refers to hopping amplitudes).

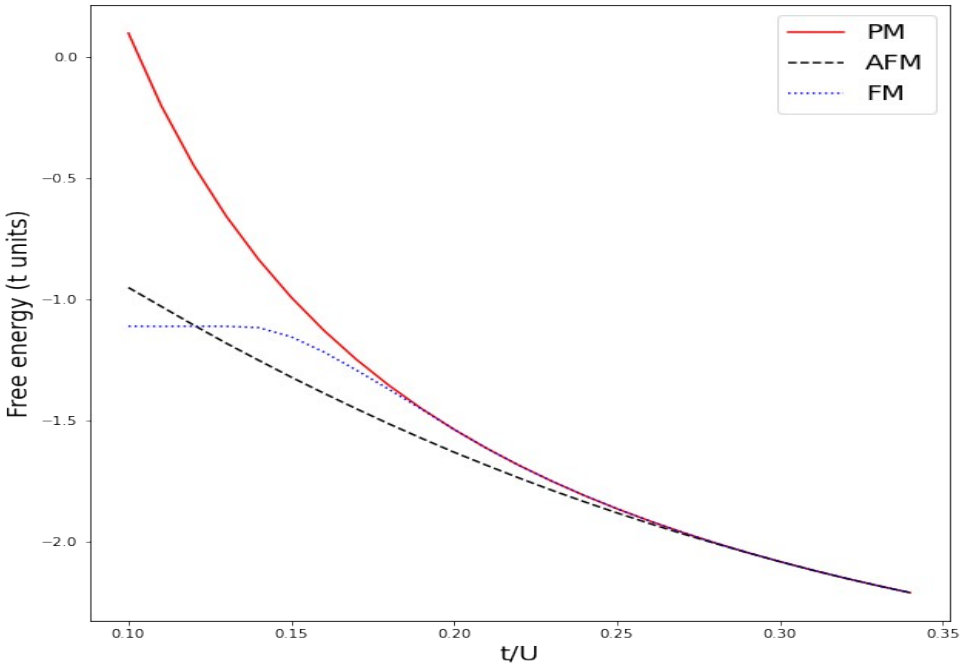

Figure 2: . A phase transition occurs where magnetic-energy curves cross each other. For n=0.8 the system becomes ferromagnetic below t/U = 0.13.

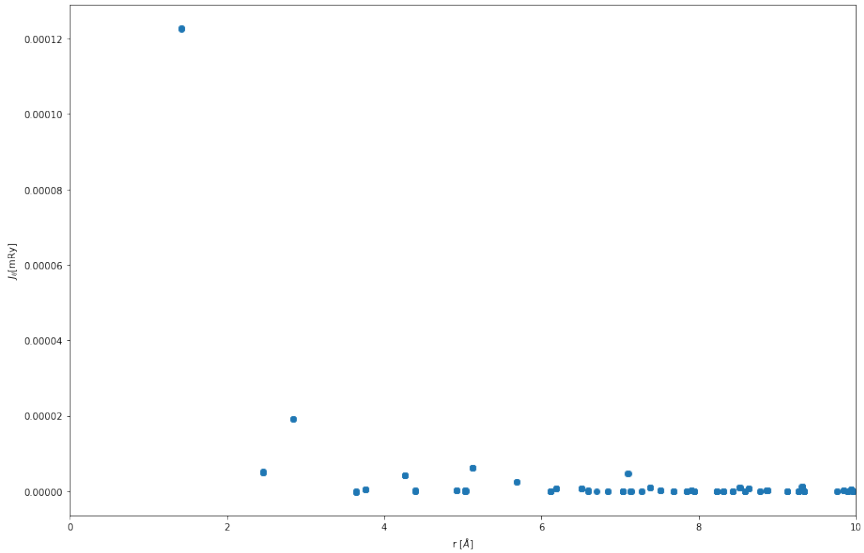

Figure 3: Calculated exchange coupling of the surface atoms of ABC graphene, based on reference ground state obtained from a first principles calculation performed by SIESTA.

Technical background:

1. Hubbard model.

Itinerant, interacting spin $\frac{1}{2}$ electrons hopping on a set of spatially confined orbitals are described by the Hubbard model. The Hamiltonian is written as:

$$\hat{H}_H = -\sum_{ij\sigma} t_{ij} \hat{C}^{\dagger}_{i\sigma} \hat{C}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$\hat{C}^{\dagger}_{i\sigma}$ is an operator that represents the creation of a spin electron σ at site i, $\hat{C}_{i\sigma}$ is an operator that represents the annihilation of a spin electron at site j, and t_{ij} is the process' amplitude, the so-called hopping amplitude from site j to site i where the electron is generated. Finally, the sum over ij , and $t_{ij} = (t_{ij})^*$, implying that the Hamiltonian is hermitian, as it should be. ***U*** represent the on-site Coulomb repulsion.

To obtain the complete mean-field solution, we first discuss the tight-binding solution for U = 0, and then examine the action of the H term in mean-field. In both cases, we can apply a Fourier transform to the k-space to fully exploit the 2-dimensional periodicity.

2. Mapping to Heisenberg model.

A lattice of localized classical spins is defined by unit vectors $\vec{e}_i$, where i denotes lattice (or atomic) sites, in the classical Heisenberg model. The spin-spin interactions are represented by isotropic exchange parameters J_{ij} , which inserted in the spin Hamiltonian.[2]

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} \vec{e}_i \vec{e}_j$$

The magnetic force theorem allows us to extract the exchange parameter J_{ij} from the effective single-particle Hamiltonian $\hat{H}$ resulting from a self consistant calculations. We write $\hat{H}$ in terms of a basis set of localized orbitals centered at lattice locations, using a collinear-spin reference frame. As a result, in the spin indices, the Hamiltonian is diagonal. The corresponding spin-dependent and site-indexed Hamiltonian blocks are indicated by H^{σ}_{ij} for all the base functions assigned to one site and, the same basis functions are taken into account for the two spin-channels. Then it is possible to derive the exchange parameters from the expression.

$$J_{ij} = \frac{2}{\pi} \int_{-\infty}^{\epsilon_F} d\,\epsilon\, Tr_L [H^s_{ii} \widetilde{G}^{\uparrow}_{ij}(\epsilon) H^s_{jj} \widetilde{G}^{\uparrow}_{ji}(\epsilon)]$$

where ϵ_F is the Fermi energy, Tr_L denotes the trace of matrices in orbital space, with H^s_{ii} is the local, part of the Hamiltonian that corresponds to the exchange splitting.

$$H_{ii}^{s}=\frac{\left(H_{ii}^{\uparrow}-H_{ii}^{\downarrow}\right)}{2}$$

and the Green's function

$$\widetilde{G}_{ij}^{\sigma}=\left[\left(zS-H\right)^{-1}\right]_{ij}^{\sigma}$$

Description of research work carried out in the current semester:

This semester, My work this semester was based on three points.

1) became acquainted with the numerical procedure to obtain the J_{ij} Heisenberg interactions (exchange energy).

During this phase I studied how to find a way for first-principle calculations of J_{ij} , and it was a good choice to use the Green's function formalism to obtain the exchange energy. Then applying this to the tools I have (the code in hand), running through the it and matching it with the system in hand.

2) Calculate ABC graphene DFT, and Hubbard Hamiltonian J_{ij}

I ran the the code for different ABC graphene configuration. I tried it for 3,5,8,15 layers. All runs were performed using the computer cluster made available by KIFÜ.

3) Complete the code with J_{ij} from mean-field solution of the Hubbard model for carbon ribbons, but the calculations are still in progress.

The Hubbard Hamiltonian obtained from were used with the same algorithm for calculating the J_{ij} . This work is still in progress, and we hope to publish our findings as soon as possible. We are currently finalizing the work that will be published.

Studies in current semester:

1. solid state theory (FIZ/1/022E)

In the field of condensed materials I got to know about the newest findings and research. The main focus was on Molecular dynamics, empirical potentials, many particle potential, first principle methods, Phase field theories, Continuum theory of defects. Those which have extended my theoretical skills.

2. Many body problems (FIZ/KUT-S4)

The purpose of this lecture is to introduce many body descriptions to the field-theoretical formalism based on perturbative expansion through Feynman's diagrams.

Workshops and seminars during my studies:

- 2020 Joint Conference of the Condensed Matter Divisions of EPS (CMD) and RSEF (GEFES) ,CMD2020GEFES, which held Madrid spain between 31 AUG -4 SEP, 2020. during this workshop I attended number of lectures, including:

1. Modern trends in topological quantum matter.

2. Quantum thermoelectrics and heat currents at the nanoscale each of these talks were held by multiple talker, where they talked about their work in this subject field

- 4th Graphene and 2D Hetero structure Workshop, which held at BME between 24-25. OCTOBER, 2019. during this workshop I attended number of lectures, including:

1. Theory of induced spin-orbit coupling and its twist-angle dependence in graphenetransition metal dichalcogenide heterostructures, by Andor Kormányos.

2. Spin-orbit induced phase shift in Josephson junctions, by Assouline Alexandre

3. Simulating transport through mono- and bilayer graphene nanoconstrictions, by Thomas Fabian

Seminar under the title: accurate numerical calculations for strongly correlated ultracold few-fermion systems with the trans correlated approach. This seminar was held at BME, and given by Peter Jeszenszki, on 2019. 10. 07

Acknowledgment:

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References :

1. Y.Claveau et al Eur. J. Phys. **35** 035023 (2014)

2. L.Oroszlány, J.Ferrer, A.Deák, L.Udvardi, and L.Szunyogh Phys. Rev. B **99**, 224412 (2019)

3. O.Gröning, S.Wang, X.Yao. Engineering of robust topological quantum phases in graphene nanoribbons. *Nature* **560**, 209–213 (2018)

4. S.Slizovskiy, E.McCann, M.Koshino. Films of rhombohedral graphite as two-dimensional topological semimetals. *Commun Phys* **2**, 164 (2019).