Third Semester Report

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Ph.D. Thesis topic:

Electronic and magnetic properties of exotic nanomaterials

Monday January 22nd 2021

Introduction:

During this semester, I carried on my previous work. We have focused our work on a specific material, Graphene, trying to describe physical phenomena for different structures, using computer models. What is new in this semester that there was some cooperation with other teams, specifically with Topology in Nanomaterials Research Group (lead by Péter Nemes-Incze). Where we tried to confirm their findings on Graphene ABC stacking. Our part was to find a model that explain their findings. Which will be described later in the report.

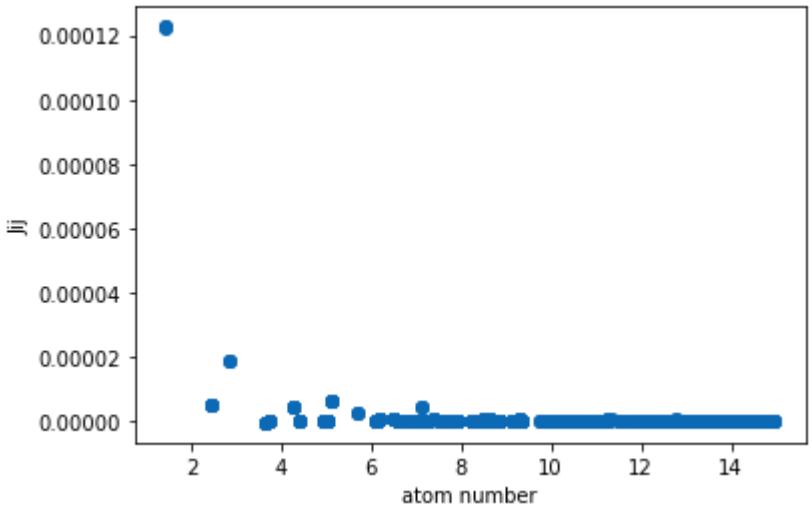

Figure 1: Coupling convergence

Figure 1 shows the convergence of the electrons coupling as a function of distance from atoms at the edge layer.

Description of research work carried out in the current semester:

My work this semester was divided into two parts:

1. Graphene nan-oribion: where we wanted to progress our work with self consistent Hubbard model, into Graphene nanao-ribbons. We started by building the Hamiltonian that includes the spins, we were interested in studying the exchange interactions. For this job to be done I used some python code, which was based on previous research, (Oroszlány, L., Ferrer, J., Deák, A., Udvardi, L. and Szunyogh, L., 2021. *Exchange Interactions From A Nonorthogonal Basis Set: From Bulk Ferromagnets To The Magnetism In Low-Dimensional Graphene Systems*.)

But we had to pause due to new work that had emerges, which will be in the second category .

2. An experimental physics team at Wigner research institute, had observed a critical temperature for a possible magnetic phase transition in 15 layers Graphene, they came to us asking for our help to

build a model to describe what they see. We first used a self consistent Hamiltonian generated using DFT calculation, done using the SIESTA code. Then extracting Heisenberg model parameters from the ab initio calculations hopping to see some results. Altho the Heisenberg model confirmed that the considered magnetic configuration is the true ground state, the calculated critical temperature was considerably lower than the experimentally observed one.

At this stage we have done further DFT calculations which suggest that one possibly can not describe the system by a simple Heisenberg model. At this stage we are searching for a model that would be a good use for our case.

Studies in the current semester:

During this semester I enrolled in two courses:

1. Quantum information theory: we have been introduced to the foundation of quantum information theory, and how it was linked to quantum mechanics. It has covered the treatment of the system state using the the concept of the density matrix, and how it determines important properties of th system. We usied some dervations to reach some results in a much eseir way. Then we have used this knowledge to connect it to quantum computers, and its keywords, such as qubits, entaglments, teleportation, quantum bank notes, ...etc.

2. Transmission electron microscopy and electron diffraction: this course covers the fundementals of Transmission electron microscop, from how it work to how we analyze the results, and how to defrenciate the planes from a picture. Using this analysis we could tell what kind of crystal sturcture a material could have, where are the defficts, and all other important information we could gather from it.

Workshops and seminars in the current semester:

During this semester I attended one workshop.

The workshop was under the title: 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

Each other week there is an extra work that is required from each member of the group, that we review the arxive published papers on condensed matter physics. The work is divided that, for each date on the calendar its responsibility of one of the group members to do the review.