First Semester Report

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Ph.D. Thesis topic:

Electronic and magnetic properties of exotic nanomaterials

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Introduction:

The research in solid state physics and materials physics has been in the heart of now a day's new technologies. The discovery of new exotic materials such as graphene, topological insulators, semimetals, and single molecular magnets, has introduced a big advancement leap in these fields. In these materials, the constituting electronic and magnetic degrees of freedom give rise to emergent quantum states with intriguing properties that make them ideal candidates for several innovative applications, from molecular sensors to nanoscaled energy harvesters, from ultra-dense and ultra-fast classical computer memories to architectural elements in a future quantum computer.

Due to those exotic materials electronic structure they will play a crucial role in developing solid-state quantum computer architectures, as tthey are robust against environmental effects, also it is easy to integrate them in current technologies.

Exotic material shows an interesting magnetic pattern in real space that we can benifit in information storage technologies. On the other hand, on quantum computer architecture using molecular magnets will lead to a new alternative architecture. During my PhD work I will try to develop a new theoretical tools to try to understand the results that arises from the experiments related to the exotic materials. The research work will be based on tree pillars: 1. First-principles modelling of exotic nanomaterials, 2. Development of simple analytic toy models and effective theories, 3. Calculation of experimentally relevant electronic and magnetic properties.

Description of research work carried out in the current semester:

I started my work by working on some known systems Hamiltonians. In particular the Hubbered model. During this work I got myself more familiarized with python modeling for such systems. The reason for choosing the Hubbered model is that it is an excellent tool to stimulate my reflections towards the treatment of realistic magnetic interactions. By studying a detailed analytical and numerical calculations of how to find the mean-field solution of the model on a square lattice. In this work I'm trying to reproduce the results from this paper: Mean-field solution of the Hubbard model: the magnetic phase diagram (Y Claveau, B Arnaud and S Di Matteo , 2014, European Journal of Physics)

By doing this I managed to construct magnetic phase diagram and understand in this way why ferromagnetism or antiferromagnetism can be determined by the interplay of Coulomb repulsion.

Studies in the current semester:

During this semester I enrolled in two courses:

1. Topological insulators: which held at BME. This course is an introduction for the field of topological insulators, it covers several core subjects in the field such as: electrons in solids: the tight-binding model, simple 1D and 2D models of topological insulators, Berry phase, Chern number, adiabatic charge pumping, edge states and their topological protection, topological invariants, bulk-boundary correspondence, disorder and conductance quantization in topological insulators, quantum anomalous and spin Hall effects.

   We have attacked each of these subjects in a detailed way, where at each class we were required to read the about a pre-advertised subject, and then a discussion would start to reach a common understanding of the concept. This course has been a good review for my understanding of quantum mechanics, as it takle some fundamental concepts and require the student to connect all the points to reach a good level of understanding.

2. Mesoscopic systems: which held at ELTE. During this course we have been introduced to micro-nanoscal systems, we have learned how to construct a Hamiltonian for a lattice and how to introduce the electrons hopping between lattice sites. Also, we have learned how to benefit from the Greens function in a way we can gather information of systems of interest. At the end of the course we were required to develop a code of one of several given problems, where we had to construct the Hamiltonian and then using the Greens function, we can represent the requested results. My project was Graphene focusing, where a monolayer of graphene on a PN junction, has a different potential at each half. If we introduce an electron current on one of the halves, the difference of potential will cause the electron current to focus on one point on the other half. I managed to represent my results graphically using python code.

Workshops and seminars in the current semester:

During this semester I attended one seminar and one workshop.

The seminar was 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. where he presents his group work, they have improved the existing exact denationalization approach with two distinguished steps. During the seminar he has present some numerical example of their approach for few firmions 1d and 3d systems. Where their calculation has shown an improved error, value compared to the standard re normalization approach.

The workshop was under the title: 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 graphene-transition 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

Every week there was a group meeting, where we discuss what each member advancement had in their work, also what is new and interesting in the field. An extra work 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.