Doctoral School of Physics - Eötvös Loránd University (ELTE)

Semester Report 1

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Ph.D. Thesis title: Investigation of Layered Topological Insulators

Introduction

Layered materials – crystals consisting only one or few atomic layers – are in the forefront of the solid state physics research ever since the first successful isolation of graphene in 2004 [1]. Many similar materials have been synthesized or isolated over the last 15 years showing a large variety of properties: there are semiconductors, semimetals, insulators, half-metals, half-semiconductors, ferromagnetic or antiferromagnetic systems among them.

Topological insulators (TIs) represent a new quantum state of matter characterized by robust gapless states inside the insulating bulk gap [2]. The topological edge states of a two-dimensional (2D) TI carry dissipationless current because of the robustness against backscattering [3], and this may lead to low-power-consumption electronic devices [4]. The Nobel Prize in Physics 2016 was awarded "for theoretical discoveries of topological phase transitions and topological phases of matter" [5] – which clearly reflects the interest and importance of TIs. Graphene can be thought as the prototype of 2D TIs [3] albeit the non-trivial gap is too small thus the 2D TI state is not accessible for practical use. Therefore, research groups around the world are looking for alternative materials with non-trivial gaps above the room temperature – both theoretically and experimentally.

Primary concern in this research is to build tight binding models and fit models to DFT calculations on small systems and subsequently calculate properties of interest.

Description of research work carried out in current semester

I was on learning stage during the first term of the doctoral school. I have attended three lectures to expand my knowledge in physics and get to know computational stuff. One of the most important courses was Computational Studies of Electron Systems which is directly connected to density functional theory (DFT) based on quantum chemical tools (e.g. SIESTA [6], VASP [7]) to calculate properties of various 2D crystals. The first time I met SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) and VASP (The Vienna Ab initio Simulation Package). I have done a project about Fermi velocity of quasiparticles in graphene [8]. By this project l had a chance to gain a deep knowledge on SIESTA (for instance, how to generate pseudopotential files, convergence of K points and Mesh-Cutoff for a finite 3D grid calculation), as well as how to use a Linux operating system and practice some Bash commands.

The another lecture was Mesoscopic Systems which gave me deeper knowledge of Python programming language. I took a project about QWZ model dirty edge local density for finishing the course. By this l could built up Hamiltonian, calculate Green function [9] and DOS in Python. I strongly believe that obtaining hands-on experience in Python programming along with Linux and Bash is quite useful as my studies involve complex computations where results must be precise. Apparently, the utilization of such tools will speed up the computations and certainly, will avoid possible human miscalculations. The third lecture was Topological Insulators I, which taught about band structure and edge states in one and two dimensions. All these courses provided the opportunity to highlight initials use of a new active courses in next term.

Moreover, l started to assess the priorities of various tasks during the active semester period and examine Fundamentals of the Physics of Solids [10] and Introduction to quantum mechanics [11] books time by time. I review new submission articles on https://arxiv.org/ weekly. I have participated a weekly group seminar which consider on about interesting articles, conferences and discussion on PhD students duties during the week and future educational plan.

Additionally, reviewed articles which is mainly related to my thesis research such as High quality transport in exfoliated jacutingaite crystals [12], Prediction of a Large-Gap and Switchable Kane-Mele Quantum Spin Hall Insulator [13], Dual topology in jacutingaite Pt2HgSe3 [14] and etc.

Conference in current semester

4th Graphene and 2D heterostructure Workshop - Budapest University of Technology and Economics, MTA-BME Quantum Electronics Research Group. Budapest, 24-25. October, 2019.

Awards

Stipendium Hungaricum Scholarship

Hungarian Quantum Technologies Excellence Project

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