Quantum and classical physics of molecule size and two dimensional systems

Final Report

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Principal Investigator: Dr. Dávid Visontai

During the time of research we managed to accomplish many of the goals, that we aimed for in the submitted research plan. The funding covered travel expenses to visit our collaborators and present our work at a workshop. As a direct result of this funding no work was published yet but in all 3 topics, that are detailed below, much work was done and we are preparing papers and codes for publishing.

1. Development of the transport code (Gollum[1] and EQuUs[2] package) Our aim was (and still is) to create and develop tools that enable us to extend our numerical calculations with new physics and to make it possible to study experimentally relevant sample sizes. Our efforts took us into two directions. One is the EQuUs (Eötvös Quantum Transport Utilities), which is a highly efficient code using the latest algorithms suited for the mathemathics in our calculations and for the high performance computing environment. The other direction is the Gollum project, where we develop a package for a much wider community and try to facilitate the usage for non experts.

Both of these packages are designed for electronic transport calculations implementing the equilibrium Green's function formalism developed in Ref. [3] and in the spirit of Landauer's formalism[4]. Many physical properties of the 0D, 1D, 2D and 3D materials can be obtained that are related to electronic transport. With these tools we investigated novel nanostructures, that are already used in experiments or have potential use for future applications.

Since the previous version of Gollum[5], we collected many ideas to implement new physics into the code, to make it more user friendly, faster and decrease memory usage.

The extra modularites are:

- Kondo & Coulomb blockade physics
- Magnetic field
- Scripts to handle multiscale simulations
- Interface to plane-wave codes using Wannier90 code

The major part of the work was done during two different shifts, 2 weeks in Oviedo, Spain and 1 week in Lancaster, England. After the semester finishes will we be able to run an extra round of tests and release the code for public use.

From this OTKA funding my travel expenses were covered to Spain.

2. Optical properties of 2D crystals with disorder and/or defects Part of this deliverable was to create an efficient and parallelized solver for the time dependent Schrödinger equation for non-interacting systems[6]. By calculating real time correlation functions via the Kubo formula based on the kernel-polynomial method[7, 8] and Green's-function techniques[9] it is able to give predictions for experimentally relevant system sizes. Using C and python languages with

the PETSC[10] library we compiled a code that does the abovementioned calculation and it is available on Github[11], so anyone can reproduce our findings and calculations later on.

The purpose of this code is to study the effect of defects and optical properties on large sizes of 2D crystals such as BiTeI or BiTeI-graphene-BiTeI heterostructures. In order to do that we need the smallest but accurate enough model for our material.

We created a simplified model Hamiltonian for such systems, that concentrates on an effective description of the electronic states near the Fermi level, and investigated its properties as the function of various parameter values. We mapped the phases of the system that can behave as an insulator, metal or topological insulator (Fig. 1). With VASP, a package for density functional theory calculations, we calculated the band structure of this system and by fitting our model parameters (indicated with a star on Fig. 1 (b) panel) we know which parameters are close to the realistic ones and can relate points on the phase diagram to the electronic structure of the heterostructure. This way it is easier to see how do we need to alter the system, if it is possible at all, to behave as a specific device.

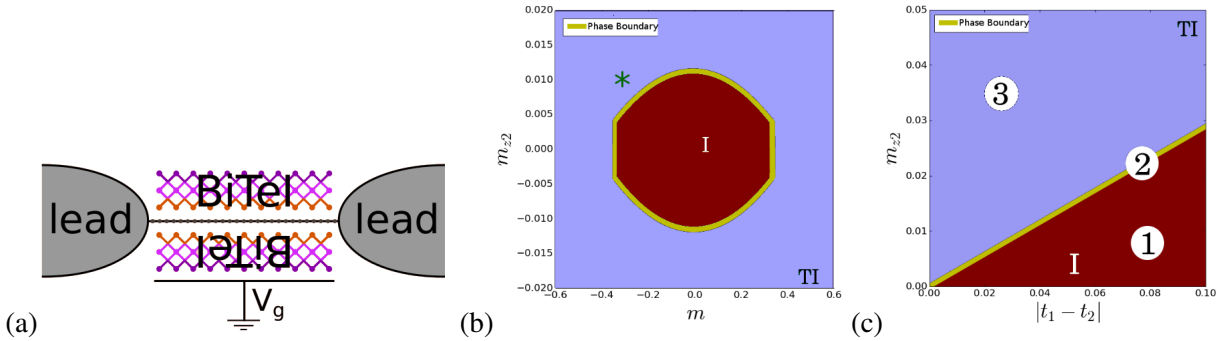

Fig. 1: (a) Structure of BiTeI-graphene-BiTeI in a transport measurement setting. (b and c) Phase diagrams of the system. All units are in eV. If the parameters of the system are in the light blue region then the system is topological insulator, when in the dark red region it is a trivial insulator. On the phase boundary the system is metallic.

Then we used this simplistic model to calculate transport characteristics on a micrometer sized sample (Fig. 2). Our results can be used as guidance to interpret future experiments.

A paper covering this simplistic model and transport calculations is ready for submission[12].

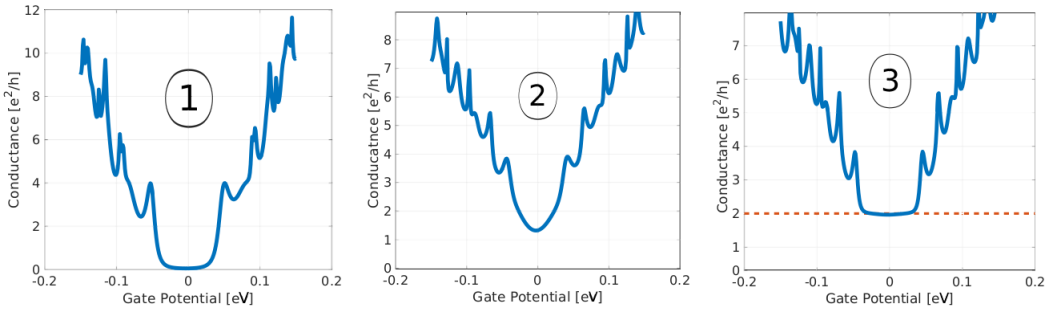

Fig. 2: Transport properties of the model for different phases. The phases are indicated with the same number on the phase diagram in the (c) panel of Fig. 1.

3. Carbon based nanostructures Following the idea in Ref. [13], we created a model of bilayer graphene with two gate on both top and bottom sides (shown on Fig. 3) and calculated the Josephson current with the EQuUs code on fairly large, about 20nm long and 60nm wide samples.

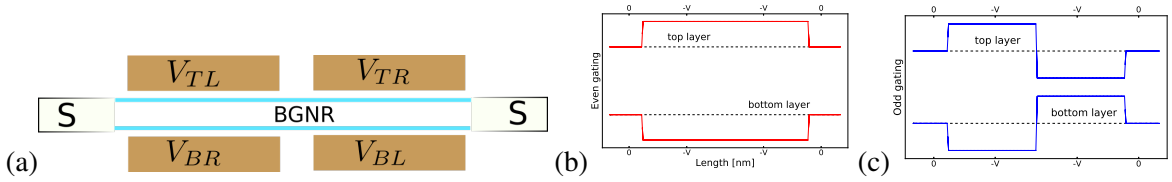

Fig. 3: Setup of the gated Superconductor electrode - Bilayer graphene - Superconductor electrode system. With the voltages on the top and bottom gates as shown on (c) panel one can create a topological state (TS) that is perpendicular to the direction of the current.

In the gapped system the states in the gap (Fig. 4) propagate along the edges of the graphene. These states have a certain extension and for narrow samples the opposite edge states overlap.

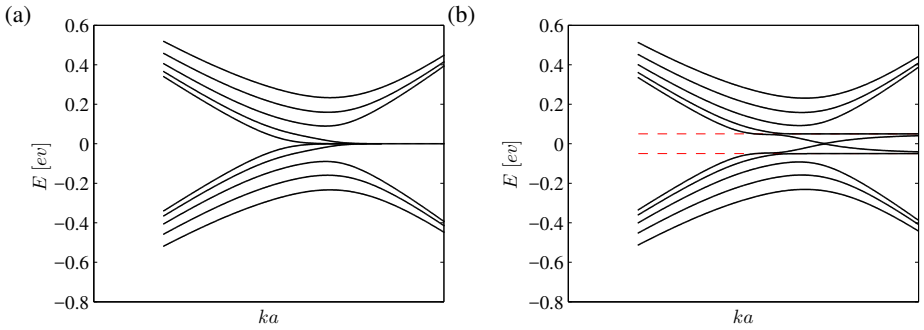

Fig. 4: Band structure of a (a) non-gapped and (b) gapped bilayer graphene calculated for a W = 21 nm wide, zigzag edged ribbon in the K valley. The gate potentials were chosen to (a) $V = 0$ and (b) $V = 50$ meV. The horizontal dashed lines in (b) represent the bulk band gap.

Josephson current without magnetic field When the TS is present it causes a backscattering and the critical current is lower by one order of magnitude compared to the case when no TS is present (Fig. 5).

We investigated the effect of edge disorders as well. Unfortunately, we choose too large defects on the edges and it is not so surprising that the critical current changed signicantly regardless of having a TS. This part is non-conclusive and calculations are still running.

Josephson current with perpendicular magnetic field In case of narrow BGNR up to 21nm the edge states are overlapping. When TS is present the Current-Phase Relation (CPR) is shifted by π and the magnitude of the critical current I_c varies as a function of the B magnetic field. When NTS is present the opposite happens, I_c remains constant and CPR shifts as a function of the perpendicular B magnetic field (Fig. 6).

We are still running calculations on large samples and analyse the results. This setup proves to be an exciting example for testing the code, because there is motivation to calculate on large samples and this way we are forced to try to do that on different high performance supercomputer environments such as the NIIF (National Infrastructure Development Programme) clusters.

With the OTKA funding I managed to participate on the IX TRNM (Towards Reality in Nanoscale Materials) workshop, where I introduced our work on Josephson Current calculations and presented a poster.

4. Other international collaborations not covered by OTKA We finally finished our work on "Formation of two-dimensional micelles on graphene"[14], which was a multi-scale theoretical and experimental study in collaboration with Lancaster and Durham University.

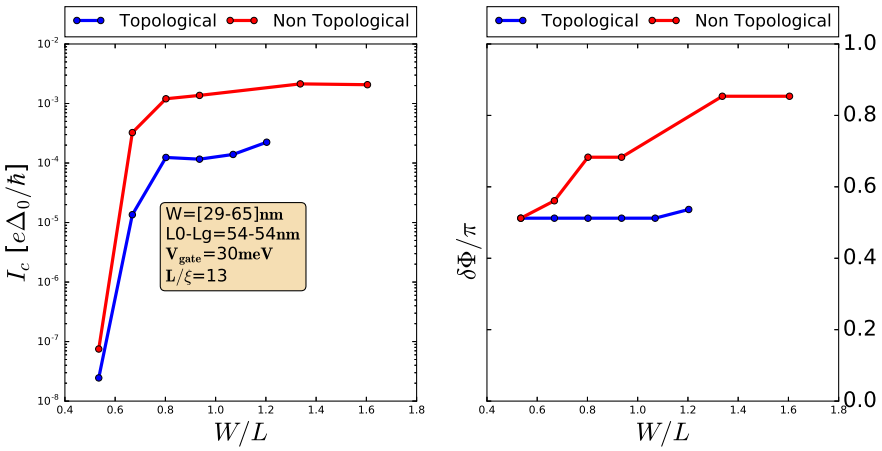

Fig. 5: Left plot: I_c critical current , right plot: CPR. Critical-current I_c is an order of magnitude lower with Topological state present due to scattering between the edge states. $W = 24$nm. The CPR is skewed for the system where no TS is present.

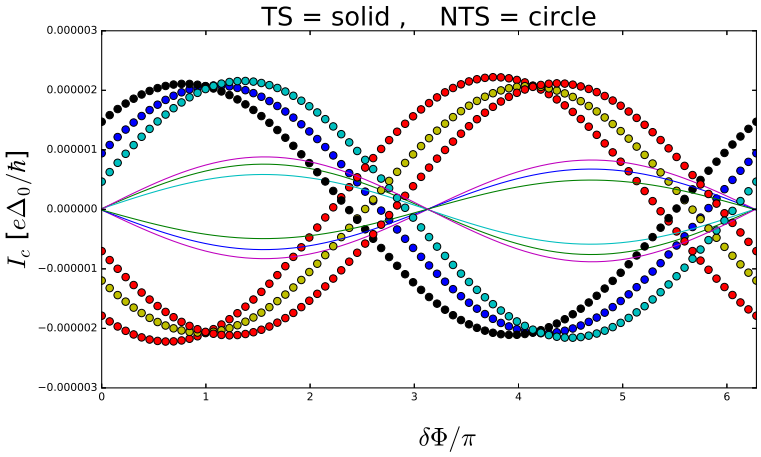

Fig. 6: Left hand side: curves correspond to different B both TS and NTS . There is a π- Josephson effect with a TS and CPR shifts when NTS is present.

I also participated on a CECAM School on Static and Dynamic methods for the study of photoinitiated processes. The scope of this school was beyond the static

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