STSM Report
Workshop on the Response Iteration Method to solve Kohn-Sham equations

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General

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STSM Topic: Workshop on the Response Iteration Method to solve Kohn-Sham equations
Host: Esa Räsänen, Tampere University of Technology, Department of Physics, 33101 Tampere(FI), esa.rasanen@tut.fi
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1 Purpose of the STSM

The short-term scientific mission is part of a project to develop a fast quantum chemistry simulation code based on a finite element discretization of the Kohn-Sham equations of Density Functional Theory (DFT). Our main focus is the simulation of two-dimensional systems containing a large number of electrons, prevalent in semiconductor technology. Our approach uses a novel way to treat the non-linearity of the Kohn-Sham equations via a so-called response-iteration scheme.

The group of Prof. Esa Räsänen is well established in the field of simulations of low-dimensional electron systems. In collaboration with his group, we plan to study very large (i.e., many-electron) quantum dots and artificial graphene flakes. Here, Prof. Räsänen is collaborating with an experimental group that has obtained peculiar and hard-to-explain measurement results on such dots and flakes, which are too large to be accessible by the simulation codes currently in use at Prof. Räsänen's group. The first task would be to study these system.

The visit was mainly planned as a workshop to exchange knowledge about the experimental system and its setup and to get a basic understanding of the involved physics.

2 Work carried out during the STSM

Since the STSM was mainly planned to exchange knowledge on the simulation of low-dimensional electron systems, we discussed this topic at length on several occasions during the week of my visit. On March 8 2016 I gave a talk at the Quantum Control and Dynamics group meeting at the Tampere University of Technology on the topic of our Response Iteration scheme for solving Kohn-Sham equations.

Furthermore, we made such good progress that it was even possible for us to start calculating band structures of Kekulé-distorted molecular graphene flakes [1] of various different sizes experiencing a homogenous magnetic field. We were able to obtain results for several small systems and analyze those results while I was staying in Tampere.

3 Main results obtained during the STSM

Due to the mainly informational character of this STSM, knowledge about the physics involved in low-dimensional electronic systems on the one side, and about the most suitable algorithms to handle the challenges on the other side, was exchanged and several ideas were discussed.

During these conversations, we decided to focus our joint research on calculating the band structure of finite, Kekulé-distorted molecular graphene flakes [1] experiencing a homogenous magnetic field. This is a continuation of a previous collaboration between my institution and Prof. Räsänen's group, where molecular graphene flakes without distortions were investigated [2], with the goal to observe a band gap opening for increasing distortions.

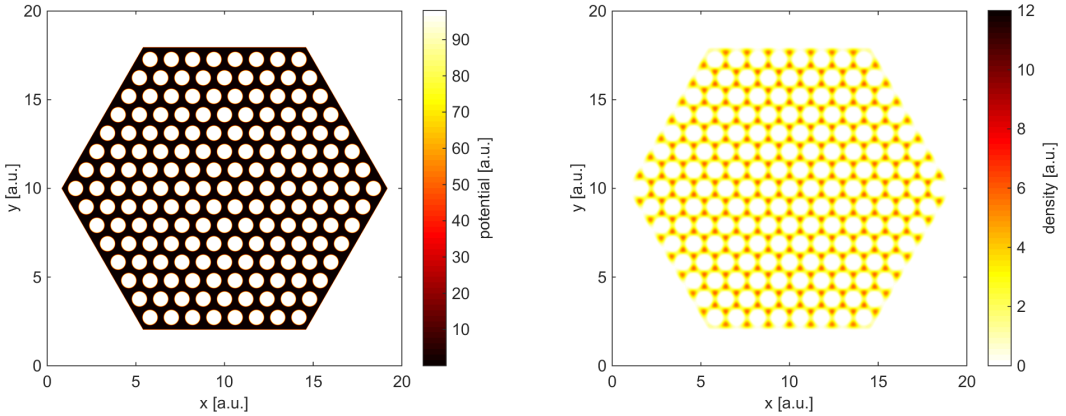
During my visit, the lowest-lying eigenvalues for a few such systems could be calculated as function of the magnetic field. The largest of the systems so far is the L07-Flake, which edges consist of 6×7 scattering centers. The scalar potential describing this system is depicted in Fig. 1 alongside the corresponding electronic density for vanishing magnetic fields.

Fig. 2 shows the scalar potential of the same system with small Kekulé distortion together with its resulting electronic density for vanishing magnetic fields. Compared to the case without distortions, see Fig. 1, the electron density locally becomes higher due to the narrowing of certain channels between the scattering centers.

In Fiq. 3 the single-electron eigenenergies as well as the density of states (DOS) of the L07 flake are plotted. To obtain the DOS, we have broadened the eigenenergies with Gaussian functions. It can be clearly seen that a gap emerges between the two larger bands, which is in contrast to the undistorted L07 flake that does not have this band gap [2]. The position of the emerging band gap is at the Dirac point of the undisturbed system. The formation of the additional smaller bands is suspected to be due to localized states on the edges of the system, as more detailed analysis of smaller flakes show.

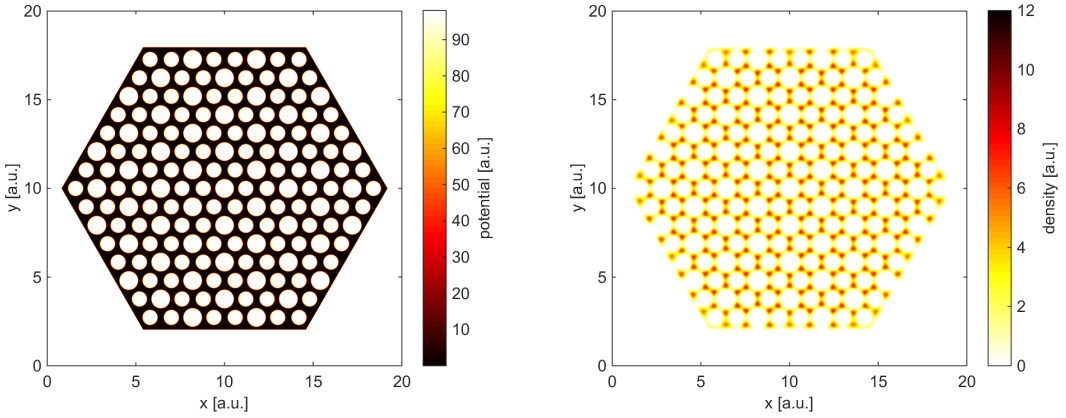
4 Future collaboration with the host institution

During my visit to Tampere further collaborations were discussed. In the next few month we will focus on molecular graphene flakes with Kekulé distortions with an special focus on possible gap openings in the band structure of this material. Afterward, the original idea of investigating



(a) scalar potential **(b)** electronic density

Figure 1: Plot of the scalar potential used to model the L07 molecular graphene flake (6×7 scattering centers on the edges) without Kekulé distortion (left) and the corresponding electron density with magnetic field $B = 0$ (right).



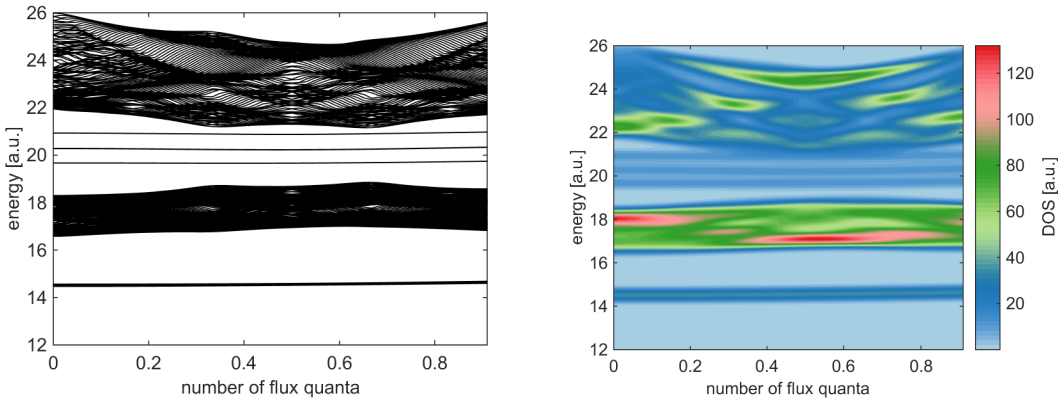
(a) scalar potential **(b)** electronic density

Figure 2: Same as Fig. 1 but with small Kekulé distortion.

very large quantum dots using our Response Iteration Method to solve Kohn-Sham equations will be further pursued.

5 Foreseen publications to result from the STSM

The ongoing collaboration of my institution with Prof. Räsänen's group already lead to several publications in peer-reviewed journals. The Workshop on the Response Iteration Method to solve Kohn-Sham equations was the first step in a new project that will hopefully lead to several joint publications. Additionally, the results obtained during this mission concerning molecular



(a) single-electron eigenenergies **(b)** density of states

Figure 3: Plot of the single-electron eigenenergies (left) and the density of states (right) of the L07 molecular graphene flake as function of flux quanta per unit area.

graphene will be subject of at least one article in a scientific journal.

6 Conformation by the host institution of the successful execution of the STSM

The confirmation by the host will be sent via email.

References

[1] K.K. Gomes and W. Mar and W. Ko and F. Guinea and H.C. Manoharan, *Nature* **483**, 306 (2012)

[2] M. Aichinger and S. Janecek and I. Kylänpää and E. Räsänen, *Phys. Rev. B* **89**, 235433 (2014)