Final report, ESF Exchange grant

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The purpose of my visit was to work with Andreas Honecker to investigate the influence of finite geometry on magnetic properties of graphene in a numerical approach. Graphene is a two dimensional material with honeycomb lattice. We can distinguish two types of edges in graphene, armchair edge and zigzag edge. The importance of the geometry in finite size system have already been shown for the electronic properties of graphene (see for example [1]).

We have used a Hubbard model and studied the problem in direct space where we can compute expectation values for a particular site. We have used a mean-field approximation which allows us to rewrite the Hamiltonian of the Hubbard model as a sum of one term corresponding to spin up, one term corresponding to spin down and a constant:

$$H^{MF} = H_\uparrow + H_\downarrow + C$$

$$\begin{aligned} H_\uparrow &= -t \sum_{<i,j} c^+_{i,\uparrow} c_{j,\uparrow} + U \sum_i n_{i,\uparrow} \langle n_{i,\downarrow} \rangle \\ H_\downarrow &= -t \sum_{<i,j>} c^+_{i,\downarrow} c_{j,\downarrow} + U \sum_i \langle n_{i,\uparrow} \rangle n_{i,\downarrow} \\ C &= -U \sum_i \langle n_{i,\uparrow} \rangle \langle n_{i,\downarrow} \rangle \end{aligned}$$

This form is easier to be diagonalised and allows us to study bigger systems than with exact diagonalisation of the Hubbard model.

We compute with the help of the Lappack library in a self consistent way the average density and the energy of the ground state. We use for initial condition an average density of 0.5. To solve some convergence problem we use for the first iteration in place of the ground state a thermal state compatible with Fermi-Dirac one particle energy distribution at a given temperature [2].

To evaluate the accuracy of the mean-field approximation we have compared some results obtained with the approximation with the one obtained with exact diagonalisation. For exact diagonalisation computations we have used the ALPS application suite [3]. The

systems studied are small since the exact diagonalisation could be performed only for a small system.
Below we show some results for a system of ten sites (fig.1).

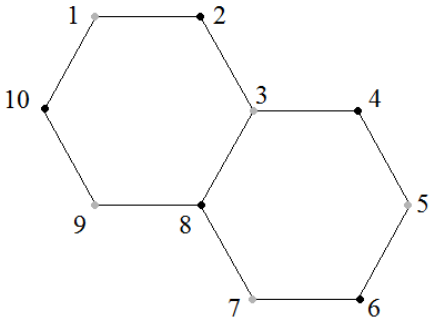

Figure 1: System of 10 sites

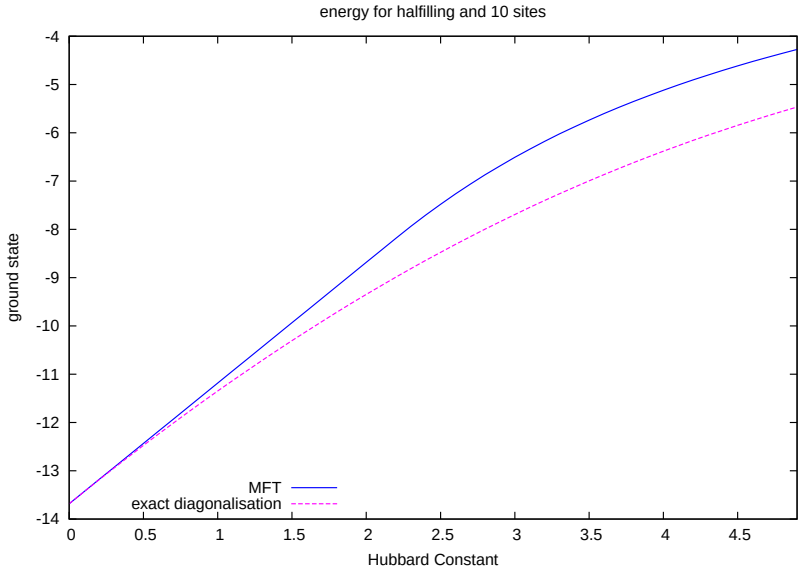

Figure 2: Energy for 10 sites and half-filling

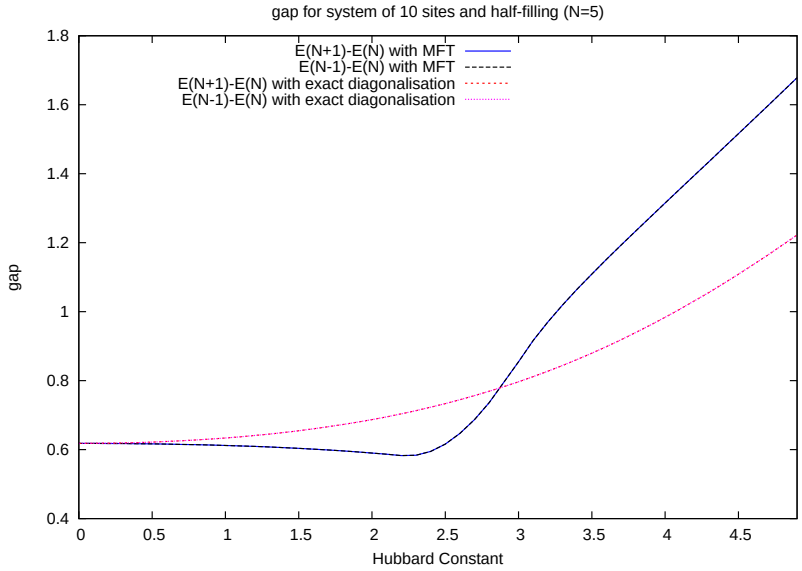

Figure 3: Charge-gap for 10 sites and half-filling

In the first results obtained for a system with periodic boundary conditions we can see a transition paramagnetic-antiferromagnetic (see fig.4) for a critical value of U (the Hubbard constant) equal to 2.4 (with the hopping integral t equal to 1). This results is a bit higher than the value of 2.23 find by [5].

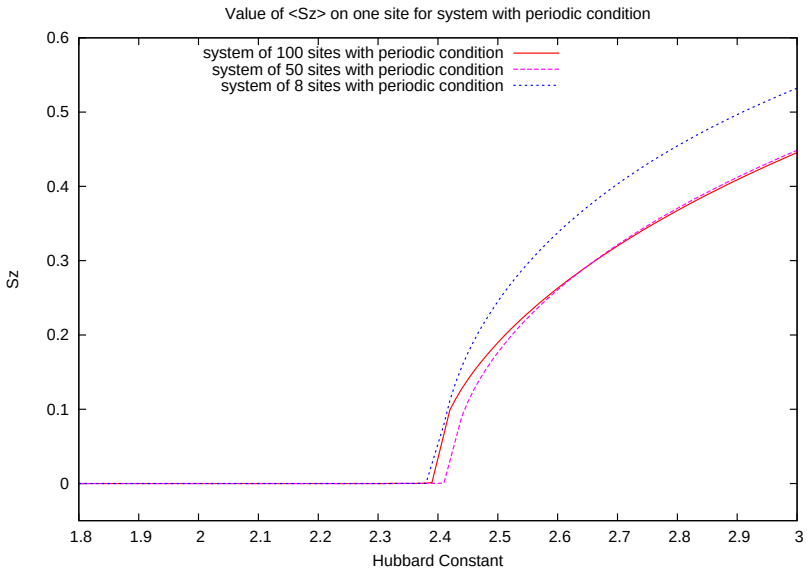

Figure 4: Local magnetization fonction of U

Since experimentally large graphene sheets do not show any magnetic ordering, the

value of U in graphene should be smaller than the critical value. So we use $U = 2.0$ as in [4].
Furthermore, we have studied the magnetic properties of a ribbon and we found that no magnetic ordering appears in a ribbon geometry with armchair edge for U lower than the critical value. On the other hand a ribbon with zigzag edge shows edge magnetism (see fig.5).

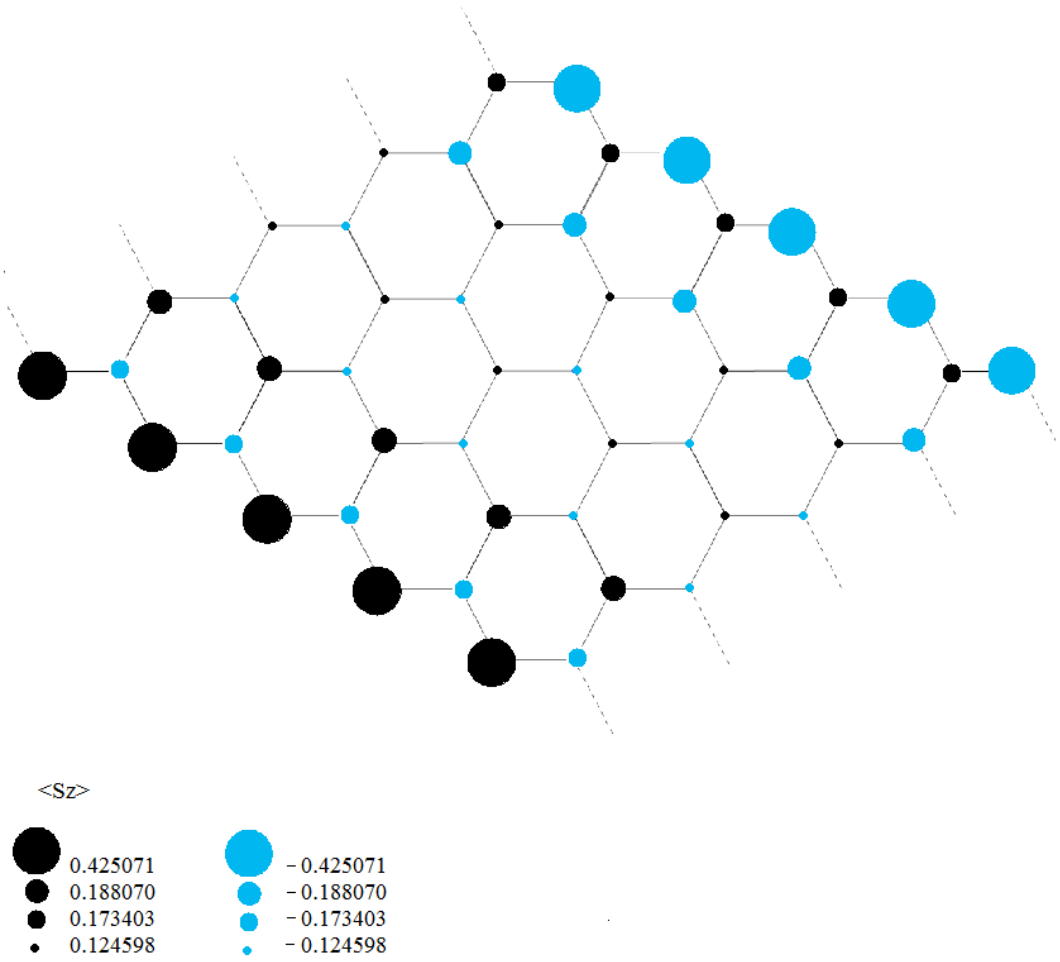

Figure 5: Edge magnetism in graphen ribbon with zigzag edge (U=2.0)

We have also looked at the influence of geometry on a quantum dot, and we have observed the appearance of edge-magnetism for a zig-zag edge.

We have planed to write a paper centered around the comparison of the mean-field theory and Exact Diagonalisation, we just need to have some results for bigger system, and in the future we plan to look at the possibility of spin transport in graphene devices.

I wish to thank ESF and especially the INSTANS program for providing this grants.

References

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[5] "Semi-Metal-Insulator Transition of the Hubbard Model in the Honeycomb Lattice", S. Sorella and E. Tosatti, Europhys. Lett. 19 699-704 (1992)