Hybrid Monte Carlo simulations of emergent magnetism in graphene in presence of hydrogen adatoms

M. V. Ulybyshev, M. I. Katsnelson

Regensburg University, Universitatsstrasse 31, Regensburg, Germany
Maksim.Ulybyshev@physik.uni-regensburg.de

Abstract

We perform quantum Monte Carlo simulations of graphene in presence of hydrogen adatoms. We employ Hybrid Monte Carlo algorithm broadly used in particle physics, for example in Lattice Quantum Chromodynamics. For a given quantum Hamiltonian this method produces exact results up to controllable statistical errors. Its application for tight-binding model of graphene was described in the paper [1]. The basic advantage of this method is the possibility to take into account even very strong electron-electron interaction without any physical simplifications or assumptions. In this work we study emergent magnetic moments arising in graphene due to strong electron-electron interaction in presence of hydrogen adatoms. We base on the tight-binding model for electrons at π-orbitals with static Coulomb interaction. Screening of Coulomb interaction at short distances by σ-electrons is also taken into account in a way described in the paper [2]. Thus we have realistic inter-electron potentials both at short (like on-site interaction and interactions with the nearest neighbors) and long distances. We calculate spin distribution (see fig.1) and energies of midgap states, concentrated near adatoms (see table 1). Emergent antiferromagnetism is observed in the vicinity of adatoms. We calculate magnetic moment associated with one isolated adatom and several typical configurations of adatoms. In the latter case we observe large interference between magnetic moments of close adatoms (see table 2). For example, two adatoms at the distance of 1 lattice step have magnetic moment 1.5 times larger than two isolated adatoms.

References

[1] M. V. Ulybyshev *et al.*, Phys. Rev. Lett., **111** (2013) 056801.
[2] T. O. Wehling *et al.*, Phys. Rev. Lett., **106** (2011) 236805.

Figures

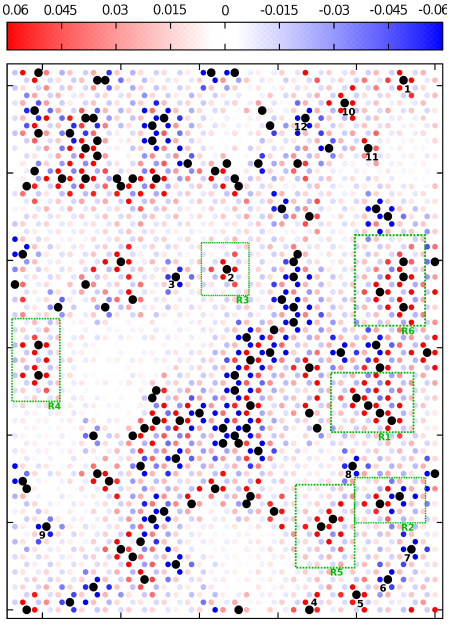

Figure 1. Distribution of average spin. Red points correspond to spin up and blue ones correspond to spin down. Adatoms are marked as black circles, concentration is 5%. Electron-electron interaction corresponds to suspended graphene.

	Center 1	Width 1	Center 2	Width 2	Gap
Ordinary potentials	0.76	0.40	-0.69	0.22	1.1 ± 0.17
Screened potentials	0.52	0.16	-0.49	0.18	0.74 ± 0.12

Table 1. Midgap states form 2 energy bands above and below the Fermi-level. Parameters of these two bands (their centers, widths and gap between them) are presented in case of suspended graphene ("ordinary potentials") and graphene on boron nitride ("screened potetials"). Concentration of adatoms is 5% in both cases.

Region on the map	$M = 2 S_z$
R3	0.530 ± 0.016
R4	1.330 ± 0.026
R5	1.542 ± 0.026
R6	2.70 ± 0.04
R1	3.20 ± 0.04

Table 2. Magnetic moment of different configurations of adatoms. All these configurations are marked with green lines at the figure 1. R3 corresponds to one isolated adatom, R4 corresponds to 2 adatoms at the distance of 2 lattice steps, R5 contains 2 adatoms at the distance of 1 lattice step, R1 and R6 contain 4 adatoms (denser configuration in case of R1).