Simulating graphene impurities

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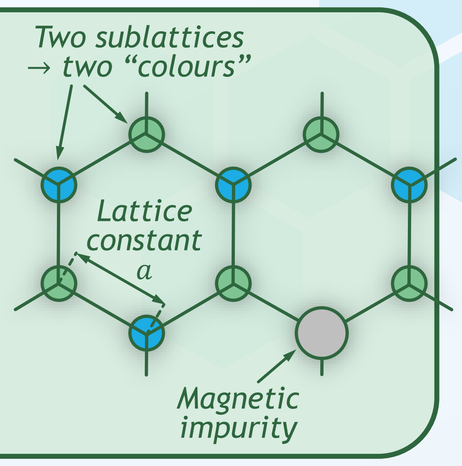
INTRODUCTION
Graphene and its impurities

Consider a honeycomb graphene lattice. It can be divided into two sublattices.

Graphene impurities are randomly spread atoms on a graphene lattice. Also, magnetic adatoms are placed on top of carbon atoms.



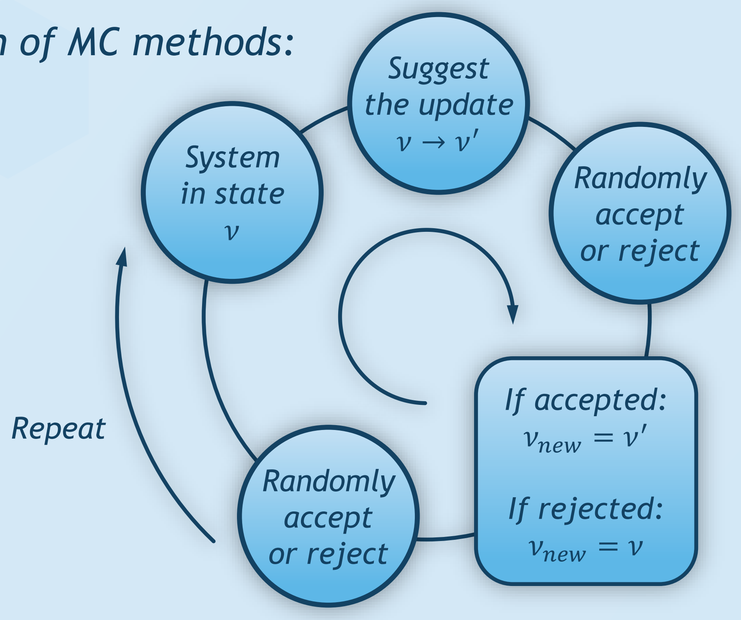
OBJECTIVE
Simulating graphene impurities

The project had a simple goal: to study a model of magnetic graphene impurities by the means of computer simulations. Impurities are expected to have a long-range ordering [1] and we are curious how this can change the transport properties of graphene.

THEORETICAL METHOD
Monte Carlo methods

A physical system in finite temperature will fluctuate between possible states of the system. Monte Carlo methods uses this mechanism in form of repeated random updates of the system.

Mechanism of MC methods:

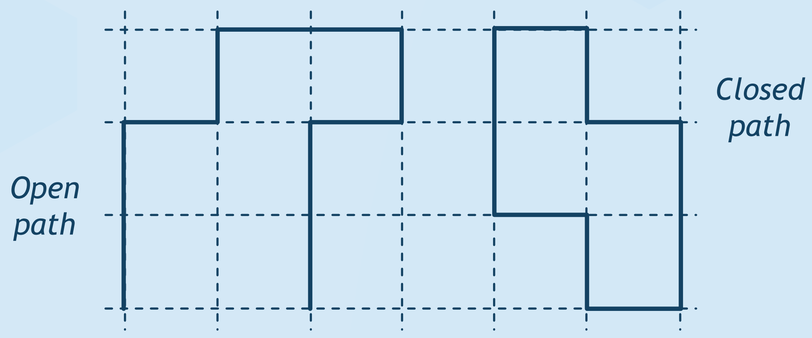


The probability of accepting the updates is calculated using the balance equation, which is the heart of all MC methods[2]:

$$W_\nu \sum_{\nu',u} p_u P_u^{acc}(\nu \to \nu') = \sum_{\nu',u} W_{\nu'} p_u P_u^{acc}(\nu' \to \nu)$$

where W_ν – weight of configuration ν, p_u – probability of choosing update $u = (\nu \to \nu')$ over any other, $P_u^{acc}(\nu \to \nu')$ – probability of accepting update u.

The worm algorithm is one of MC methods, that represents the system as bonds. Using open/closed paths, one can calculate statistical quantities.

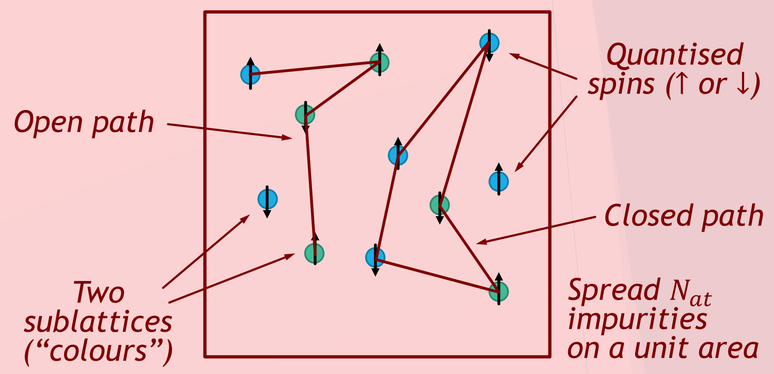


SIMULATION USING THE METHOD
Building the model of impurities

Introduce the following simplifications:

- *Lattice constant a is much smaller than the distances between impurities → neglect the underlying lattice structure and consider a continuous case: a graph.*
- *The interaction between impurities is mediated by conduction electrons. The theory suggests that it should be proportional to r^{-3}.*
- *Impurities can only have spin "up" and "down" (↑ or ↓).*

With those simplifications, the system can be pictured as:



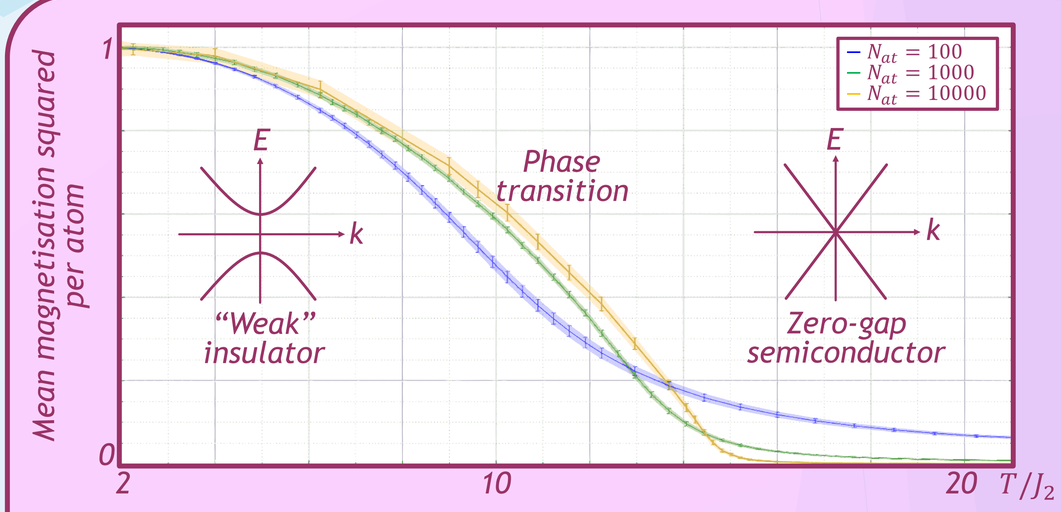
Hamiltonian of the system:

$$H = \sum_{i,j} s_i s_j \frac{J_1 - J_2 c_i c_j}{r_{ij}^3}$$

Investigated case: $J_1 = 0$.

s_i, s_j – spins $(= \pm 1)$, c_i, c_j – "colours" of the sublattices $(= \pm 1)$, J_1, J_2 – interaction constants, r_{ij} – the distance between sites i and j.

RESULTS & CONCLUSIONS
Ordering of adatoms on graphene



The ordering of magnetic impurities is indeed possible on graphene lattice. The critical temperature is estimated:

$$T_C = (15.37 \pm 0.41)\, J_2$$

It is consistent with theoretical approximation [1]. Magnetic susceptibility was also determined and is consistent with theoretical prediction [3]:

$$\chi = \frac{c_0}{T} \sum_{n=1}^{\infty} C_n \left(\frac{T_0}{T}\right)^{\frac{2}{3}(n-1)}$$

Perspectives:

- *Determine dependence $T_C(J_1, J_2)$*
- *Phase transitions in other models*
- *Experiments needed for determining J_1, J_2*

[1] Cheianov, Syljuåsen, Altshuler, Fal'ko, EPL 89, p. 56003 (2010).
[2] Prokof'ev, Lecture notes on Monte Carlo methods, unpublished, http://mcwa.csi.cuny.edu/umass/lectures.html, retrieved 2013-06-10.
[3] Cheianov, Szyniszewski, Burovski, Sherkunov, Fal'ko, Phys. Rev. B 86(5) 054424 (2012).

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