Magnetic field nanosensor based on Mn impurities

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I. Graphene – from fundamental to future applications
There’s plenty of room at the bottom

Lecture at American Physical Society meeting, Caltech, December 29, 1959

Richard P. Feynman
Types of nanostructures

1. 

2. 

3.
Properties

Graphene

- Strong
- Tiny
- Almost transparent
- Impermeable
- Thermal conductivity
- Extreme flexibility
Space Applications

A. Bresson, Y. Bidel, P. Bouyer, B. Leone, E. Murphy, P. Silvestrin, Quantum mechanics for space applications, *Applied Physics, B*, 84, Issue 4, ISSN 0946-2171 (eISSN 1432-0649), pp. 545-550, 2006:

a new direction of research launched by **European Space Agency (ESA)** and lead by **Office National d'Études et de Recherches Aérospatiales (ONERA)**
ESA/ONERA’s top research directions:

1) atomic clocks
2) atomic inertial sensors
3) detectors of low temperature and magnetic flux with an energy sensitivity unequalled by any other device
4) superfluidity or quantum transition
5) advanced nanodevices based using state-of-the-art semiconductor technology
Other potential applications

- graphene transistors
- integrated circuits
- graphene capacitors
- biodevices
- composites
From real world …
... to nanostructures

butterfly’s wing $\rightarrow$ scales $\rightarrow$ microribs

(Morpho sp.)
Gecko’s foot (Gekko gecko)
gecko toe → lamellae → setae → spatulæ
II. Few words about spintronics
Spintronics $\rightarrow$ Spin Transport Electronics
(magnetic and electrical fields manipulation)
Electron spin

- Spin – the rotation of a particle around its axis
Spin polarization

- Ferromagnetic (a)
- Antiferromagnetic (b)
III. Physical model of the nanosensor
Graphene Nanoribbon - GNR

Unit cells

Scattering region

Electrodes
GNRs with Mn impurities
IV. Mathematical modeling and numerical simulations
Kohn-Sham formalism using Density Functional Theory

From multi-particles Schrödinger equation...

\[ H \Psi(r_1, r_2, \ldots, r_N) = E \Psi(r_1, r_2, \ldots, r_N) \]

where the Hamiltonian is given by

\[ H = -\frac{1}{2} \sum_{i=1}^{N} \nabla_i^2 + V_{\text{ext}} + \sum_{i<j}^{N} \frac{1}{|r_i - r_j|} \]
...to uni-particle Kohn-Sham equations

\[
\left( -\frac{1}{2} \nabla^2 + V_{KS}(r) \right) \Psi(r) = E \Psi(r)
\]

with the Kohn-Sham potential

\[
V_{KS}(r) = V_{\text{ext}}(r) + \int \frac{\tilde{\rho}(r_1)}{|r_1 - r|} \, dr_1 + V_{xc}(r), \quad \tilde{\rho}(r) := \sum_i \Psi_i^*(r) \Psi_i(r)
\]
V. Results and discussion
• The all-spins-up configuration “++++” as well as the all-spins-down configuration “−−−−” have the closest energies to the ground state at ~100 meV

• The other configurations assume at least one pair of spins at a certain edge with AFM coupling, which raises the energy of the system.

• The largest energy difference compared to the ground state is about ~500 meV

• These values have been obtained in the absence of the magnetic field.
Transmission functions - T

AFM polarization

FM polarization
VI. Conclusions
Conclusions:

• Presented paper enrolls in a current topic of great interest, including space and aerospace fields

• More specifically, the paper is about nanomaterials, spintronics, nanosensors etc., applications that will revolutionize future technologies
Conclusions:

• The spin transport properties were investigated in graphene nanoribbons (GNR) with Mn impurities.

• The numerical simulation data of Kohn-Sham equations using SIESTA package.

• The presence of a magnetic field is likely to give the pronounced variations of the total energy.

• So GNR with Mn impurities constitutes a magnetic field sensor.
Conclusions:

- Energy levels involved belong to infrared radiation, important for the satellites equipments
- Research in this field are in progress, as reflected by the scientific conferences and bibliography
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VII. References


Thank you very much for your attention!