Numerical simulation of graphene in an external magnetic field

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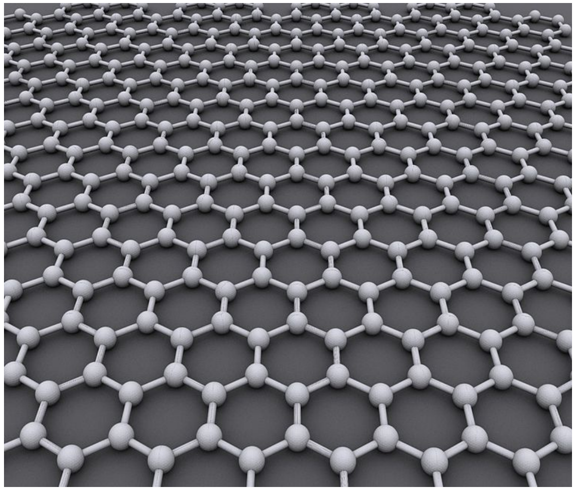
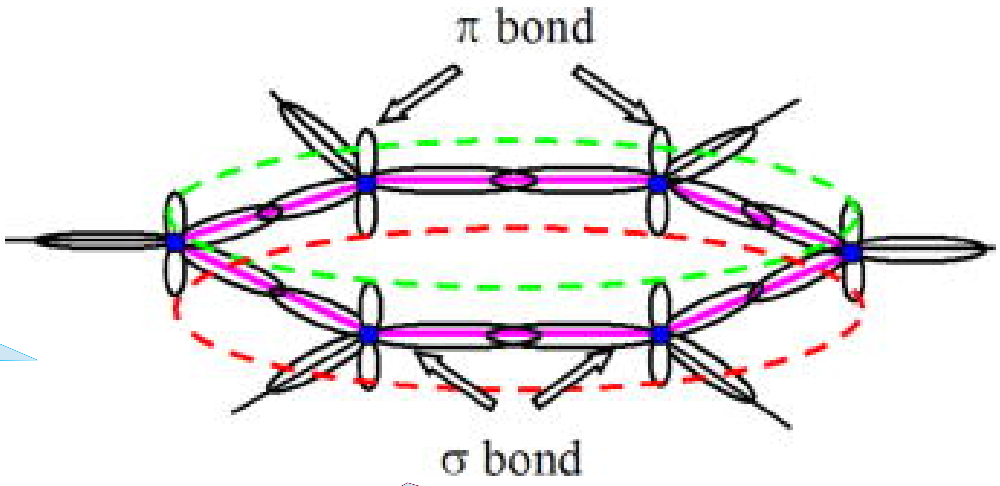
Basic properties of graphene



Graphene is a monolayer honeycomb lattice of carbon atoms



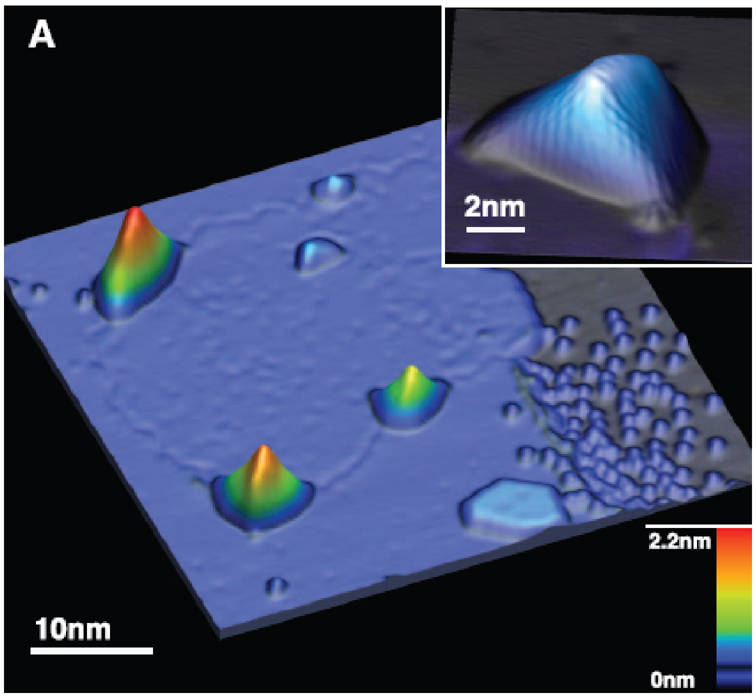
3 electrons of carbon form chemical bonds (σ-orbitals), 1 forms π-orbital

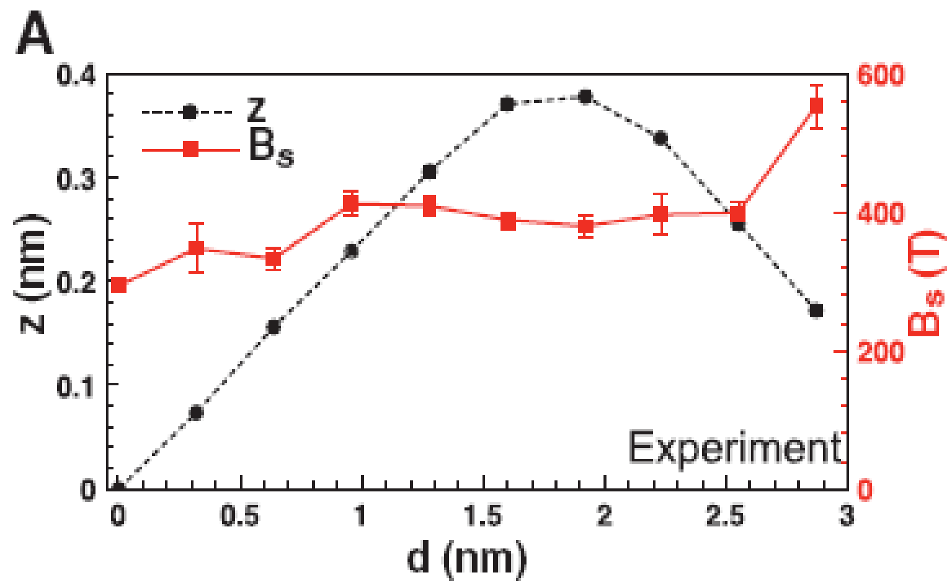
Electrons on π-orbitals are responsible for electric properties of graphene.
They can jump from site to site.

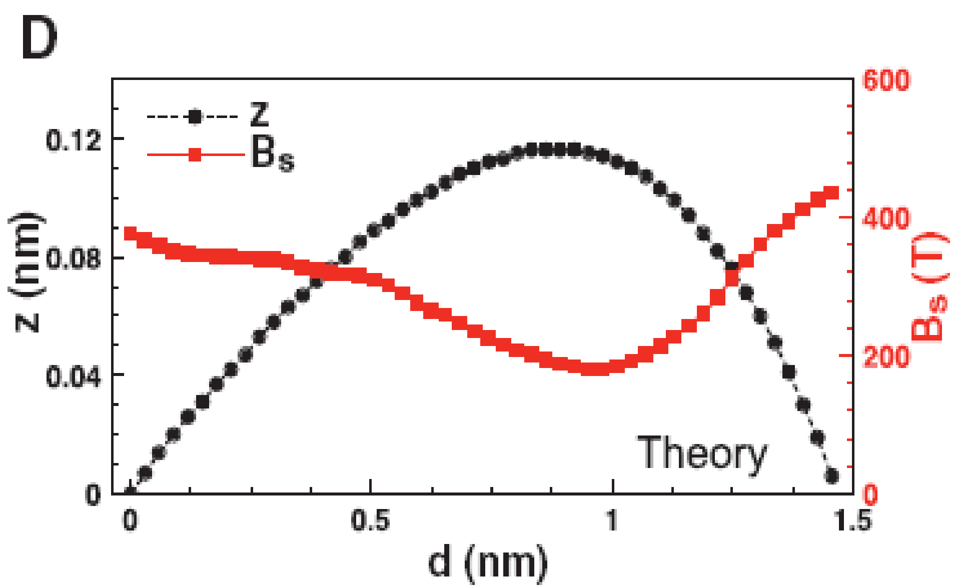
Usually graphene is placed on some substrate (SiO2,...) which effectively screens interactions. This screening is characterized by dielectric permitivity ε of substrate.

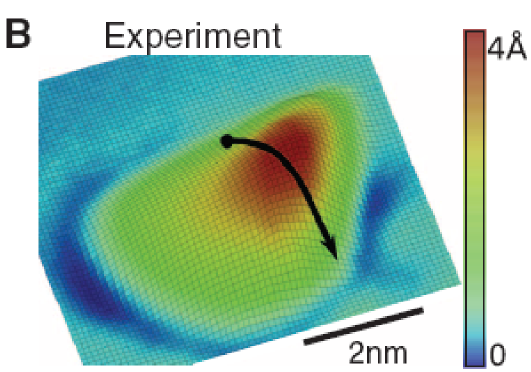
«Artificial» magnetic field

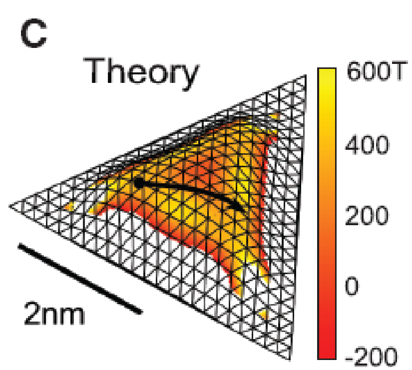
N. Levy et. al., Science 329 (2010), 544











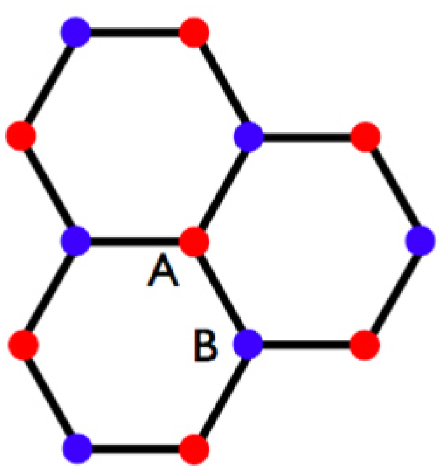
Tight-binding model of graphene

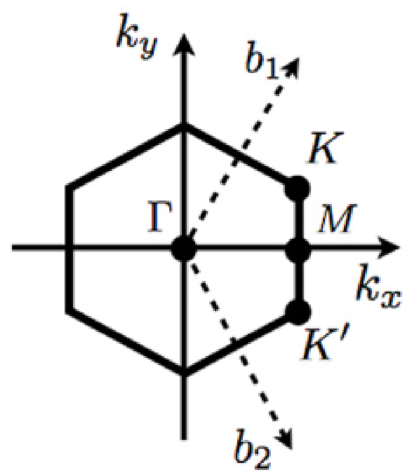
Only hoppings to the **nearest** sites are allowed:

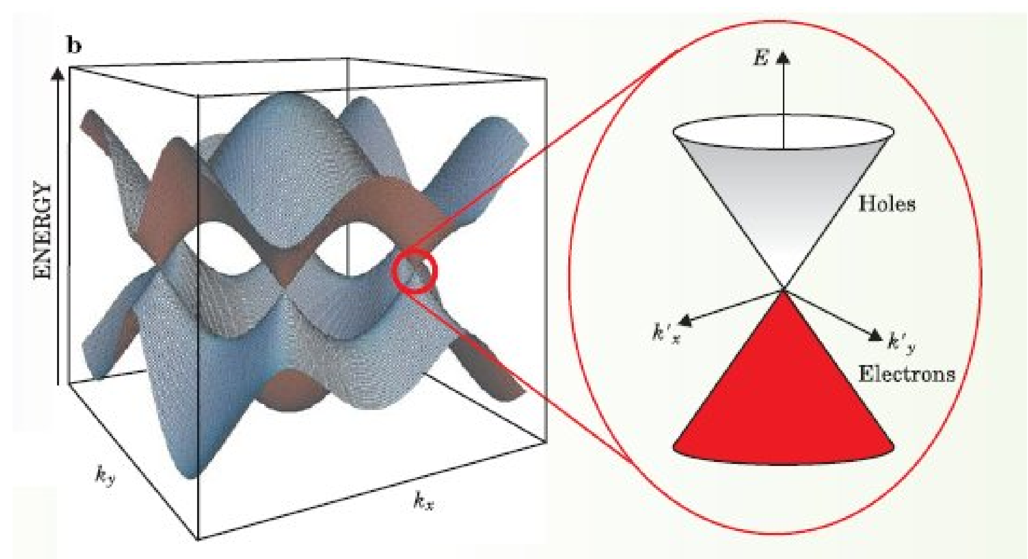
$$\hat{H}_{tb} = -\kappa \sum_{<x,y>,s} \left(\hat{a}^{+}_{y,s}\hat{a}_{x,s} + \hat{a}^{+}_{x,s}\hat{a}_{y,s} \right) \qquad s = \pm 1$$

$$\kappa = 2.7eV \qquad \{\hat{a}_{x,s}\hat{a}^{+}_{x',s'}\} = \delta_{xx'}\delta_{ss'}$$

Dispersion relation contains 2 independent conical points K and K' with **linear law** in their vicinity with Fermi velocity **vF = c/300**







Tight-binding model connects 2 sublattices of honeycomb lattice: A and B

Effective field theory

While dispersion relation in vicinity of K-points is linear, one can obtain an effective low-energy field theory from tight-binding model:

We couple fermions to electromagnetic field. Due to smallness of Fermi velocity, magnetic part is supressed and we can neglect it

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi\mathcal{D}A_0 \exp\left(-\frac{1}{2}\int d^4x\,(\partial_i A_0)^2 - \right.$$
$$\left. - \int d^3x\,\bar{\psi}_f\left(\Gamma_0\,(\partial_0 - igA_0) - \sum_{i=1,2}\Gamma_i\partial_i\right)\psi_f\right)$$

2 flavors of massless 2+1 Dirac fermions correspond to 2 possible spin orientations of electrons in graphene

$$g^2 = 2\alpha_{em}/(v_F(\epsilon + 1))$$

Takes into account screening by substrate

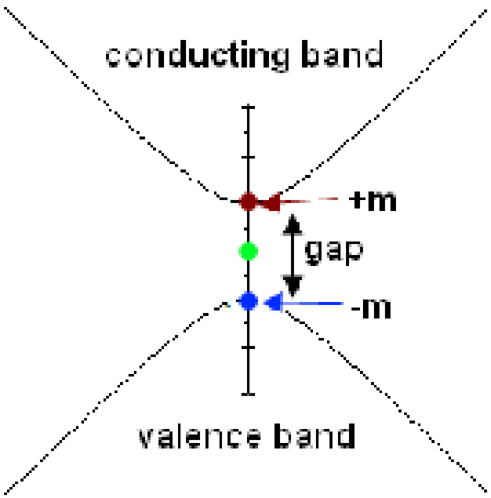
Effective field theory 2

Continuum theory has U(4) symmetry which can be broken in different ways.

We will focus only on one possibility which corresponds to nonzero chiral condensate:

$$\bar{\psi}_a \psi_a$$

When condensate is nonzero, mass gap in spectrum of electronic excitations will open.



This will directly effect on electronic properties of graphene, for instance, on its electric conductivity.

Effective field theory is good for **qualitative studies**

Why lattice?

$$g^2 = 2\alpha_{em}/(v_F(\epsilon + 1))$$

Coupling constant g ~ 300/127 = 2

We need nonperturbative first-principle calculations!

Lattice regularization

- Rectengular lattice with a = 0.142 nm (step of graphene honeycomb lattice)
- 1 taste of 2+1 staggered fermions wich gives us exactly 2 flavors of continuum fermions:

$$S_\Psi\left[\bar{\Psi}_x, \Psi_x, \theta_{x,\mu}\right] = \sum_{x,y} \bar{\Psi}_x D_{x,y}\left[\theta_{x,\mu}\right] \Psi_y =$$

$$= \sum_x \delta_{x_3,0}\left(\sum_{\mu=0,1,2} \frac{1}{2}\bar{\Psi}_x \alpha_{x,\mu} e^{i\theta_{x,\mu}} \Psi_{x+\hat{\mu}} - \sum_{\mu=0,1,2} \frac{1}{2}\bar{\Psi}_x \alpha_{x,\mu} e^{-i\theta_{x,\mu}} \Psi_{x-\hat{\mu}} + m\bar{\Psi}_x \Psi_x\right)$$

- Non-compact 3+1 action for gauge fields to avoid non-physical condensation of monopoles:

$$S_g\left[\theta_{x,\mu}\right] = \frac{\beta}{2}\sum_x \sum_{i=1}^{3}\left(\theta_{x,0} - \theta_{x+\hat{i},0}\right)^2, \qquad \beta \equiv \frac{1}{g^2} = \frac{v_F}{4\pi e^2}\,\frac{\epsilon+1}{2}$$

- External magnetic field is introduced in a usual way and it's qauntized:

$$H = \frac{2\pi}{eL_s^2} n$$

Observables

We study chiral condensate and electric conductivity:

$$\langle\bar{\psi}\psi\rangle = \frac{1}{8L_0L_1L_2}\sum_{x,t}\langle\bar{\Psi}_x\Psi_x\rangle.$$

Chiral condensate

Condactivity can be extracted from current-current correlator

$$G(\tau) = \frac{1}{2}\sum_{i=1,2}\int dx^1 dx^2 \langle J_i(0)J_i(x)\rangle,$$

via Green-Cubo relation

$$G(\tau) = \int_0^\infty \frac{dw}{2\pi} K(w,\tau)\sigma(w),$$

with kernel

$$K(w,\tau) = \frac{w\ \cosh\left[w\left(\tau - \frac{1}{2T}\right)\right]}{\sinh\left(\frac{w}{2T}\right)}$$

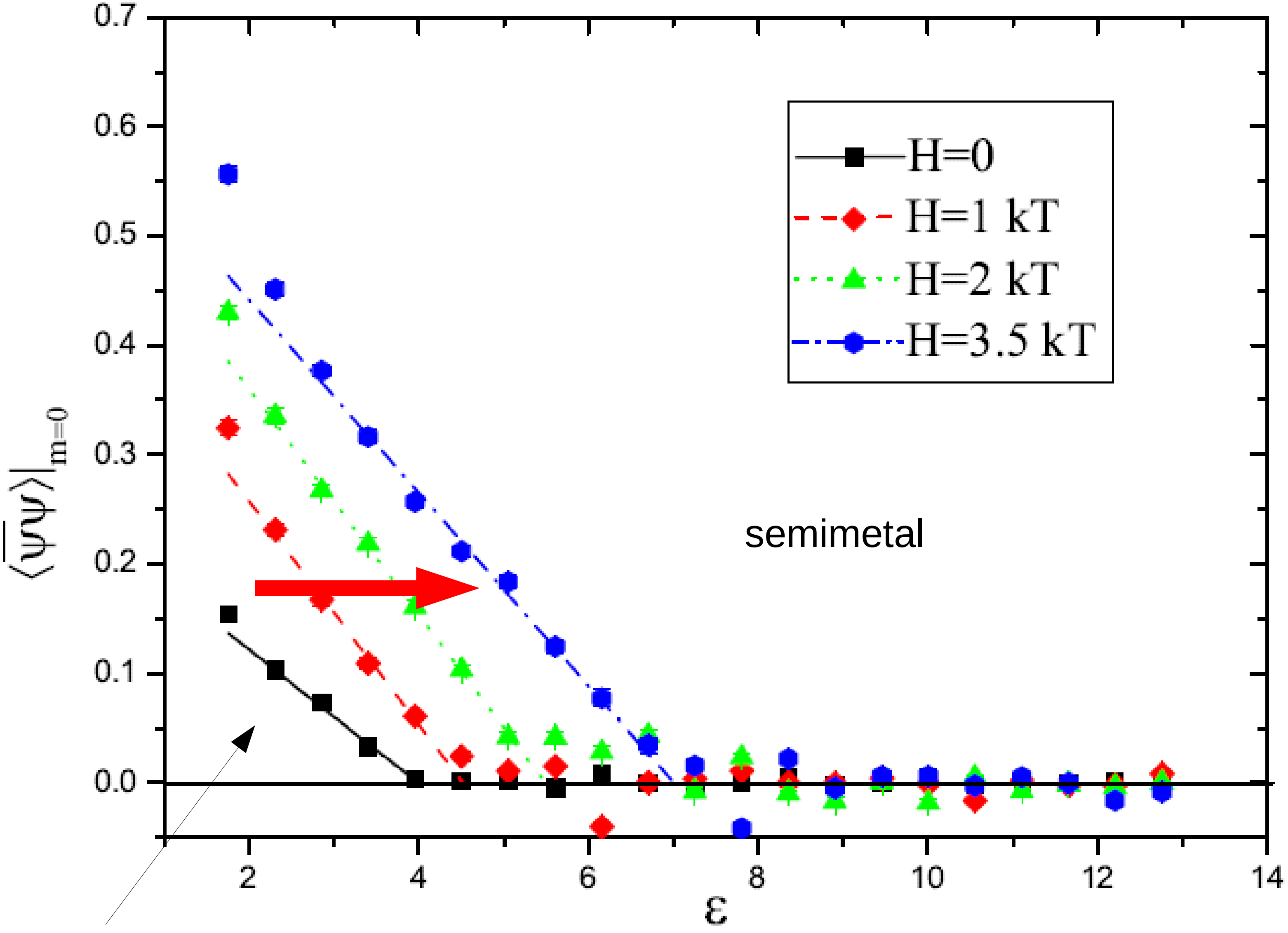
Simulation parameters

- Lattice size: 20^4
- Values of dielectric permitivity: 1.75 ... 12.75
- Magnetic field: 0.5 … 3.5 kT
- Masses: 0.01, 0.02, 0.03

We calculate each observable in a limit of vanishing fermion mass

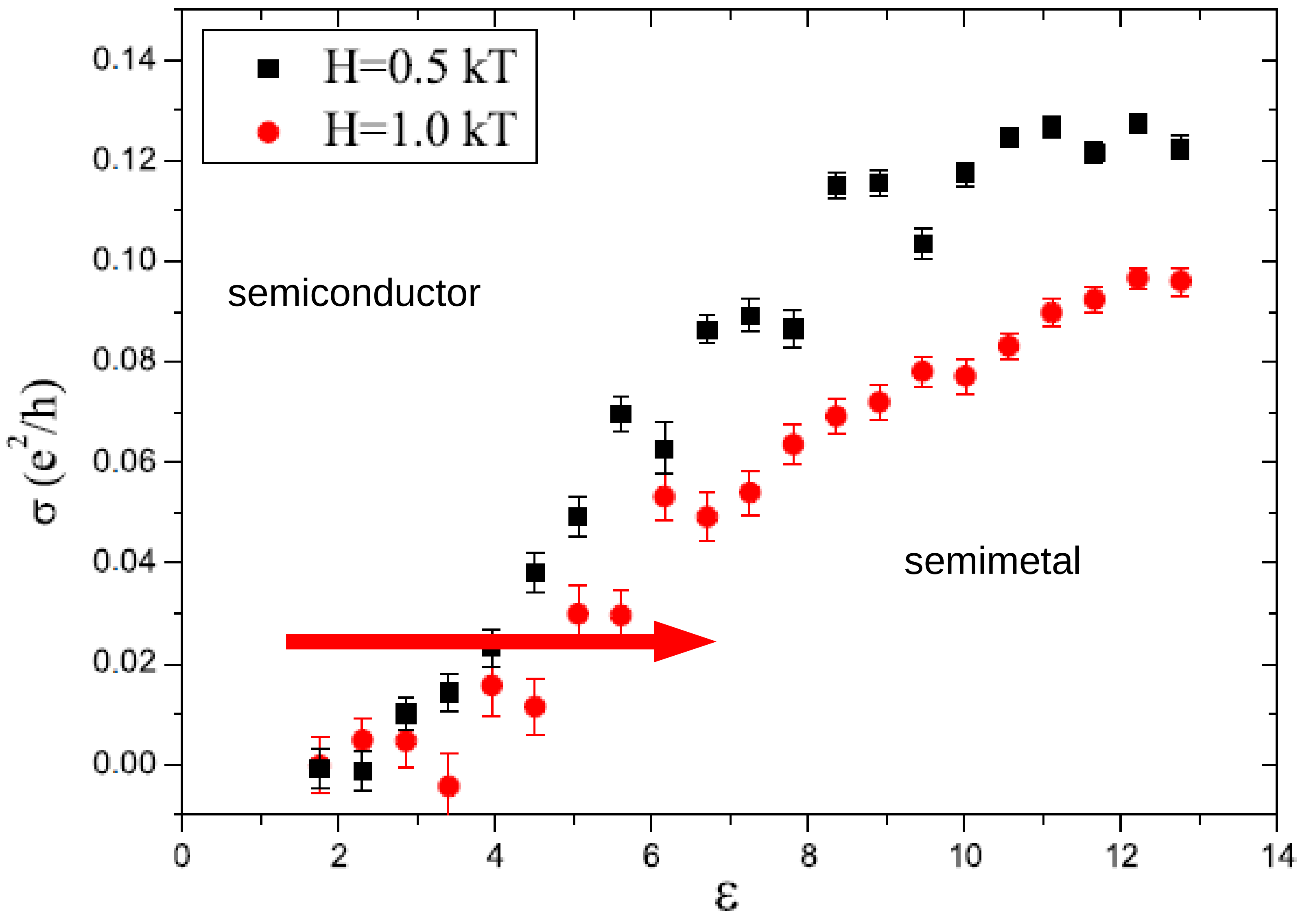
$T = 0.2$ eV, which is the temperature of electron exitations (not a crystal temperature), is small in comparision with typical energy scale ~3 eV.

Results: condensate

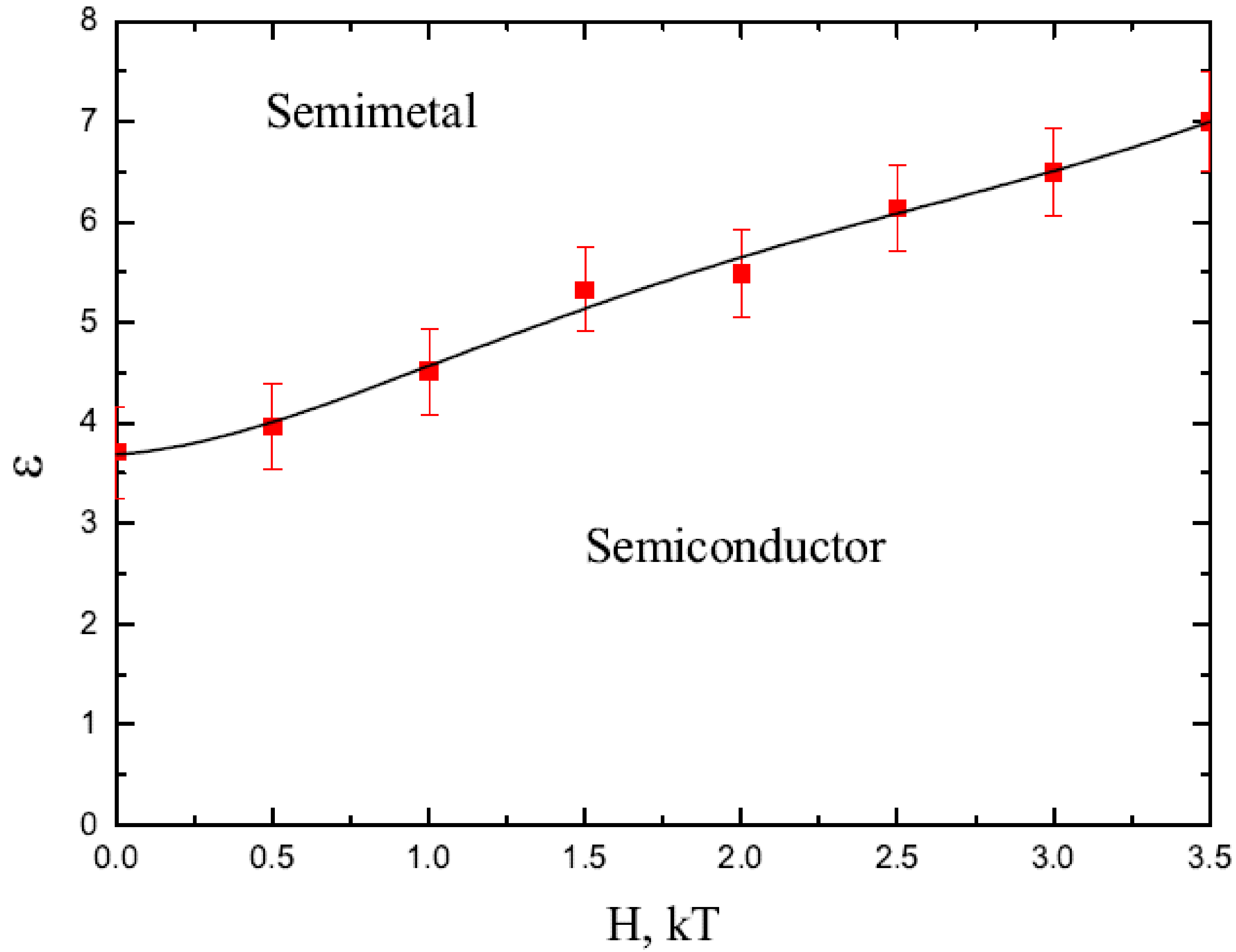


semiconductor

Results: conductivity



Results: phase diagram



Conclusions

- Phase diagram of graphene in an external magnetic field is obtained
- Results for conductivity is in agreement with behavior of chiral condensate
- These results also might be important for understanding physics of ripples on a graphene sheet where huge artificial magnetic fields are observed.

Thank you!