Possible Ordered States in Graphene Systems

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Final Defense : May 19, 2008

Projects done during the Ph.D program

1. Charge and spin Hall conductivity in metallic graphene
N. A. Sinitsyn, J. E. Hill, Hongki Min, Jairo Sinova, A. H. MacDonald
Phys. Rev. Lett. **97**, 106804 (2006)

2. Intrinsic and Rashba spin-orbit interactions in graphene sheets
Hongki Min, J. E. Hill, N. A. Sinitsyn, B. R. Sahu, L. Kleinman, A. H. MacDonald
Phys. Rev. B **74**, 165310 (2006)

3. Ab initio theory of gate induced gaps in graphene bilayers
Hongki Min, B. R. Sahu, Sanjay K. Banerjee, A. H. MacDonald
Phys. Rev. B **75**, 155115 (2007)

4. Pseudospin magnetism in graphene
Hongki Min, Giovanni Borghi, Marco Polini, A. H. MacDonald
Phys. Rev. B **77**, 041407 (R) (2008)

5. Chiral decomposition in the electronic structure of graphene multilayers
Hongki Min, A. H. MacDonald
Phys. Rev. B **77**, 155416 (2008)

6. Energy gaps, magnetism, and electric field effects in bilayer graphene nanoribbons
B. R. Sahu, Hongki Min, A. H. MacDonald, Sanjay K. Banerjee
Phys. Rev. B **78**, 045404 (2008)

7. Room-temperature superfluidity in graphene bilayers?
Hongki Min, Rafi Bistritzer, Jung-Jung Su, A. H. MacDonald
Phys. Rev. B **78**, 121401 (R) (2008)

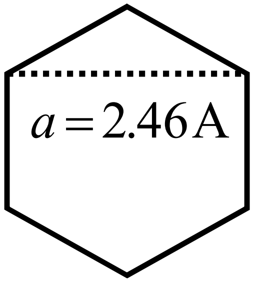
Possible ordered states in graphene systems

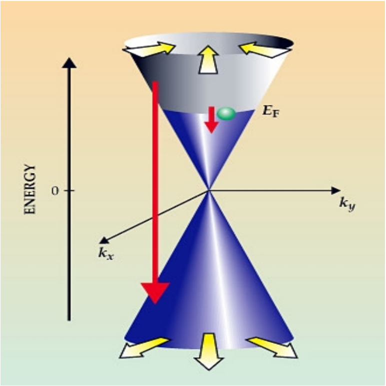
Outline

1. Introduction
2. Exciton condensation in graphene bilayers
3. Coupled graphene stacks
4. Pseudospin magnetism in graphene bilayers
5. Conclusion

Introduction

- What is graphene?
- Why is it important?



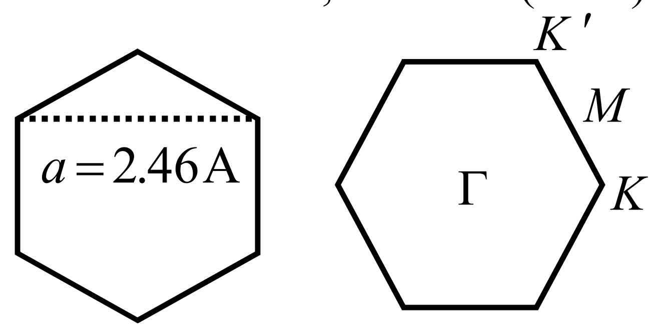


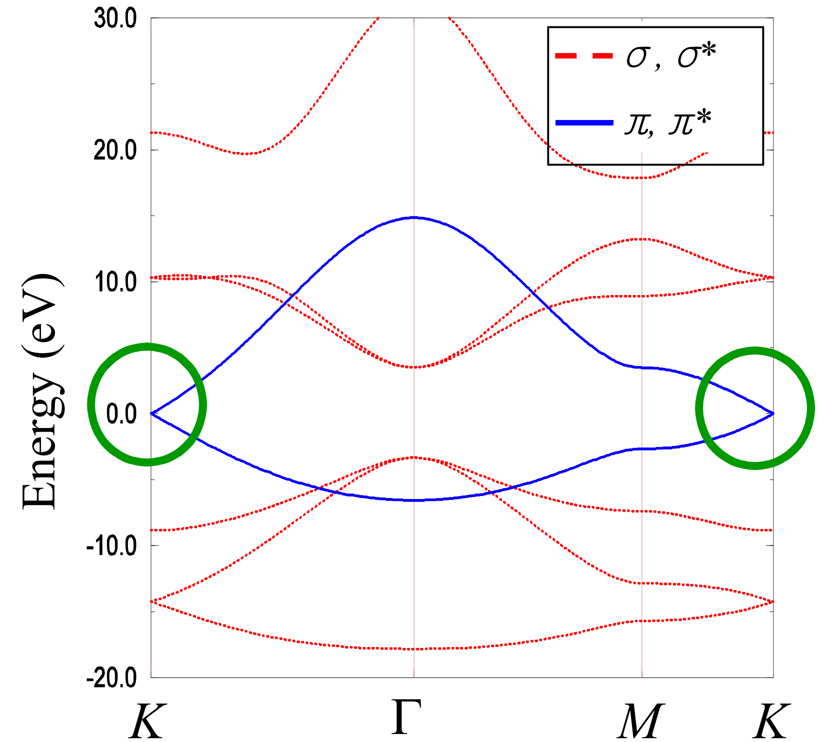
1. Introduction

1) Graphene

- Two-dimensional honeycomb lattice of carbon atoms.
- 2D Dirac-like equation with linear dispersion near *K*/*K'*.
- New electron-electron interaction physics? Example: magnetism, superconductivity

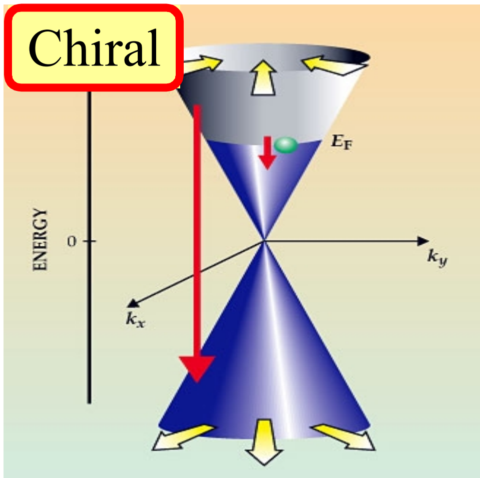
Min et al. PRB **74**, 165310 (2006)





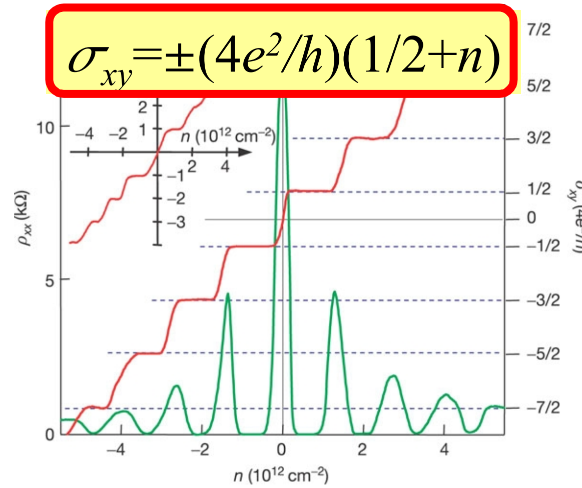
1. Introduction

2) Extraordinary properties of graphene



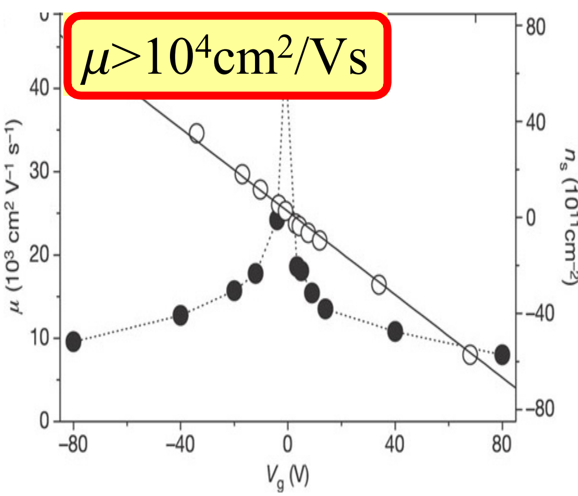
Dirac-like equation

Wallace,
Phys. Rev. (1947)



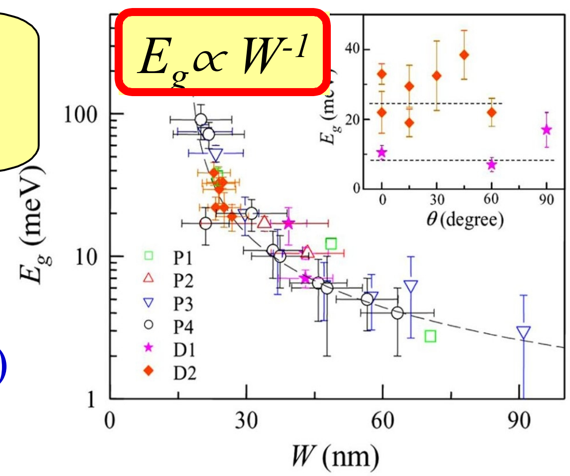
Quantum Hall effect

Novoselov et al.
Nature (2005)



High mobility

Zhang et al.
Nature (2005)

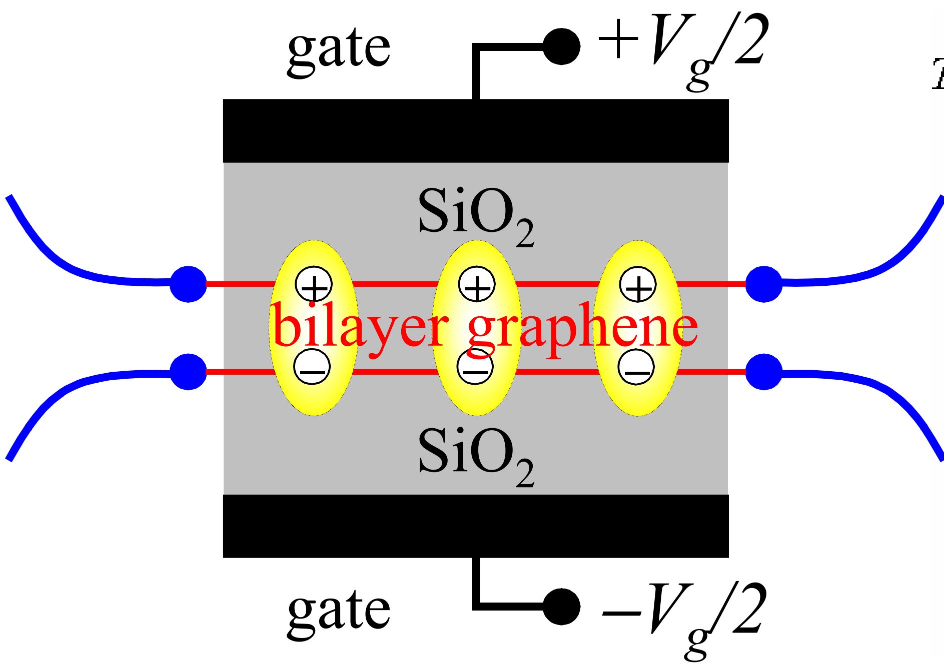


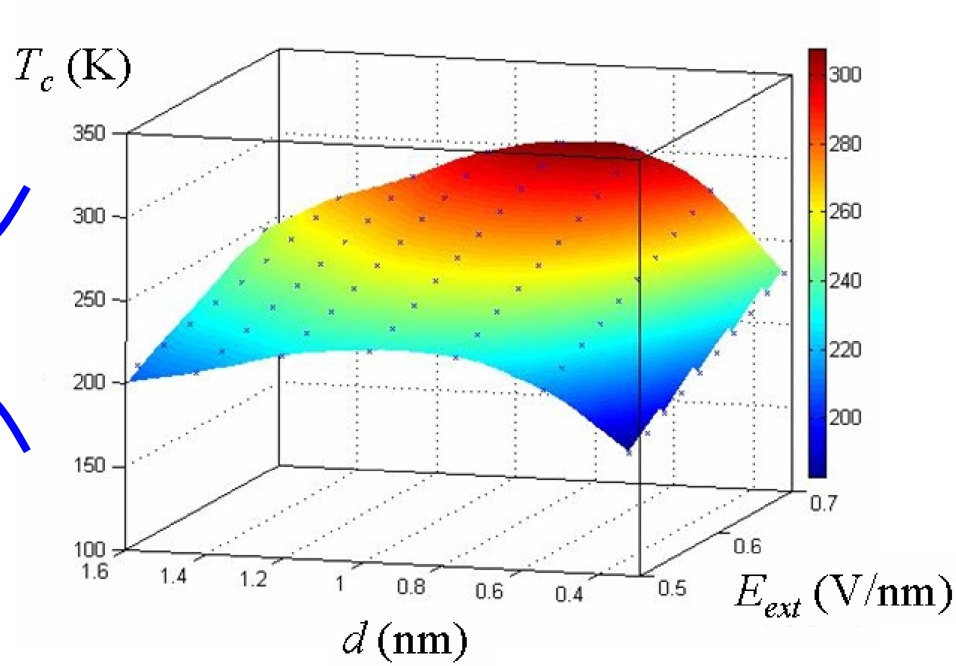
Device application

Han et al.
PRL (2007)

Possible ordered states in graphene systems

Exciton condensation in graphene bilayers



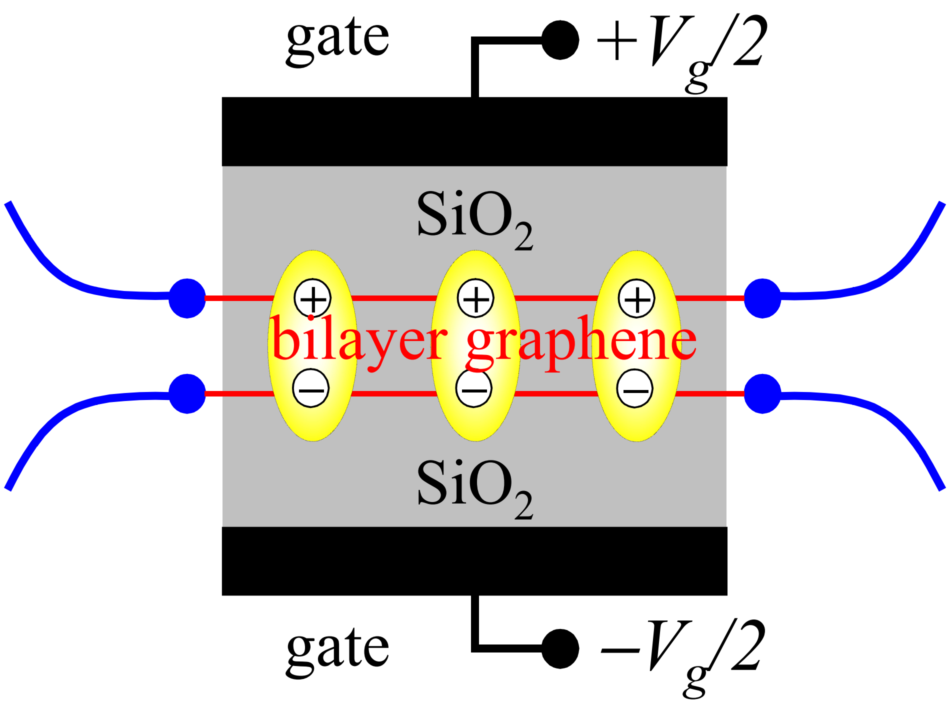


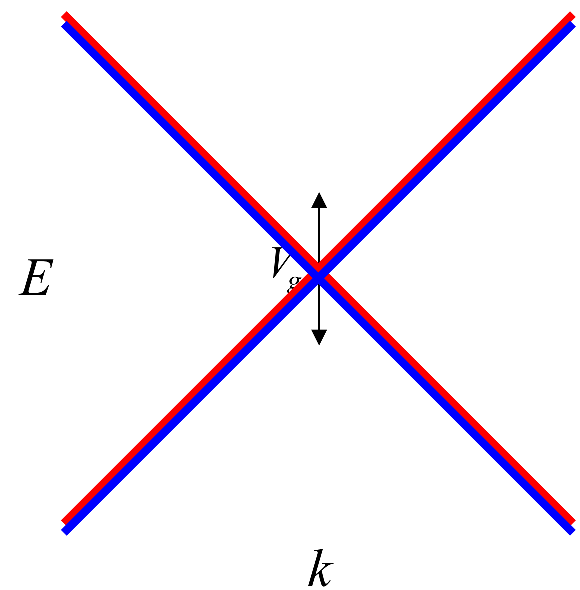
$\Rightarrow$ Room-temperature superfluidity

2. Exciton condensation in graphene bilayers

1) System

- Two single-layer graphene sheets separated by SiO_2 dielectric barrier in the no tunneling limit.





$\Rightarrow$ High-temperature exciton condensation

2. Exciton condensation in graphene bilayers

2) Pair condensation

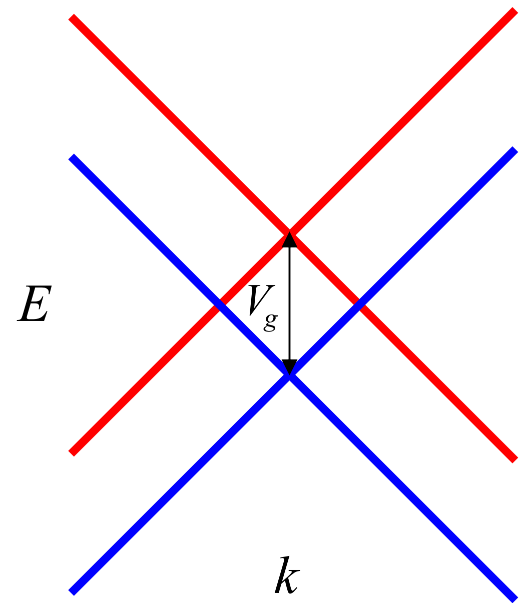
$$\boxed{\left\langle \hat{\psi}_{\uparrow}(\mathbf{r})\hat{\psi}_{\downarrow}(\mathbf{r})\right\rangle \neq 0}$$ Cooper pairs

$$\boxed{\left\langle \hat{\psi}_{t}^{+}(\mathbf{r})\hat{\psi}_{b}(\mathbf{r})\right\rangle \neq 0}$$ Bilayer excitons

$\Rightarrow$ Exciton condensation is spontaneous interlayer coherence.

3) Why graphene?

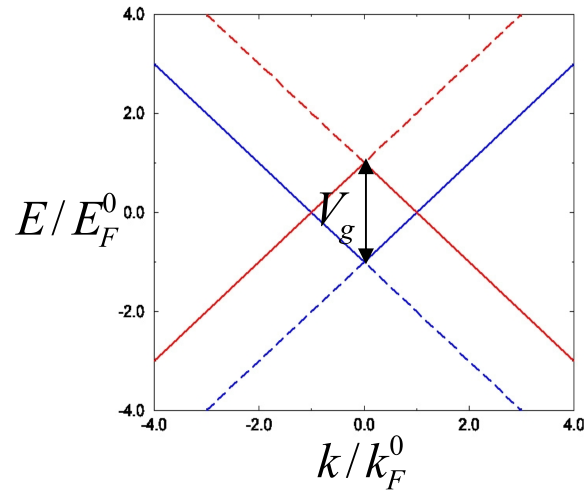
- Gapless semiconductor
- Perfect particle-hole symmetry
- Atomically two-dimensional

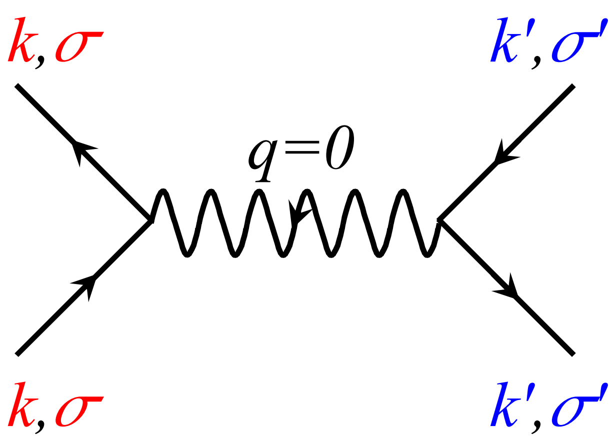


Possible ordered states in graphene systems

4) Numerical calculation

- A self-consistent mean-field theory neglecting remote bands





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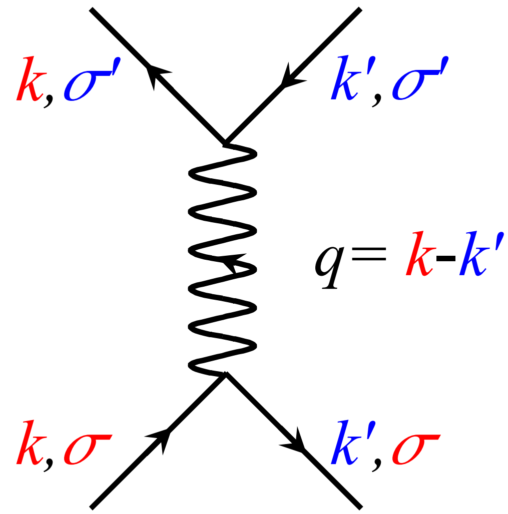
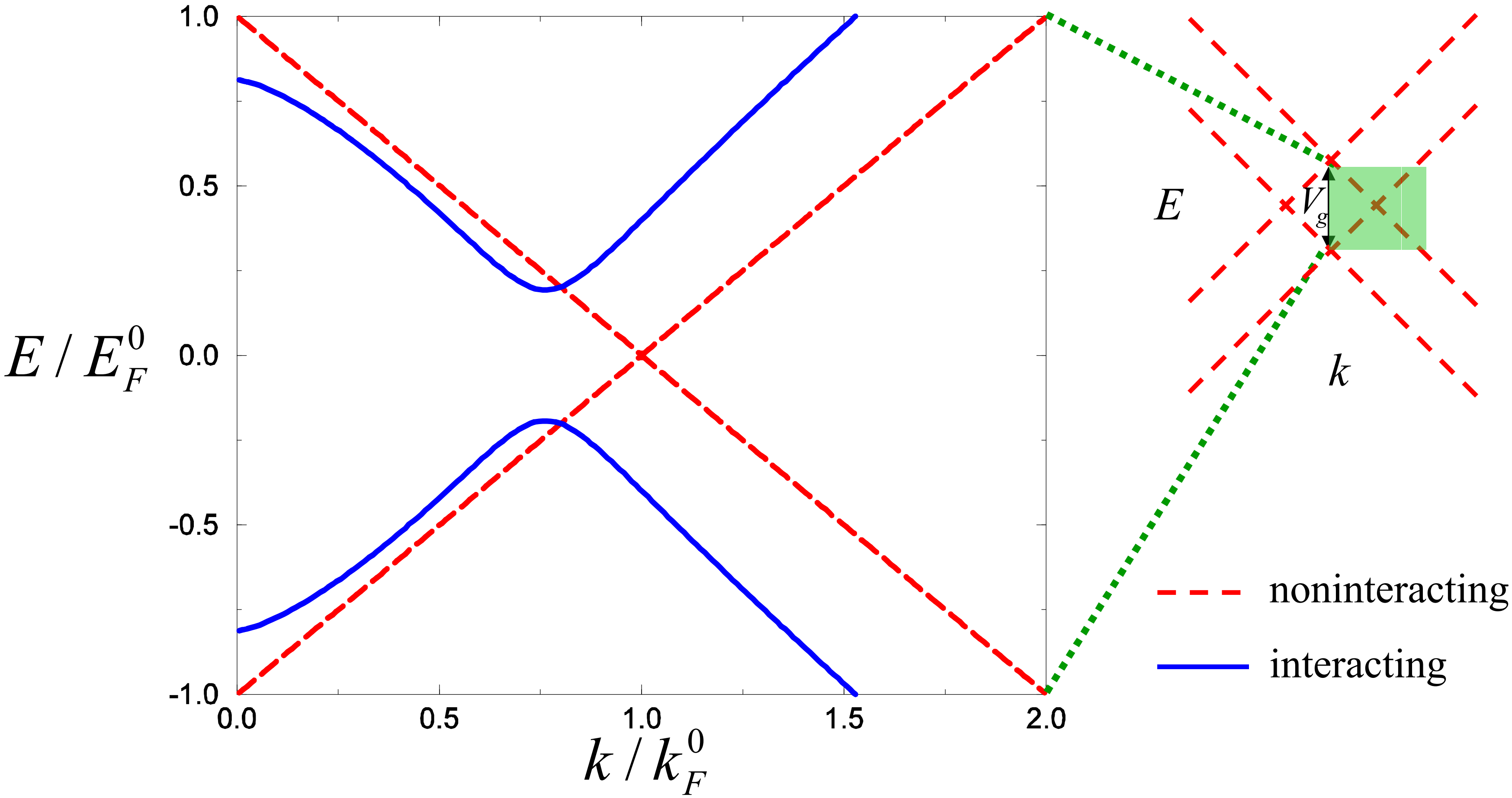


5) Energy band structure

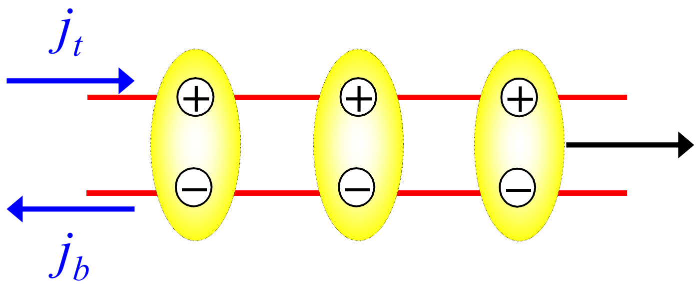
Min et al. PRB **78**, 121401(R) (2008)

- Cooper instability



6) Exciton superfluidity

- Counter-flow current



$$j_Q = \frac{e}{\hbar}\rho_s Q$$

exciton momentum

7) Kosterlitz-Thouless (KT) transition

- In 2D, superfluidity is destroyed by vortex proliferation.

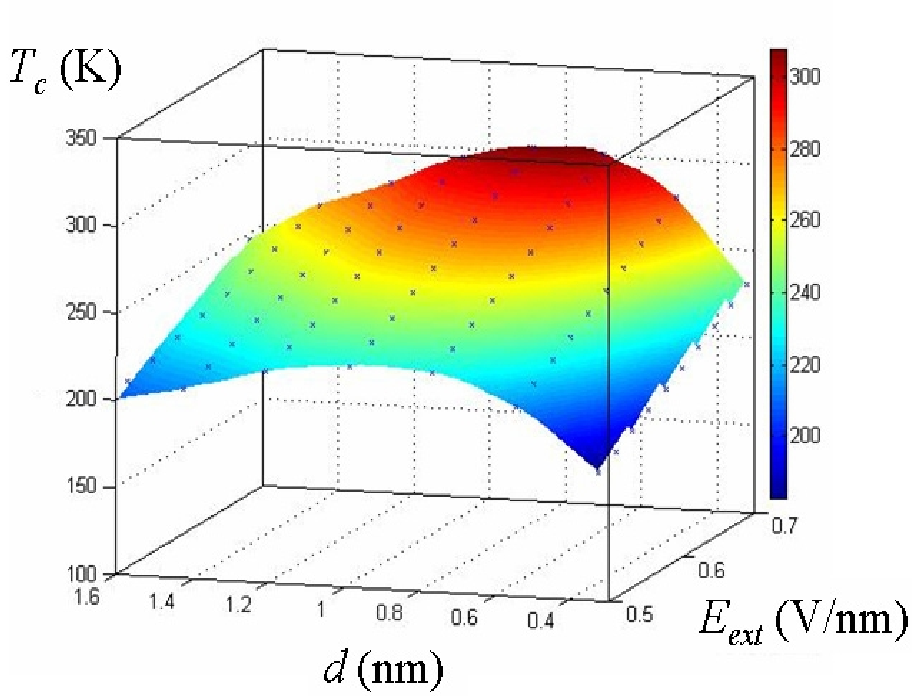
$$k_B T_{KT} = \frac{\pi}{2}\rho_s(k_B T_{KT})$$

8) Phase diagram

Min et al. PRB **78**, 121401(R) (2008)

- $T_c \uparrow$ as $E_{ext} \uparrow$
- Optimal layer separation
- $E_{ext} \sim 0.7$ V/nm, $d \sim 1$ nm

$\Rightarrow$ $T_c \sim 300$ K



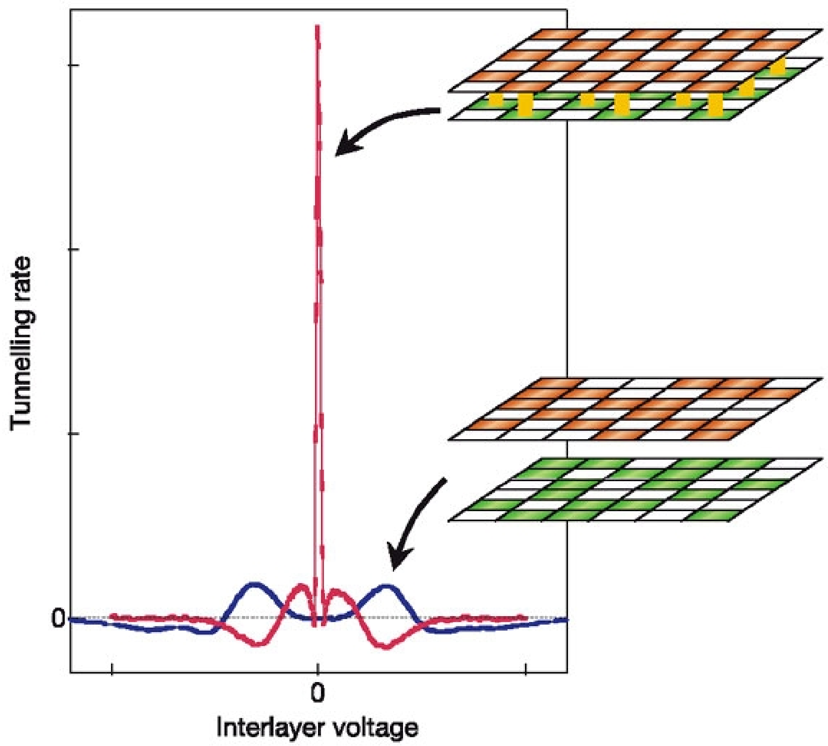
- Comparison with BCS superconductivity

Cooper pair : limited by ω_D $\Rightarrow$ $T_c \sim 10$ K

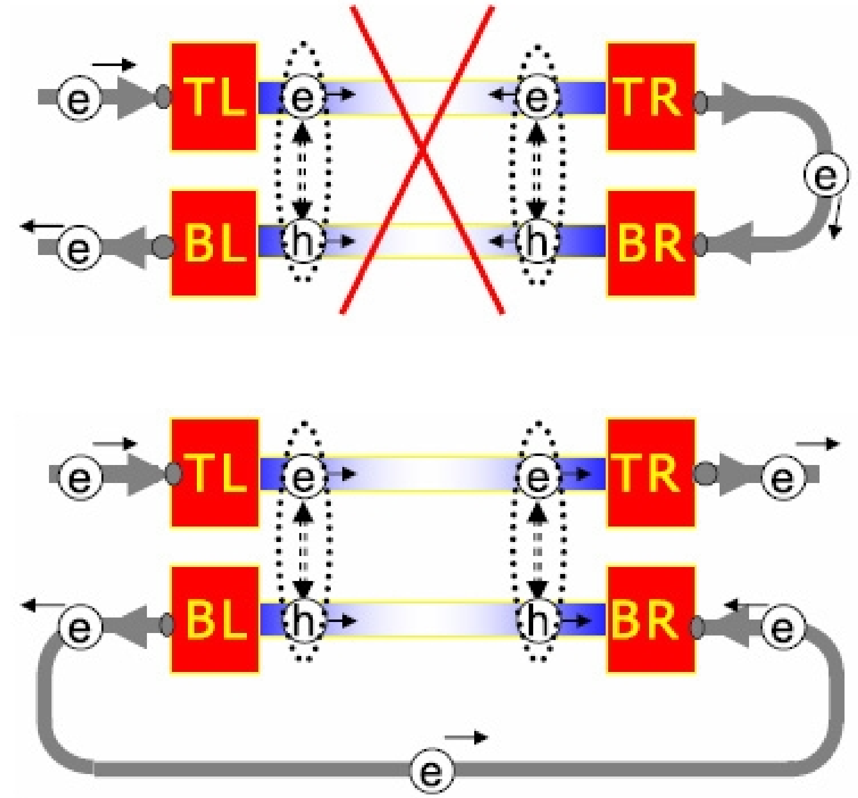
Bilayer exciton : limited by v_F/d $\Rightarrow$ $T_c \sim 300$ K

9) Experimental search

Tunneling



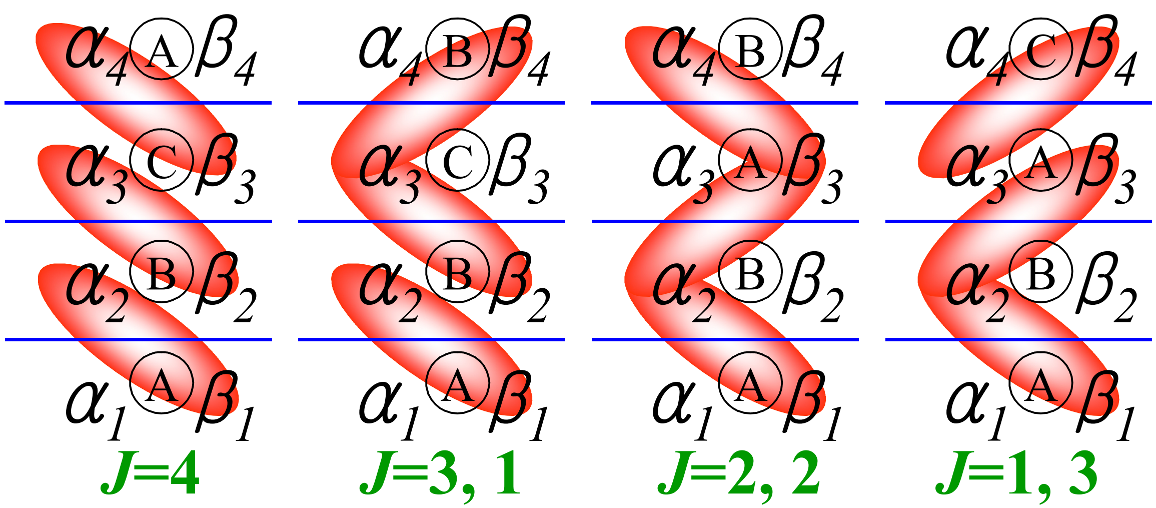
Transport

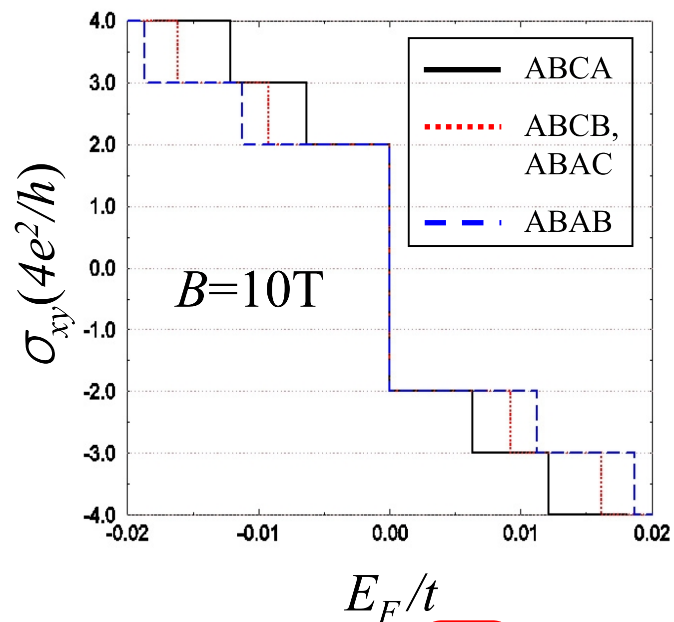


Eisenstein and MacDonald, Nature **432**, 691 (2004)

Su and MacDonald, arXiv:0801.3694

Coupled graphene stacks





$\Rightarrow$ New quantum Hall effects

$$\sigma_{xy} = \pm \frac{4e^2}{h}\left(\boxed{\frac{N}{2}} + n\right)$$

3. Coupled graphene stacks

1) Effective theory

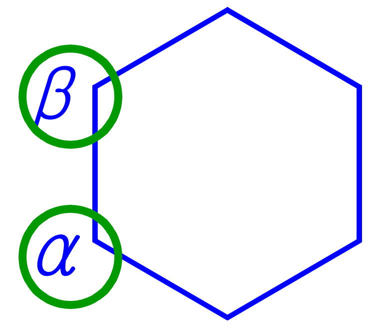
- Monolayer

$$H_B^{mono} = v_F \begin{array}{c} \begin{array}{cc} \quad\alpha & \qquad\beta \end{array} \\ \begin{pmatrix} 0 & pe^{-i\phi_{\mathbf{p}}} \\ pe^{i\phi_{\mathbf{p}}} & 0 \end{pmatrix} \end{array}$$

$$E(\mathbf{p}) = \pm v_F\, p$$

$v_F =$ in-plane velocity

$\phi_{\mathbf{k}} = \tan^{-1}(k_y / k_x)$

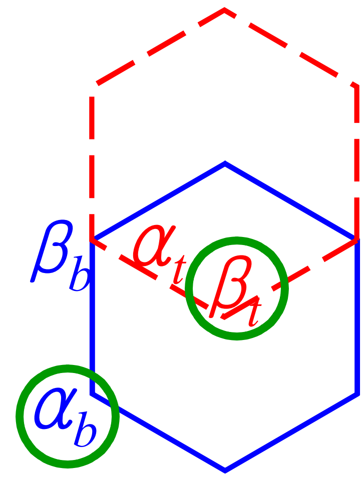


- Bilayer

$$H_B^{bi} = -\frac{1}{2m} \begin{array}{c} \begin{array}{cc} \quad\alpha_b & \qquad\beta_t \end{array} \\ \begin{pmatrix} 0 & p^2 e^{-i2\phi_{\mathbf{p}}} \\ p^2 e^{i2\phi_{\mathbf{p}}} & 0 \end{pmatrix} \end{array}$$

$$E(\mathbf{p}) = \pm \frac{p^2}{2m}$$

$m = \gamma_1 / 2v_F^2$



3. Coupled graphene stacks

2) Chirality

- A projection of spin (**σ**) on the direction of motion (**n**).

$$H_J = \varepsilon_0 \begin{pmatrix} 0 & p^J e^{-iJ\phi_{\mathbf{p}}} \\ p^J e^{iJ\phi_{\mathbf{p}}} & 0 \end{pmatrix} = \varepsilon_0 p^J \boldsymbol{\sigma} \cdot \mathbf{n}_J(\phi_{\mathbf{p}})$$

$$\mathbf{n}_J(\phi_{\mathbf{p}}) = (\cos J\phi_{\mathbf{p}}, \sin J\phi_{\mathbf{p}})$$

$$\phi_{\mathbf{p}} = \tan^{-1}(p_y / p_x)$$

- Energy spectrum $E_J(\mathbf{p}) = \pm\varepsilon_0 p^J$

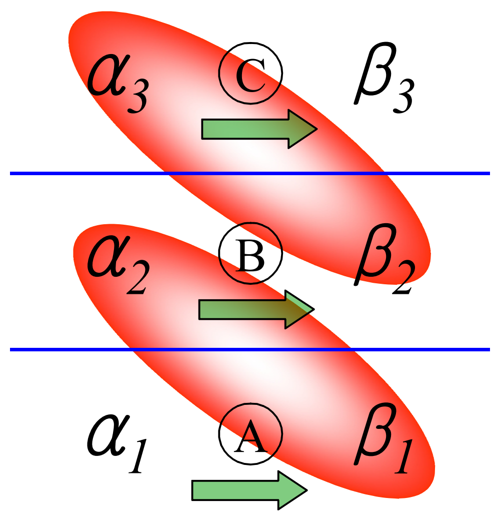
$\Rightarrow$ Monolayer graphene : J=1 chiral 2D electron gas
Bilayer graphene : J=2 chiral 2D electron gas

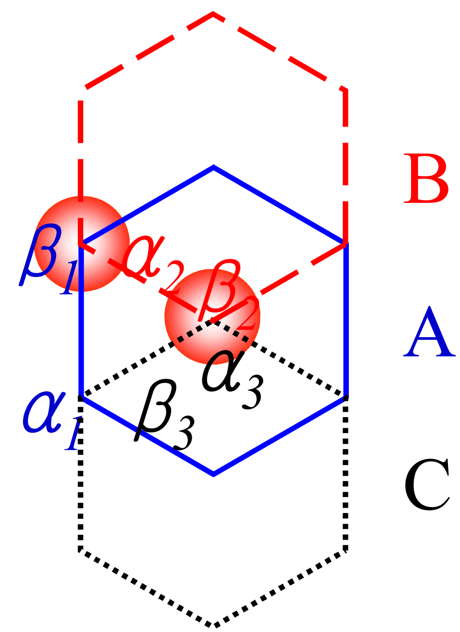
3. Coupled graphene stacks

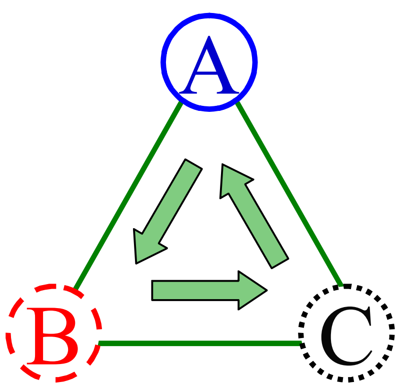
3) Stacking diagram

Min and MacDonald, PRB **77**, 155416 (2008)

- Example: ABC trilayer







***J*=3** chiral 2D electron gas

4) Effective theory (ABC)

Min and MacDonald, PRB **77**, 155416 (2008)

- Identify zero-energy states from the stacking diagram.

$\Rightarrow$ Ex: isolated α_1 and β_N are zero-energy states.

Ex: ABC stacked N-layer

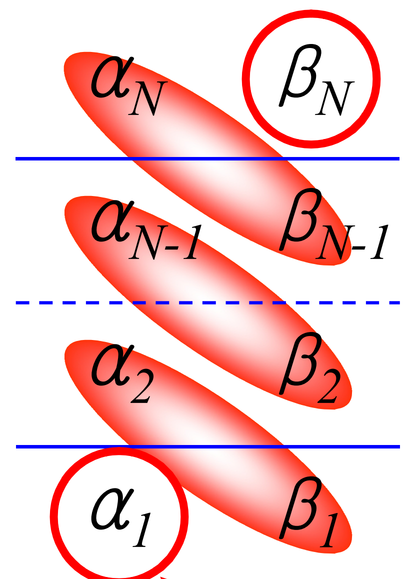
- Obtain the effective theory using degenerate state perturbation theory.

$$\boxed{H = H_{\perp} + H_{\parallel}}$$

$$\boxed{\langle \Psi_r | H | \Psi_{r'} \rangle = \langle \Psi_r | H_{\parallel} \left[\hat{Q}(-H_{\perp}^{-1})\hat{Q} H_{\parallel} \right]^{n-1} | \Psi_{r'} \rangle}$$

$\Rightarrow$ Ex: $\boxed{\langle \alpha_1 | H | \beta_N \rangle = -t_{\perp}(v_F p e^{-i\phi_{\mathbf{p}}} / t_{\perp})^N}$

N-chiral system

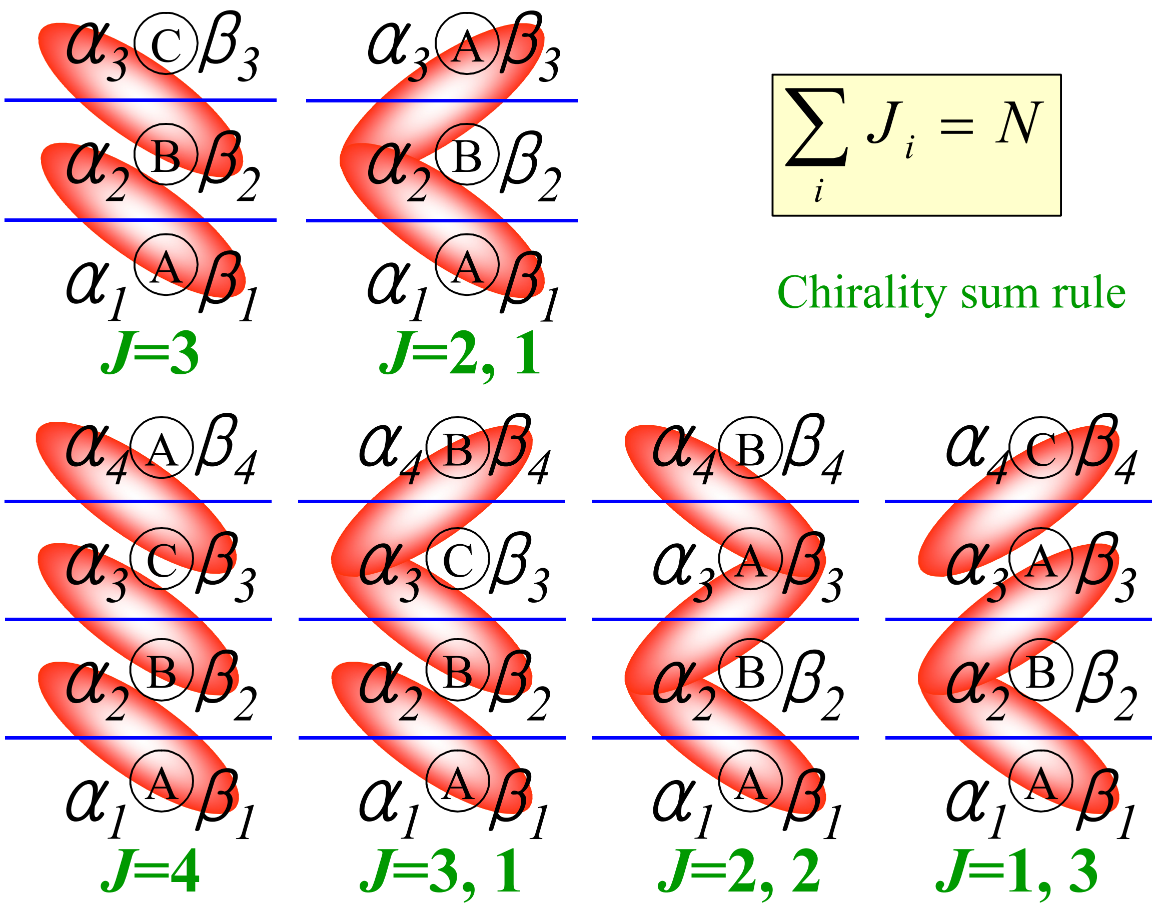


zero-energy states

5) Chiral decomposition

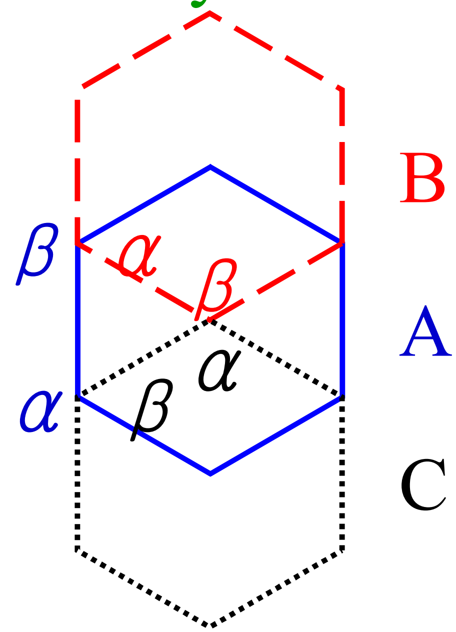
Min and MacDonald, PRB **77**, 155416 (2008)

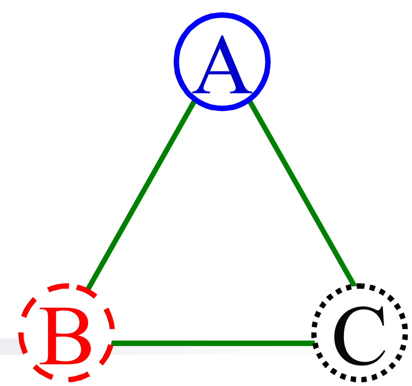
- The system is decomposed to different chiral systems.



$$\boxed{\sum_i J_i = N}$$

Chirality sum rule





Possible ordered states in graphene systems

6) Energy band structure

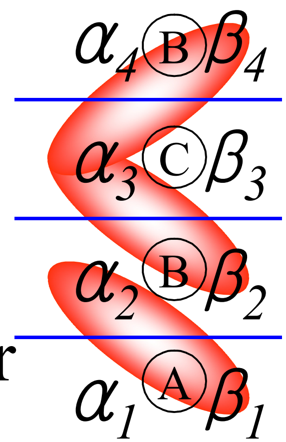
Min and MacDonald, PRB **77**, 155416 (2008)

- Energy spectrum for *J*-chiral system

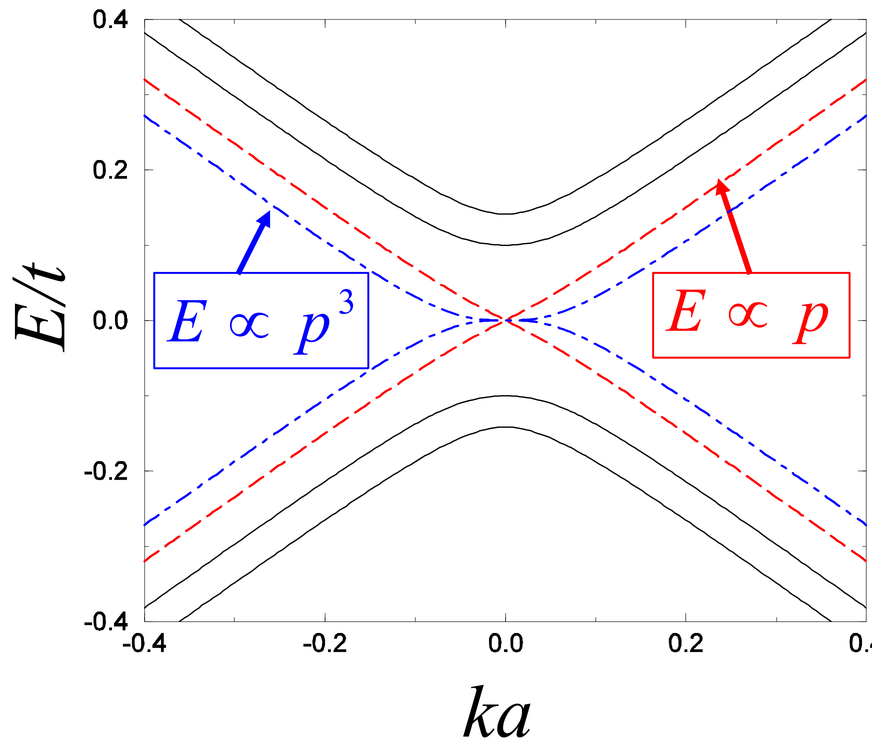
$$\boxed{E_J(\mathbf{p}) \propto p^J}$$

- Example: ABCB tetralayer

$$\boxed{E_{ABCB}(\mathbf{p}) \propto p,\, p^3}$$



***J*=3, 1**



$$\Rightarrow \boxed{H_N^{eff} = H_{J_1} \otimes H_{J_2} \otimes \cdots \otimes H_{J_{N_D}}}$$

$$\boxed{\sum_{i=1}^{N_D} J_i = N}$$

Chirality sum rule

7) New quantum Hall effects

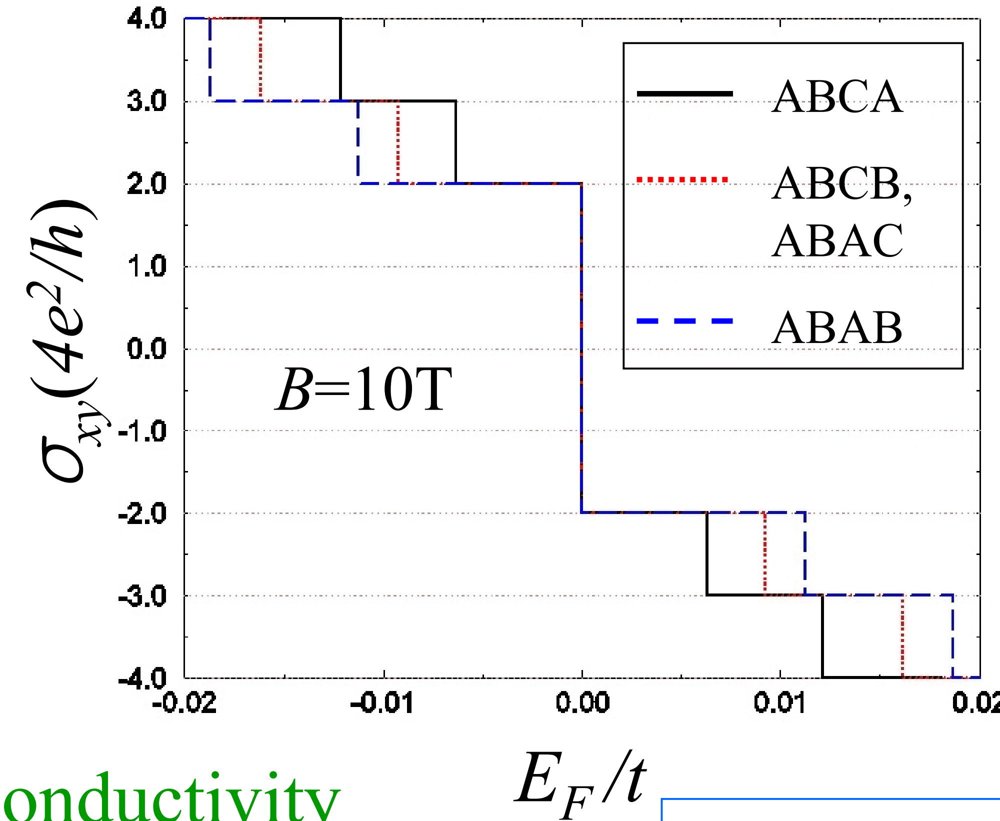
Min and MacDonald, PRB **77**, 155416 (2008)

- Quantum Hall conductivity

$$\boxed{\sum_{i=1}^{N_D} J_i = N}$$

$$\Rightarrow \boxed{\sigma_{xy} = \pm \frac{4e^2}{h}\left(\boxed{\frac{N}{2}} + n\right)}$$

n=0,1,2,3,…

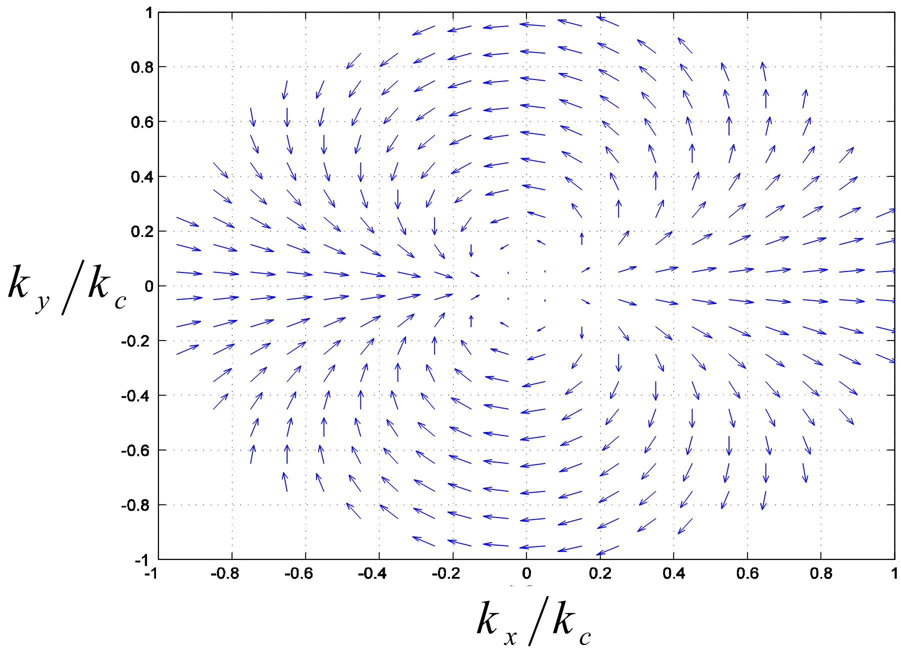


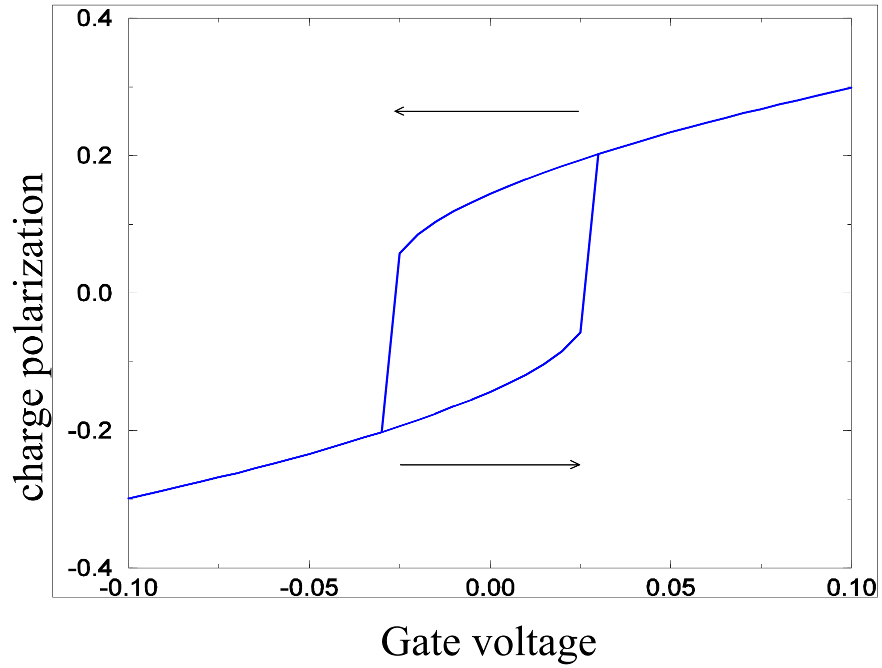
- Example: Tetralayer

$\Rightarrow$ N=4 quantum Hall conductivity

E_F = Fermi energy
t = intralayer hopping

Pseudospin magnetism in graphene bilayers





$\Rightarrow$ Spontaneous charge polarization

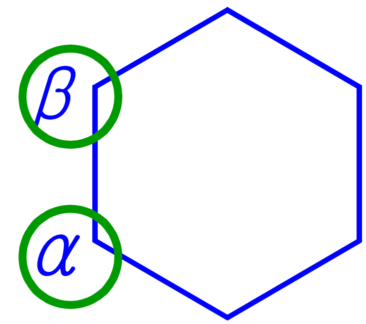
4. Pseudospin magnetism in graphene bilayers

1) Pseudospin $\Rightarrow$ Two-valued quantum degrees of freedom

- Monolayer

$$\begin{array}{cc} & \begin{array}{cc} \alpha & \beta \end{array} \\ H_B^{mono} = v_F & \begin{pmatrix} 0 & pe^{-i\phi_{\mathbf{p}}} \\ pe^{i\phi_{\mathbf{p}}} & 0 \end{pmatrix} \end{array}$$

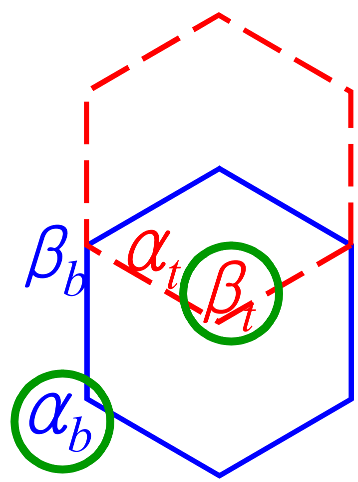
$$\text{“}\uparrow\text{”} = \alpha$$
$$\text{“}\downarrow\text{”} = \beta$$



- Bilayer

$$\begin{array}{cc} & \begin{array}{cc} \alpha_b & \beta_t \end{array} \\ H_B^{bi} = -\frac{1}{2m} & \begin{pmatrix} 0 & p^2 e^{-i2\phi_{\mathbf{p}}} \\ p^2 e^{i2\phi_{\mathbf{p}}} & 0 \end{pmatrix} \end{array}$$

$$\text{“}\uparrow\text{”} = \alpha_{\mathrm{b}}$$
$$\text{“}\downarrow\text{”} = \beta_{\mathrm{t}}$$



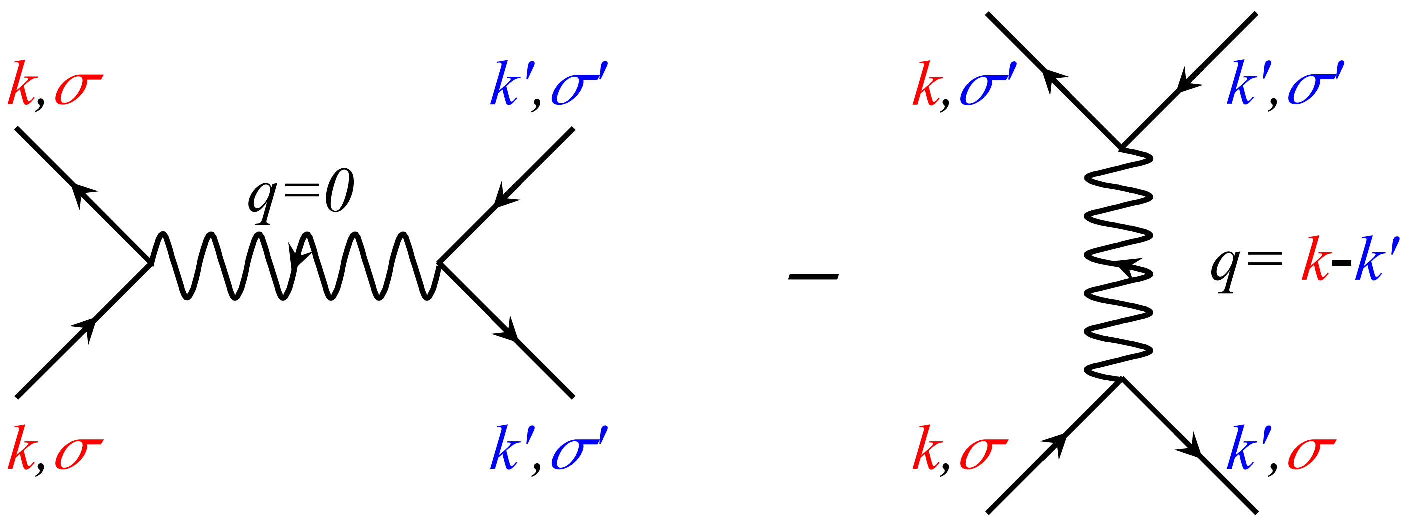
4. Pseudospin magnetism in graphene bilayers

2) Numerical calculation

- A self-consistent mean-field theory

$$\boxed{H_{MF} = -\mathbf{B}(\mathbf{k})\cdot\boldsymbol{\sigma}}$$

$\mathbf{B}(\mathbf{k})$: effective magnetic field
$\boldsymbol{\sigma}$: pseudospin

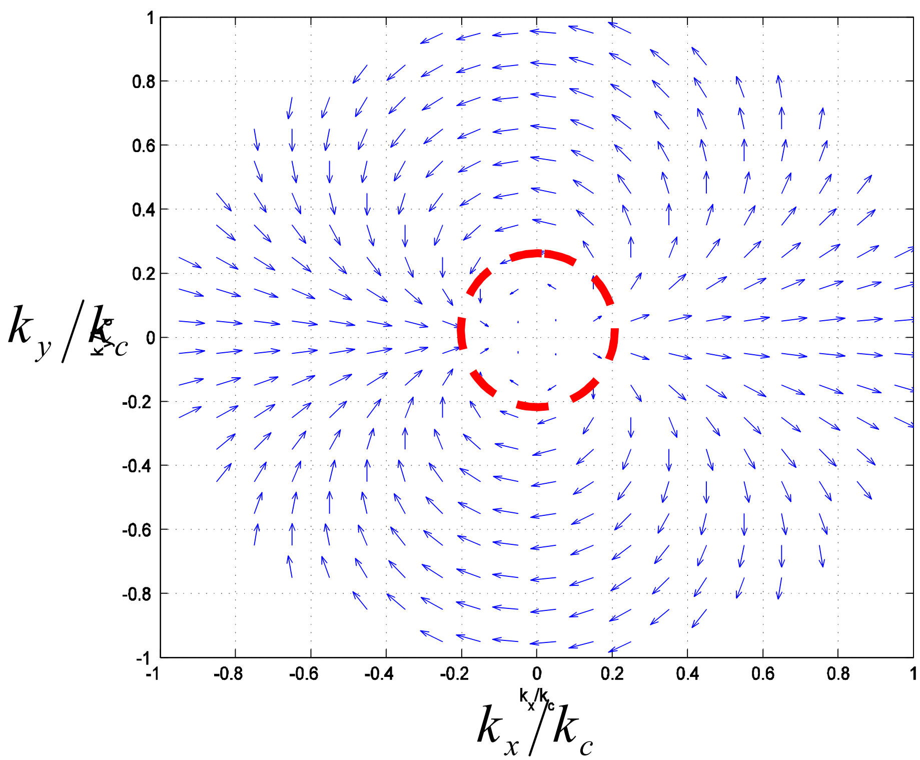


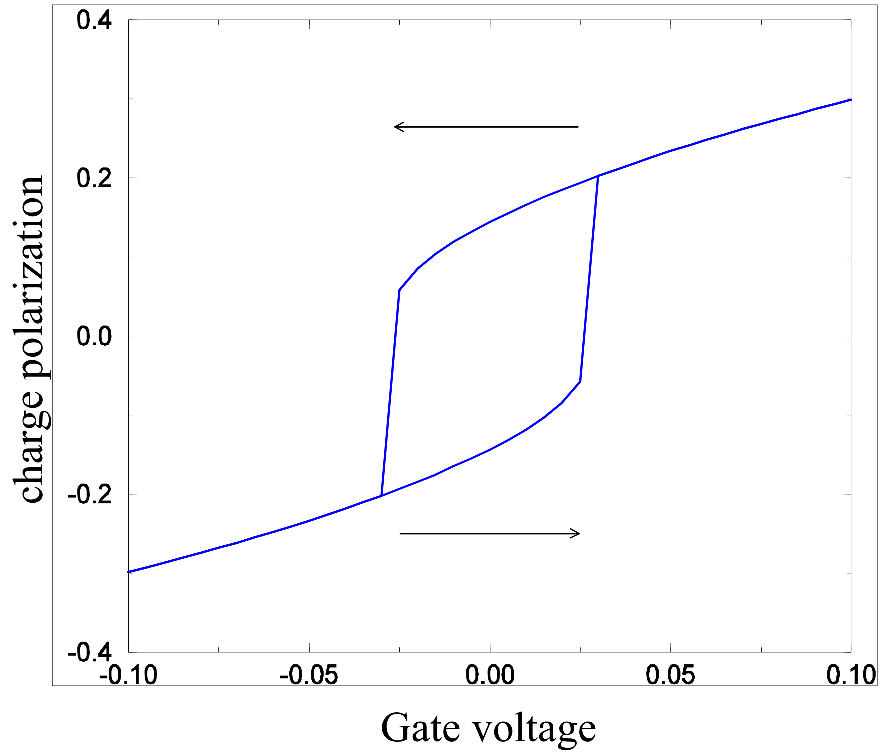
Direct   Exchange

4. Pseudospin magnetism in graphene bilayers

3) Example: Bilayer graphene (J=2)

Min et al. PRB **77**, 041407(R) (2008)





$$\boxed{H_{MF} = -\mathbf{B}(\mathbf{k})\cdot\boldsymbol{\sigma}}$$

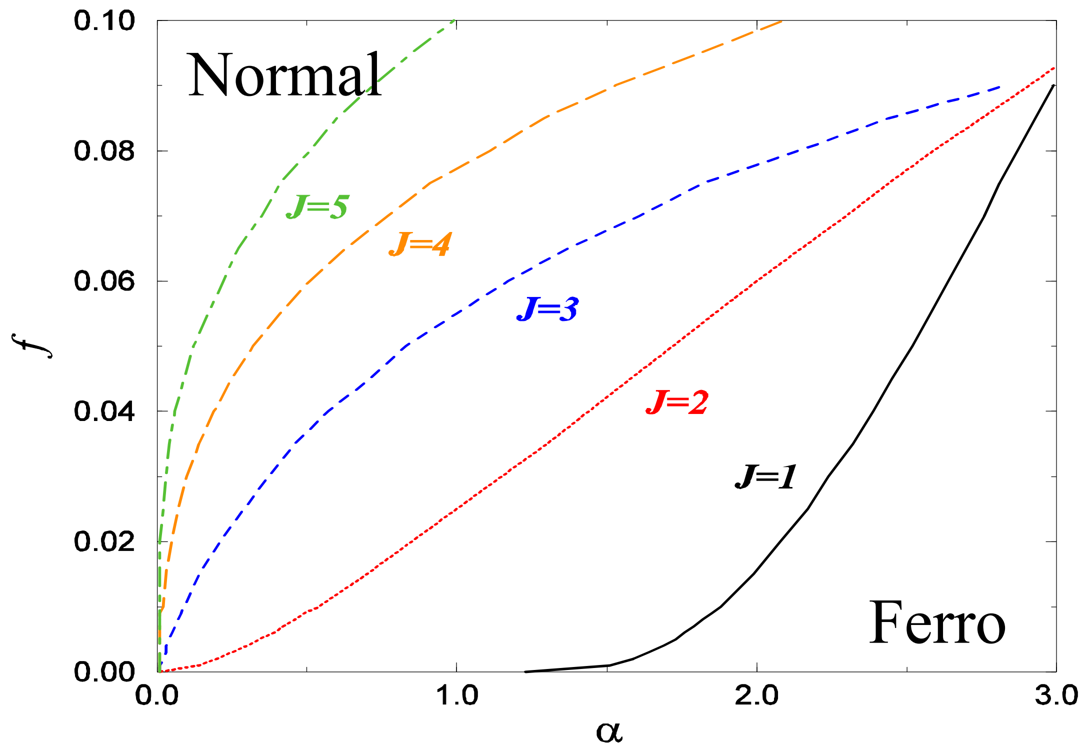
$$\boxed{\mathbf{B}(\mathbf{k}) = (B_\perp \cos J\phi_{\mathbf{k}}, B_\perp \sin J\phi_{\mathbf{k}}, B_z)}$$

$\Rightarrow$ Spontaneous charge transfer between two layers

4. Pseudospin magnetism in graphene bilayers

4) Phase diagram

Min et al. PRB **77**, 041407(R) (2008)



J : chirality

α : interaction strength

f : doping

- Pseudospin magnetism is stable for stronger interaction strength, for smaller doping, for larger chirality.

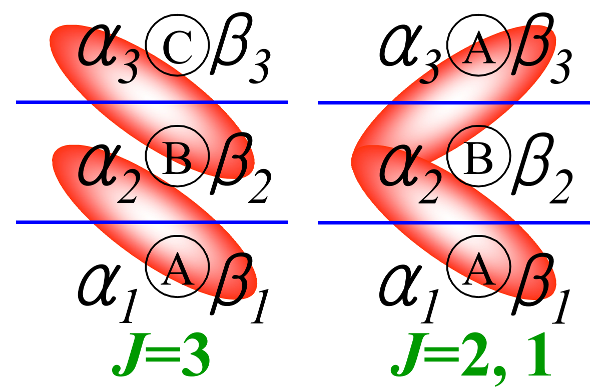
5) Chiral decomposition revisited

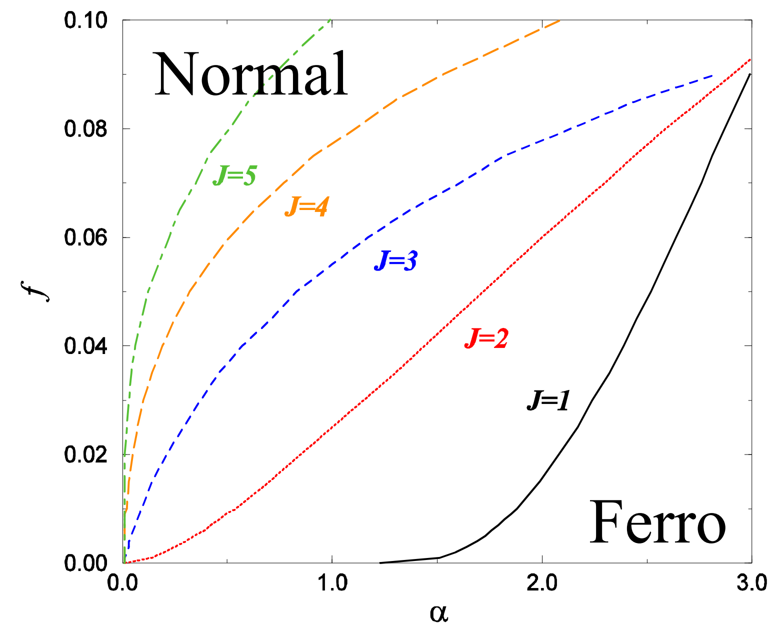
- Chiral decomposition in the electronic structure

$$H_N^{eff} = H_{J_1} \otimes H_{J_2} \otimes \cdots \otimes H_{J_{N_D}}$$

$$\sum_{i=1}^{N_D} J_i = N$$

$\Rightarrow$ ABC stacked multilayers are excellent candidates.





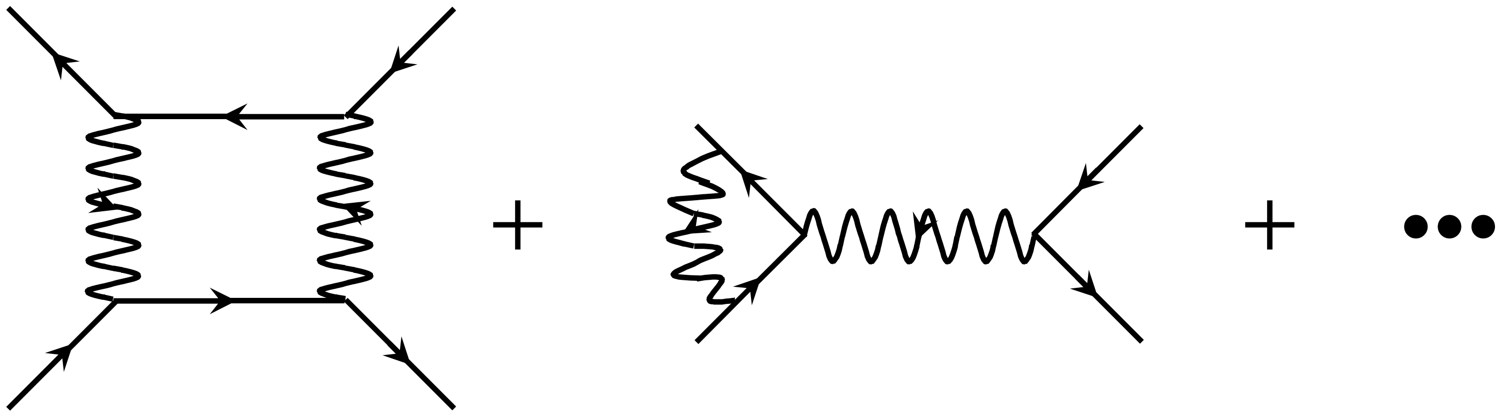
Possible ordered states in graphene systems

4. Pseudospin magnetism in graphene bilayers

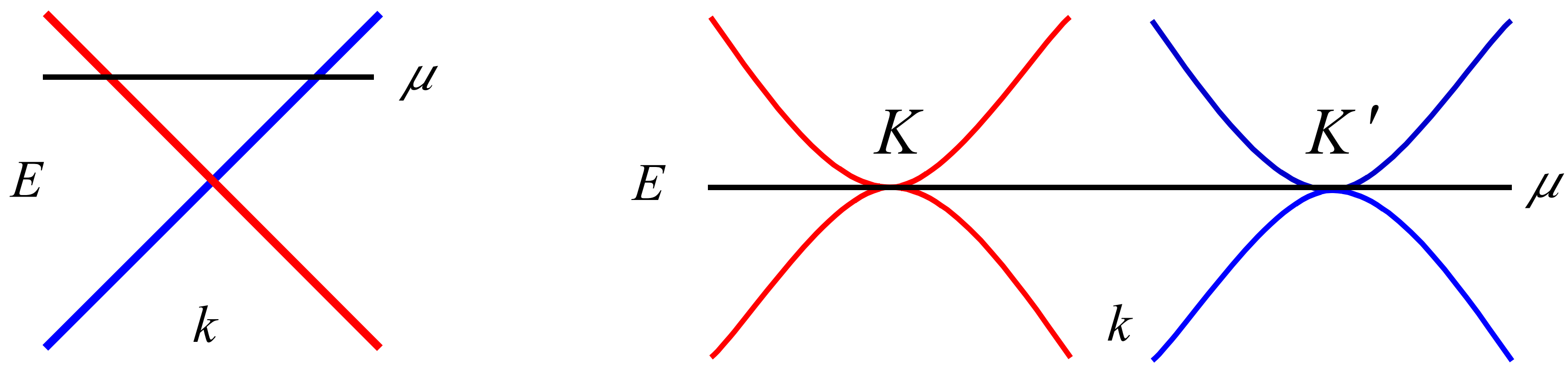
6) Future work

Electron-electron interactions in graphene bilayers
F. Zhang, Hongki Min, M. Polini, A.H. MacDonald
Manuscript in preparation

- Beyond Hartree-Fock

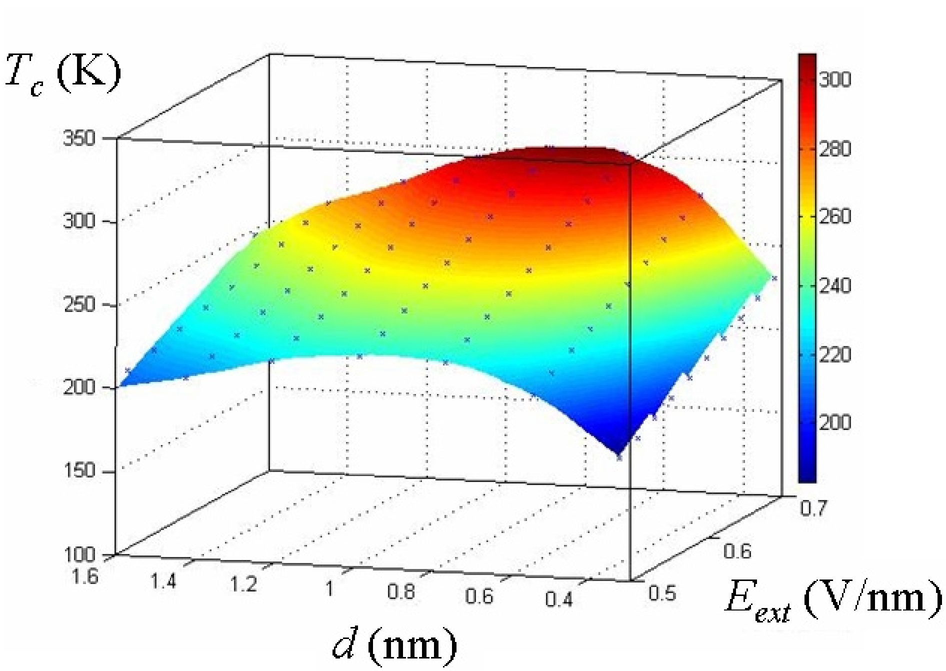


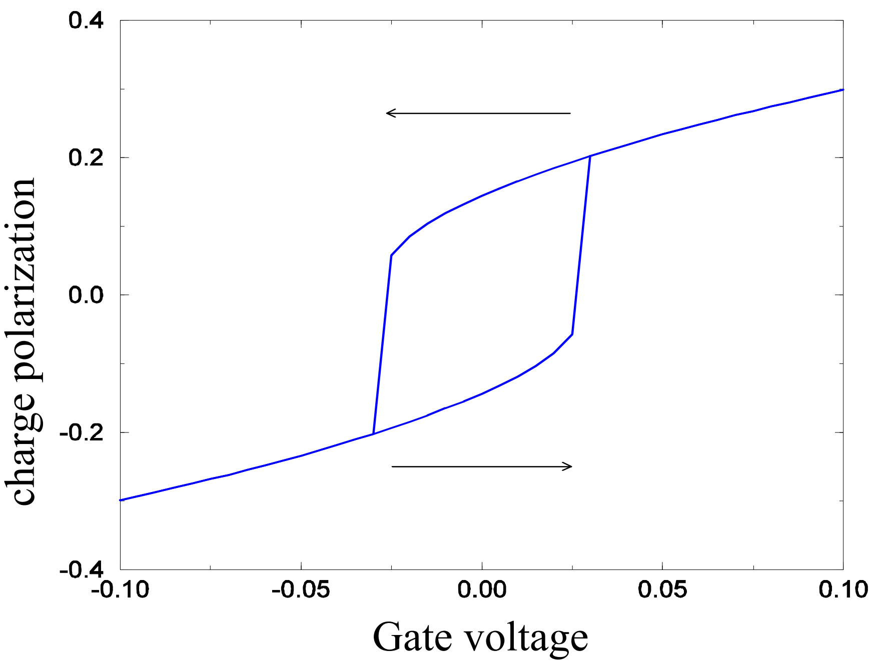
- 1D system vs neutral graphene bilayers



Possible ordered states in graphene systems

Conclusion





$\Rightarrow$ New electronic device scheme?

5. Conclusion

1) Search for new ordered states in graphene systems

Relativistic Dirac-like wavefunction

+

Non-relativistic electron-electron interaction

$\Rightarrow$ Possible ordered states in graphene systems

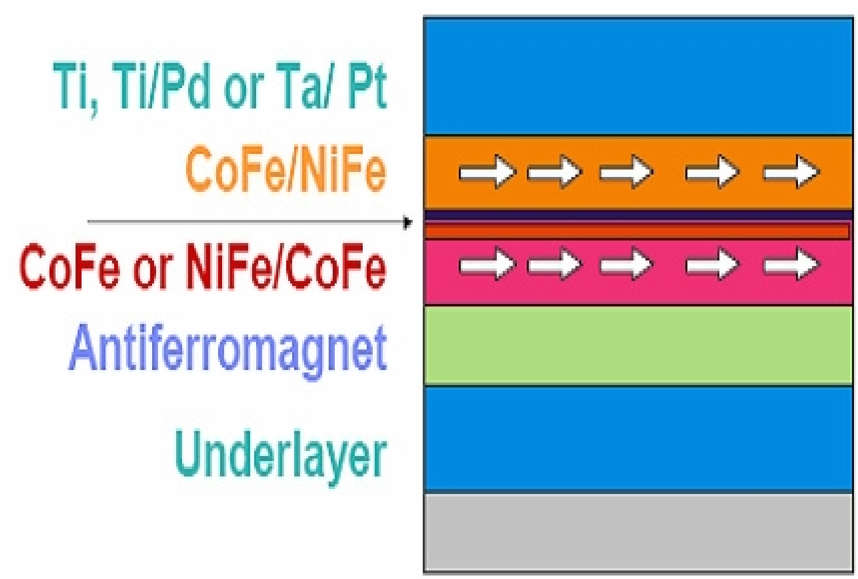
Exciton condensation in decoupled graphene bilayers

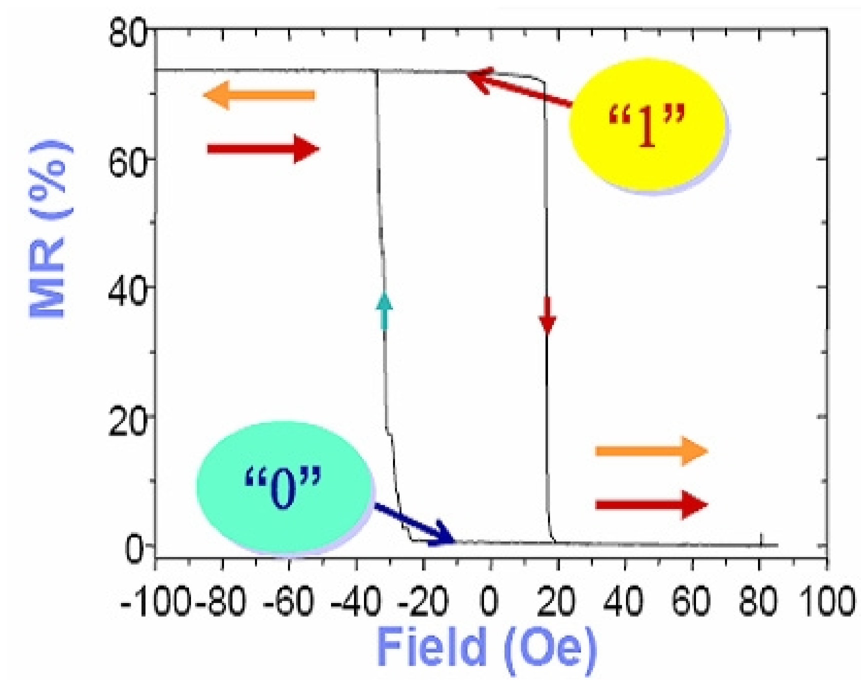
Pseudospin magnetism in coupled graphene bilayers

5. Conclusion

2) Collective field effect transistor (FET) vision

- Giant magnetoresistance (GMR)





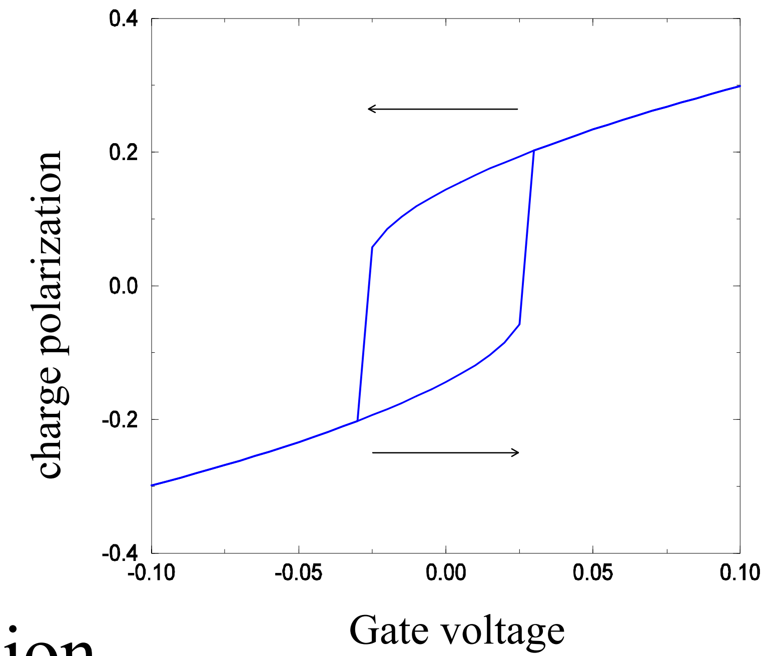
⇒ Collective behavior of many electrons

5. Conclusion

3) New electronic device scheme

Example: Pseudospin magnetism

- Collective behavior of many electrons
- Can be switched with gate voltages using much less power .
- Can exhibit a pseudospin version of GMR and spin-transfer torque.



Pseudospintronics!

References and collaborators

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