Pseudospintronics: a new electronic device scheme in graphene systems - 연필심 위의 물리학

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Motivation



• How can we overcome the barrier efficiently between the text book and real research problems?

What is graphene?

Graphene is 2D honeycomb lattice of carbon atoms



Adapted from Wikipedia

 $a = 0.246 \,\mathrm{nm}$

How to make graphene?

Scotch tape method







Adapted from NIST

Other methods: epitaxial growth, chemical vapor deposition, ...

Why graphene?

Graphene is described by relativistic wavefunction



Relativistic wavefunction in a low energy system

P. R. Wallace, Phys. Rev. **71**, 622 (1947)

Graphene has high electron mobility



100 times faster than conventional semiconductors at room temperature

Y. Zhang *et al*, Nature **438**, 201 (2005)

Why graphene?

Bilayer graphene is a band gap tunable semiconductor



Band gap opening by an external electric field

E. McCann, Phys. Rev. B **74**, 161403 (2006)

Graphene can be used as touch screen and flexible display



Atomically thin and conducting

S. Bae *et al*, Nat. Nanotech. 5, 574 (2010)

Why graphene?

Graphene is an excellent thermal conductor



Graphene is 200 times stronger than steel



NEMS application

C. Lee *et al*, Science 321, 385 (2008)

Outline

- 1. Electronic structure
 - Tight-binding model
- 2. Transport and optical properties
 Boltzmann transport theory
- 3. Electron-electron interactions
 - Mean-field theory
- 4. Conclusion and future work— New electronic device scheme

Electronic structure – Tight-binding model

- What is the model Hamiltonian for graphene?
- What is the effective theory near the Fermi energy?
- What is the effect of stacking sequence?

Hamiltonian

Time independent Schrödinger equation

 $H(\mathbf{k})|\Psi_n(\mathbf{k})\rangle = E_n(\mathbf{k})|\Psi_n(\mathbf{k})\rangle$

- \mathbf{k} = wave vector
- E_n = energy band
 - n = band index

Tight-binding model

Example: 1D chain composed of two kinds of atoms



$$f(\mathbf{k}) = t \left[e^{ik(a/2)} + e^{-ik(a/2)} \right] = 2t \cos\left(\frac{ka}{2}\right)$$

Monolayer graphene



 ${}^{6}\text{C}=1s^{2}2s^{2}2p^{2}$

Expand around K

Monolayer graphene

Monolayer graphene has a linear dispersion at low energies Effective theory around *K*

$$\begin{array}{ccc} \boldsymbol{\alpha} & \boldsymbol{\beta} \\ H = v_0 \begin{pmatrix} 0 & \pi^* \\ \pi & 0 \end{pmatrix} = v_0 \mathbf{p} \cdot \boldsymbol{\sigma} \end{array}$$

$$\pi = p_x + ip_y$$

$$v_0 = \text{ in-plane velocity}$$

$$\mathbf{p} = \hbar \mathbf{k}$$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

 $E(\mathbf{p}) = \pm v_0 p$



Monolayer graphene

Pseudospin, chirality and Berry phase





 $H = \mathbf{B} \cdot \boldsymbol{\sigma}$

Bilayer graphene

Bilayer graphene is composed of a pair of coupled graphene





Electronic structure of bilayer graphene

Bilayer graphene is composed of a pair of coupled graphene 4-band model around *K*



Band gap opening in bilayer graphene

Band structure control by an external electric field 4-band model around *K*







Band gap opening in bilayer graphene

Band structure control by an external electric field

⇒ Tunable energy gap semiconductor Possible application to a switch device



Min, Sahu, Banerjee, and MacDonald, Phys. Rev. B 75, 155115 (2007)

Bilayer graphene is composed of a pair of coupled graphene 4-band model around *K*



Bilayer graphene has a parabolic dispersion at low energies Effective theory around *K*



Pseudospin, chirality and Berry phase



Pseudospin, chirality and Berry phase



Pseudospin and Chirality

66本99

Effective theory of a general chiral system

66 | 99

$$H_{J} = \varepsilon_{0} \begin{pmatrix} 0 & \pi^{*J} \\ \pi^{J} & 0 \end{pmatrix} = \varepsilon_{0} p \left(\mathbf{\sigma} \cdot \mathbf{n}_{J} (\mathbf{\phi}_{\mathbf{p}}) \right), \quad \sigma_{x} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_{y} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

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

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

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

McCann & Fal'ko , Phys. Rev. Lett. **96**, 086805 (2006) Min & MacDonald, Phys. Rev. B **77**, 155416 (2008)

Pseudospin: Two-valued quantum degrees of freedom Example: sublattice, layer

Chirality: Projection of pseudospin to momentum direction

Monolayer graphene : 2D chiral system with chirality J=1Bilayer graphene : 2D chiral system with chirality J=2

Multilayer stacking

Three distinct stacking arrangements, labeled A,B,C







Electronic structure

Important lessons Min and MacDonald, Phys. Rev. B 77, 155416 (2008)

Electronic structure strongly depends on the stacking sequences. \Rightarrow Electronic structure engineering by stacking sequences

Low-energy band structure is described by a set of chiral systems.

Ex: ABA trilayer
$$(J=1,2)$$

$$H_{eff} \sim \begin{pmatrix} 0 & \pi^* \\ \pi & 0 \end{pmatrix} \oplus \begin{pmatrix} 0 & \pi^{*2} \\ \pi^2 & 0 \end{pmatrix}$$



High-energy band structure follows that of monolayer graphene.

Transport and optical properties – Boltzmann transport theory

- What is the effect of impurities?
- What is the response to light?
- How can we identify the stacking sequence?

Model

Boltzmann transport theory

• Non-equilibrium distribution function

$$dn = \frac{d\mathbf{k}}{(2\pi)^d} f(\mathbf{k}, t)$$
$$\mathbf{J} = (-e) \int \frac{d\mathbf{k}}{(2\pi)^d} f(\mathbf{k}, t) \mathbf{v}(\mathbf{k})$$

electrical conductivity

• Relaxation time approximation

$$\frac{df(\mathbf{k},t)}{dt} = \frac{\partial f(\mathbf{k},t)}{\partial \mathbf{k}} \cdot \frac{d\mathbf{k}}{dt} + \frac{\partial f(\mathbf{k},t)}{\partial t} \qquad \qquad \hbar \frac{d\mathbf{k}}{dt} = (-e)\mathbf{E}$$

$$\approx -\frac{f(\mathbf{k},t) - f_0(\mathbf{k})}{\tau_{\mathbf{k}}} \qquad \qquad f_0(\mathbf{k}) = \begin{array}{c} \text{equilibrium} \\ \text{equilibrium} \\ \text{distribution function} \\ \tau_{\mathbf{k}} = \end{array}$$

Model

Boltzmann transport theory

• Relaxation time

$$\frac{1}{\tau_F} = \frac{2\pi}{\hbar} n_{imp} V_{imp}^2 v(\varepsilon_F)$$
DOS

Fermi's Golden rule

• Electrical conductivity
$$\mathbf{J} = (-e) \int \frac{d\mathbf{k}}{(2\pi)^d} f(\mathbf{k}, t) \mathbf{v}(\mathbf{k}) = \sigma \mathbf{E}$$

$$\sigma = e^2 \left[g_s g_v v(\varepsilon_F) \right] \left[\frac{1}{2} \mathbf{v}_F^2 \tau_F \right] \qquad \mathbf{v}_F = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial k} \Big|_{\varepsilon = \varepsilon_F}$$

DOS Diffusion constant in 2D Fermi velocity

$$\Rightarrow \sigma \propto \frac{v_F^2}{n_{imp}V_{imp}^2}$$

Density dependence of conductivity

Short-range scatterers

Min et al. Phys. Rev. B 83, 195117 (2011)

Short range scatterers



 $A \rightarrow J=1$, $AB \rightarrow J=2$, $ABC \rightarrow J=3$, $ABA \rightarrow J=1,2$

Optical conductivity measurements

Transmittance of graphene



$$T(\omega) = \left(1 + \frac{2\pi}{c}\sigma(\omega)\right)^{-2}$$

$$R(\omega) = 1 - T(\omega)$$

Optical conductivity of bilayer graphene

High frequency limit



At high frequencies, each decoupled layer gives σ_{uni} , thus optical conductivity approaches to $N\sigma_{uni}$.

Optical conductivity of bilayer graphene

Intermediate frequency regime (t_{\perp} =0.3~0.4 eV)



At intermediate frequencies, optical conductivity shows characteristic peaks depending on the stacking sequence.

Optical conductivity of bilayer graphene

Low frequency limit



At low frequencies, optical conductivity approaches to $N\sigma_{uni}$.

Optical conductivity of graphene multilayers

Low frequency limit

• Monolayer graphene (J=1)

$$\sigma_{uni} = \frac{\pi}{2} \frac{e^2}{h}$$

• J-chiral system



• Chirality sum is the number of layers

$$\sigma = \sum_{i} \sigma_{J_{i}} = N \sigma_{uni}$$

At low frequencies, optical conductivity approaches to $N\sigma_{uni}$.





Optical conductivity measurements provide a useful way to identify the number of layers and stacking sequences.

Comparison with experiments

Optical conductivity and stacking sequence



Mak *et al*, PRL **104**, 176404 (2010)

Min and MacDonald, PRL **103**, 067402 (2009)

Electron-electron interactions - Mean-field theory

- What is the effect of electron-electron interaction?
- How can we treat the electron-electron interaction?
- Is there a pseudospin version of ferromagnetism?

Electron-electron interaction

Interaction-induced ordered states

• Magnetism

. . .

• Superconductivity

• Exciton-condensation





Mean-field theory

Weiss molecular-field approximation

$$\begin{split} H &= -\frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \\ \mathbf{S}_i &= \langle \mathbf{S}_i \rangle + \delta \mathbf{S}_i \\ \mathbf{S}_i \cdot \mathbf{S}_j &= \left(\langle \mathbf{S}_i \rangle + \delta \mathbf{S}_i \right) \cdot \left(\langle \mathbf{S}_j \rangle + \delta \mathbf{S}_j \right) \\ &= \langle \mathbf{S}_i \rangle \cdot \left\langle \mathbf{S}_j \right\rangle + \delta \mathbf{S}_i \cdot \left\langle \mathbf{S}_j \right\rangle + \left\langle \mathbf{S}_i \right\rangle \cdot \delta \mathbf{S}_j + \delta \mathbf{S}_j \delta \mathbf{S}_j \\ &\approx \langle \mathbf{S}_i \rangle \cdot \mathbf{S}_j + \left\langle \mathbf{S}_j \right\rangle \cdot \mathbf{S}_i - \left\langle \mathbf{S}_i \right\rangle \cdot \left\langle \mathbf{S}_j \right\rangle \\ H^{MF} &\approx -\sum_i \mathbf{B}_i^{MF} \cdot \mathbf{S}_i \qquad \mathbf{B}_i^{MF} = \sum_j J_{ij} \left\langle \mathbf{S}_j \right\rangle \end{split}$$

Mean-field theory

Weiss molecular-field approximation



Mean-field theory

Hartree-Fock approximation



Interacting electrons

Non-interacting electrons in an effective potential

Pseudospin magnetism

Pseudospin \Rightarrow Two-valued quantum degrees of freedom Bilayer graphene (chirality *J*=2)



Ferromagnetism means spontaneous spin polarization.

Is there spontaneous charge polarization in the presence of electron-electron interactions?

 \Rightarrow Pseudospin magnetism

Pseudospin magnetism in bilayer graphene

In-plane pseudospin direction Min et al. Phys. Rev. B 77, 041407(R) (2008)



No electron-electron interaction

Pseudospin magnetism in bilayer graphene

In-plane pseudospin direction Min et al. Phys. Rev. B 77, 041407(R) (2008)



 \Rightarrow VoÆecfromelieotrioninteractionssprecturned on Spontaneous charge transfer between the two layers

Pseudospin magnetism in multilayer graphene



Pseudospin magnetism is more stable for larger chirality. \Rightarrow ABC stacked multilayers are excellent candidates. Ex) AB, ABC, ABCA, ABCAB,... Conclusion and future work – New electronic device scheme

- How can we use the ordered states in devices?
- Are there other interaction-induced ordered states?
- Ongoing work

Search for ordered states in graphene systems

Interplay between chirality, e-e interaction and disorder

Dirac-like chiral wavefunction

+ Electron-electron interaction

Disorder

 \Rightarrow New ordered states in graphene systems

Energy band structure and stacking sequences

Pseudospin magnetism in coupled graphene bilayers

High-quality sample with low disorder

Prospects

Current electronic device scheme \Rightarrow Future electronic device scheme

Single particle behavior

 \Rightarrow Collective behavior of many particles

Classical/semi-classical phenomena

 \Rightarrow Quantum phenomena in macroscopic scale

Collective electron device scheme

Example: Giant magnetoresistance (GMR)



⇒ Collective behavior of many electrons Magnetic field control of ordered states

Collective electron device scheme

Example: Pseudospin magnetism

- Collective behavior of many electrons
- Can be switched with a small gate voltage change using much less power
- Electrical control of ordered states
- Can exhibit a pseudospin version of GMR and spin-transfer torque

Pseudospintronics!



Conclusion

Text book examples vs research problems

