# Electronic and Transport Properties of Graphene

Tsuneya ANDO

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2. **Singular diamagnetic susceptibility**
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   - Spatially varying magnetic field
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4. **Multi-layer graphene**
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*Nara, Jun 4 (Tue) 2013*

IWCE Nara Japan 2013

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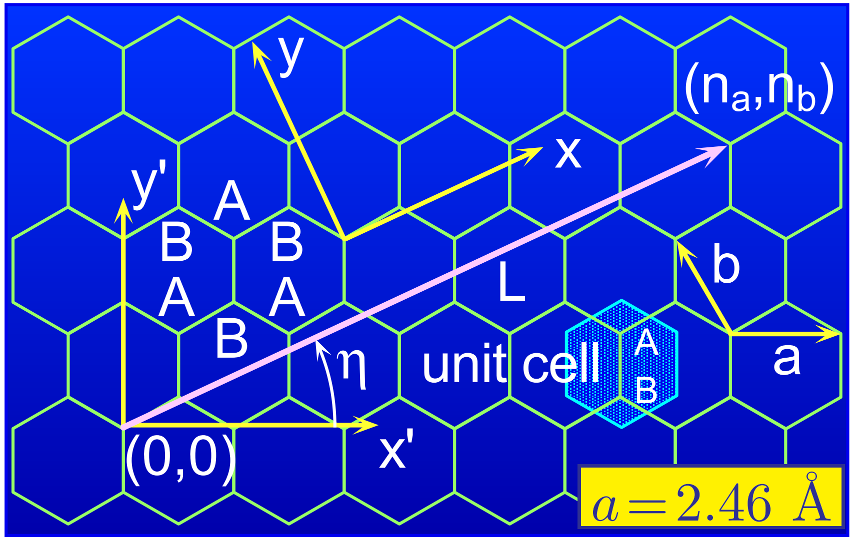
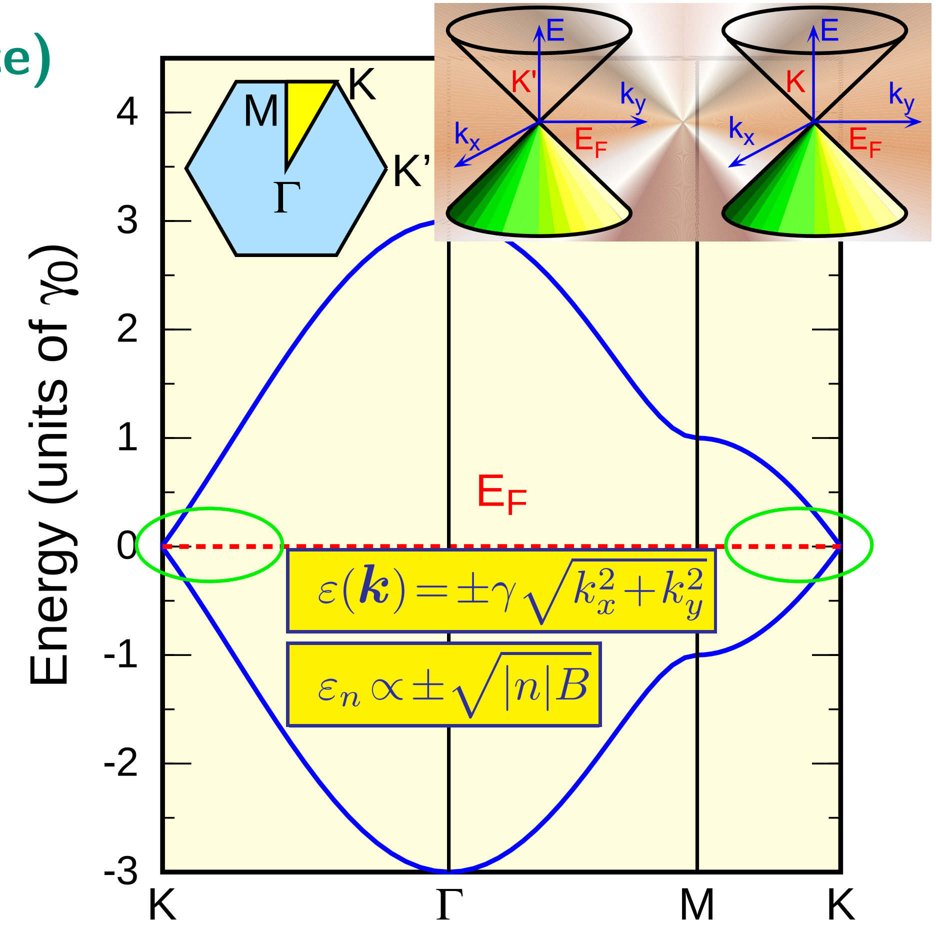
16th International Workshop on Computational Electronics, Nara Prefectural New Public Hall
Jun 4 (Tue) – 7 (Fri) 2013 [13:30–14:30 (50+10)]

# Effective-Mass Description: Neutrino or Massless Dirac Electron

## Graphene (Triangular antidot lattice)




## Weyl's equation for neutrino (K)

$$\Leftrightarrow\ \gamma(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{k}})\boldsymbol{F}(\boldsymbol{r})=\varepsilon\boldsymbol{F}(\boldsymbol{r})$$

$$\Leftrightarrow\ \gamma(\sigma_x\hat{k}_x+\sigma_y\hat{k}_y)\boldsymbol{F}(\boldsymbol{r})=\varepsilon\boldsymbol{F}(\boldsymbol{r})$$

$$\begin{pmatrix} 0 & \gamma(\hat{k}_x-i\hat{k}_y) \\ \gamma(\hat{k}_x+i\hat{k}_y) & 0 \end{pmatrix}\begin{pmatrix} F^A(\boldsymbol{r}) \\ F^B(\boldsymbol{r}) \end{pmatrix}=\varepsilon\begin{pmatrix} F^A(\boldsymbol{r}) \\ F^B(\boldsymbol{r}) \end{pmatrix}$$

$\hat{\boldsymbol{k}}=-i\vec{\nabla}$
**Velocity:** $v_F=\gamma/\hbar$
**K':** $\boldsymbol{\sigma}\to\boldsymbol{\sigma}^*$

$v_F\sim c/300\ (\gamma_0\sim 3\,\text{eV})$

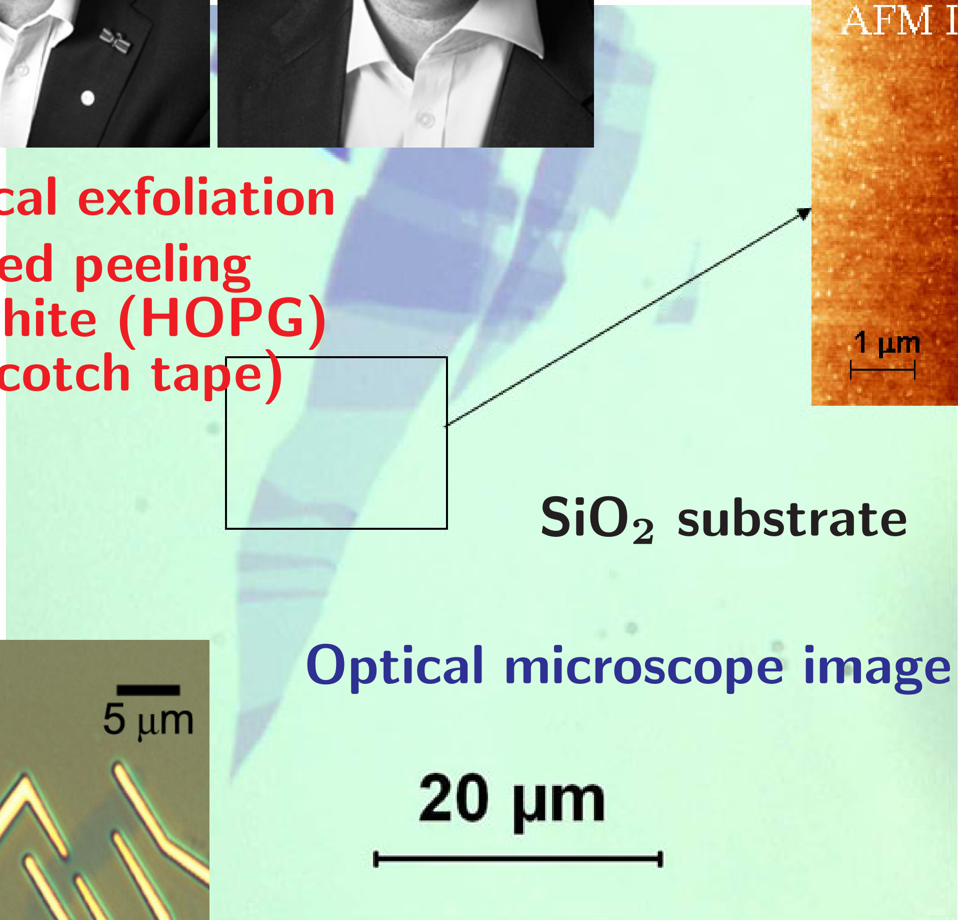
**Massless (Dirac)**
**Constant velocity (∼light, cannot stop)**
**Topological anomaly**

$\gamma=\sqrt{3}\gamma_0 a/2$ ($\gamma_0$: **Hopping integral**)

# A.K. Geim & K.S. Novoselov – Nobel Prize Physics 2010 –

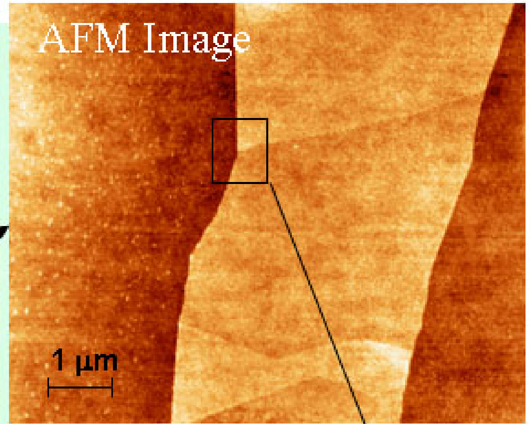
*K.S. Novoselov et al., Science 306, 666 (2004)*

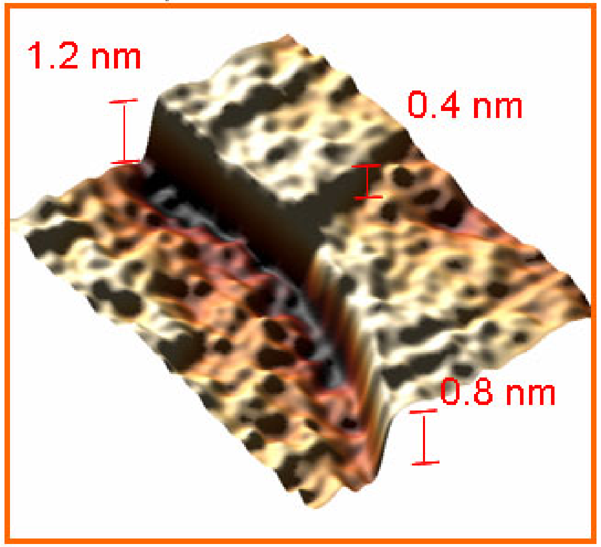
**Mechanical exfoliation (Repeated peeling of graphite (HOPG) using scotch tape)**

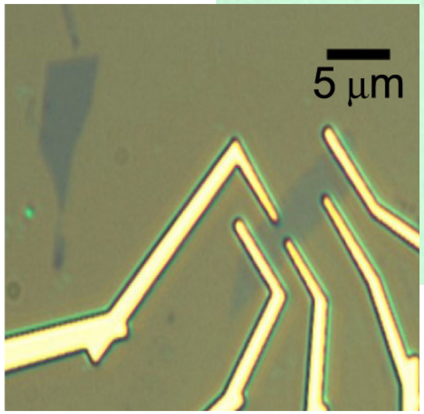



$SiO_2$ substrate

Optical microscope image



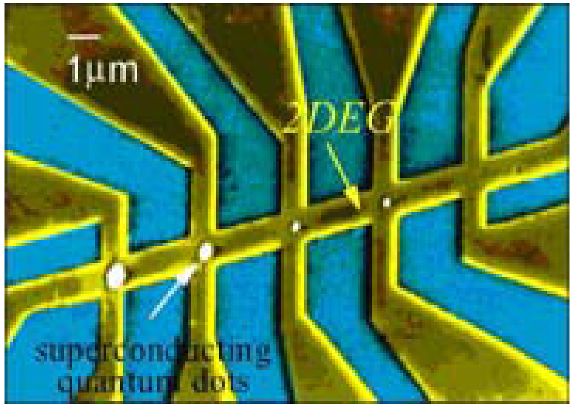



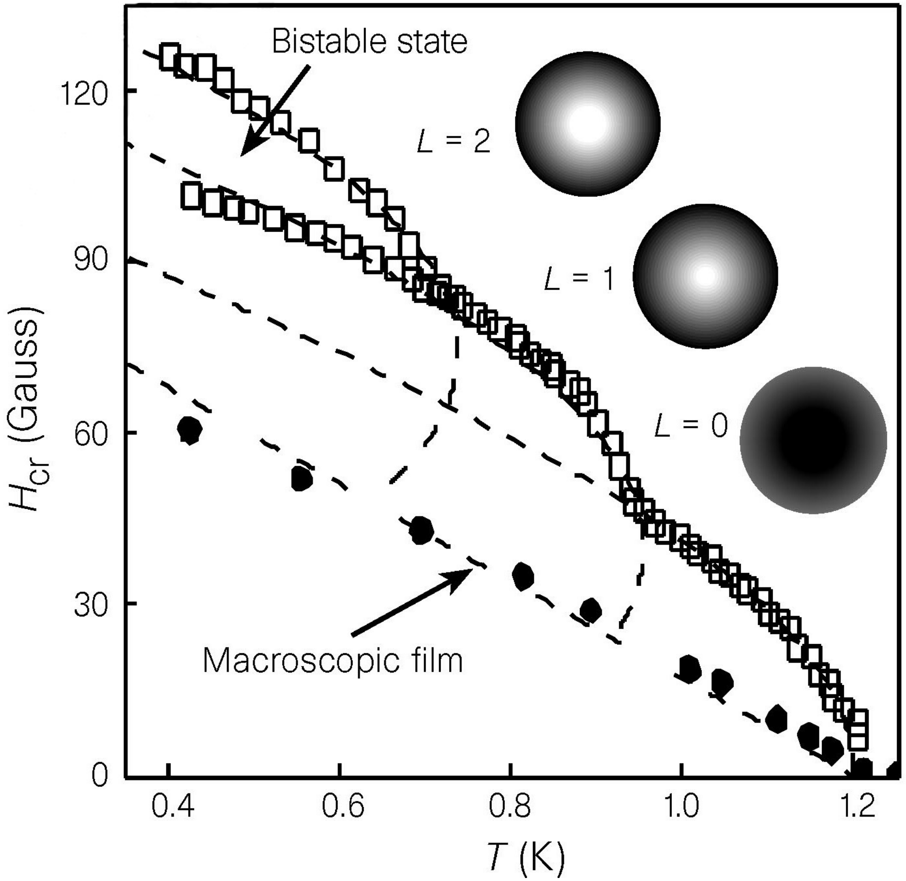



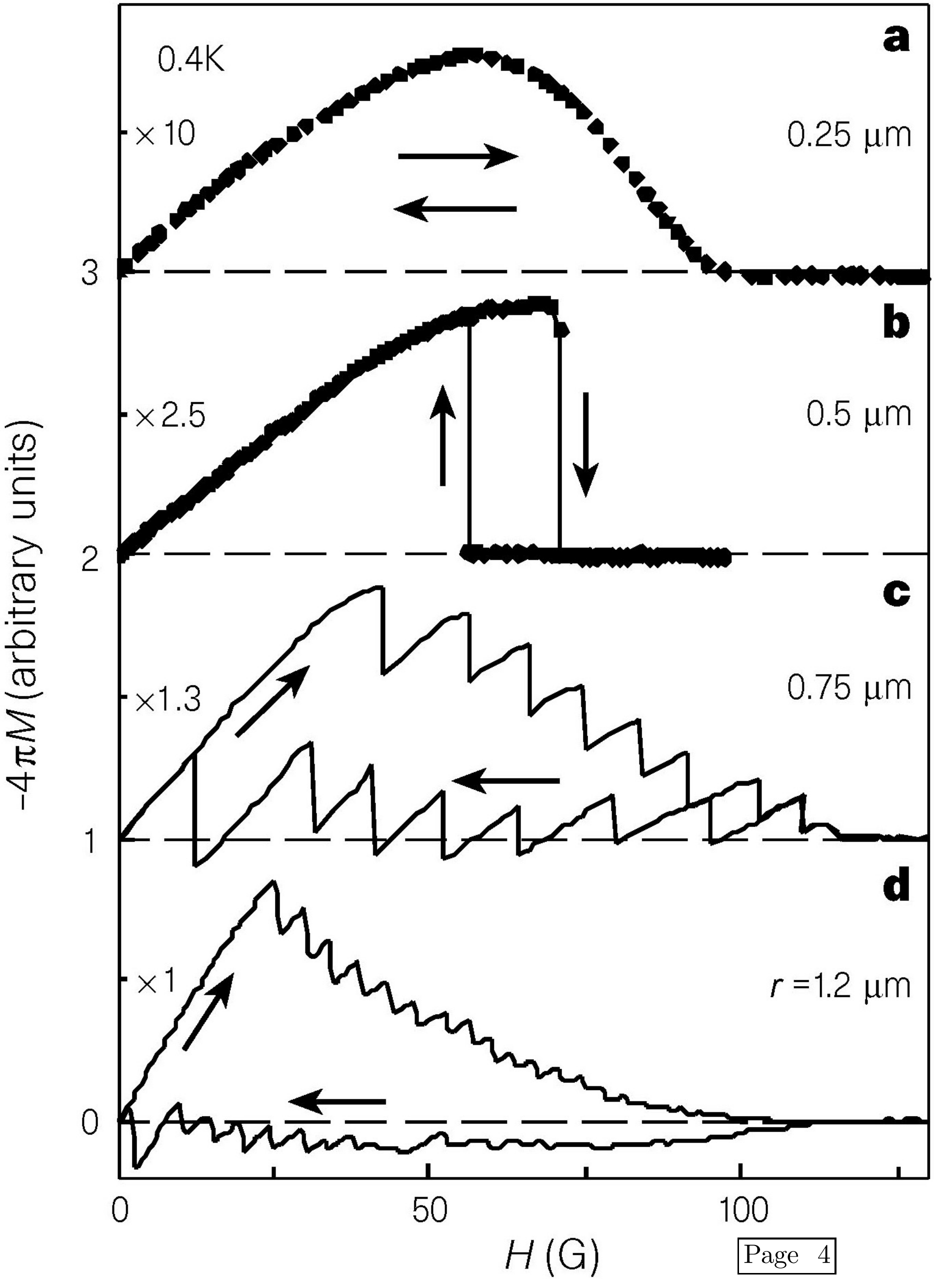

**FET: Field Effect Transistor**

$(n_s < 5\times 10^{13}\,\mathrm{cm}^{-2})$

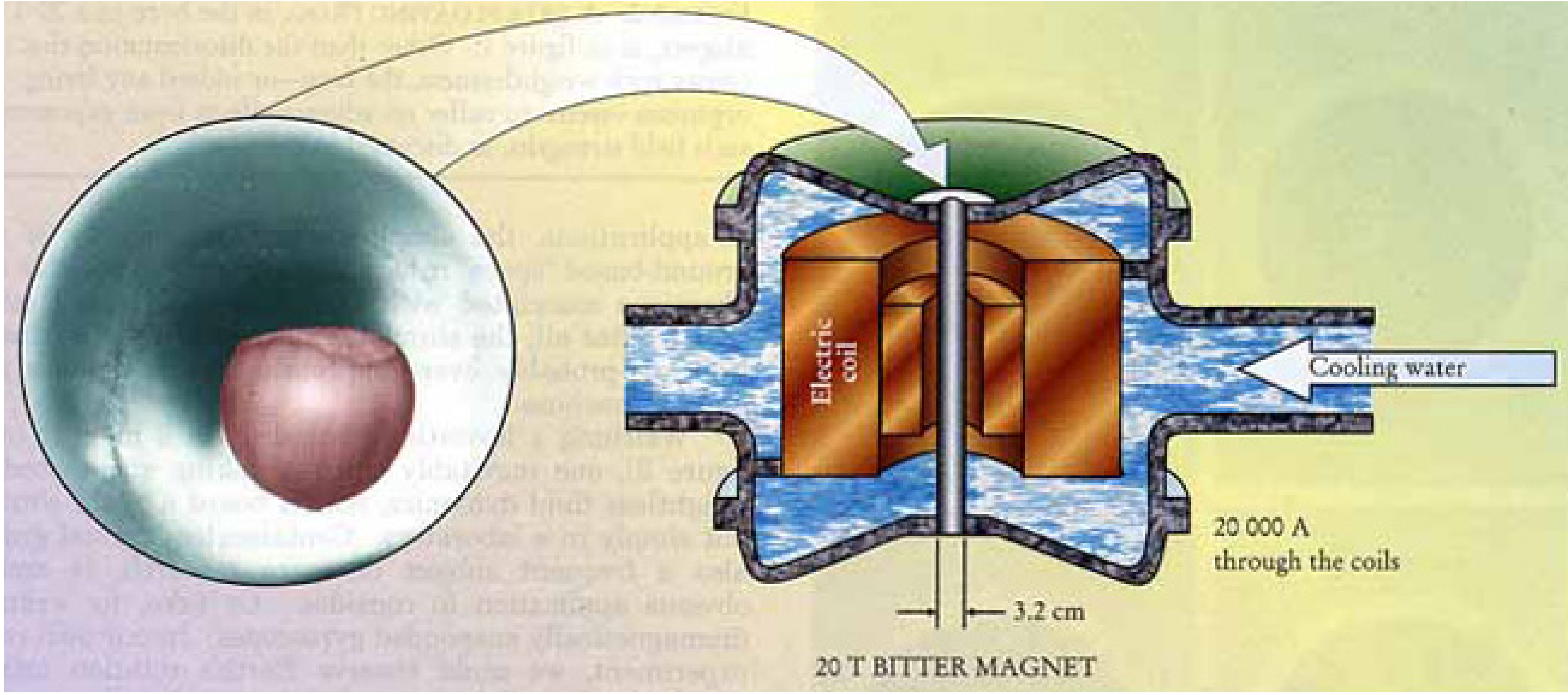
# ‘Phase Transitions’ in Small Superconductors (Nijmegen, ∼1997)



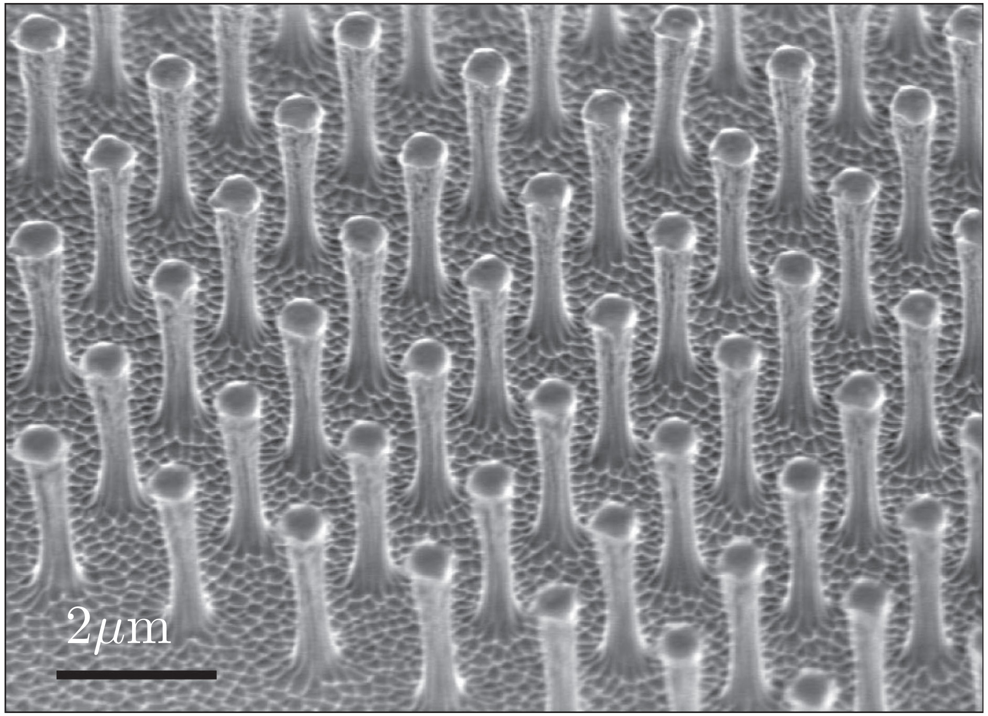



# Magnetic Levitation (Nijmegen, ∼1998)




# Gecko Tape (Manchester, ∼2003)




**Gecko (やもり)**

# Topological Anomaly and Berry's Phase

$$R(\theta) = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$

**Weyl's equation : Neutrino ⇔ Helicity ($\boldsymbol{\sigma} \leftrightarrow \boldsymbol{k}$)**

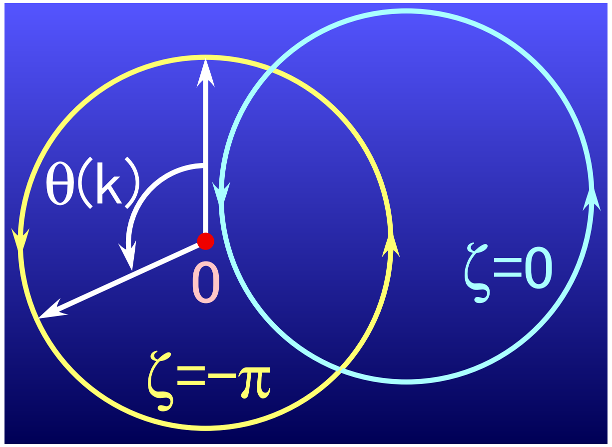
$$\gamma(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{k}})\,\boldsymbol{F}_{s\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon_s(\boldsymbol{k})\,\boldsymbol{F}_{s\boldsymbol{k}}(\boldsymbol{r}) \qquad \boldsymbol{F}_{s\boldsymbol{k}}(\boldsymbol{r}) = \frac{e^{i\varphi_{\boldsymbol{k}}}}{\sqrt{2L^2}}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})\,R^{-1}[\theta(s\boldsymbol{k})]\big|s)$$

$$R(\theta\pm 2\pi) = -R(\theta) \qquad R(-\pi) = -R(+\pi)$$

$$\varepsilon_s(\boldsymbol{k}) = s\gamma|\boldsymbol{k}| \quad s=\pm 1 \qquad \psi(T) = e^{-i\zeta}\psi(0)$$

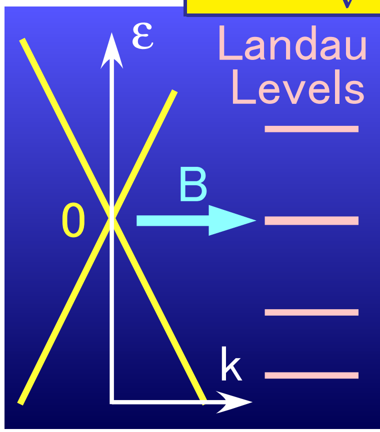
**Pseudo spin ⇒ Berry's phase**

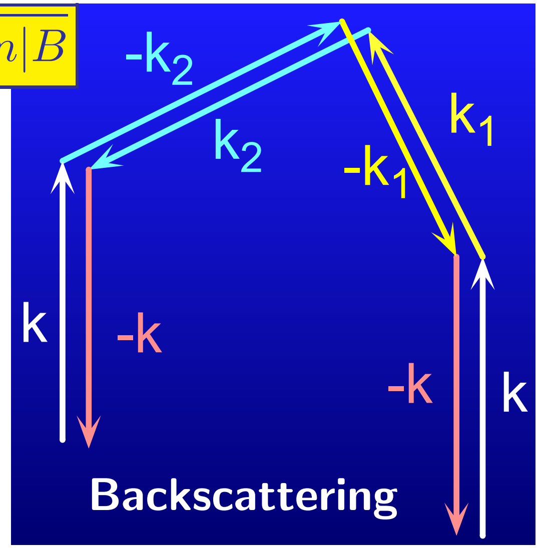
$$\zeta = -i\int_0^T dt \Big\langle s\boldsymbol{k}(t)\Big|\frac{d}{dt}\Big|s\boldsymbol{k}(t)\Big\rangle = -\pi \qquad \frac{1}{\sqrt{2}}\begin{pmatrix} s \\ e^{i\theta} \end{pmatrix}$$




**Landau levels at** $\varepsilon=0$ [*J.W. McClure, PR* 104*, 666 (1956)*]

$$\chi = -\frac{g_{\rm v} g_{\rm s}\gamma^2}{6\pi}\left(\frac{e}{c\hbar}\right)^2\int\left(-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right)\delta(\varepsilon)\,d\varepsilon \qquad \varepsilon_n \propto \pm\sqrt{|n|B}$$



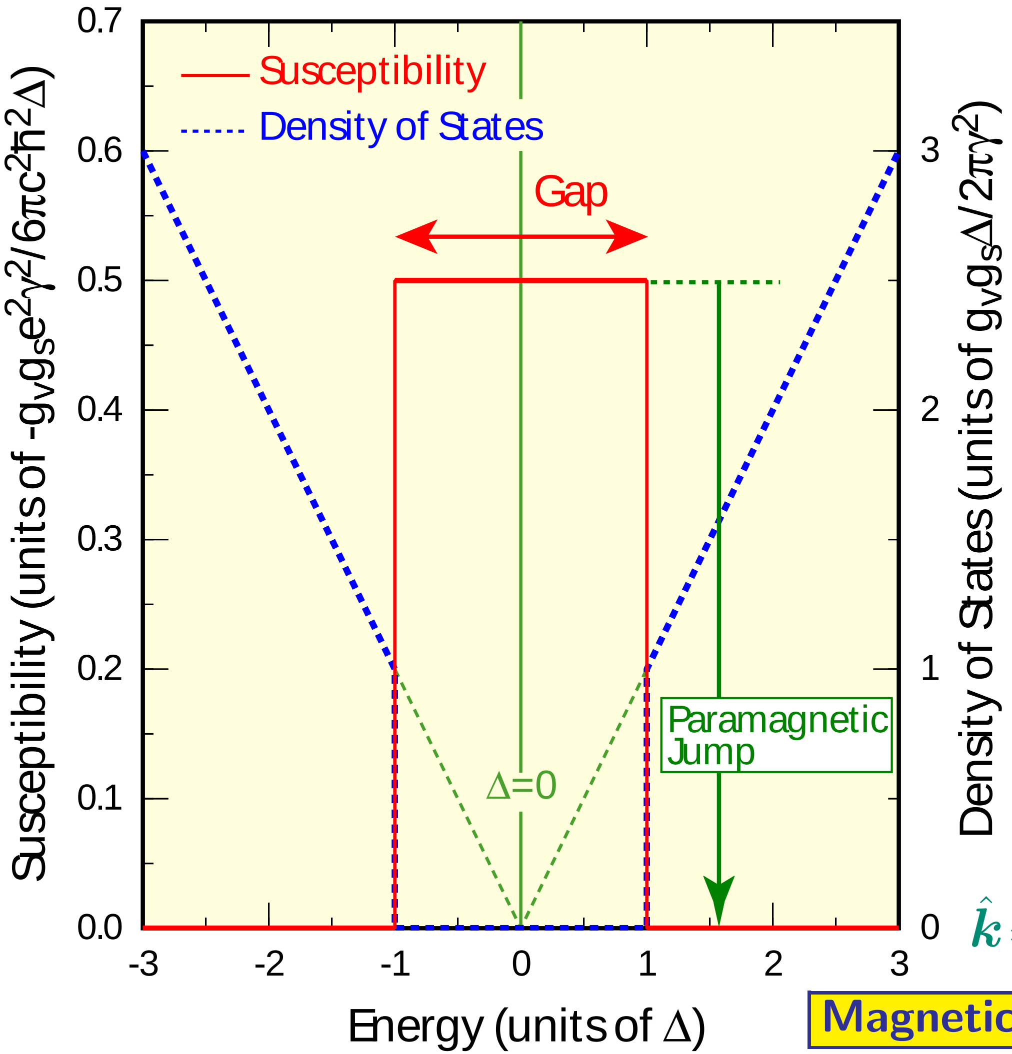

**Absence of backscattering**

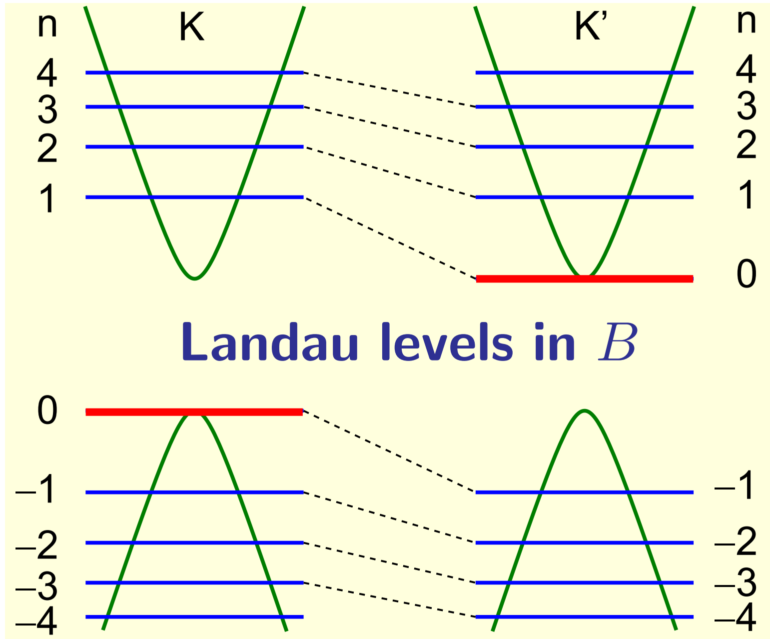
**Metallic CN with scatterers**

**⇒ Perfect conductor**

*T. Ando & T. Nakanishi, JPSJ* 67*, 1704 (1998)*

# Band-Gap Effect [*M. Koshino & T. Ando, PRB* 81*, 195431 (2010)*]




**Landau levels in $B$**

**Hamiltonian at band edge**

$$\mathcal{H} = \frac{\hbar^2 \hat{\boldsymbol{k}}^2}{2m^*} \pm \frac{e\hbar}{2m^* c} B \qquad m^* = \frac{\hbar^2 \Delta}{\gamma^2}$$

$$\hat{\boldsymbol{k}} = \frac{\vec{\nabla}}{i} + \frac{e\boldsymbol{A}}{c\hbar}$$

**Magnetic moment**

$$\chi_P(\varepsilon) = +\left(\frac{e\hbar}{2m^* c}\right)^2 D(\varepsilon)$$

**Pauli**

$$\chi_L(\varepsilon) = -\frac{1}{3}\left(\frac{e\hbar}{2m^* c}\right)^2 D(\varepsilon)$$

**Landau**

$$D(\varepsilon) = \frac{g_s g_v m^*}{2\pi\hbar^2}$$

**Graphene with a gap**

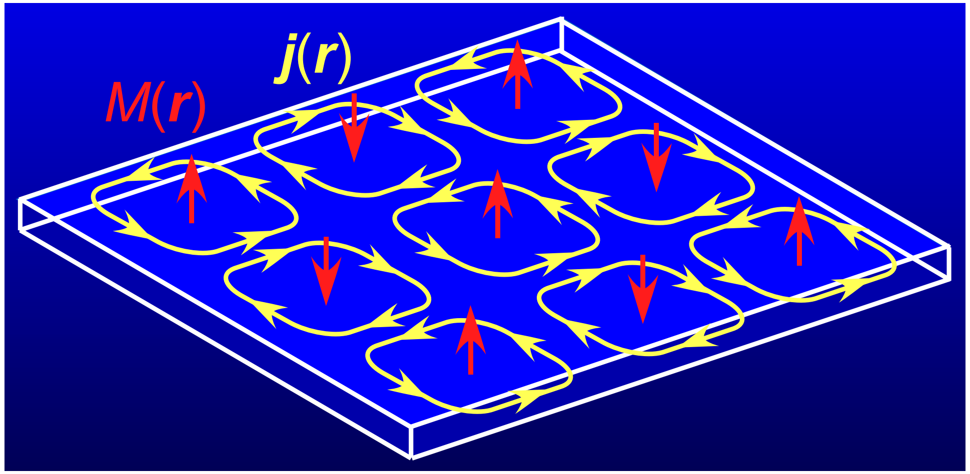
$$\begin{pmatrix} \Delta & \gamma \hat{k}_- \\ \gamma \hat{k}_+ & -\Delta \end{pmatrix} \Rightarrow \chi(\varepsilon) = -\frac{g_v g_s e^2 \gamma^2}{6\pi c^2 \gamma^2} \overbrace{\frac{\theta(\Delta - |\varepsilon|)}{2\Delta}}^{\to\, \delta(\varepsilon)}$$

# Diamagnetic Susceptibility of Spatially Varying Field

**Induced current** $\hat{K}(\boldsymbol{r}) = (K_{\mu\nu}(\boldsymbol{r}))$

$$\boldsymbol{j}(\boldsymbol{r}) = \int \hat{K}(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{A}(\boldsymbol{r}')\,d\boldsymbol{r}'$$

$$\Leftrightarrow \boldsymbol{j}(\boldsymbol{q}) = \hat{K}(\boldsymbol{q})\boldsymbol{A}(\boldsymbol{q})$$




**Gauge invariance**
**Current conservation**

$$K_{\mu\nu}(\boldsymbol{q}) = K(q)\left[\delta_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right]$$

**Magnetic moment:** $M(\boldsymbol{r}) \Leftrightarrow \boldsymbol{j}(\boldsymbol{r}) = c\,(\boldsymbol{\nabla}\times\hat{z})M(\boldsymbol{r}) \quad H(\boldsymbol{r}) = \boldsymbol{\nabla}\times\boldsymbol{A}(\boldsymbol{r})$

**Diamagnetic susceptibility:** $\chi(\boldsymbol{q}) = \frac{1}{cq^2}K(q) \Leftrightarrow M(\boldsymbol{q}) = \chi(\boldsymbol{q})H(\boldsymbol{q})$

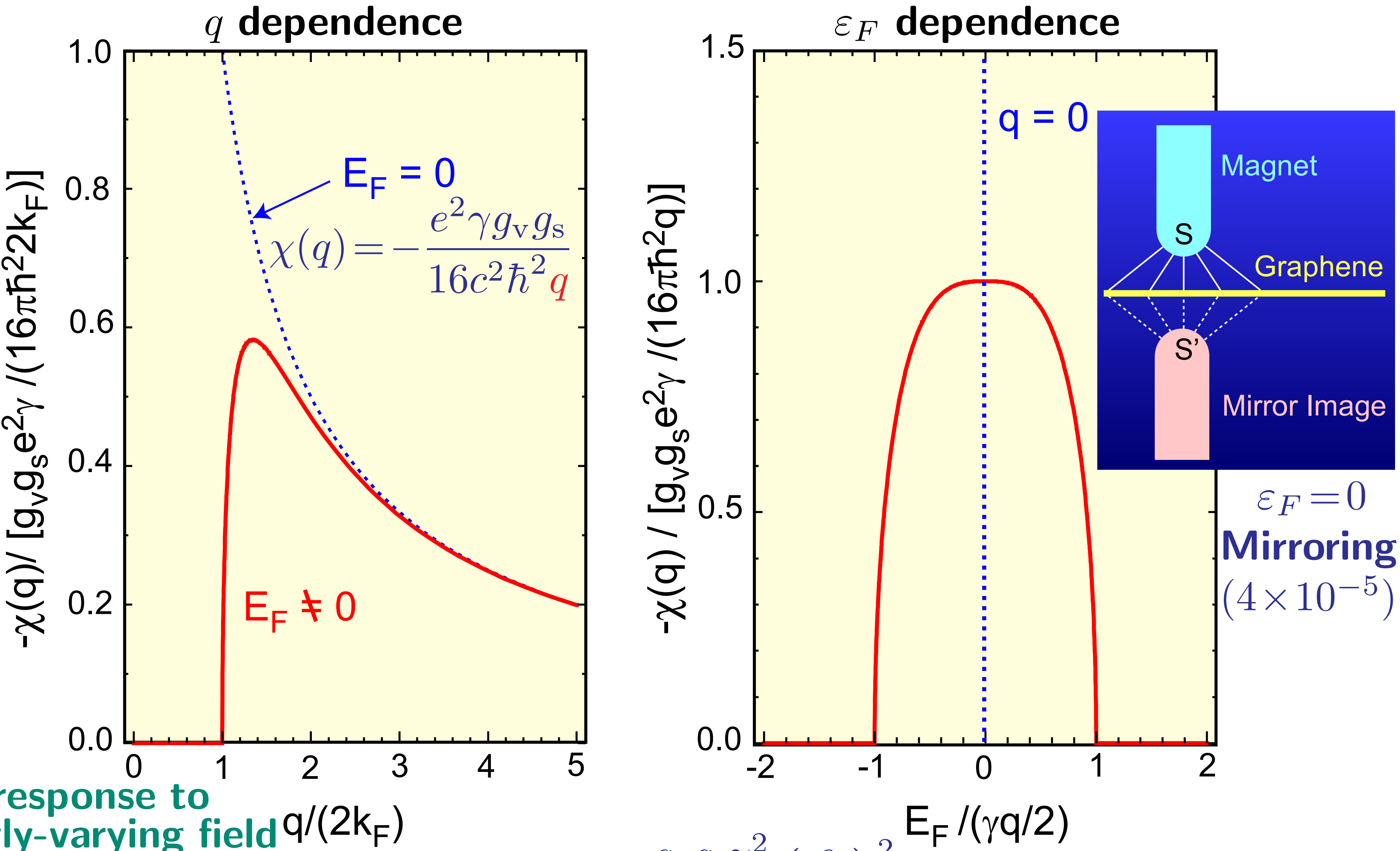
$$\chi(q) = -\frac{e^2\gamma g_{\rm v} g_{\rm s}}{16c^2\hbar^2}\frac{1}{q}\theta(q-2k_F)\left[1 + \frac{2}{\pi}\frac{2k_F}{q}\sqrt{1-\left(\frac{2k_F}{q}\right)^2} - \frac{2}{\pi}\sin^{-1}\left(\frac{2k_F}{q}\right)\right]$$

$$\Rightarrow \chi(q) = \begin{cases} 0 & (q < 2k_F) \\ \sim q^{-1} & (q > 2k_F) \end{cases} \qquad \int_{-\infty}^{\infty}\chi(q;\varepsilon_F)d\varepsilon_F = -\frac{g_{\rm v} g_{\rm s}\gamma^2}{6\pi}\left(\frac{e}{c\hbar}\right)^2$$

**2DEG:** $\chi(q) = -\frac{e^2 g_{\rm v} g_{\rm s}}{24\pi m^* c^2}\left(1-\left[1-\left(\frac{2k_F}{q}\right)^2\right]^{3/2}\theta(q-2k_F)\right)$

# Diamagnetic Susceptibility $\chi(q)$ of Spatially Varying Field

*M. Koshino, Y. Arimura, and T. Ando, PRL 102, 177203 (2009)*




$\varepsilon_F = 0$

**Mirroring**

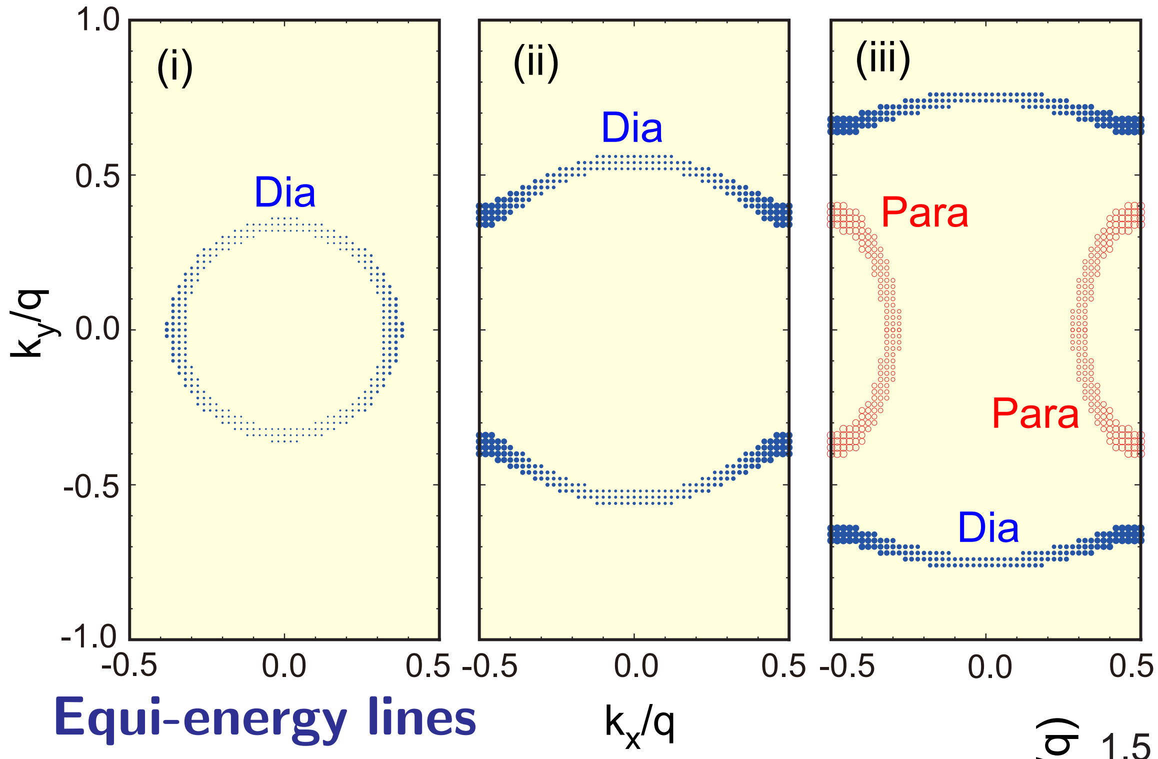
$(4\times10^{-5})$

**No response to slowly-varying field**

**Uniform limit:** $\lim_{q\to 0} \chi(q) = -\frac{g_v g_s \gamma^2}{6\pi}\left(\frac{e}{c\hbar}\right)^2 \delta(\varepsilon_F)$

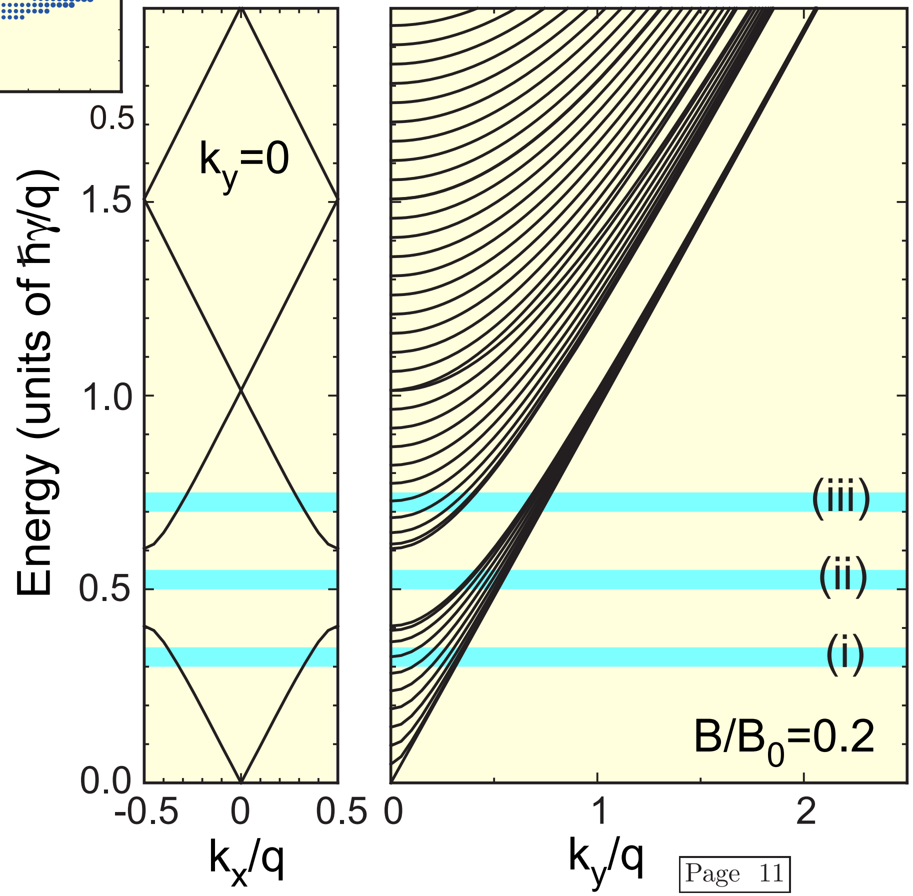
**Magnetic Superlattice**
*M. Koshino & T. Ando, Solid State Commun. 151, 1054 (2011)*

*cf. C.H. Park et al., PRL 101, 126804 (2008), . . .*

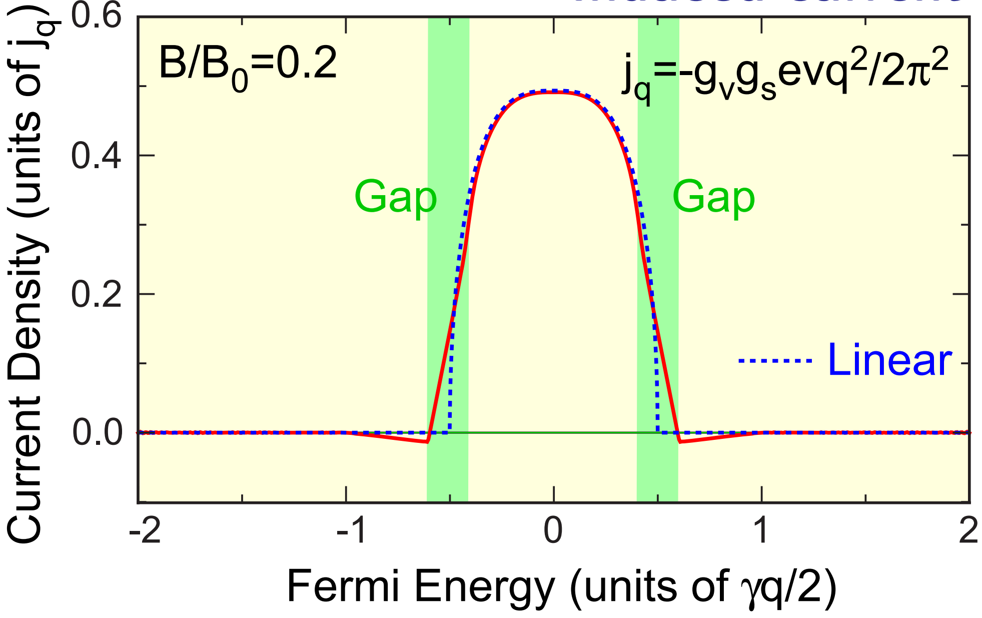



## Equi-energy lines

## Energy bands




## Induced current



# Zero-Mode Anomaly in Conductivity

**Density of states:** $D(\varepsilon) = \frac{|\varepsilon|}{2\pi\gamma^2}$ $\Rightarrow$ **Zero-gap semiconductor**

**Boltzmann conductivity**

$$\sigma(\varepsilon_F) = g_s g_v e^2 D^* D(\varepsilon_F) = \frac{g_s g_v}{4} \frac{e^2}{\pi^2 \hbar} \frac{1}{W}$$

**Einstein relation**

$$D^* = v_F^2 \tau = \frac{\gamma^2}{\hbar^2}\tau \qquad W = \frac{n_i u^2}{4\pi\gamma^2} \ll 1$$

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} n_i u^2 D(\varepsilon_F) \propto 2\pi W |\varepsilon_F|/\hbar$$

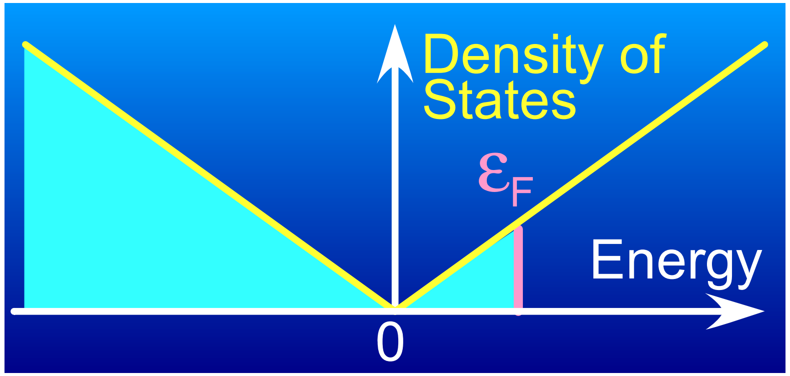
$$\tau \propto D(\varepsilon_F)^{-1}$$

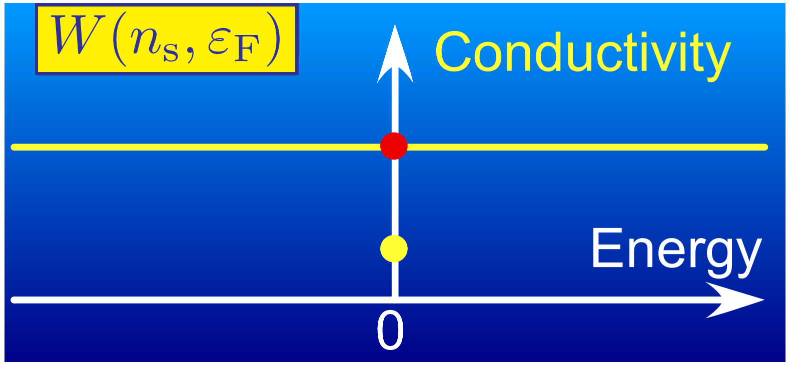
$u$ **Impurity strength**
$n_i$ **Impurity density**

**Short-range** $(k_F d \ll 1)$

$\Rightarrow$ **Metal!**

$\Rightarrow$ $\sigma(0)$ for $D(0)=0$ $\quad (\Rightarrow 2e^2/\pi^2\hbar)$




**Singularity at the Dirac point** $(\varepsilon_F = 0)$ $\Leftrightarrow$ **Fermi energy scaling**

$$\sigma_{xx}(B) = \sigma_{xx}\left(\frac{\hbar\omega_B}{\varepsilon_F}\right) \qquad \hbar\omega_B \propto \sqrt{B}$$

$$\sigma_{xy}(B) = \sigma_{xy}\left(\frac{\hbar\omega_B}{\varepsilon_F}\right)$$

**Magnetoconductivity**

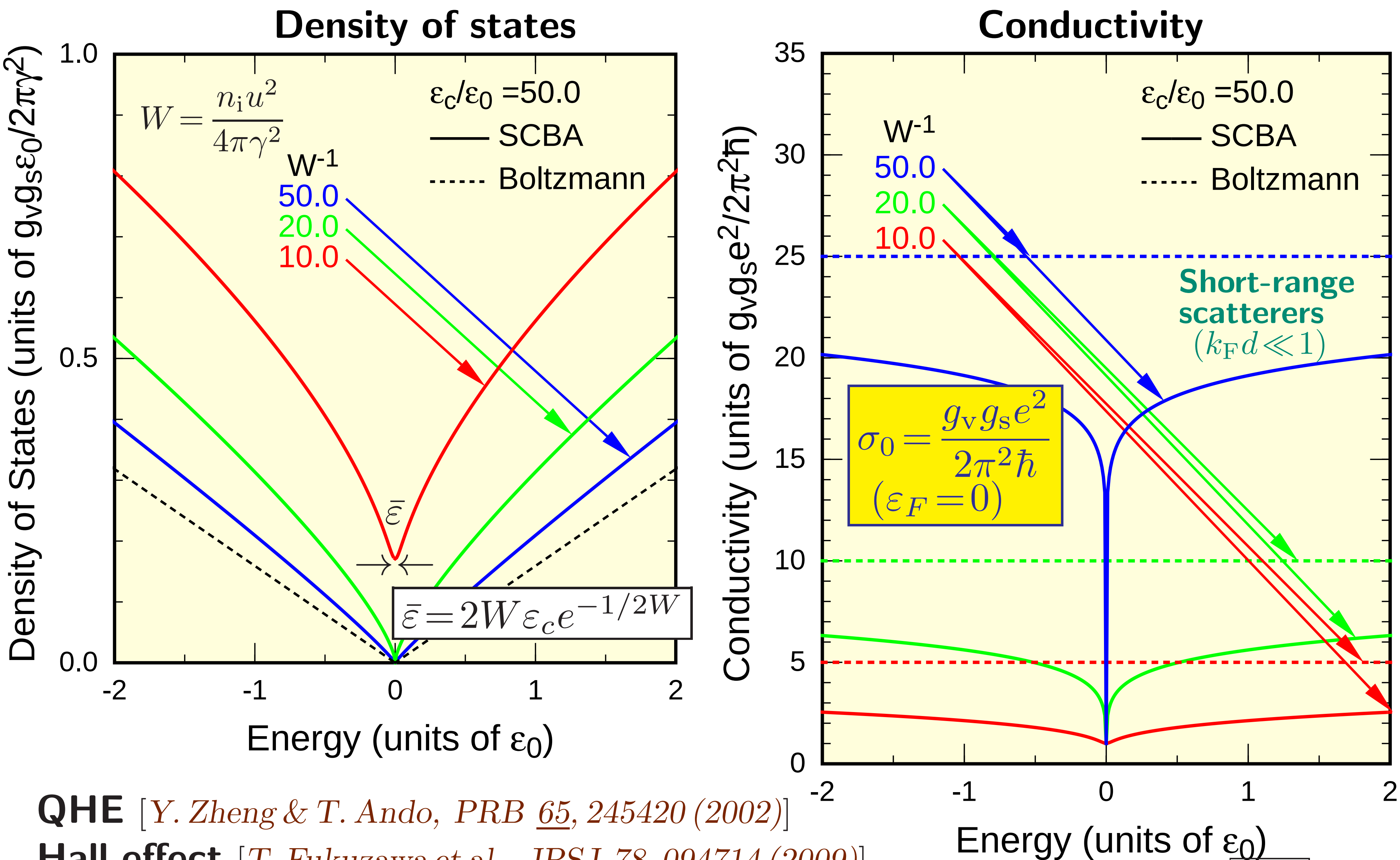
$$\sigma(\omega) = \sigma\left(\frac{\hbar\omega}{\varepsilon_F}\right) = \begin{cases} \frac{g_s g_v}{4}\frac{e^2}{2\pi^2\hbar W} & (\omega = 0) \quad \text{Intra-band} \\ \frac{g_v g_s}{4}\frac{e^2}{4\hbar} & (\hbar\omega/\varepsilon_F \gg 1) \quad \text{Inter-band} \end{cases}$$

**Dynamical conductivity**

*T. Ando et al., JPSJ 71, 1318 (2002)*

# Self-Consistent Born Approximation

[*N.H. Shon and T. Ando, J. Phys. Soc. Jpn.* 67, *2421 (1998)*]

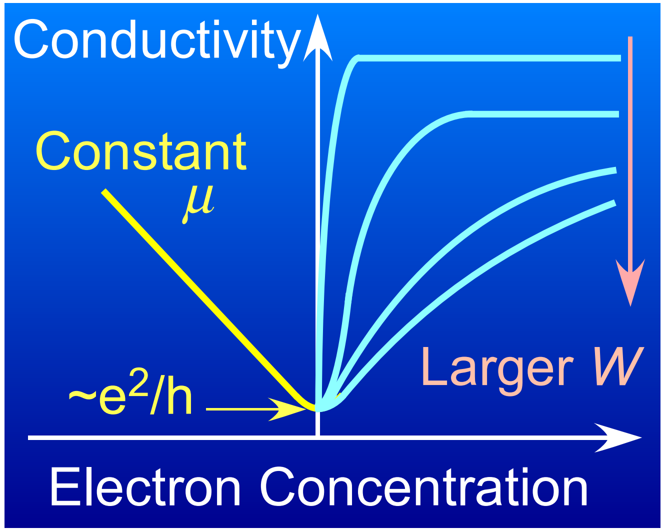



**QHE** [*Y. Zheng & T. Ando, PRB* 65, *245420 (2002)*]

**Hall effect** [*T. Fukuzawa et al., JPSJ* 78, *094714 (2009)*]

## Conductivity vs Carrier Concentration

*K.S. Novoselov et al., Nature* <u>438</u>, *197 (2005)*



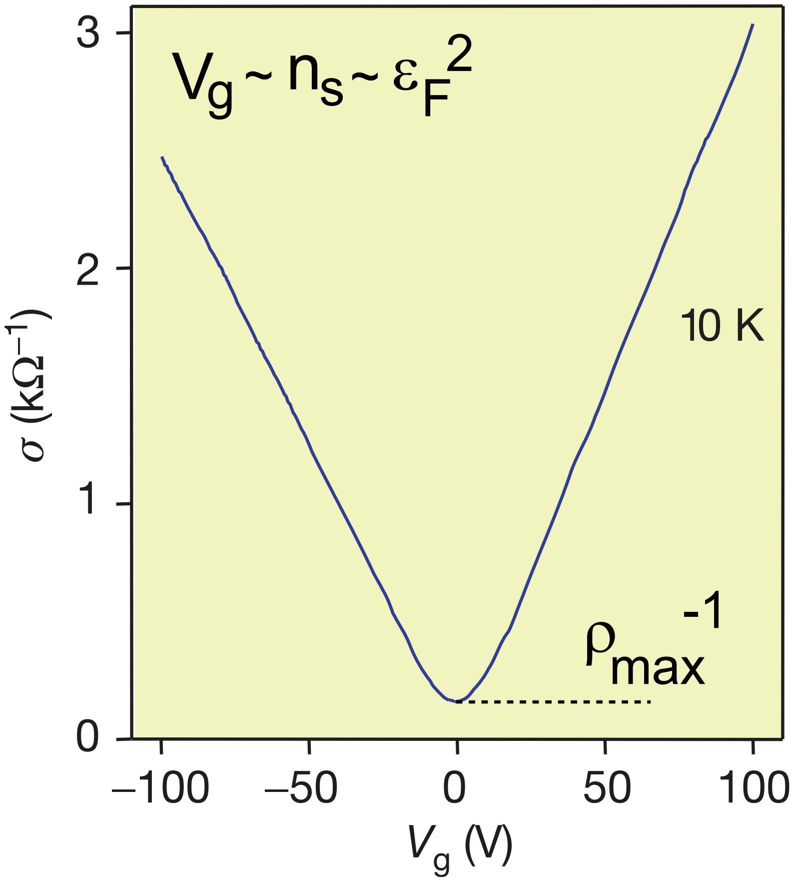

### Scattering mechanisms

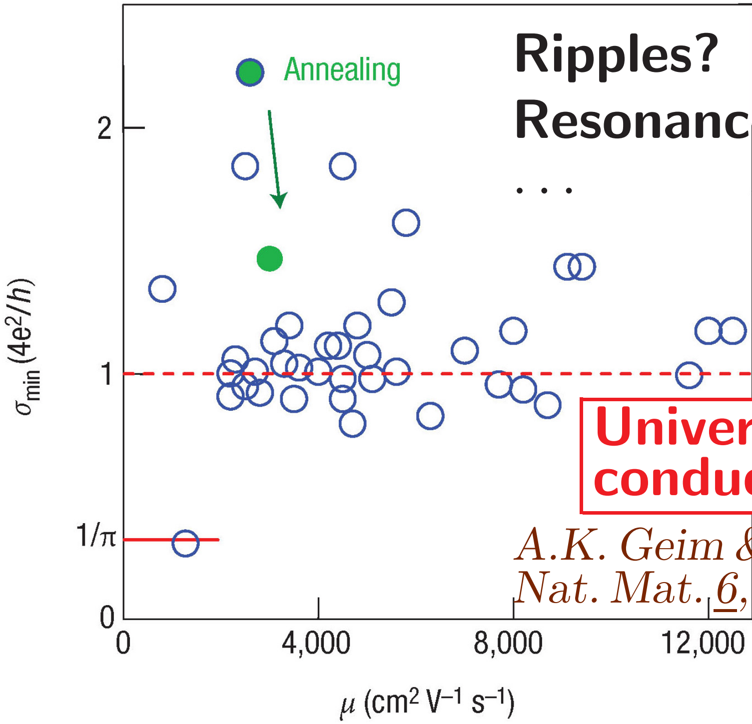
**Boltzmann conductivity** $\sigma(\varepsilon_F) = \dfrac{e^2}{\pi^2\hbar}\dfrac{1}{4W}$

**Constant mobility** $\Leftrightarrow W \propto n_s^{-1}$

**Charged impurity with screening**

- *T. Ando, JPSJ* <u>75</u>, *074716 (2006)*
- *K. Nomura & A.H. MacDonald, PRL* <u>96</u>, *256602 (2006)*




**Ripples?**

**Resonance scattering?**

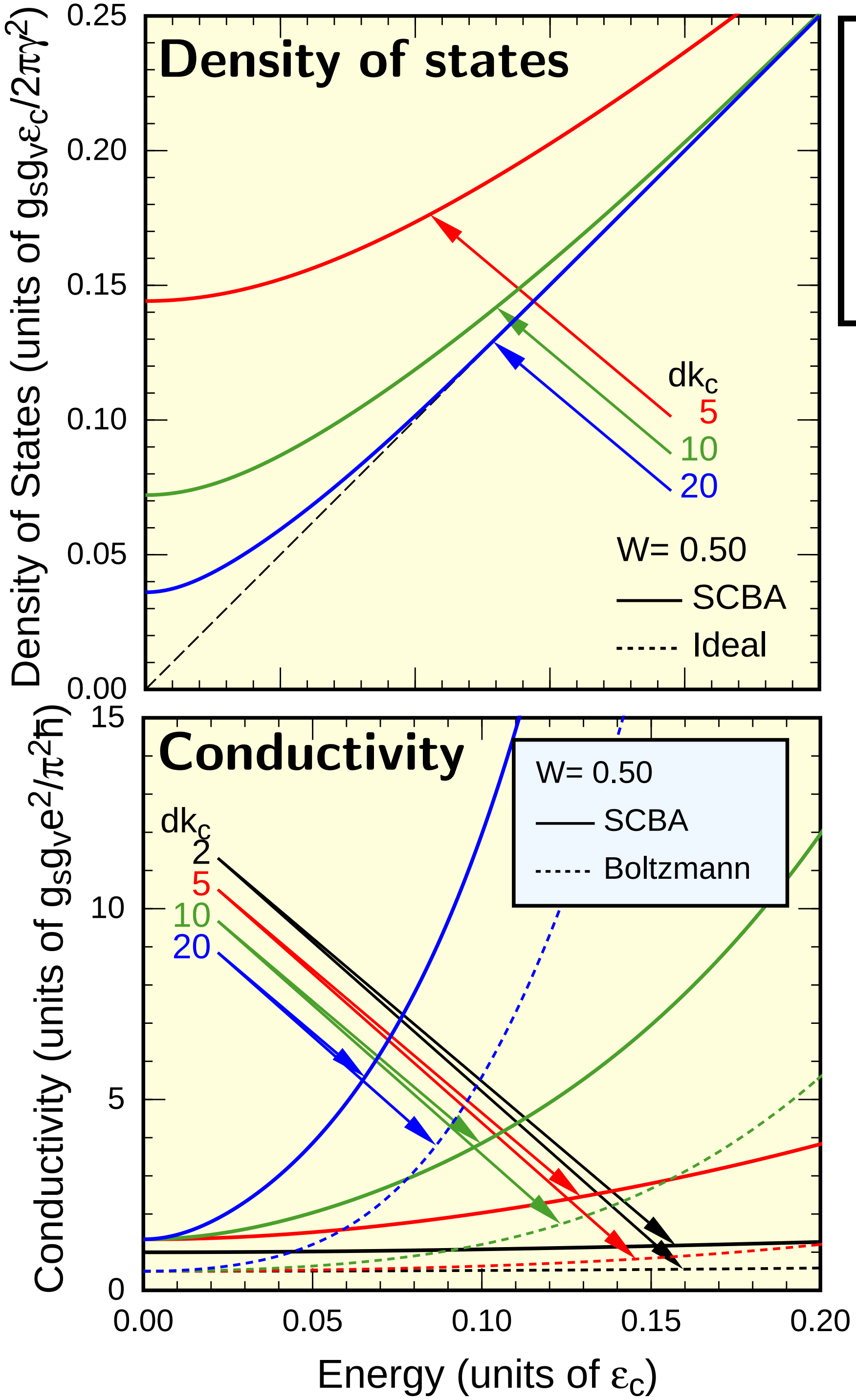
. . .

**Universal minimum conductivity?**

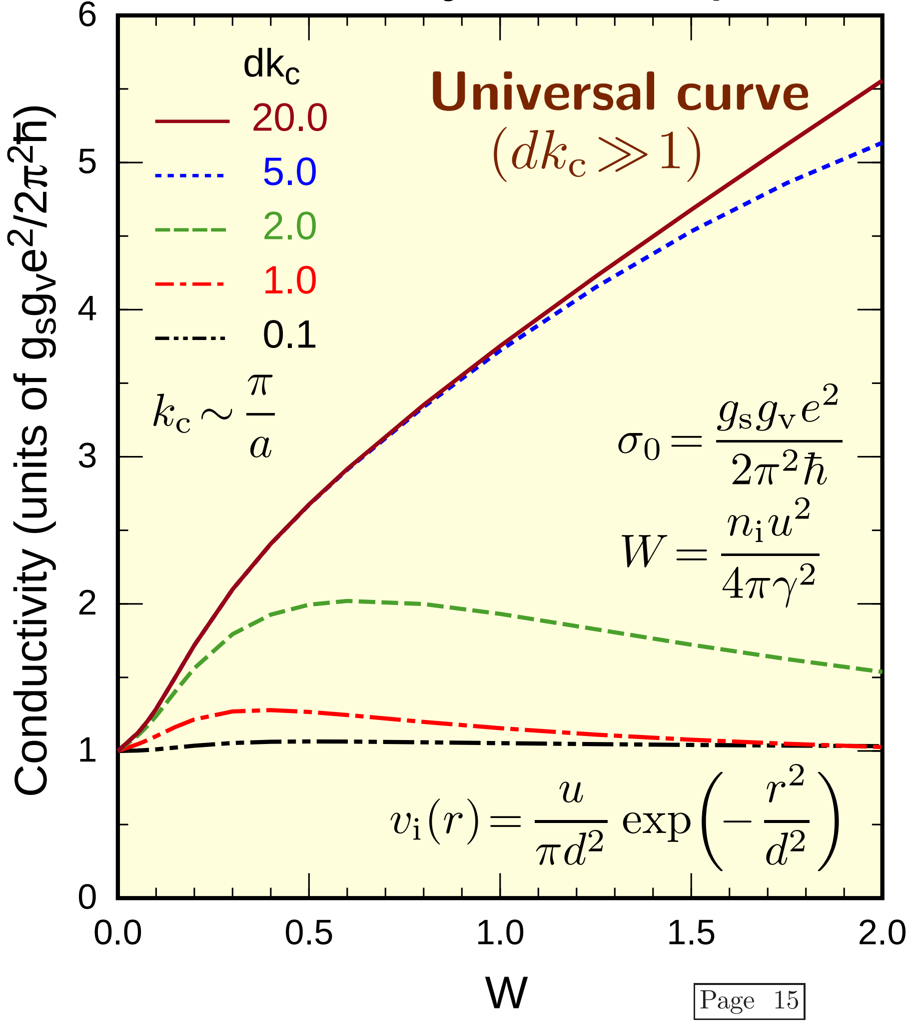
*A.K. Geim & K.S. Novoselov, Nat. Mat.* <u>6</u>, *183 (2007)*

# Scatterers with Gaussian Potential (Self-Consistent Born Approx.)

*[M. Noro, M. Koshino & T. Ando JPSJ 79, 094713 (2010)]*



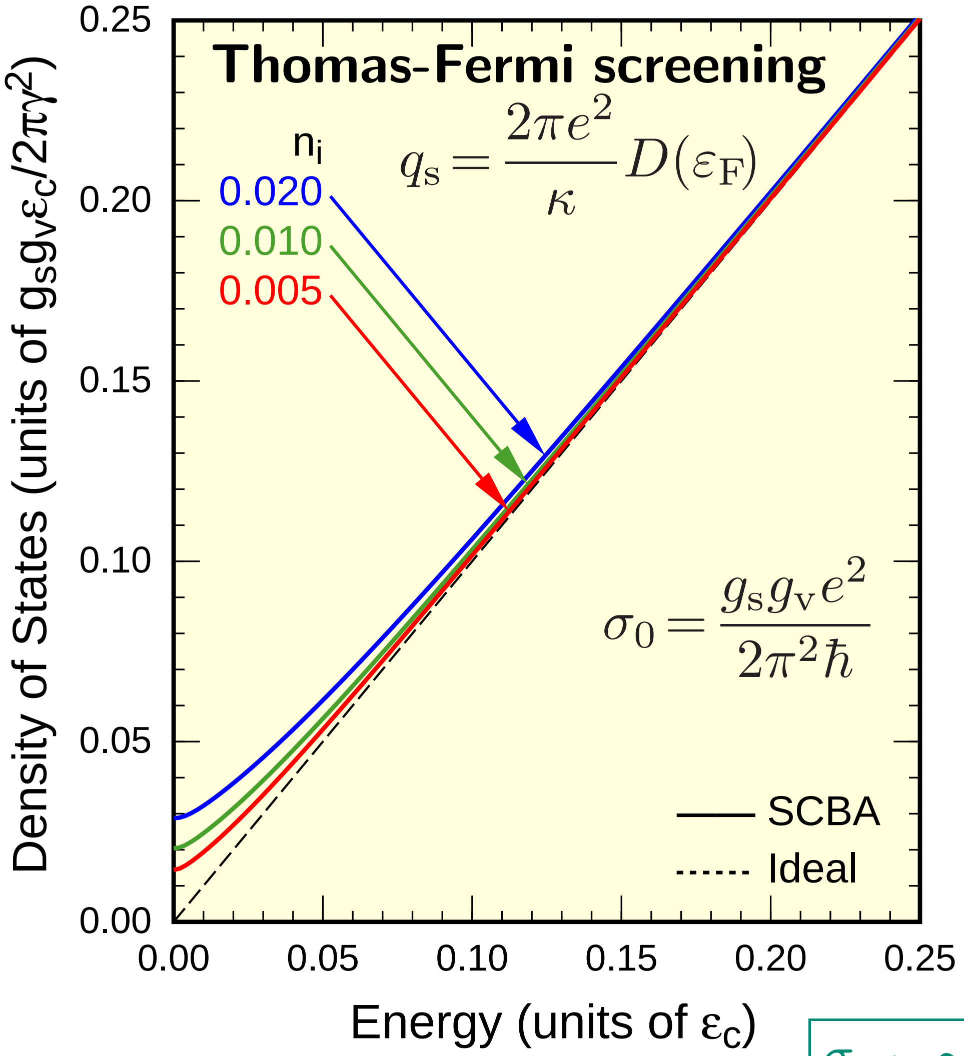

## Conductivity at Dirac point



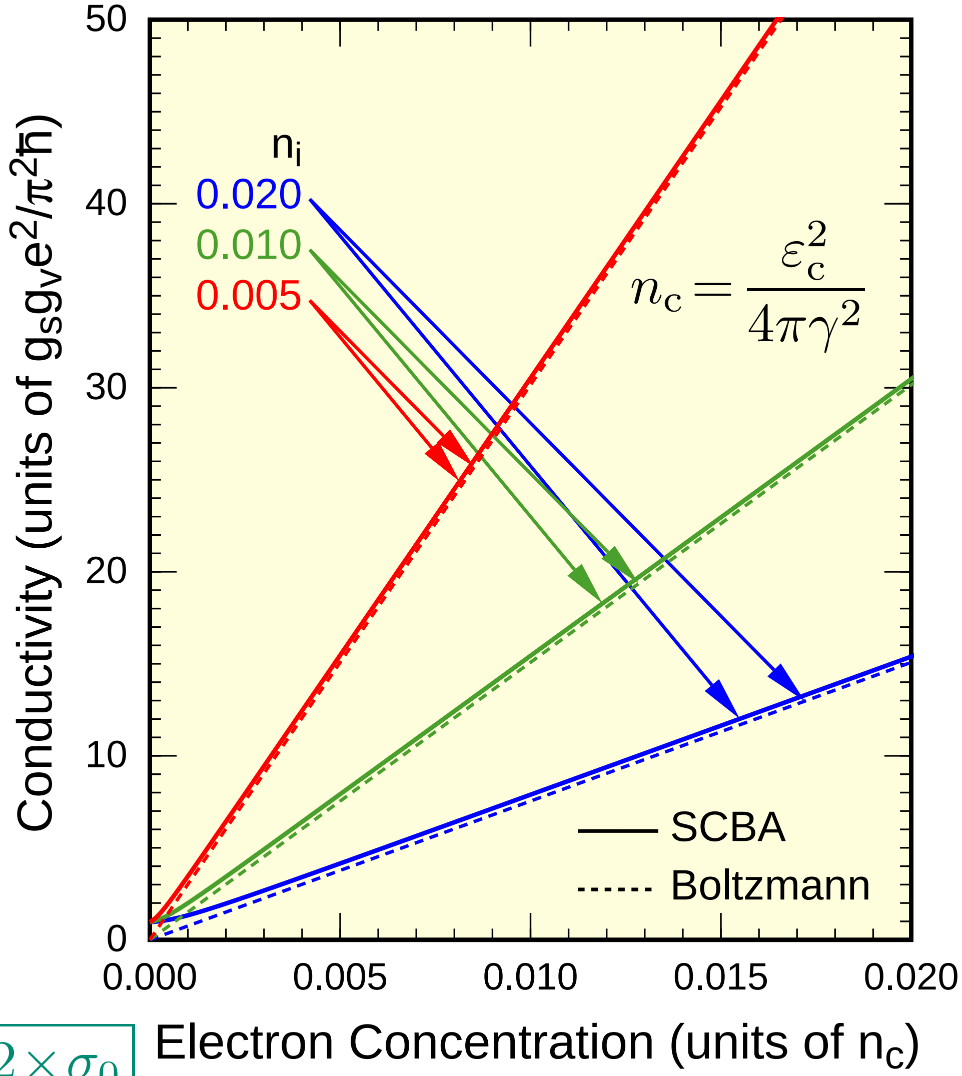
# Charged Impurities (Self-Consistent Born Approximation)

[*M. Noro, M. Koshino & T. Ando, J. Phys. Soc. Jpn.* 79, *094713 (2010)*]

## Density of states




## Conductivity vs $n_s$

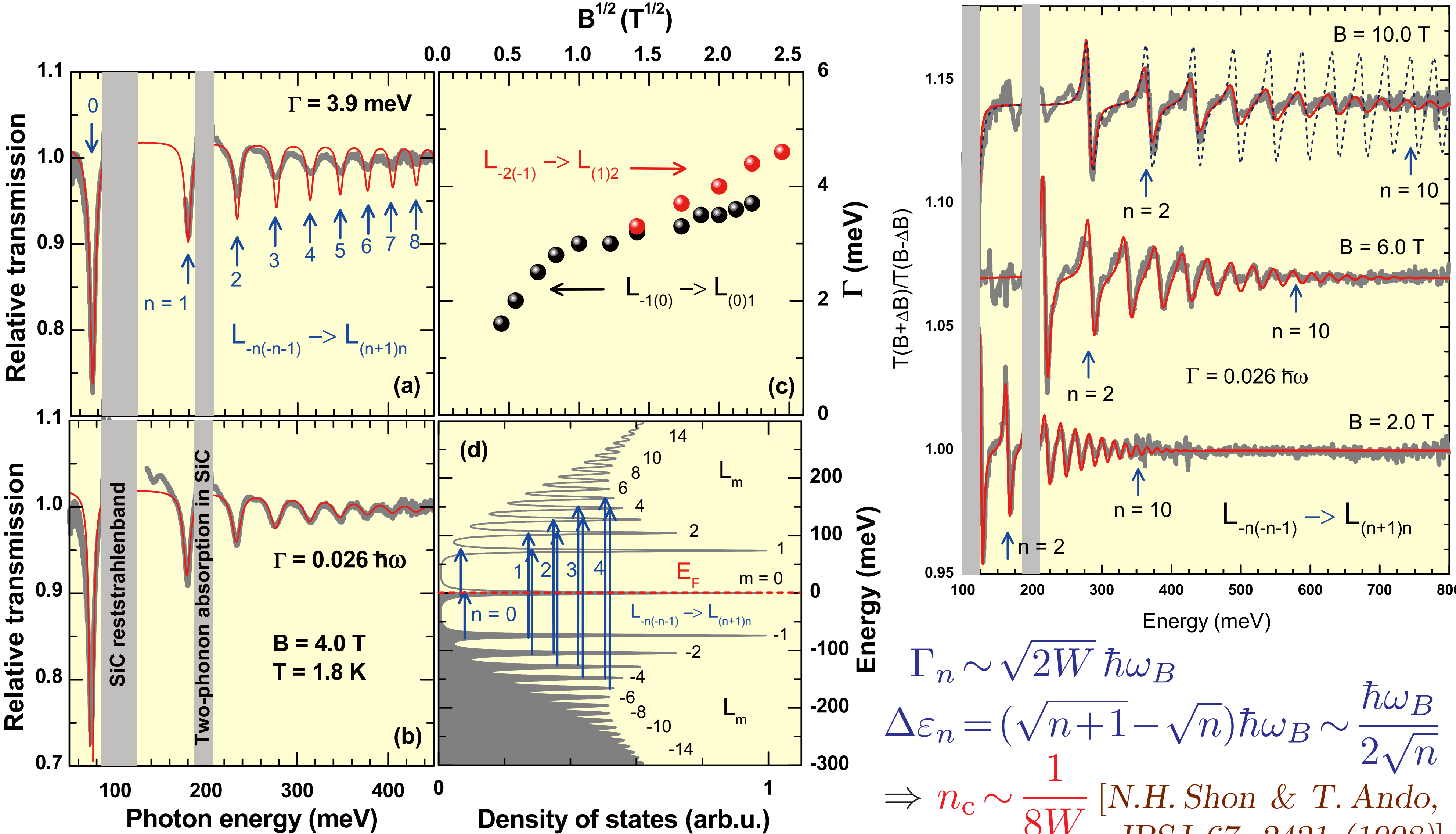



$\sigma_{\rm min} \sim 2 \times \sigma_0$

*cf: X.-Z. Yan & C.S. Ting*
*Phys. Rev. B* 80, *155423 (2009)*

# Interband Magnetoabsorption in Epitaxial Graphene

$\tau^{-1} \propto |\varepsilon|$ [*M. Orlita et al., Phys. Rev. Lett.* 107, *216603 (2011)*]




$$\Gamma_n \sim \sqrt{2W}\,\hbar\omega_B$$

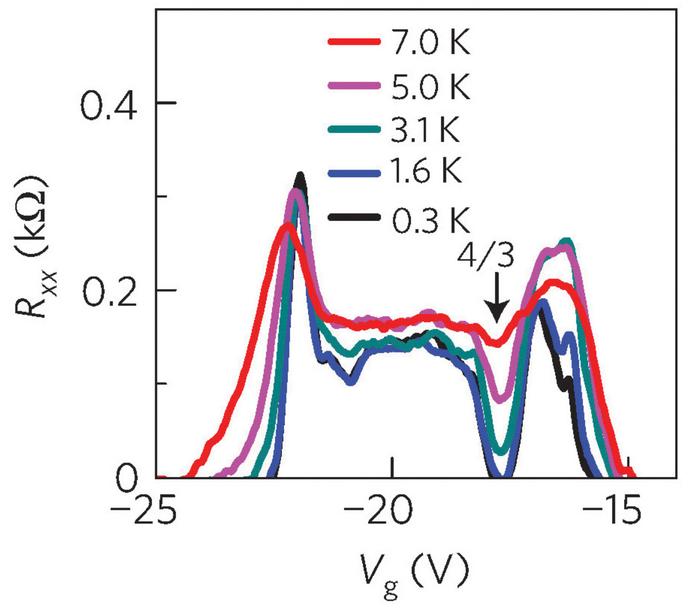
$$\Delta\varepsilon_n = (\sqrt{n+1} - \sqrt{n})\hbar\omega_B \sim \frac{\hbar\omega_B}{2\sqrt{n}}$$

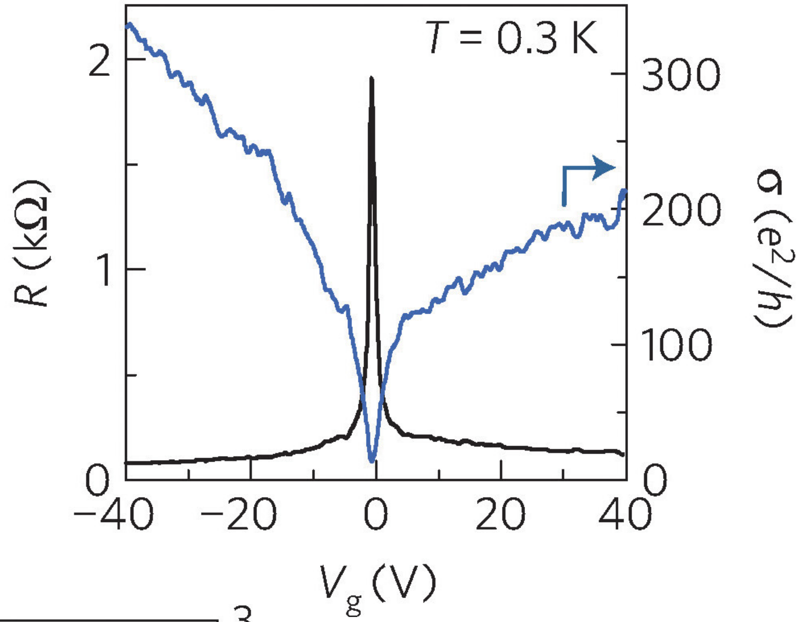
$$\Rightarrow n_c \sim \frac{1}{8W}$$ [*N.H. Shon & T. Ando, JPSJ* 67, *2421 (1998)*]

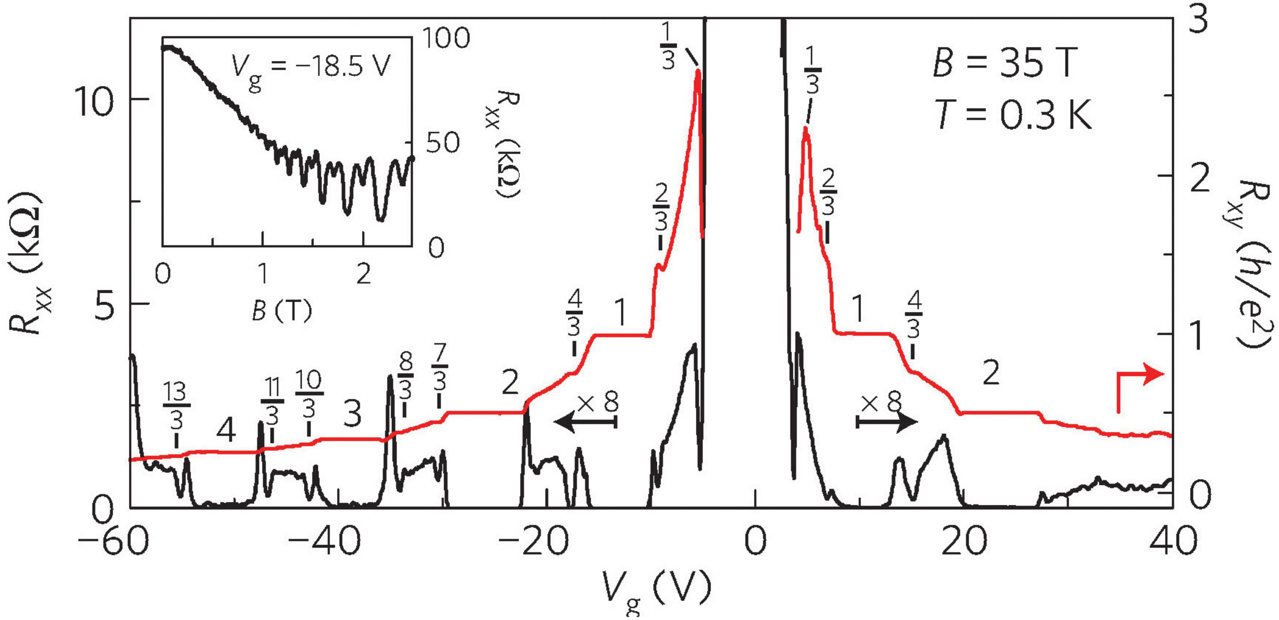
**Suspended, BN substrate, CVD grown, ⋯**

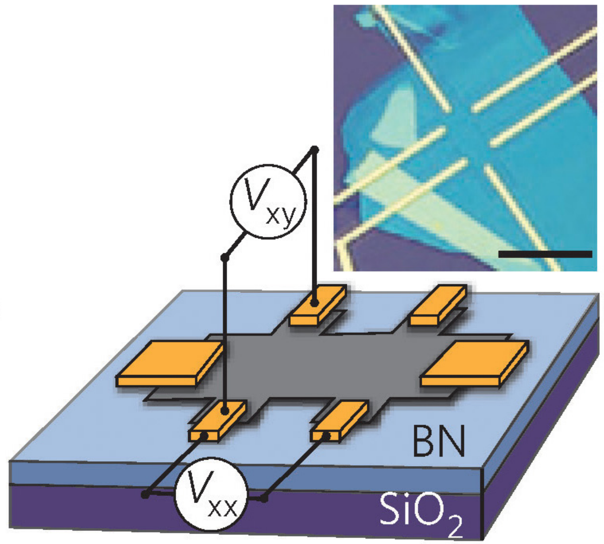
# Fractional Quantum Hall Effect (BN Substrate)

[*C.R. Dean et al., Nat. Phys.* 7, *693 (2011)*]



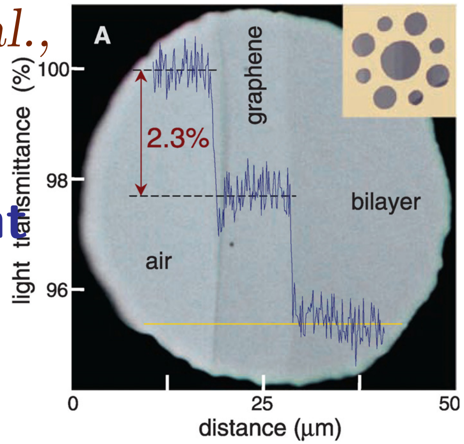



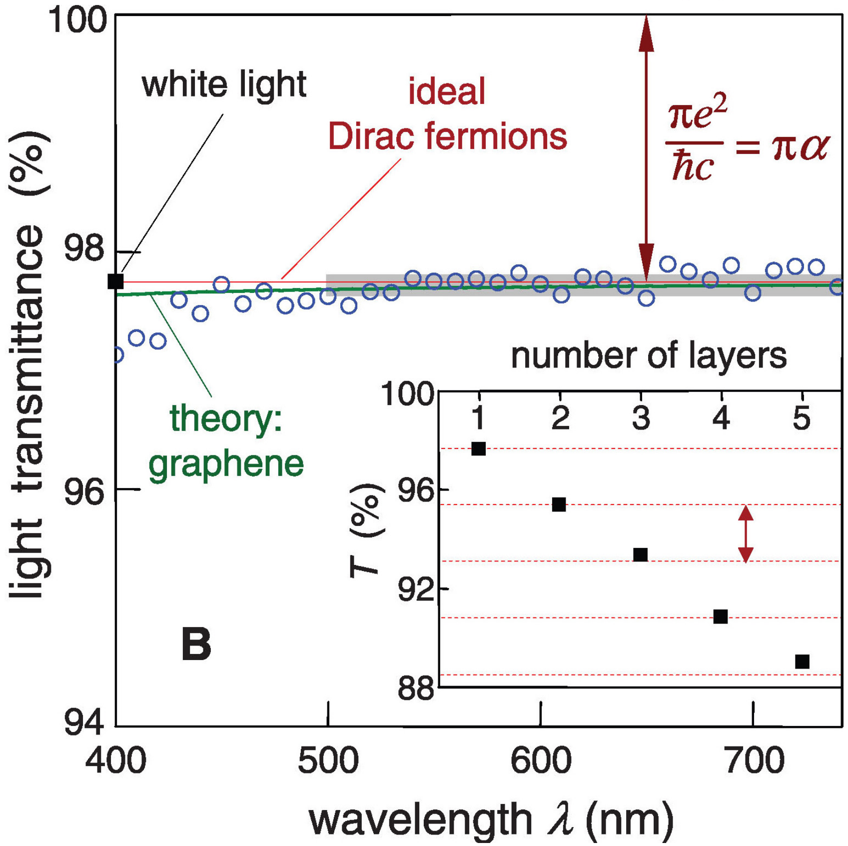



# Dynamical Conductivity: Experiments

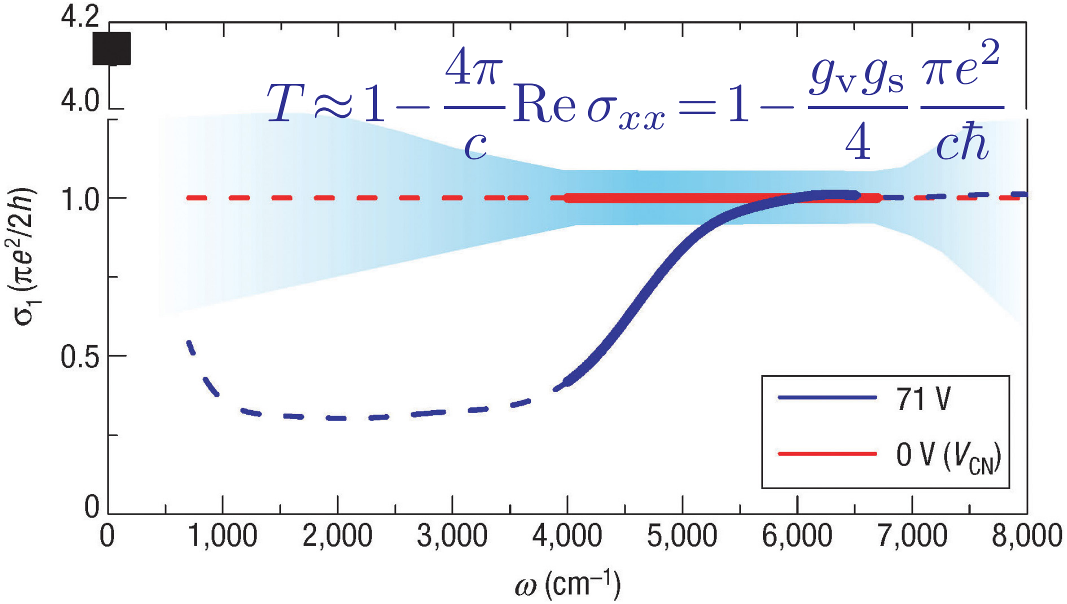
*R.R. Nair et al., Science 320, 1308 (2008)*

⇒ **Visible light**




$$T \approx 1 - \frac{4\pi}{c}\mathrm{Re}\,\sigma_{xx} = 1 - \frac{g_v g_s}{4}\frac{\pi e^2}{c\hbar}$$

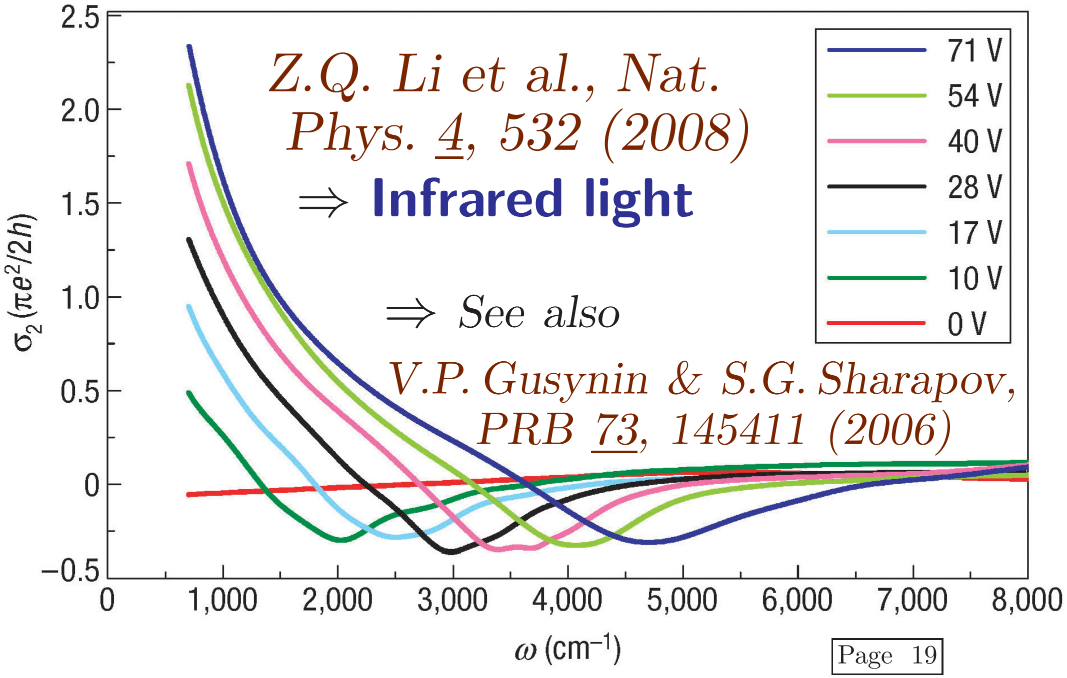



*Z.Q. Li et al., Nat. Phys. 4, 532 (2008)*

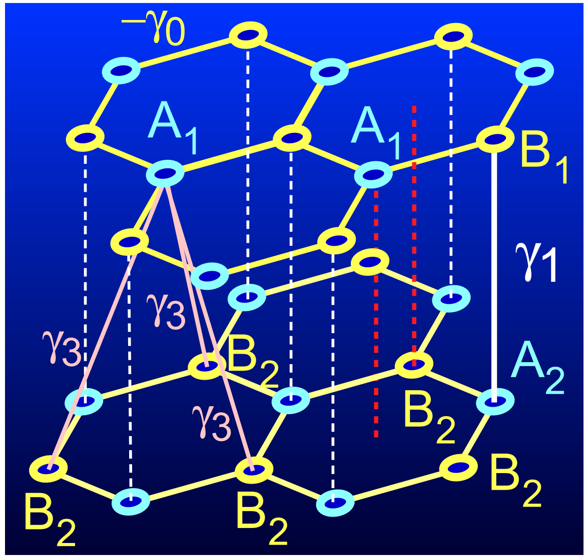
⇒ **Infrared light**

⇒ *See also*

*V.P. Gusynin & S.G. Sharapov, PRB 73, 145411 (2006)*



# Bilayer Graphene: AB Stacking (Bernal Stacking)




**Quantum Hall effect in bilayer graphene**

*K.S. Novoselov et al., Nature 438, 197 (2005)*
*K.S. Novoselov et al., Nat. Phys. 2, 177 (2006)*

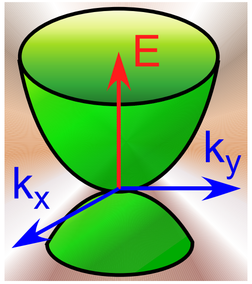
**ARPES** [*T. Ohta et al., PRL 98, 206802 (2007)*]

**Effective Hamiltonian in bilayer graphene**

$$\mathcal{H} = \begin{pmatrix} 0 & \gamma\hat{k}_- & 0 & 0 \\ \gamma\hat{k}_+ & 0 & \Delta & 0 \\ 0 & \Delta & 0 & \gamma\hat{k}_- \\ 0 & 0 & \gamma\hat{k}_+ & 0 \end{pmatrix} \quad (\text{columns: } A_1, B_1, A_2, B_2)$$

$\hat{k}_\pm = \hat{k}_x \pm i\hat{k}_y$

$\Delta = \gamma_1 \approx 0.4\,\text{eV}$

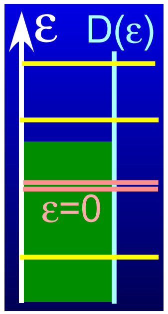



- *E. McCann and V.I. Falko, PRL 96, 086805 (2006)*
- *M. Koshino and T. Ando, PRB 73, 245403 (2006)*

$$\mathcal{H} \approx \frac{\hbar^2}{2m^*}\begin{pmatrix} 0 & \hat{k}_-^2 \\ \hat{k}_+^2 & 0 \end{pmatrix} \qquad m^* = \frac{\hbar^2\Delta}{2\gamma^2}$$

$$\varepsilon_n = \pm\hbar\omega_c\sqrt{n(n+1)} \qquad (n=0,1,\ldots)$$

$\Rightarrow$ **Two Landau levels at $\varepsilon = 0$**



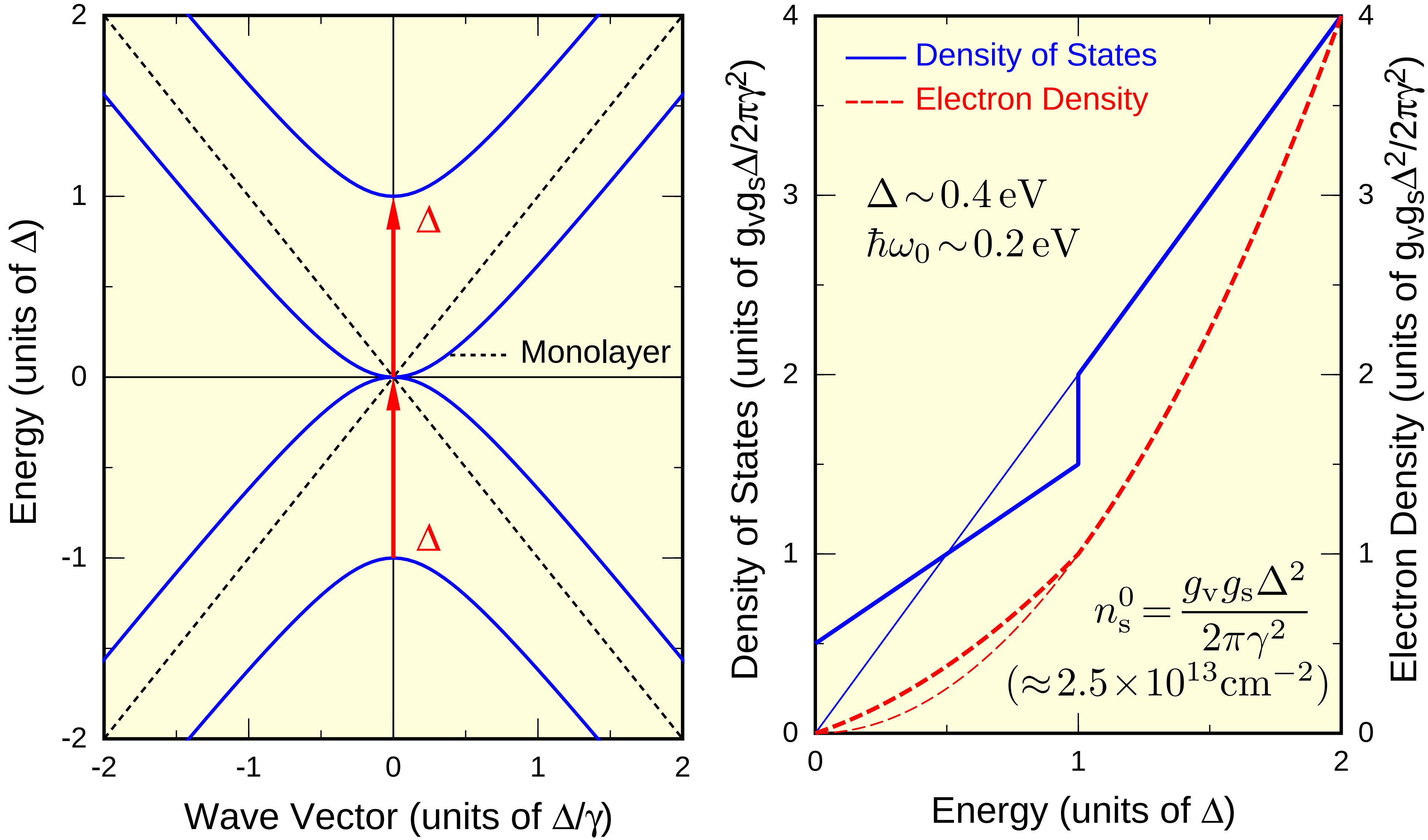

**Tight-binding models**

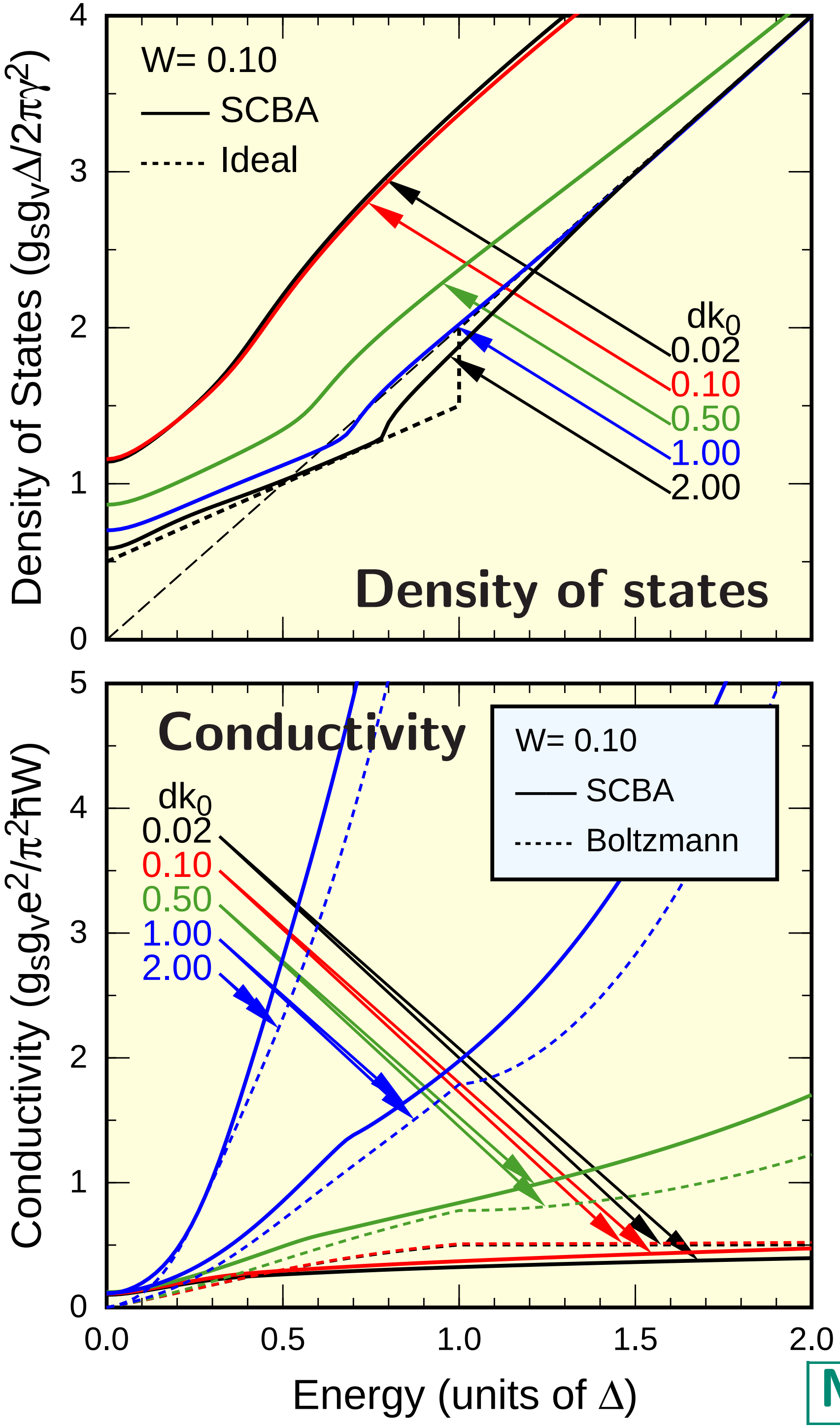
- *S. Latil and L. Henrard, PRL 97, 036803 (2006)*
- *F. Guinea et al., PRB 73, 245426 (2006), ···*

**Susceptibility** $\Rightarrow \chi(\varepsilon) = -\dfrac{g_v g_s}{4\pi}\dfrac{e^2\gamma}{c^2\hbar^2}\ln\left|\dfrac{\Delta}{\varepsilon}\right|$ [*S.A. Safran, PRB 30, 421 (1984)*]

# Energy Dispersion and Density of States of Bilayer Graphene

*T. Ando, J. Phys. Soc. Jpn. 76, 104711 (2007)*



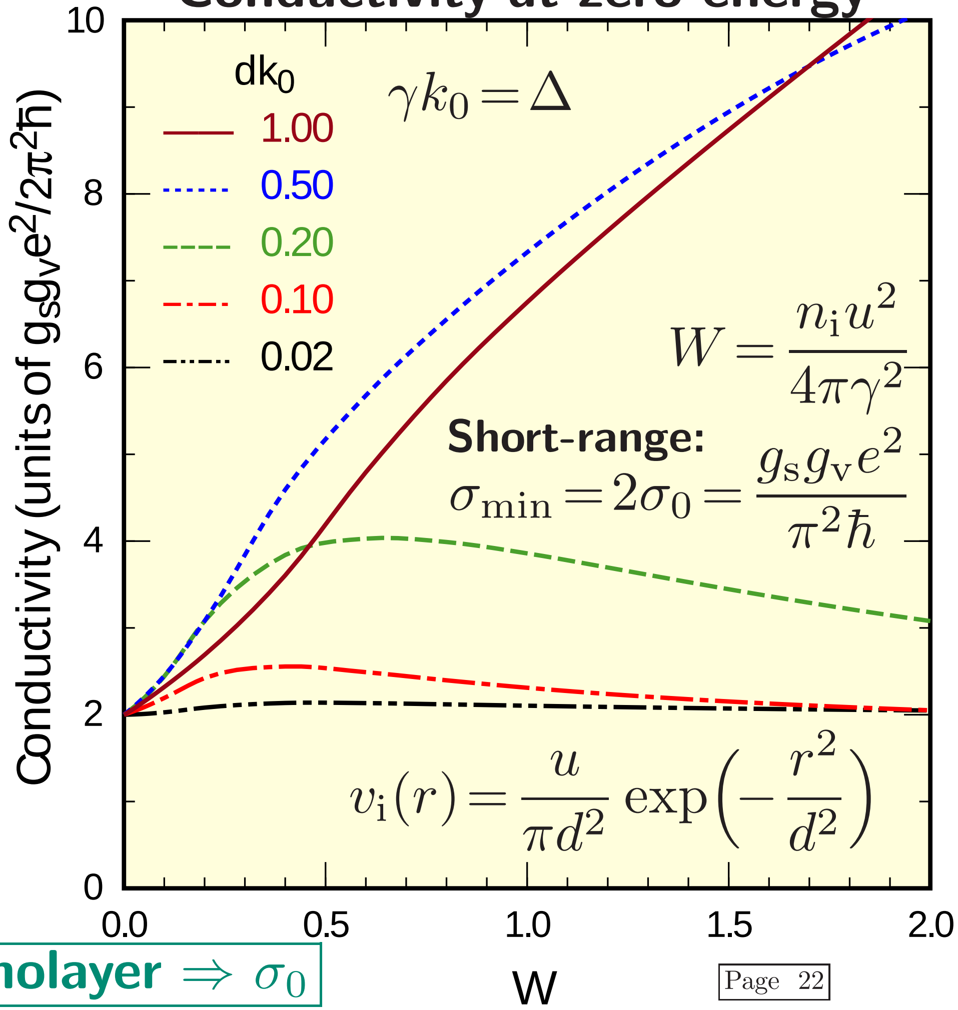



## Scatterers with Gaussian Potential (Self-Consistent Born Approx.)

[*T. Ando, JPSJ 80, 014707 (2011)*]

**Short-range:** *M. Koshino & T. Ando, PRB 73, 245403 (2006)*

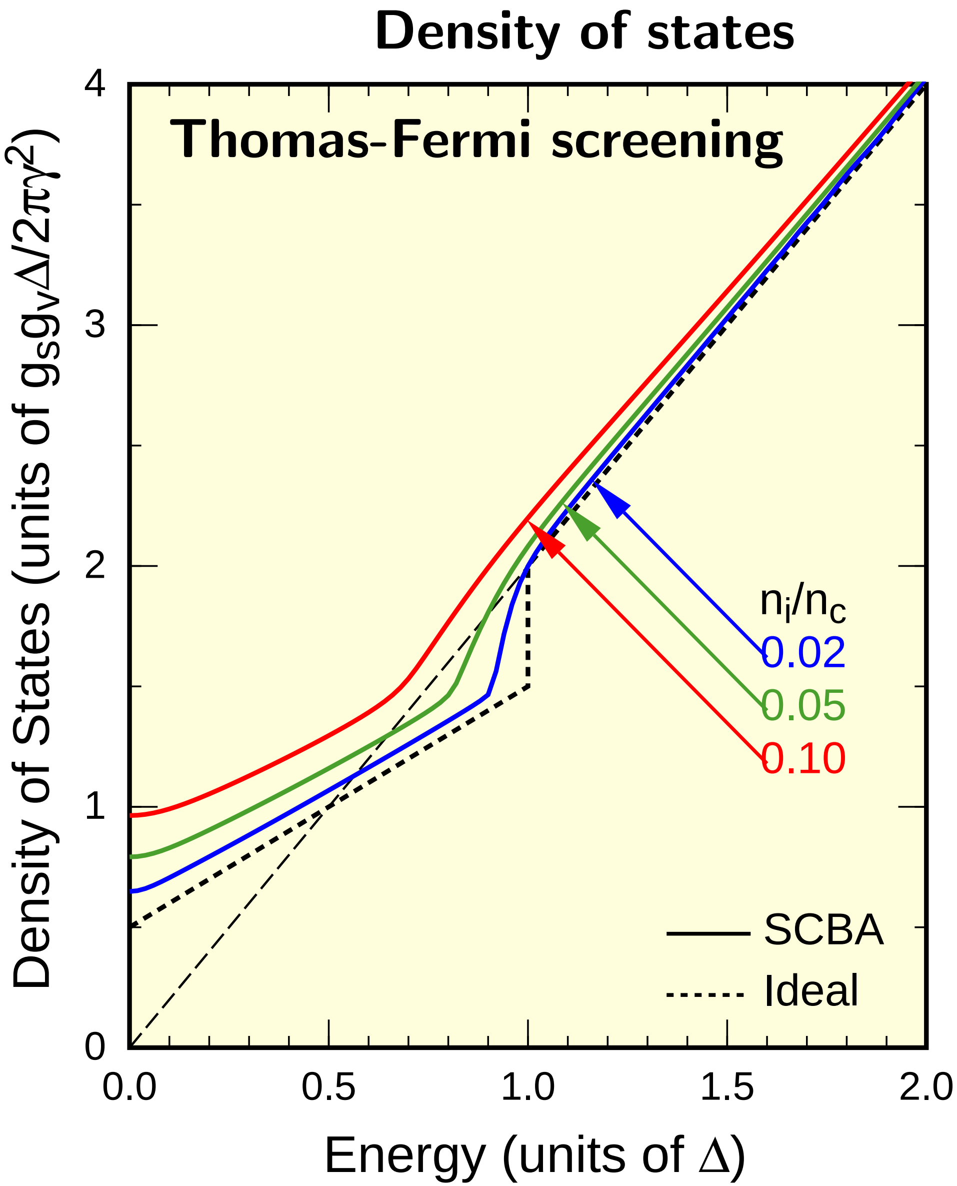
## Conductivity at zero energy

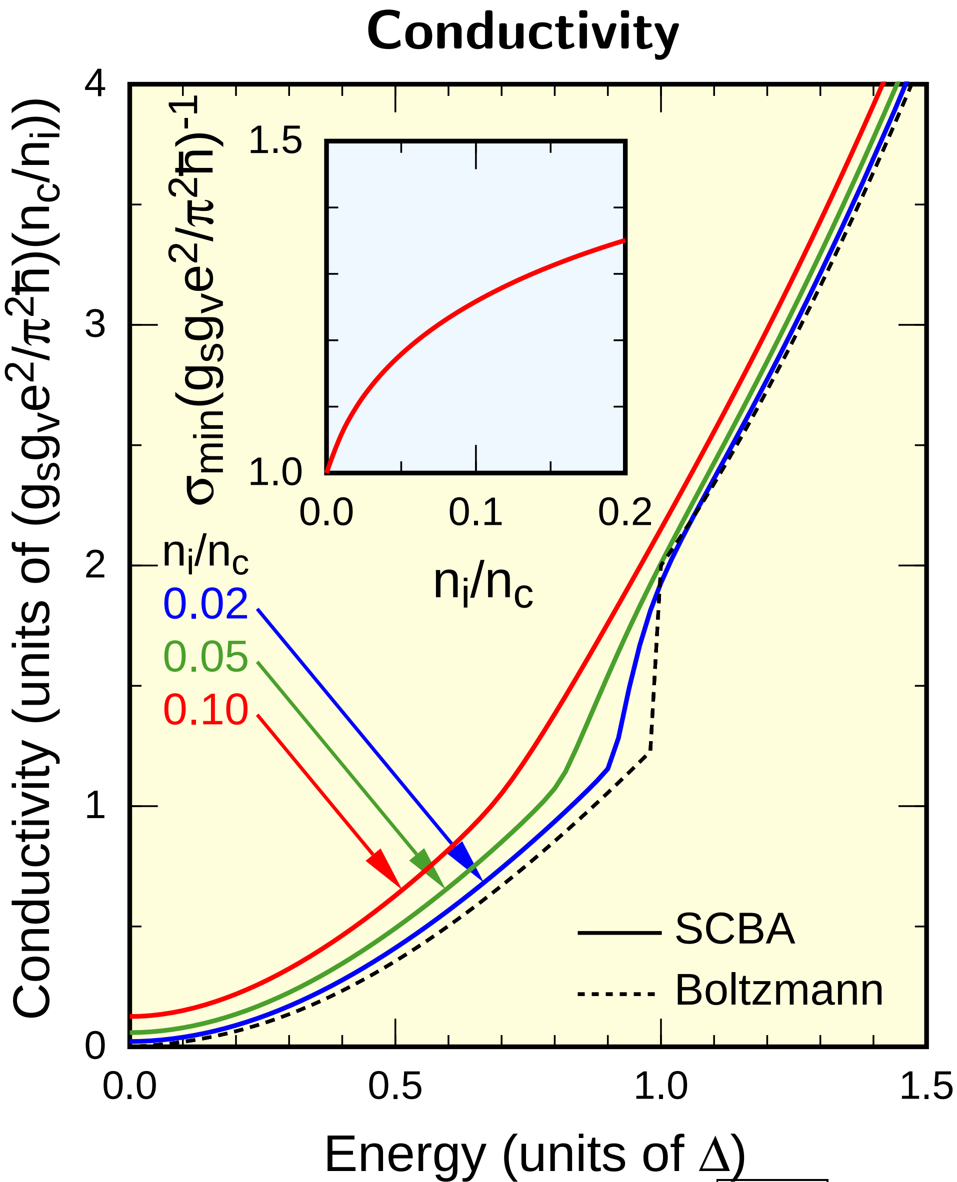



**Monolayer ⇒ $\sigma_0$**

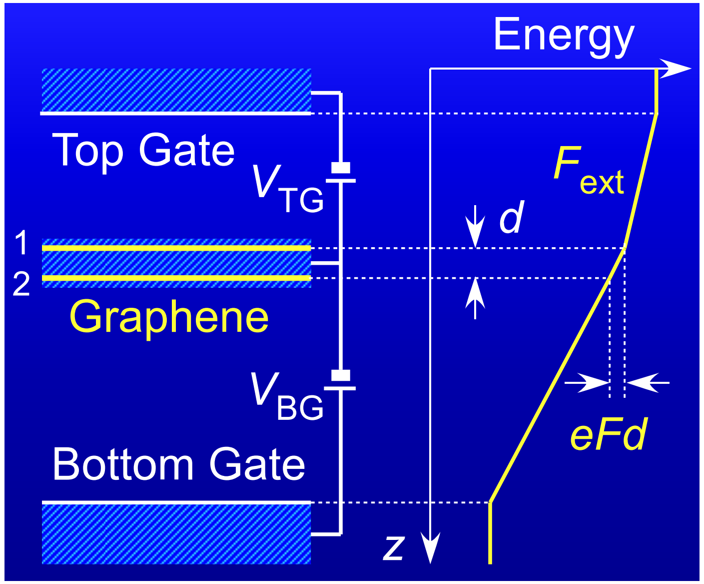
# Charged Impurities (Self-Consistent Born Approximation)

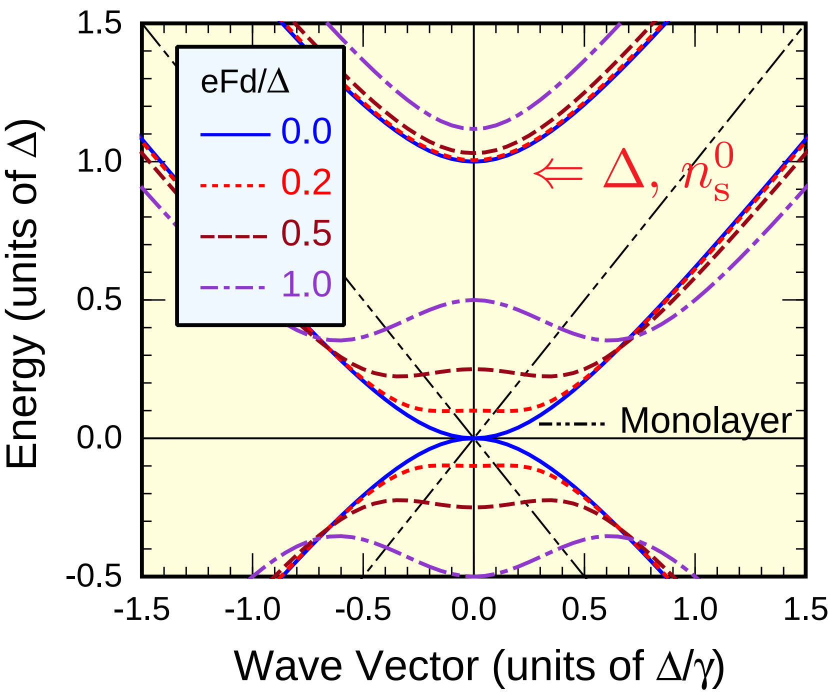
[*T. Ando, J. Phys. Soc. Jpn.* 80*, 014707 (2011)*]

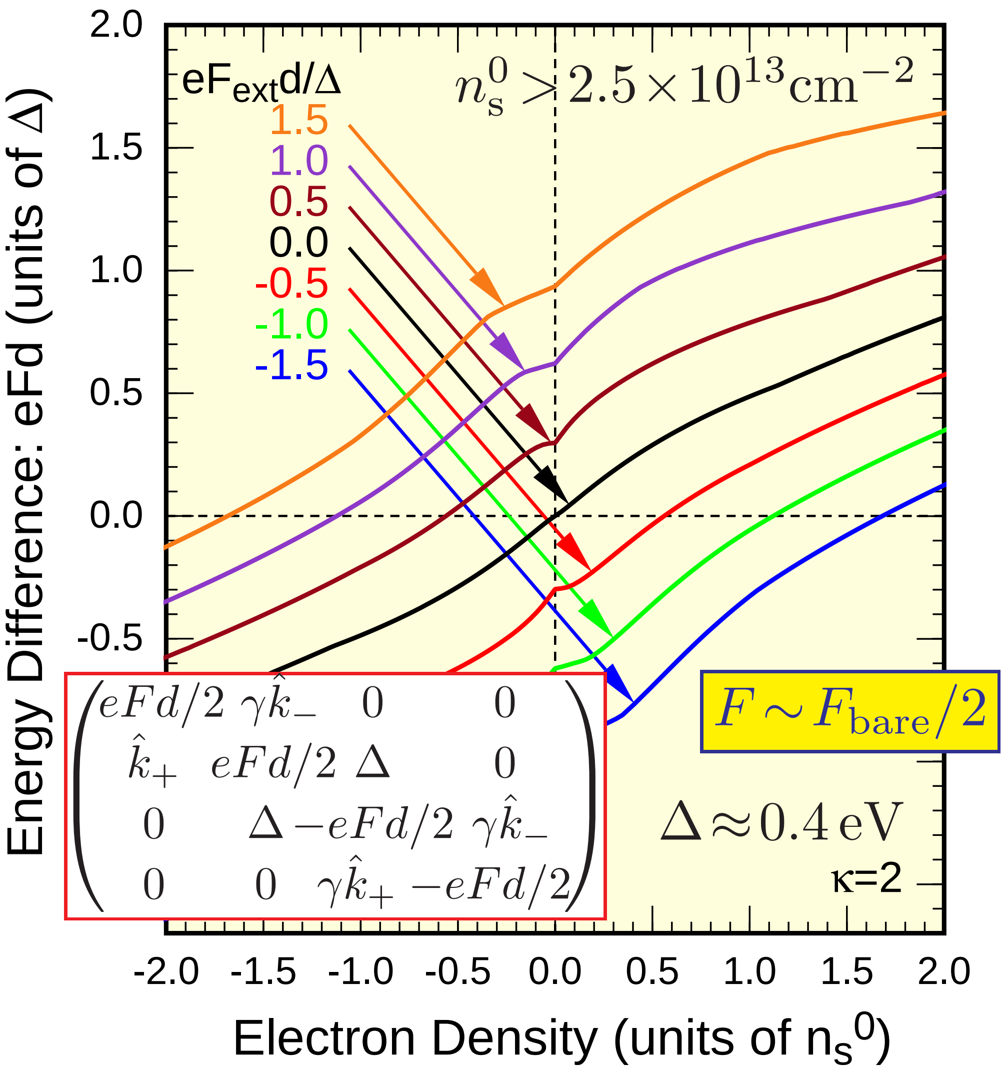


# Field Effect on Energy Spectrum in Bilayer Graphene




$$\begin{pmatrix} eFd/2 & \gamma\hat{k}_- & 0 & 0 \\ \hat{k}_+ & eFd/2 & \Delta & 0 \\ 0 & \Delta & -eFd/2 & \gamma\hat{k}_- \\ 0 & 0 & \gamma\hat{k}_+ & -eFd/2 \end{pmatrix}$$

*E. McCann, PRB 74, 161403 (2006)*
*H. Min et al., PRB 75, 155115 (2007)*
*T. Ando & M. Koshino, JPSJ 78, 034709 (2009)*

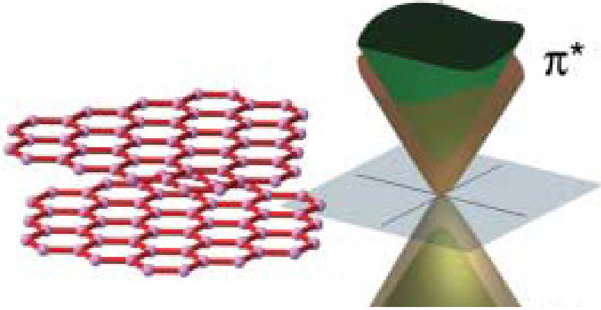
# Multi-Layer Graphene [*M. Koshino & T. Ando, PRB 76, 085425 (2007)*]

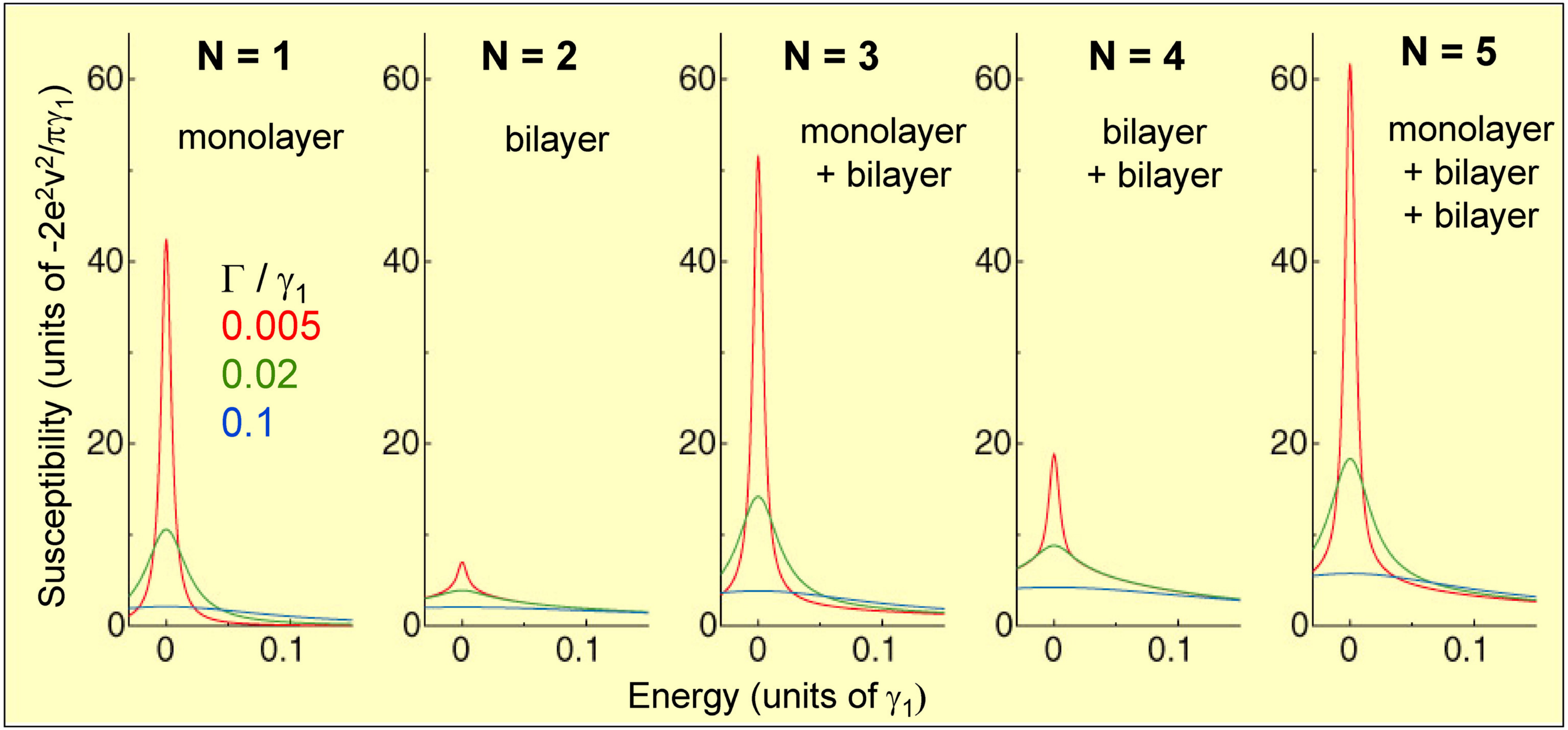
## Exact decomposition of effective Hamiltonian

$2M+1$ **Layers** $=$ $1\times$ **Monolayer** $+$ $M\times$ **Bilayers**

$2M$ **Layers** $=$ $0\times$ **Monolayer** $+$ $M\times$ **Bilayers**

**Three parameters:** $\gamma_0,\ \gamma_1,\ \gamma_3$ **(trigonal warping)**

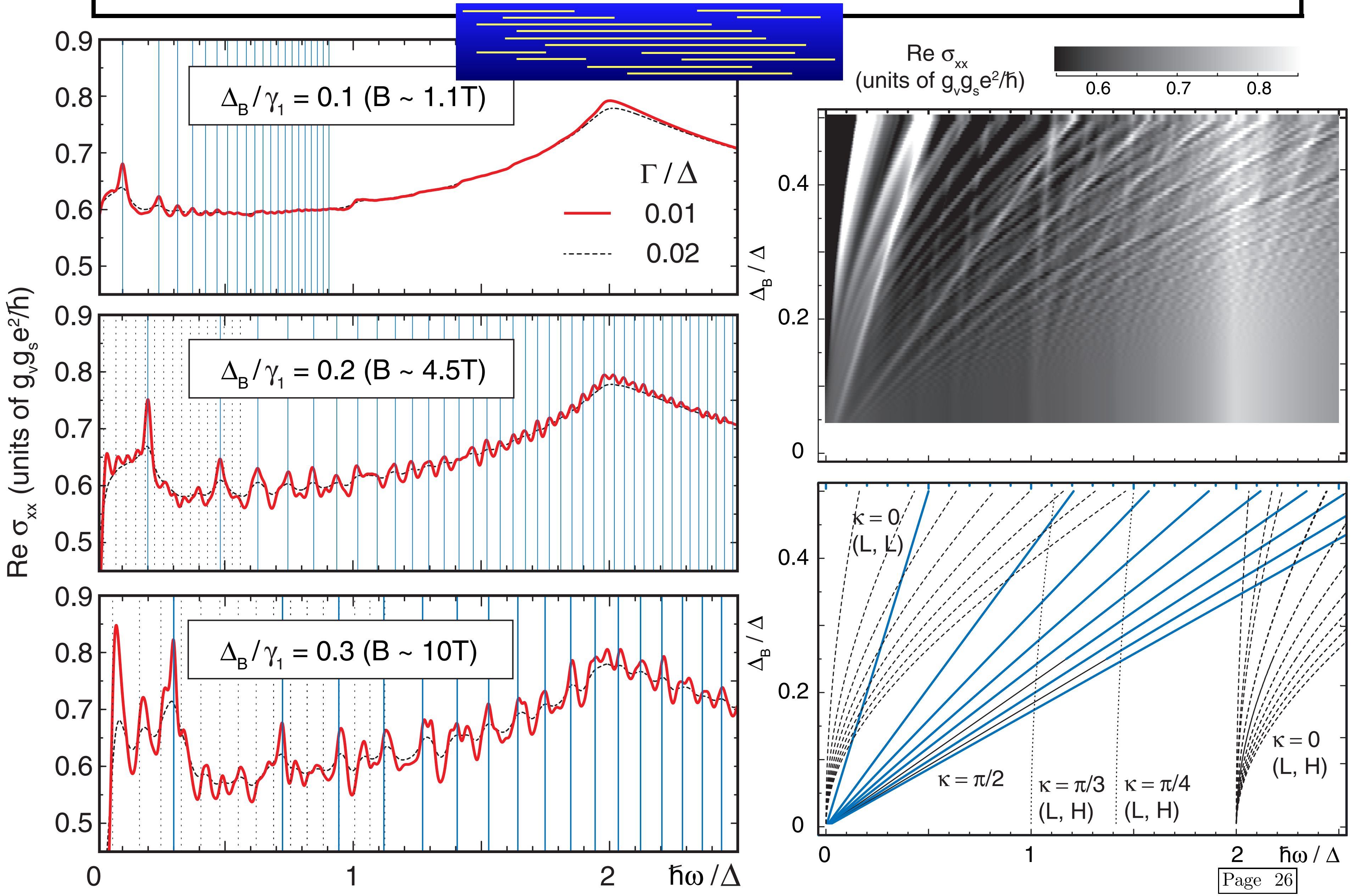


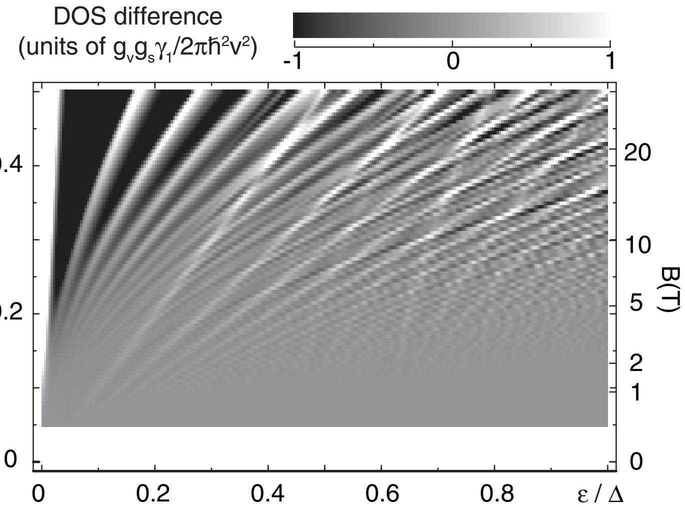




**Diamagnetic susceptibility**

# Dynamical Conductivity of Multi-Layer Graphene (Average 1–20)

*M. Koshino and T. Ando, Phys. Rev. B 77, 115313 (2008)*

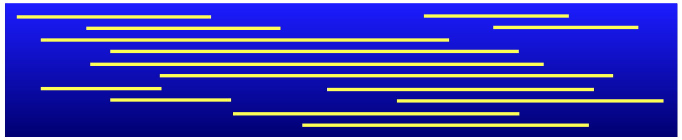


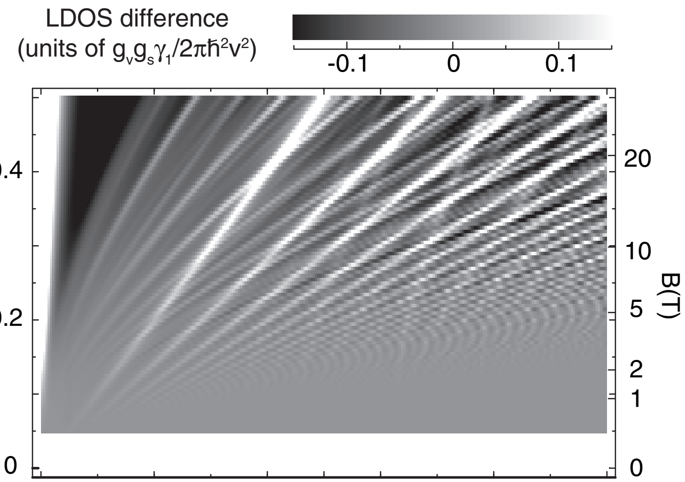


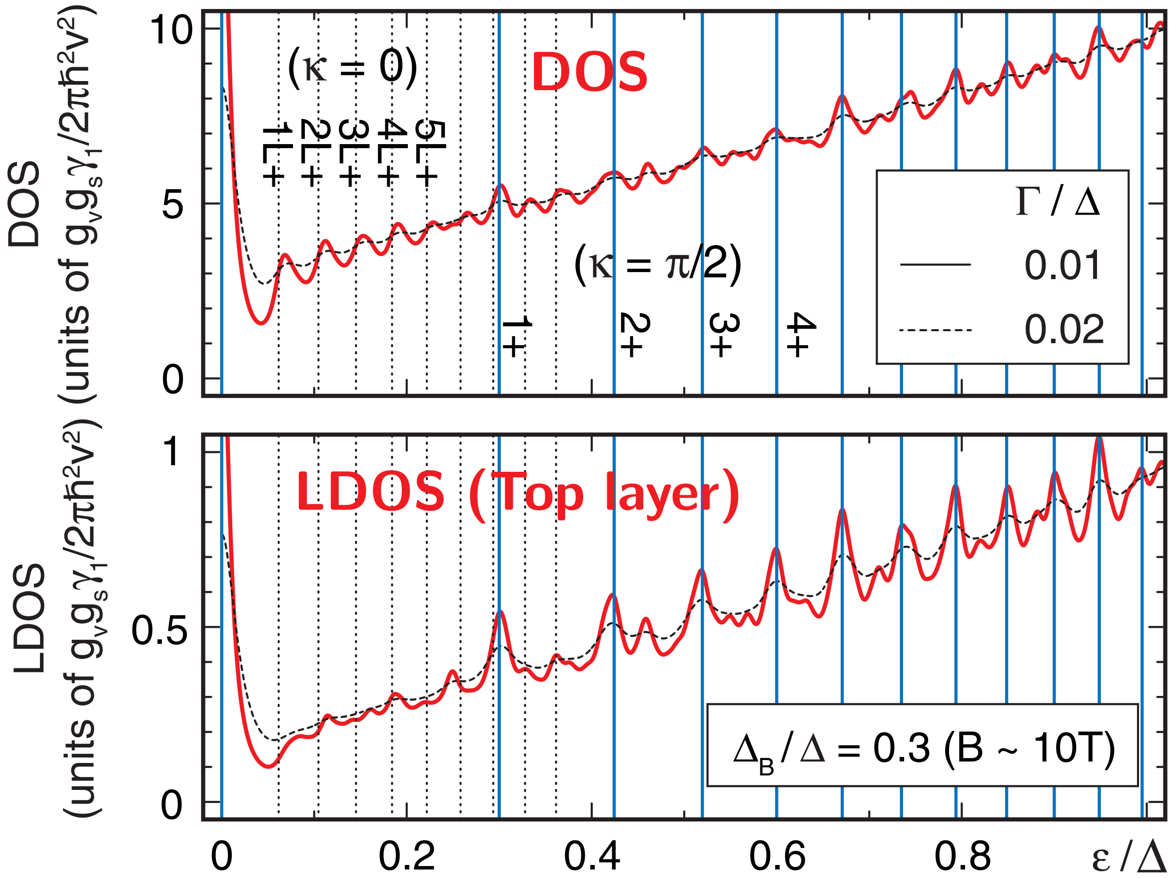

# Local Density of States of Multi-Layer Graphene (Average 1–20)

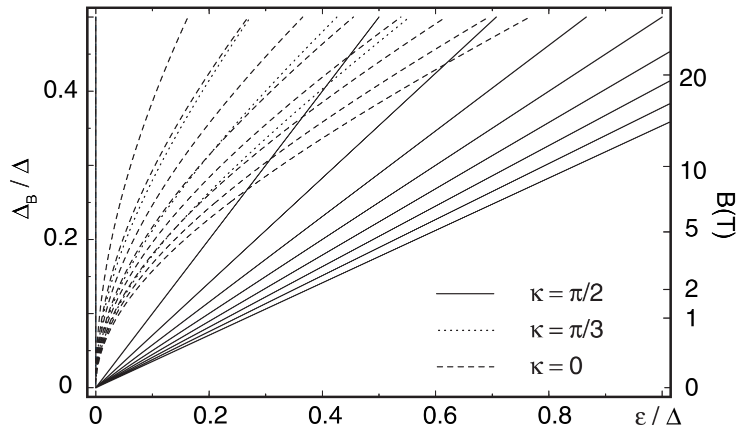
*M. Koshino and T. Ando,*

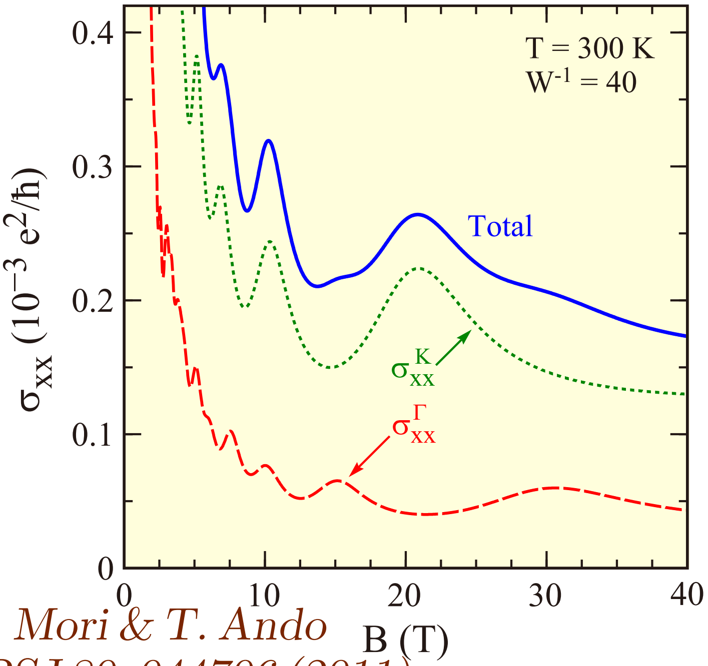
*Phys. Rev. B 77, 115313 (2008)*



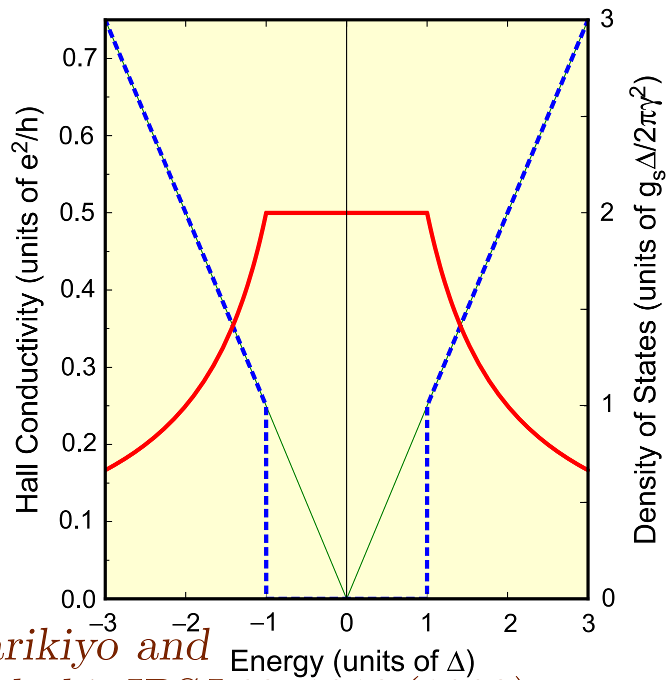





*N. Mori & T. Ando*
*JPSJ 80, 044706 (2011)*

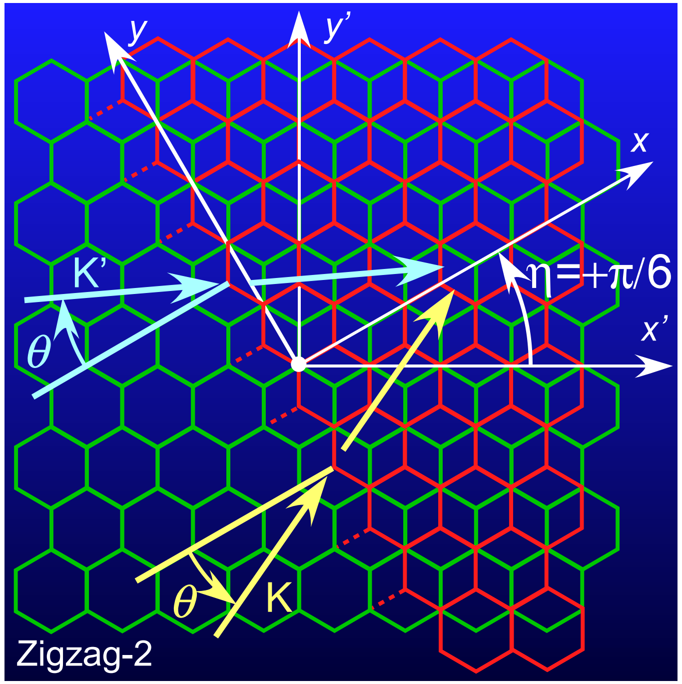



*O. Narikiyo and K. Kuboki, JPSJ 62, 1812 (1993)*

# Further Developments and Future Outlook

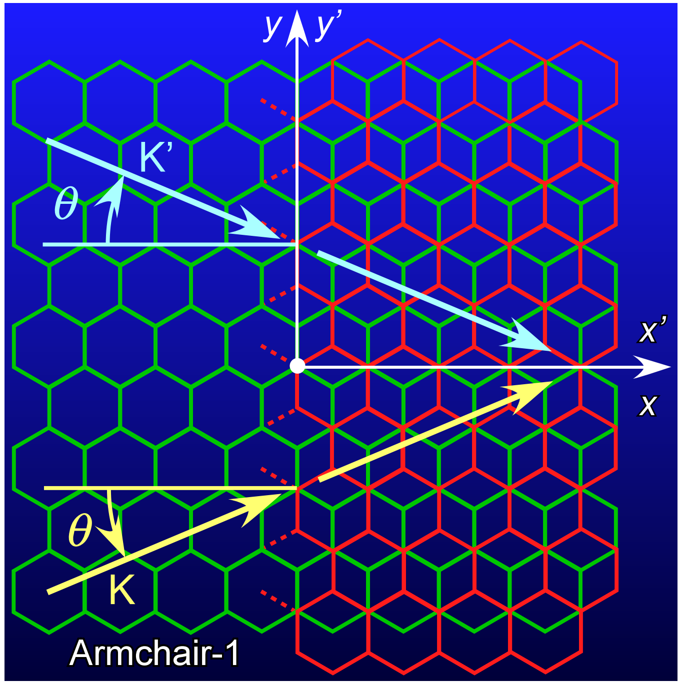
1. Time reversal symmetry and crossover
2. Electron-phonon interaction, Gauge field, instabilities, $\cdots$
   - ○ Optical phonon anomaly
   - ○ Pseudo Landau levels
   - ⇐ Magnetophonon resonances
3. Electron-electron interaction
4. Band gap and valley polarization
   - Substrate effects
   - Orbital magnetism
   - ⇐ Chiral anomaly (Hall effect without $B$, ...)
   - Chiral edge states
   - Exotic phenomena
5. Graphene ribbons
   - Chiral edge states

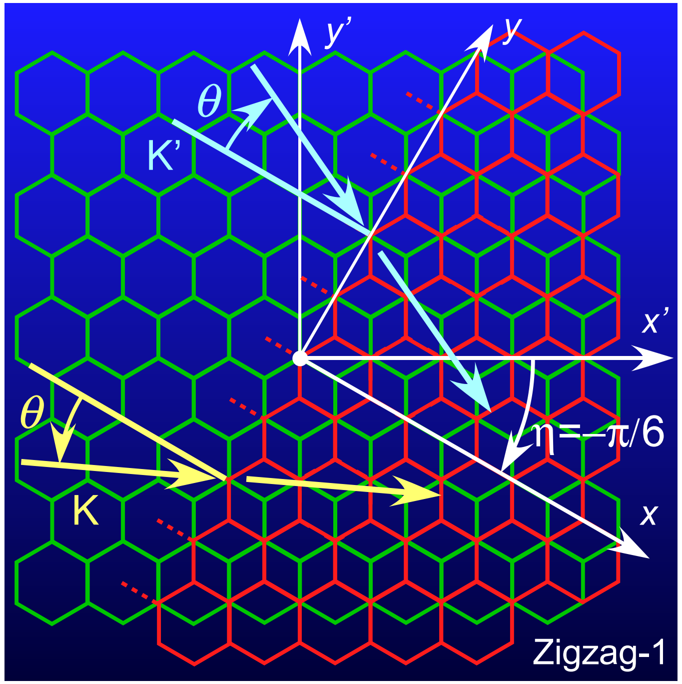
# Transmission between Mono- and Bi-Layer Graphene [*T. Nakanishi, M. Koshino, and T. Ando, PRB* 82*, 125428 (2010)*]

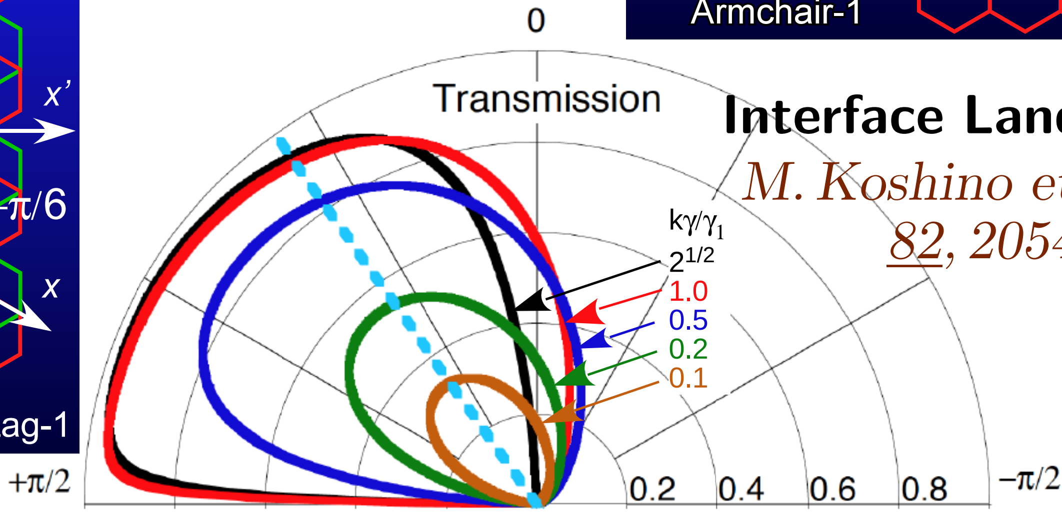



## Valley polarization

$$T_K(\theta) \gg T_{K'}(\theta)$$
$$(\theta > 0)$$




## Interface Landau levels

*M. Koshino et al., PRB* 82*, 205436 (2010)*

# Summary: Electronic and Transport Properties of Graphene

Tsuneya ANDO

1. **Introduction**
   - Weyl's equation for neutrino
   - Berry's phase and topological anomaly
2. **Singular diamagnetic susceptibility**
   - Band-gap effect
   - Spatially varying magnetic field
3. **Transport properties graphene**
   - Singularities at Dirac point
   - Long-range scatterers
4. **Multi-layer graphene**
   - Bilayer graphene
   - Hamiltonian decomposition
5. **Future outlook**
   - Gauge fields
   - Chiral edge states
6. **Summary**

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*Nara, Jun 4 (Tue) 2013*

Nara Japan 2013

**Collaborators**

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Masaki NORO (TITech)
Mikito KOSHINO (Tohoku Univ)

16th International Workshop on Computational Electronics, Nara Prefectural New Public Hall
Jun 4 (Tue) – 7 (Fri) 2013 [13:30–14:30 (50+10)]