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Theory of Quantum Transport in Graphene and Nanotubes

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Theory of Quantum Transport in Graphene and Nanotubes

- 1. Introduction
 - Weyl's equation for neutrino
 - Berry's phase & topological anomaly
- 2. Zero mode anomalies
 - Density of states and conductivity
 - Dynamical conductivity
 - Self-consistent Born approximation
- 3. Special time reversal symmetry
 - Symmetry crossover
- 4. Phonons and electron-phonon interaction
 - Acoustic phonon
 - Optical phonon
 - Zone-boundary phonon
- 5. Summary

Trieste, Aug 29 (Fri) 2008

ICTP Conference Graphene Week 2008, Trieste, Italy August 25-29, 2008 [14:30-15:20 (40+10)]

Tsuneya ANDO







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Topological Anomaly and Berry's Phase



Zero-Mode Anomaly: Boltzmann Conductivity



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Singularity at the Dirac point ($\varepsilon_F = 0$) ⇔ Fermi energy scaling Magnetoconductivity $\sigma_{xx}(B) = \sigma_{xx}\left(\frac{\hbar\omega_B}{\varepsilon_E}\right), \text{ etc.}$ **Dynamical conductivity** $\sigma(\omega) = \sigma\left(\frac{\hbar\omega}{\varepsilon_{\rm T}}\right)$ Diagonal conductivity σ_{xx} N.H. Shon and T. Ando, $\frac{g_v g_s e^2}{2\pi^2 \hbar}$ JPSJ 67, 2421 (1998) Quantum Hall effect σ_{xy} Y. Zheng and T. Ando, $4\left(n+\frac{1}{2}\right)\frac{e^2}{h}$ PRB <u>65</u>, 245420 (2002) **Dynamical conductivity** $\sigma(\omega)$ T. Ando, Y. Zheng, & H. Suzuura, JPSJ 71, 1318 (2002) Diamagnetic susceptibility $\chi(\varepsilon_F)$ M. Koshino and T. Ando, PRB 75, 235333 (2007) Page 7

3.0

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0.51.01.52.02.53.00.00.51.01.52.02.5Frequency (units of ε_0/\hbar)Frequency (units of ε_0/\hbar)

• Approximate $\hbar\omega/\varepsilon_F$ scaling except at $(\varepsilon_F, \omega) = (0, 0)$

0.0

• Experiments: Z.Q. Li et al., Nat. Phys. <u>4</u>, 532 (2008)

Conductivity vs Concentration K.S. Novoselov et al., Nature 438, 197 (2005)

Scattering mechanisms

Boltzmann conductivity $\sigma(\varepsilon_{\rm F}) = \frac{e^2}{\pi^2 \hbar} \frac{1}{4W}$ **Constant mobility** $\Leftrightarrow W \propto n_s^{-1}$ Charged impurity with screening?

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

Minimum conductivity?

- A.K. Geim & K.S. Novoselov, Nat. Phys. <u>6</u>, 183, (2007)
- Y.-W. Tan et al., PRL 99, 264803 (2007)
- K.I. Bolotin et al., SSC <u>146</u>, 2351 (2008)

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Special Time Reversal Symmetry and Universality Class

Real time reversal (K \leftrightarrow K'): T $F_K^T = \sigma_z F_{K'}^*$ $F_{K'}^T = \sigma_z F_K^*$ $T^2 = 1$ Special time reversal (within K and K'): S

$$F^{S} = KF^{*} \quad K = -i\sigma_{y} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad K^{2} = -1$$

Time reversal of $P \qquad \Rightarrow S^{2} = -1$

$$P^{S} = K^{t} P K^{-1} \Rightarrow (F_{\alpha}^{S}, P^{S} F_{\beta}^{S}) = (F_{\beta}, P F_{\alpha})$$

Time reversal		Symmetry	Matrix
Real	$T^2 = +1$	Orthogonal	Real
Special	$S^2 \!=\! -1$	Symplectic	Quaternion
None		Unitary	Complex

Reflection coefficient: $r_{\bar{\beta}\alpha} = (F_{\bar{\beta}}, TF_{\alpha}) = (F_{\beta}^{S}, TF_{\alpha}) \Leftrightarrow r_{\bar{\alpha}\beta}$ **T matrix:** $T = V + V \frac{1}{E - \mathcal{H}_{0} + i0} V + V \frac{1}{E - \mathcal{H}_{0} + i0} V \frac{1}{E - \mathcal{H}_{0} + i0} V + \cdots$ **Real** : $r_{\bar{\alpha}\beta} = (F_{\alpha}^{T}, TF_{\beta}) = (F_{\beta}^{T}, T(F_{\alpha}^{T})^{T}) = +(F_{\beta}^{T}, TF_{\alpha}) = +r_{\bar{\beta}\alpha}$ **Special:** $r_{\bar{\alpha}\beta} = (F_{\alpha}^{S}, TF_{\beta}) = (F_{\beta}^{S}, T(F_{\alpha}^{S})^{S}) = -(F_{\beta}^{S}, TF_{\alpha}) = -r_{\bar{\beta}\alpha}$ **Absence of backward scattering:** $r_{\bar{\alpha}\alpha} = 0$ (\Leftarrow **Berry's phase**) **Presence of perfect channel (Odd channel numbers) Presence of perfect channel (Odd channel numbers)** Metallic Nanotubes: Perfect Channel without Backscattering T. Ando and H. Suzuura, J. Phys. Soc. Jpn. <u>71</u>, 2753 (2002)

Symmetry Breaking Effects: Symplectic \Rightarrow Unitary

Trigonal warping (S) [H. Ajiki & T. Ando, or
$$JPSJ \underline{65}, 505 (1996)]$$

 $\mathcal{H}' = \alpha \frac{\gamma a}{4\sqrt{3}} \begin{pmatrix} 0 & (\hat{k}_x + i\hat{k}_y)^2 \\ (\hat{k}_x - i\hat{k}_y)^2 & 0 \end{pmatrix}$ one $2 \leq \beta \leq 4$
Lattice distortion [H. Suzura & T. Ando, $\delta = 0.00$
 $PRB \underline{65}, 235412 (2002)] = 0$
 $\mathcal{H}' = g_1(u_{xx} + u_{yy})$ or $2u_{xy}\sigma_y$]
 $\mathcal{H}' = g_1(u_{xx} + u_{yy})\sigma_x - 2u_{xy}\sigma_y$]
Deformation potential : $g_1 \sim 16 \text{ eV}$ one 0.000
Bond-length (b) change: $g_2 \approx \beta\gamma_0/4$ one 0.000
 $\beta = -\frac{d \ln \gamma_0}{d \ln b}, \quad \gamma = \frac{\sqrt{3}\gamma_0 a}{2}, \quad b = \frac{\sqrt{3}a}{2}$
 $u_{xx} = \frac{\partial u_x}{\partial x} + \frac{u_z}{R} \quad u_{yy} = \frac{\partial u_y}{\partial y} \quad u_{xy} = \frac{1}{2} \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right)$
Curvature: $\mathcal{H}' = p \frac{\gamma a}{4\sqrt{3}} \left[\left(\frac{\partial^2 u_z}{\partial x^2} - \frac{\partial^2 u_z}{\partial y^2} \right) \sigma_x - 2 \frac{\partial^2 u_z}{\partial x \partial y} \sigma_y \right] \gamma' = \frac{\sqrt{3}}{2} (V_{pp}^{\sigma} - V_{pp}^{\pi}) a$
Optical phonon: $\mathcal{H}' = -\frac{\beta\gamma}{b^2} \sigma \times [u_A - u_B]$
[K. Ishikawa & T. Ando, JPSJ 75, 084713 (2006)]
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Continuum models in graphene

- Acoustic phonons
- Optical phonons (zone-center)
- Zone-boundary phonon Page 17

Long-Wavelength Phonons in Carbon Nanotubes

Continuum Phonon Model and Electron-Phonon Interaction H. Suzuura and T. Ando, Phys. Rev. B <u>65</u>, 235412 (2002)

Energy functional of lattice distortion $\boldsymbol{u} = (u_x, u_y, u_z)$

 $U_{2D}[\boldsymbol{u}] = \int dx dy \, \frac{1}{2} \Big(B(u_{xx} + u_{yy})^2 + \mu \big[(u_{xx} - u_{yy})^2 + 4u_{xy}^2 \big] \Big)$ $u_{xx} = \frac{\partial u_x}{\partial x} + \frac{u_z}{R}, \quad u_{yy} = \frac{\partial u_y}{\partial y}, \quad 2u_{xy} = \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \qquad \begin{bmatrix} B : \text{Bulk modulus} \\ \mu : \text{Shear modulus} \end{bmatrix}$ Curvature **Electron-phonon interaction** $U_{\rm c}[\boldsymbol{u}] \propto \int \left[\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial u^2} + \frac{1}{B^2} \right) u_z \right]^2 d\boldsymbol{r}$ KA KB $V_{\text{el-ph}} = \begin{pmatrix} V_1 & V_2 \\ V_2^+ & V_1 \end{pmatrix} \overset{u}{\underset{a}{\longrightarrow}} \overset{u}{\underset{a^2}{\overset{a^2(u_{xx}+u_{yy})}{\overset{u}{\longrightarrow}}}}$ $V_1 = q_1 (u_{xx} + u_{yy})$ $V_2 = q_2 e^{3i\eta} (u_{xx} - u_{yy} + 2iu_{xy})$ η : Chiral angle g_1 : Deformation potential g_2 : Bond-length change [cf. (CH)_x] $(q_1 \gg |q_2|)$ No contribution of g_1 in metallic CN Page 19

Photo-relaxation: T. Hertel and G. Moos, PRL <u>84</u>, 5002 (2000) Page 20

Long-Wavelength Optical Phonon

[K. Ishikawa and T. Ando, J. Phys. Soc. Jpn. <u>75</u>, 084713 (2006)]

Optical phonon (lattice displacement u): $\mathcal{H}_{ph} = \sum \hbar \omega_0 \left(b_{\boldsymbol{q}\mu}^{\dagger} b_{\boldsymbol{q}\mu} + \frac{1}{2} \right)$

$$\boldsymbol{u}(\boldsymbol{r}) \equiv \frac{1}{\sqrt{2}} [\boldsymbol{u}_A(\boldsymbol{r}) - \boldsymbol{u}_B(\boldsymbol{r})] = \sum_{\boldsymbol{q},\mu} \sqrt{\frac{\hbar}{2NM\omega_0}} (b_{\boldsymbol{q}\mu} + b_{-\boldsymbol{q}\mu}^{\dagger}) \boldsymbol{e}_{\mu}(\boldsymbol{q}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}}$$

Electron-phonon interaction $\beta_{\Gamma} = -\frac{d \ln \gamma_0}{d \ln b}, \quad \gamma = \frac{\sqrt{3}\gamma_0 a}{2}, \quad b = \frac{\sqrt{3}a}{2}$

$$\mathcal{H}_{\mathrm{int}}^{\mathrm{K}} = -\sqrt{2} \frac{oldsymbol{eta}_{\Gamma} \gamma}{b^2} \, oldsymbol{\sigma} imes oldsymbol{u}(oldsymbol{r})$$

Dimensionless coupling constant

$$\lambda = \frac{g_{\rm v}g_{\rm s}}{4} \frac{36\sqrt{3}}{\pi} \frac{\hbar^2}{2Ma^2} \frac{1}{\hbar\omega_0} \left(\frac{\beta_{\Gamma}}{2}\right)^2$$
$$\approx 3 \times 10^{-3} \left(\frac{\beta_{\Gamma}}{2}\right)^2 \quad (4 \gtrsim \beta_{\Gamma} \gtrsim 2)$$
$$\hbar\omega_0 = 0.196 \,\mathrm{eV}$$
$$M = 1.993 \times 10^{-23} \,\mathrm{g}$$

 $\mathcal{H}_{\mathrm{int}}^{\mathrm{K}'} = +\sqrt{2} \frac{oldsymbol{\beta}_{\Gamma} \gamma}{h^2} \, oldsymbol{\sigma}^* imes oldsymbol{u}(oldsymbol{r})$ Bond length

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Frequency Shift and Broadening

[T. Ando, J. Phys. Soc. Jpn. <u>75</u>, 124701 (2006)]

Phonon Green's function $D(\boldsymbol{q}, \omega) = \frac{2\omega_0}{\omega^2 - \omega_0^2 - 2\omega_0 \Pi(\boldsymbol{q}, \omega)}$ Energy shift: $\Delta \omega = \operatorname{Re} \tilde{\Pi}(\boldsymbol{q}, \omega_0)$ Broadening : $\Gamma = -\operatorname{Im} \tilde{\Pi}(\boldsymbol{q}, \omega_0)$ Self-energy

 $\tilde{\Pi}(\boldsymbol{q},\omega) = \Pi(\boldsymbol{q},\omega) - \Pi_{\varepsilon_F=0}(\boldsymbol{q},0)$ (Avoid double counting)

 $\Rightarrow M. Lazzeri \& F. Mauri, PRL \\ \underline{97}, 266407 (2006) Page 22$

Magnetic Oscillation of Optical Phonon ($\varepsilon_{\rm F}^0/\hbar\omega_0 = 0.25$) [*T. Ando, J. Phys. Soc. Jpn.* <u>76</u>, 024712 (2007)]

Zone-Boundary Phonon

[H. Suzuura and T. Ando, JPSJ <u>77</u>, 044703 (2008)]

Highest frequency phonon: ω_K (Kekulé distortion)

High-Field Transport: Zone-Center vs Zone-Boundary Phonons

Summary: Quantum Transport in Graphene and Nanotubes

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www.stat.phys.titech.ac.jp/ando/

www.stat.phys.titech.ac.jp/~ando/reprint/graphene/reprints.htm

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