Numerical simulations of graphene conductivity with realistic inter-electron interaction potential

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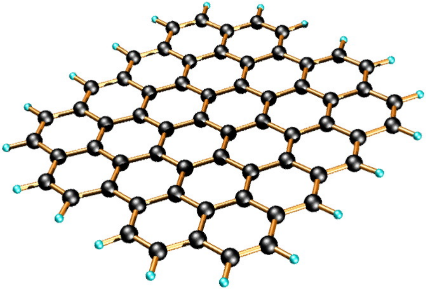
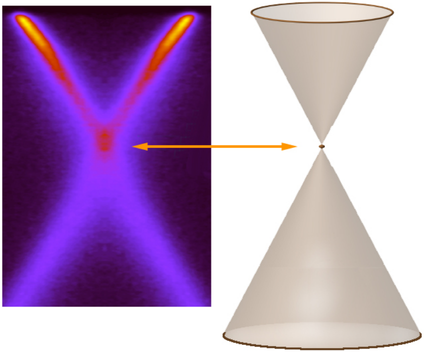
Plan

- Graphene
- Setting problem
- Model
  - Free Hamiltonian
  - Interaction Hamiltonian
  - Partition function
  - Current-current correlator
- Checking model in FREE case
- Study of finite volume effects
- Conductivity
  - Calculation scheme
  - Dependence on substrate dielectric permittivity

Graphene





$$E = v_F |\vec{p}|$$

Effects: quantum Hall effect, Klein paradox, Casimir effect

Problem

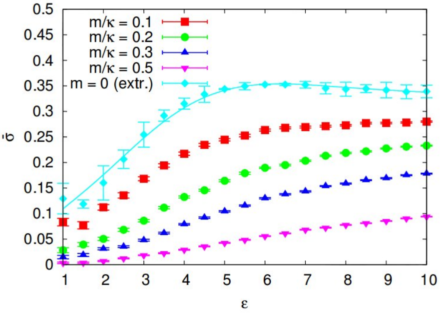
Is suspended graphene conductor or insulator ?
Can graphene conduct electric current ?

Experiments: Suspended graphene is a conductor!

$$\sigma = (1.01 \pm 0.04) \frac{1}{4} \frac{e^2}{\hbar}$$

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

A. Mayorov et. al., Nano Lett.12, 4629 (2012)



P. Buividovich et. al., Phys. Rev. B 86, 245117 (2012)

Goal: Carry out direct Monte-Carlo simulations of graphene conductivity taking into account Coulomb interaction screening

Model: free Hamiltonian

Free charges in graphene can be described by tight biding Hamiltonian

$$\hat{H}_{tb} = -\kappa \sum_{\langle x,y\rangle ,s} (\hat{a}^{\dagger}_{x,s}\hat{a}_{y,s} + \hat{a}^{\dagger}_{y,s}\hat{a}_{x,s})$$

where $\hat{a}^{\dagger}_{x,s}$, $\hat{a}_{y,s}$− operators of creation and annihilation electron in point x with spin s, with anticommutators $\{\hat{a}^{\dagger}_i, \hat{a}^{\dagger}_j\} = \{\hat{a}_i, \hat{a}_j\} = 0$, $\{\hat{a}^{\dagger}_i, \hat{a}_j\} = \delta_{ij}$

Vacuum

$$\hat{a}_{x,\uparrow} |0\rangle = 0, \quad \hat{a}^{\dagger}_{x,\downarrow} |0\rangle = 0$$

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Operators of creation and annihilation quasiparticles

electron

$$\hat{a}_x = \hat{a}_{x,\uparrow}, \quad \hat{a}_x |0\rangle = 0$$

hole

$$\hat{b}^{\dagger}_x = \pm\hat{a}_{x,\downarrow}, \quad \hat{b}_x |0\rangle = 0$$

So we can rewrite $\hat{H}_{tb}$

$$\hat{H}_{tb} = -\kappa \sum_{\langle x,y \rangle} (\hat{a}^{\dagger}_x\hat{a}_y + \hat{b}^{\dagger}_x\hat{b}_y + \mathrm{c.c.})$$

Model: free Hamiltonian

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$$\hat{H}_{tb} = -\kappa \sum_{\langle x,y\rangle,s} (\hat{a}^\dagger_{x,s}\hat{a}_{y,s} + \hat{a}^\dagger_{y,s}\hat{a}_{x,s}) \pm m \sum_{x,s} \hat{a}^\dagger_{x,s}\hat{a}_{x,s}$$

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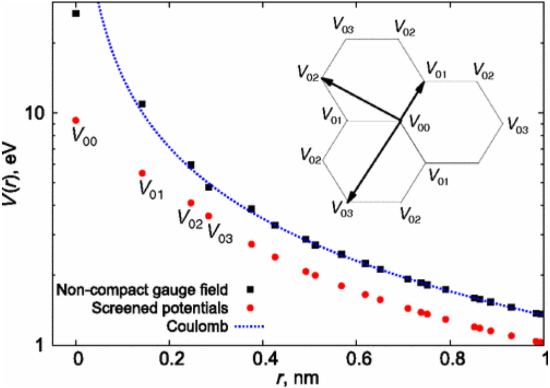
Model: Interaction Hamiltonian

Charge interaction

$$\hat{H}_C = \frac{1}{2}\sum_{x,y} \hat{q}_x V_{xy} \hat{q}_y, \qquad \hat{q}_x = \hat{a}^\dagger_x \hat{a}_x - \hat{b}^\dagger_x \hat{b}_x, \quad \hat{q}_x \left|0\right\rangle = 0$$



Screening of σ - electrons
$V_{00}, V_{01}, V_{02}, V_{03}$

T.O. Wehling et al., Phys. Rev. Lett. 106, 236805 (2011)

Screening of dielectric permittivity ϵ

$$V_{xy} \to \frac{2V_{xy}}{1+\epsilon}$$

Model: Partition function

$$\mathcal{Z} = \mathrm{Tr}\, e^{-\beta\left(\hat{H}_{tb}+\hat{H}_C\right)} = \mathrm{Tr}\, \left(e^{\delta(\hat{H}_{tb}+\hat{H}_C)}\right)^{N_t} = \quad \ldots \quad = \int \mathcal{D}\phi\, e^{-S[\phi_{x,t}]} |detM[\phi_{x,t}]|^2$$

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Action of Hubbard-Stratonovich fields

$$S[\phi_{x,t}] = \frac{\delta}{2} \sum_{x,y,t} \phi_{x,t} V^{-1}_{xy} \phi_{y,t}$$

Fermionic Matrix

$$\sum_{x,y,t,t'} \left(\psi^*_{x,t} M_{x,y,t,t'} \psi_{y,t'}\right) =$$

$$\sum_{t=0}^{N_t-1} \Big[\sum_x \psi^*_{x,2t}(\psi_{x,2t} - \psi_{x,2t+1}) - \delta\kappa \sum_{\langle x,y\rangle} (\psi^*_{x,2t}\psi_{y,2t+1} + \psi^*_{y,2t}\psi_{x,2t+1})$$

$$+ \sum_x \psi^*_{x,2t+1}(\psi_{x,2t+1} - e^{-i\delta\phi_{x,t}}\psi_{x,2t+2}) \pm \delta m \sum_x \psi^*_{x,2t}\psi_{x,2t+1} \Big]$$

Model: Current-current correlator

$$G(\tau) = \sum_{b,c} \frac{\vec{e}_b \vec{e}_c}{3\sqrt{3}a^2 L_x L_y} \sum_{x,y} \langle\, J_b\,(\tau, x)\, J_c\,(0, y)\,\rangle =$$

$$- \frac{2\vec{e}_b \vec{e}_c}{3\sqrt{3}a^2 L_x L_y} \sum_{b,c} \langle\, Re\mathrm{Tr}\, \left(j_{\uparrow,b} M^{-1}(0,\tau) j_{\uparrow,c} M^{-1}(\tau, 0)\right)\,\rangle$$

$$\sum_x J_b(x) = \sum_{x,y} \left(\hat{a}_x^\dagger j_{\uparrow,b} \hat{a}_y + \hat{b}_x^\dagger j_{\downarrow,b} \hat{b}_y\right)$$

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$$\sum_x J_b(x) = \sum_{x,y} \left(\hat{a}^\dagger_x j_{\uparrow,b} \hat{a}_y + \hat{b}^\dagger_x j_{\downarrow,b} \hat{b}_y\right)$$

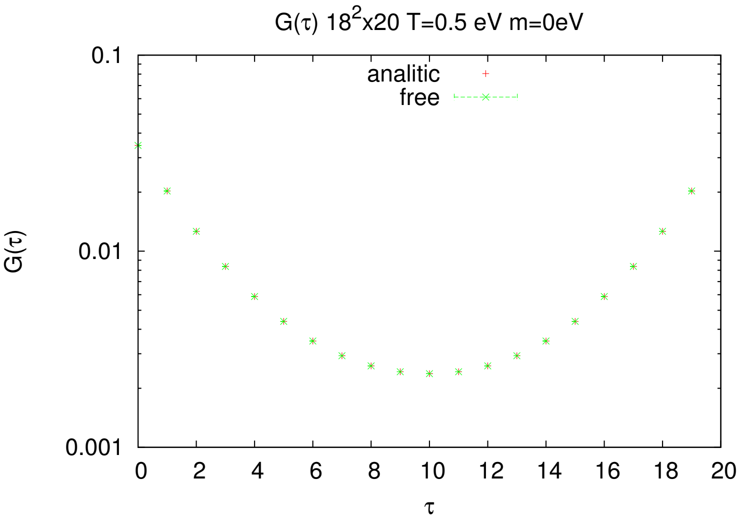
Free Case

$$G(\tau) = \sum_{b,c} \frac{2\vec{e}_b \vec{e}_c}{3\sqrt{3}a^2 L_x L_y} \frac{\kappa^2}{L_t^2} Re \sum_{\vec{k}, q_0, p_0} \frac{e^{iq_0\tau} e^{-ip_0\tau}}{\Omega(q_0, \vec{k})\Omega(p_0, \vec{k})}$$

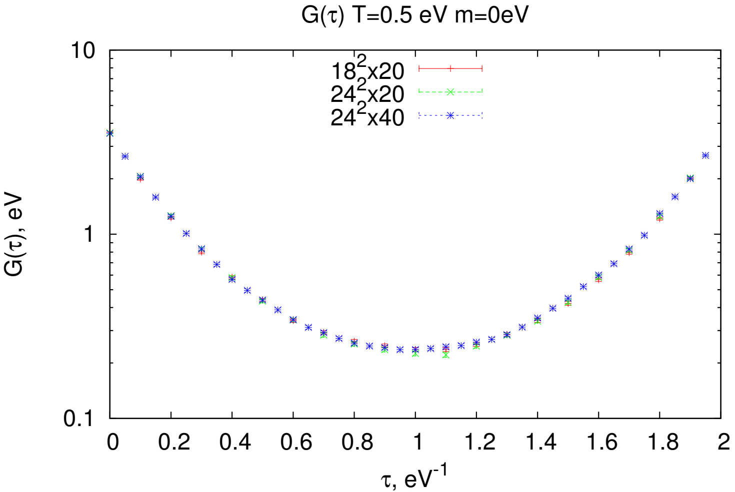
$$\left(e^{i\vec{k}(\vec{e}_b+\vec{e}_c)} \gamma(p_0, \vec{k})\gamma(q_0, \vec{k}) + e^{-i\vec{k}(\vec{e}_b+\vec{e}_c)} \beta(p_0, \vec{k})\beta(q_0, \vec{k})\right.$$

$$\left. - e^{i\vec{k}(\vec{e}_b-\vec{e}_c)} \delta(p_0, \vec{k})\delta(q_0, \vec{k}) - e^{-i\vec{k}(\vec{e}_b-\vec{e}_c)} \alpha(p_0, \vec{k})\alpha(q_0, \vec{k})\right)$$

Free case: Current-current correlator



Finite volume effects: Current-current correlator



Conductivity: calculation scheme

Green-Kubo relation

$$G(\tau) = \int_0^\infty \frac{dw}{2\pi} \frac{2w \cosh\left(w\left(\tau - \frac{1}{2T}\right)\right)}{\sinh\left(\frac{w}{2T}\right)} \sigma(w)$$

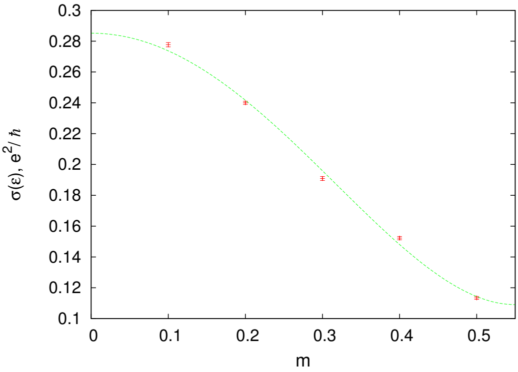
We can not get $\sigma(w)$ from this !

But!

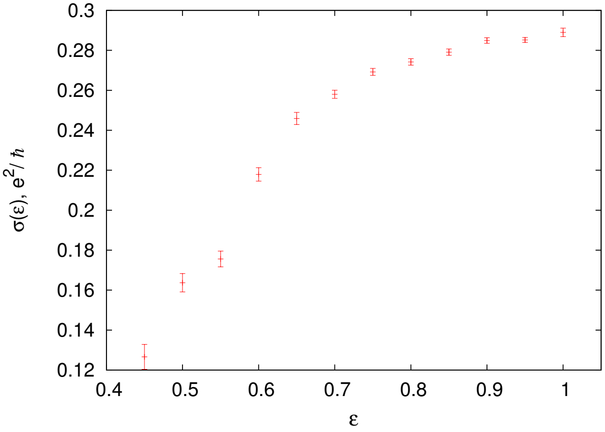
We can evaluate conductivity using average conductivity

$$\bar{\sigma} = \mathcal{N}^{-1} \int_0^\infty \frac{dw}{2\pi} \frac{2w}{\sinh\left(\frac{w}{2T}\right)} \sigma(w)$$

$$= \frac{1}{\pi T^2} G(\beta/2)$$



Conductivity: dependence on epsilon



Suspended graphene
with $\epsilon = 1$
$\sigma = 0.2890(21)\frac{e^2}{\hbar}$

Lattice $Nx = 18, Ny = 18, Nt = 20, \delta = 0.1eV^{-1}, \ T = 0.5eV$

Conclusions

- Dependence of conductivity on epsilon was calculated
- It has been shown that transition between conductive and insulator phases shifts into unphysical region of epsilon so that suspended graphene is a conductor
- Calculated conductivity agreeds with experiment
- It has ben shown that screening effects of σ - electrons plays important role

Thank you for attention!