Mitya Diakonov, 2010, Spain

Graphene conductivity: interacting fermions on 2D hexagonal lattice

P.V. Buividovich, E.V. Luschevskaya, M.I. Katsnelson, O.V. Pavlovsky, M.I.P., M.V. Ulybyshev, M.A. Zubkov,

PRL, ArXiv:1304.3660; Phys.Rev. B, ArXiv:1206.0619; Phys.Rev. B, ArXiv:1204.0921

- Introduction
- Charge carriers on hexagonal lattice
- Graphene, conductor or insulator?
- Impurity effects

Euler Symposium on Theoretical and Mathematical Physics
July 12-17, 2013, St. Petersburg, Russia

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ITEP Lattice

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Dynamics of charge carriers in graphene is described by lattice field theory of fermions on hexagonal lattice

QCD and Graphene

QCD	Graphene
1. Quarks 2. Confinement-Deconfinement 3. Chiral Condensate	1. Massless Dirac fermions 2. Insulator-conductor 3. Fermion Condensates

QCD and Graphene

QCD	Graphene
$\alpha_s \approx 1$	$\alpha_{eff} \approx 2$

Lattice QCD and Graphene

QCD	Graphene
Lattice spacing a -> 0	Lattice spacing a=0.142 nm

QCD and Graphene

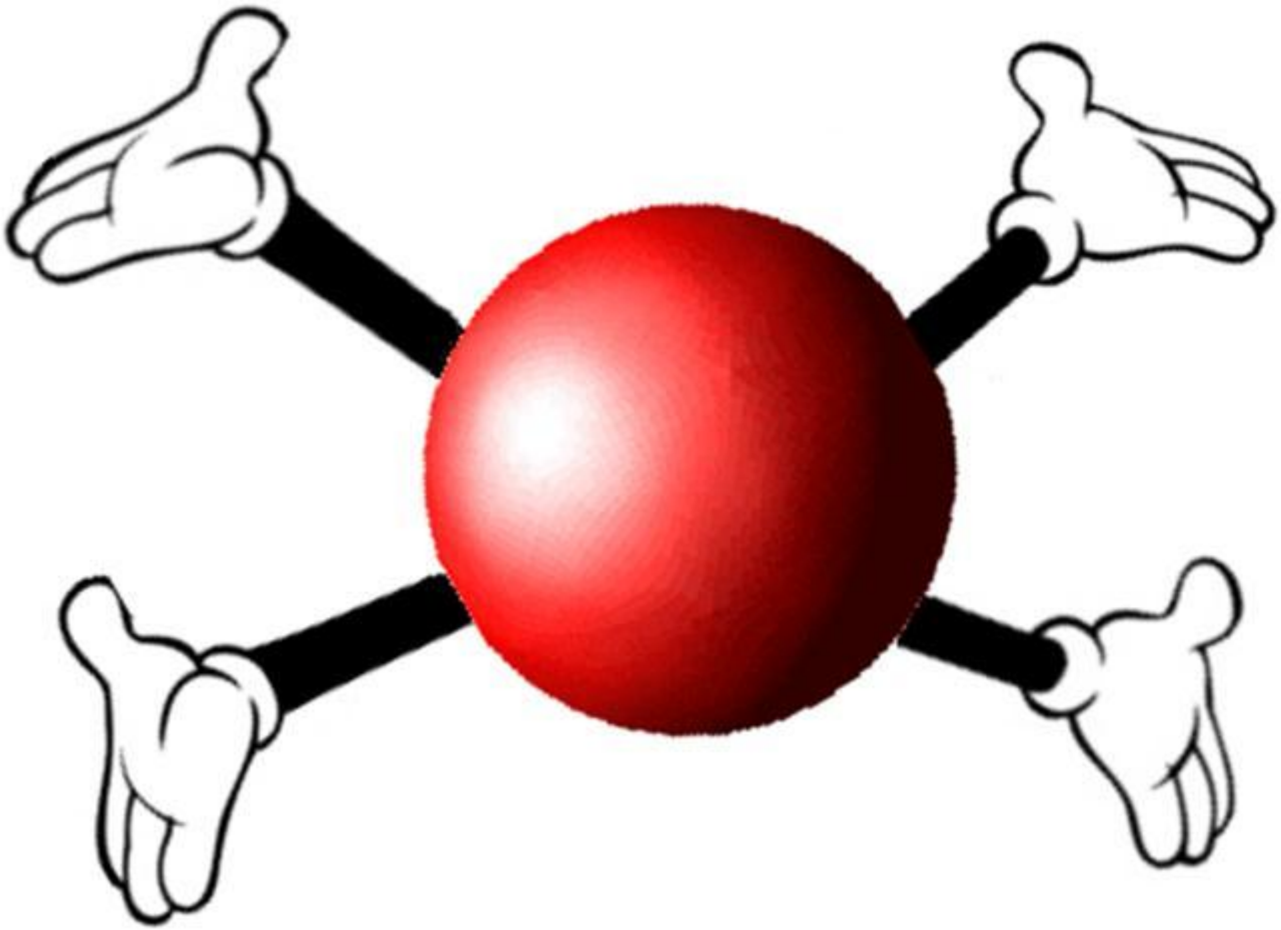
QCD	Graphene
SU(3) gauge group	Abelian theory (!)

Graphene is rather similar to lattice QCD

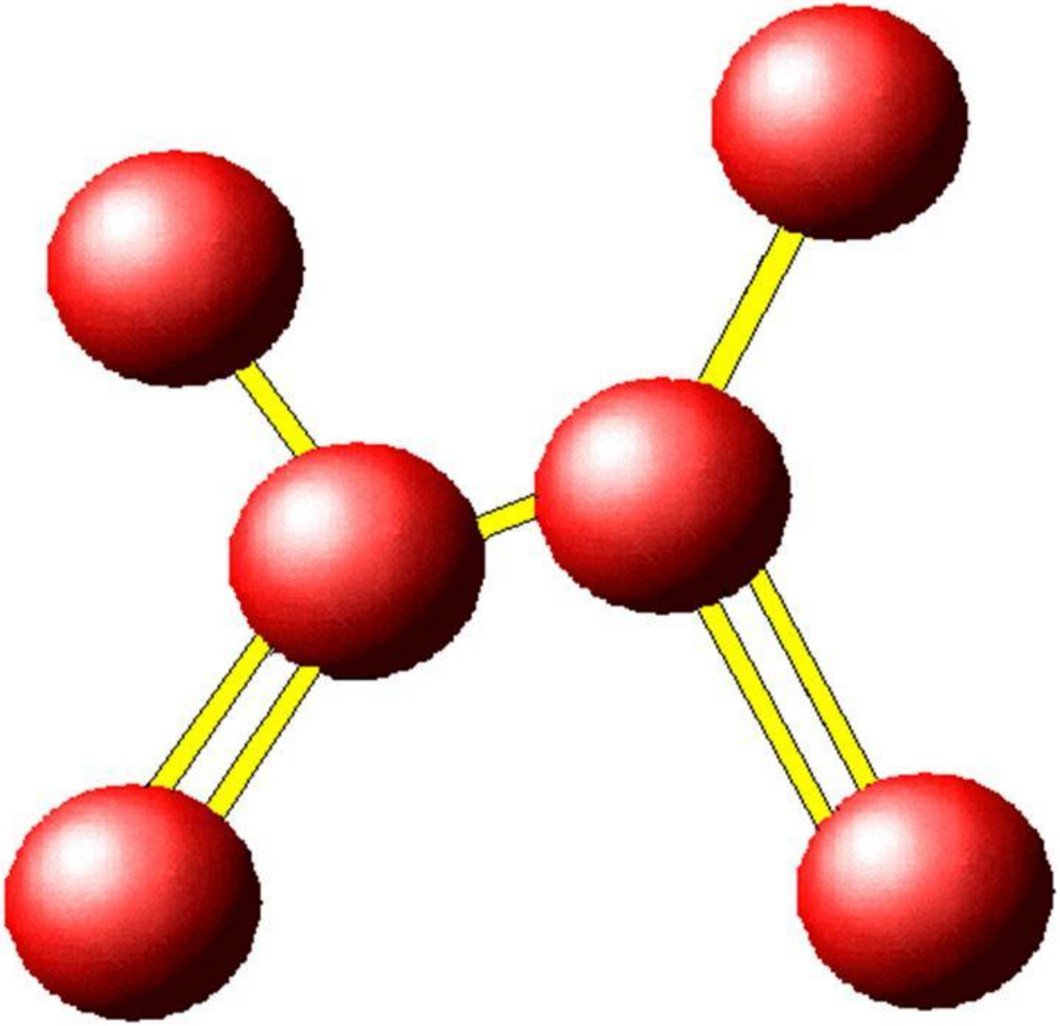
- **Strongly interacting fermions**
- **Lattice**
- **Phase transition**

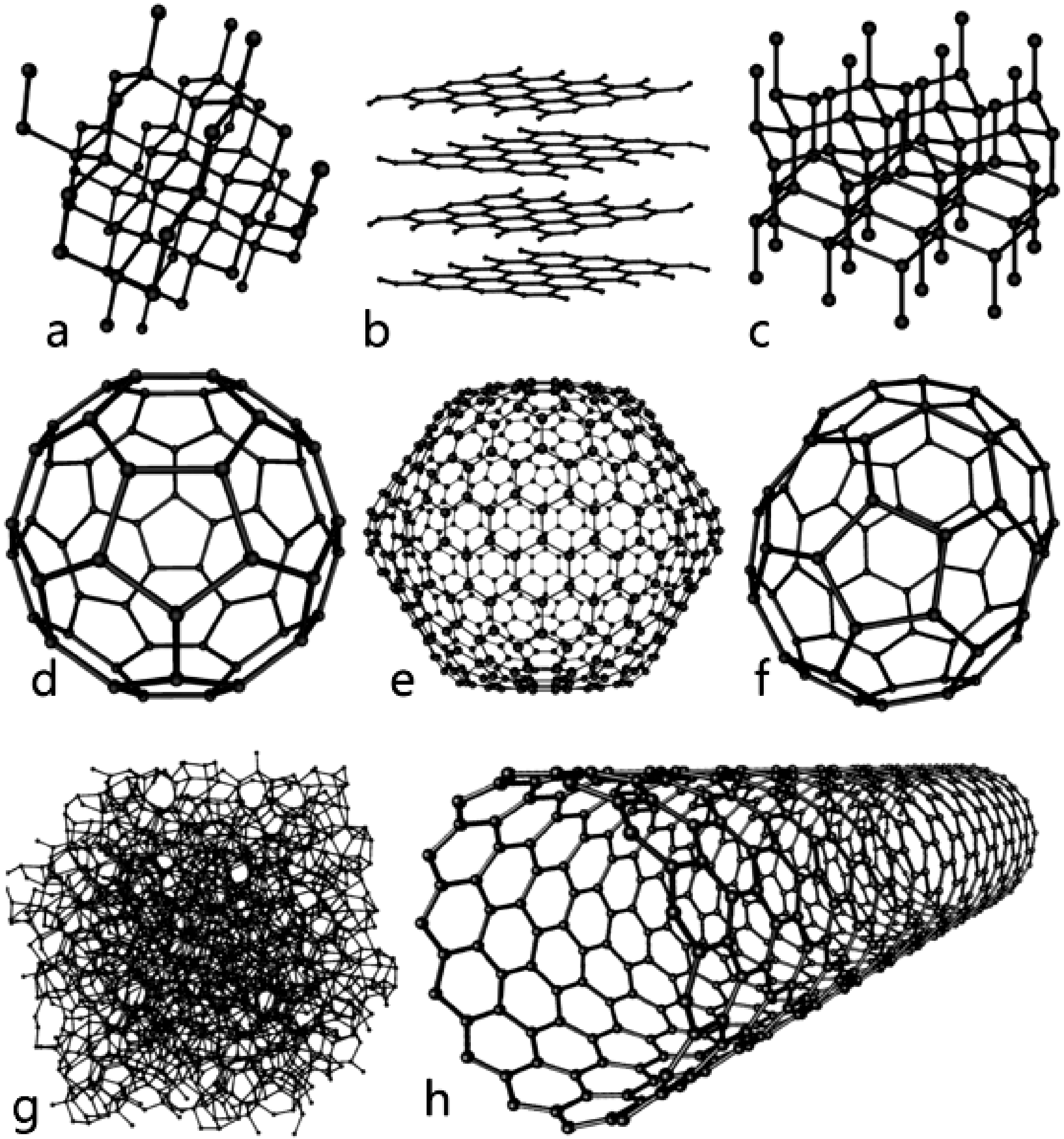
$\Rightarrow$ We apply the very well known lattice QCD methods (Monte Carlo, supercomputers) to simulate the dynamics of charge carriers in graphene

Carbon atom



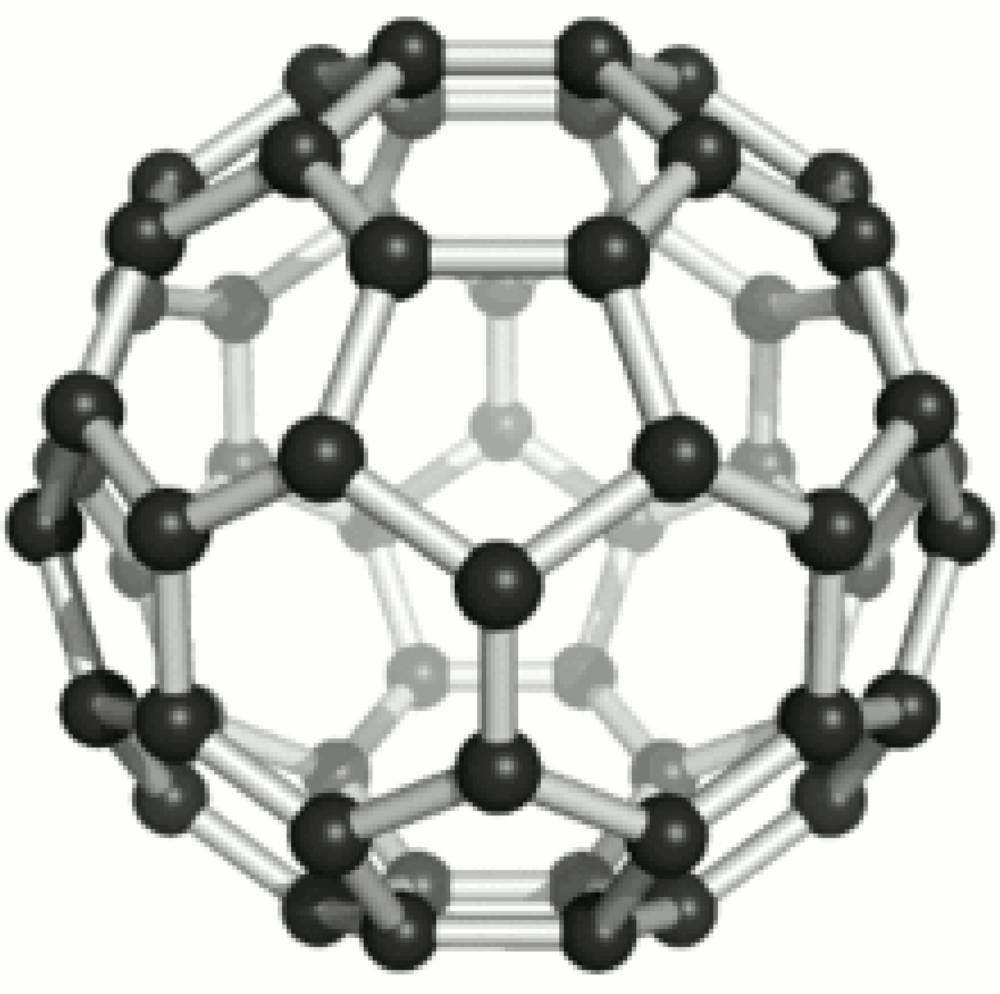
Elementary structure





Some allotropes of carbon: a) diamond; b) graphite; c)lonsdaleite; d–f) fullerenes (C_{60}, C_{540}, C_{70}); g) amorphous carbon; h) carbon nanotube.

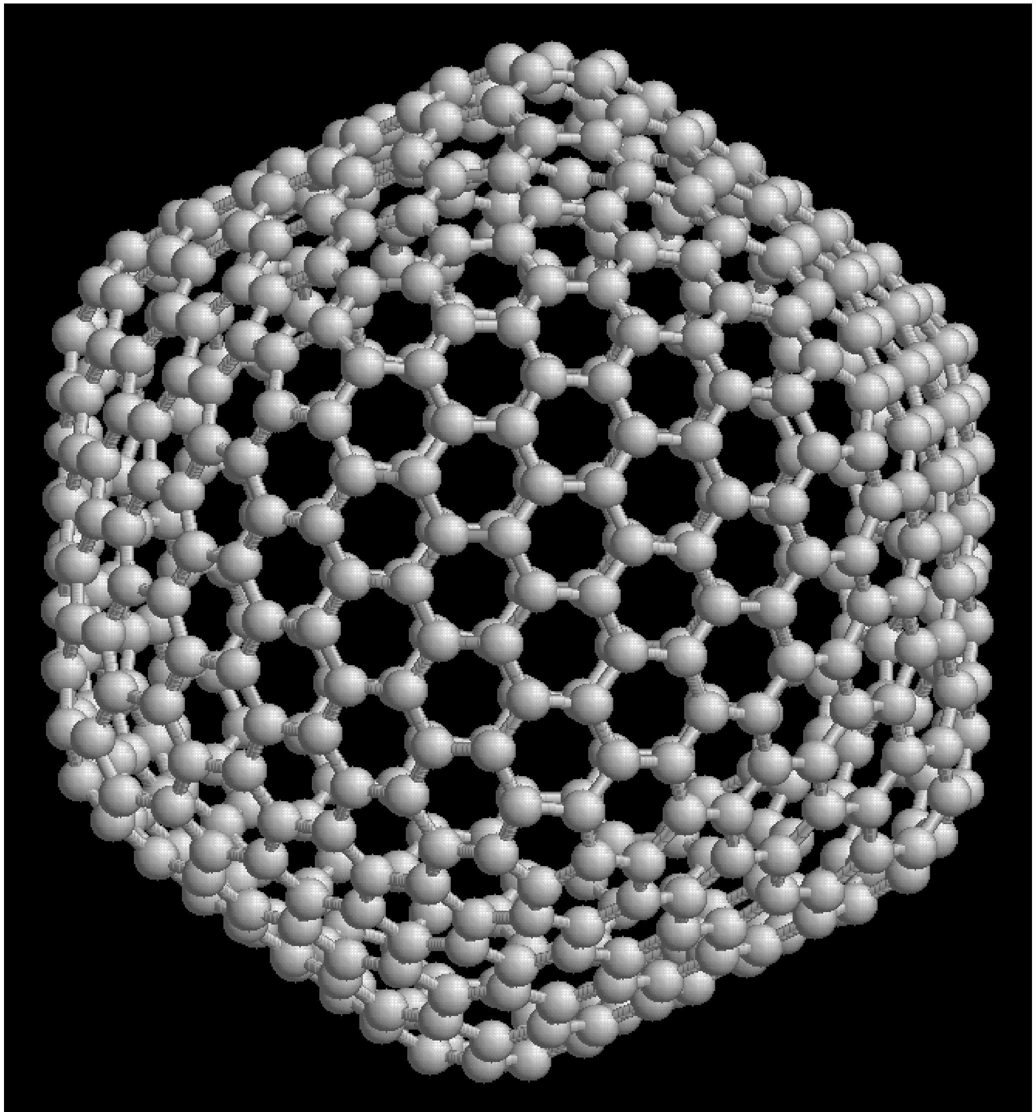
Fullerene (Buckminsterfullerene) C_{60}



Richard Buckminster Fuller
1895 -1983

The Montreal Biosphère by Buckminster Fuller, 1967

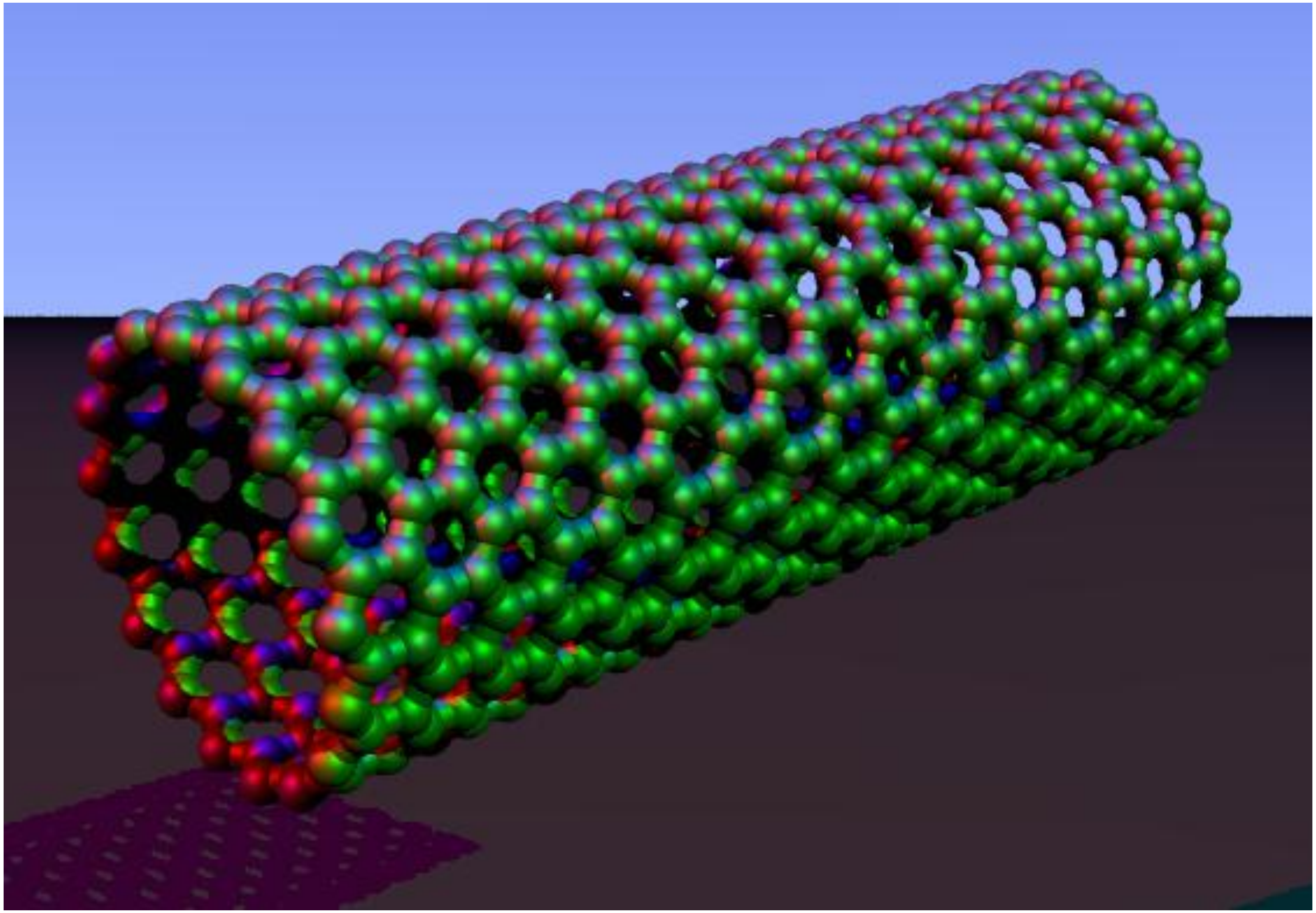
Fullerene C_{540}



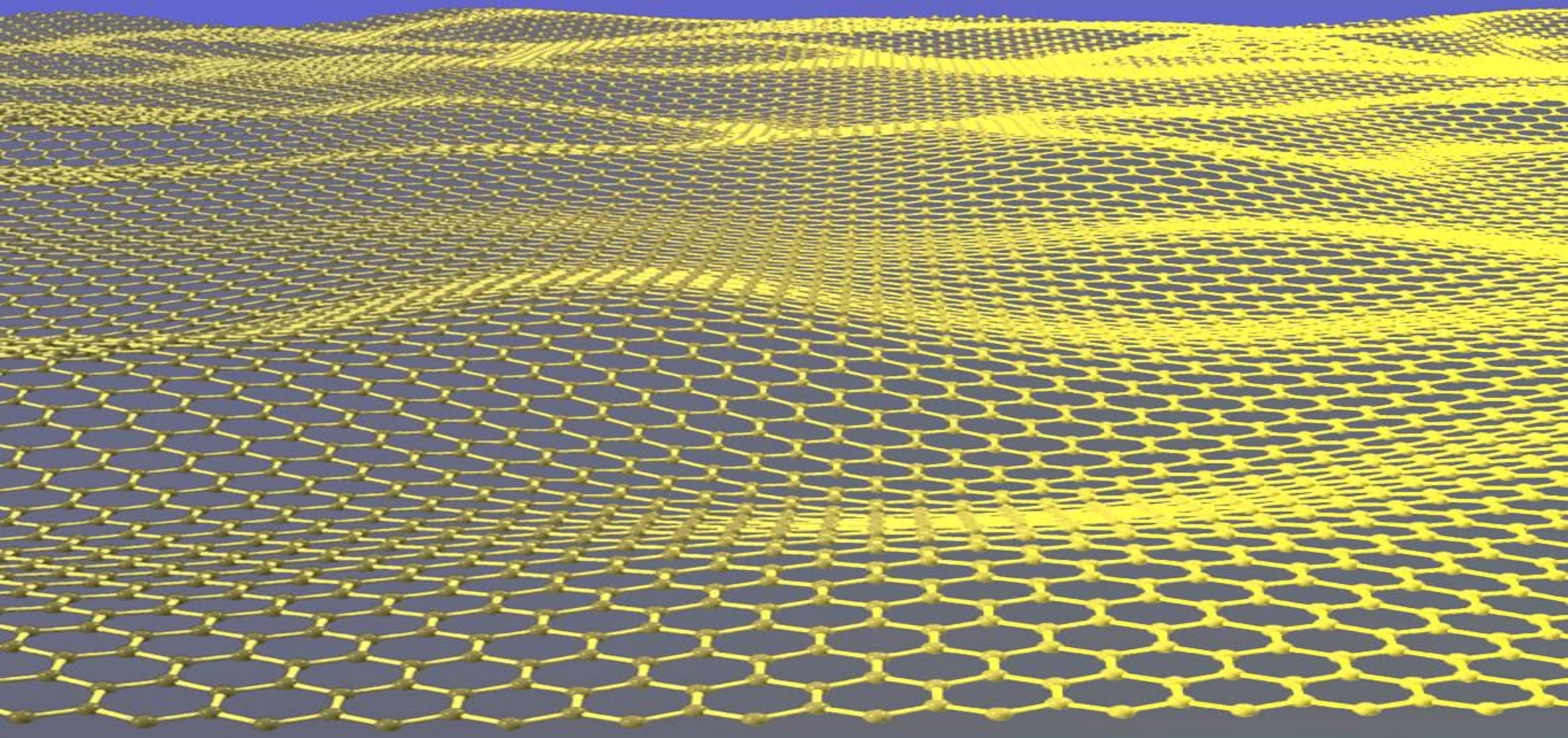
Richard Buckminster Fuller
1895 -1983

The Montreal Biosphère by Buckminster Fuller, 1967

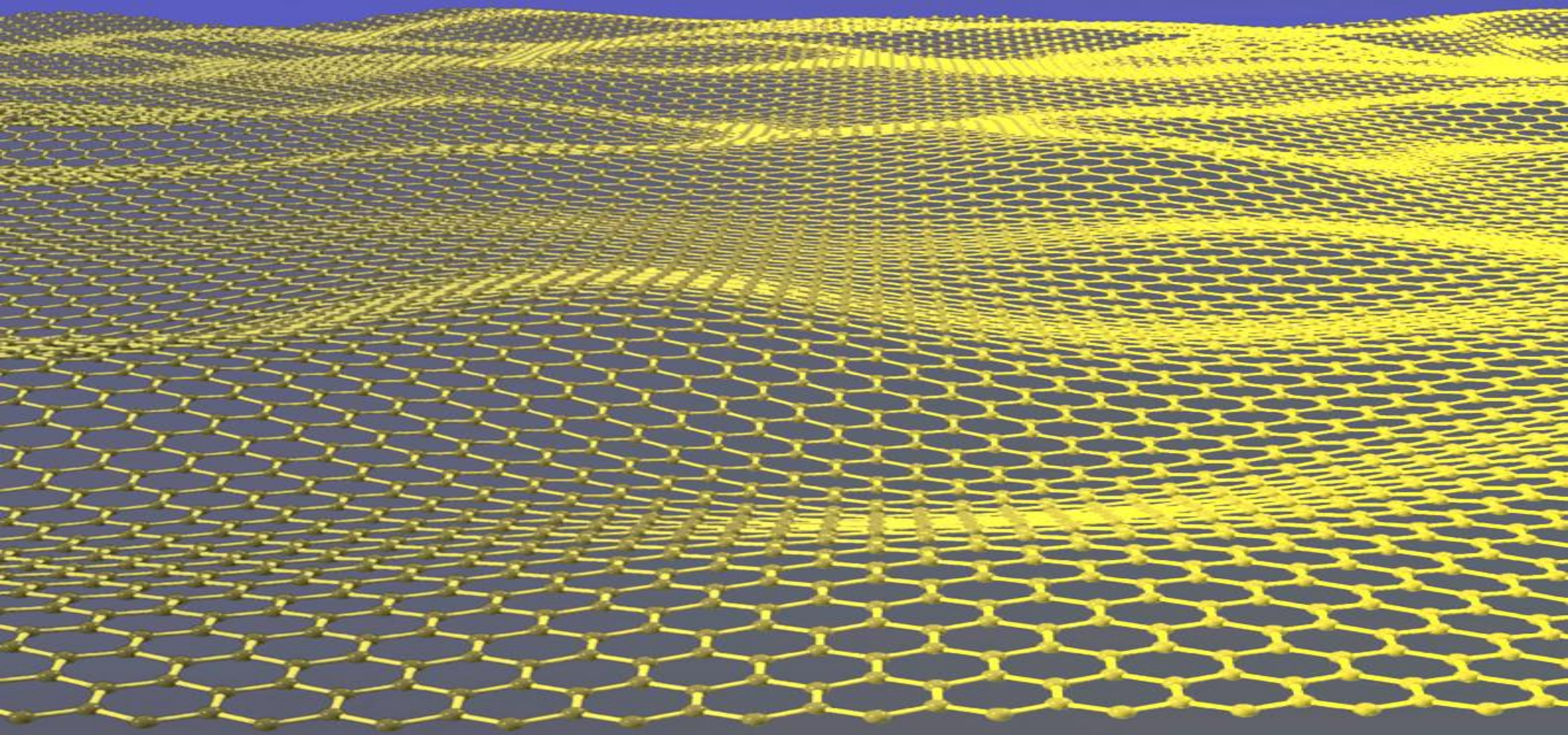
Nanotube



Graphene



The Nobel Prize in Physics for 2010 was awarded to Andre Geim and Konstantin Novoselov "for groundbreaking experiments regarding the two-dimensional material graphene"



After 2010 (Nobel prize) graphene become very popular

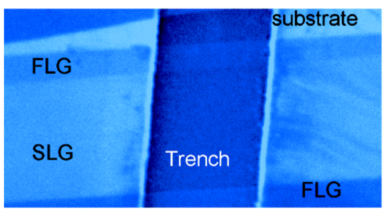
Rene Maltete

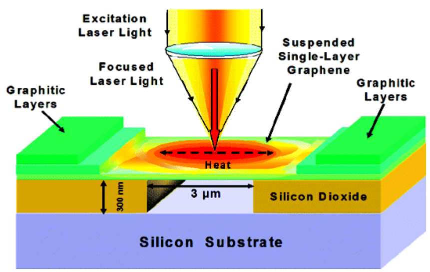
Extreme properties of Graphene

- **Superior Thermal Conductivity of Single-Layer Graphene**

Nano Lett., **2008**, *8* (3), pp 902–907

The room temperature values of the thermal conductivity in the range (4.84 ± 0.44) × 10^3 to (5.30 ± 0.48) × 10^3 W/mK





- **Giant Intrinsic Carrier Mobilities in Graphene and Its Bilayer**

Phys. Rev. Lett. 100, 016602 (2008)

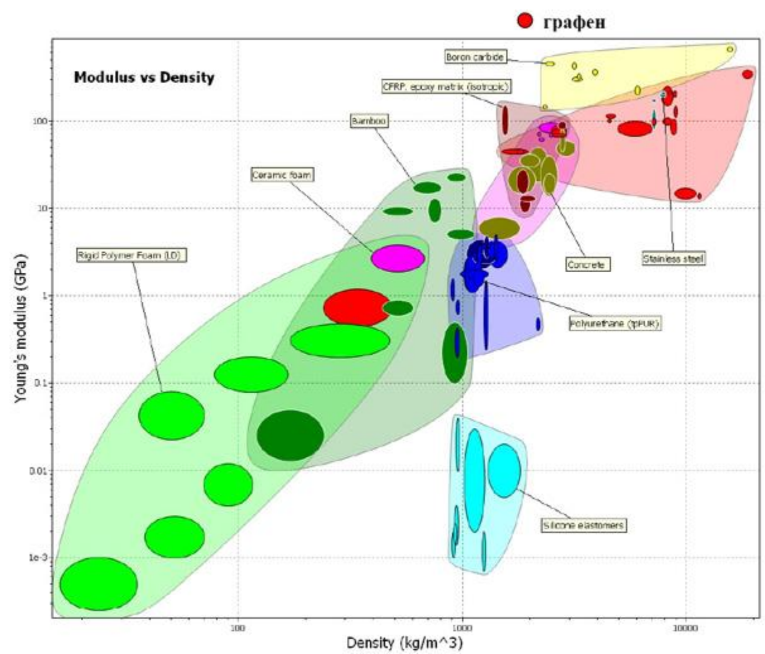
S. V. Morozov[1,2], K. S. Novoselov[1], M. I. Katsnelson[3], F. Schedin[1], D. C. Elias[1], J. A. Jaszczak[4], and A. K. Geim[1,*]

The temperature dependences of electron transport in graphene and its bilayer show extremely low electron-phonon scattering rates that set the fundamental limit on possible charge carrier mobilities at room temperature.

- **Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene**

Science 18 July 2008: Vol. 321 no. 5887 pp.385

These quantities correspond to a Young's modulus of E = 1.0 terapascals. These experiments establish graphene as **the strongest material ever measured**



Relativistic particle

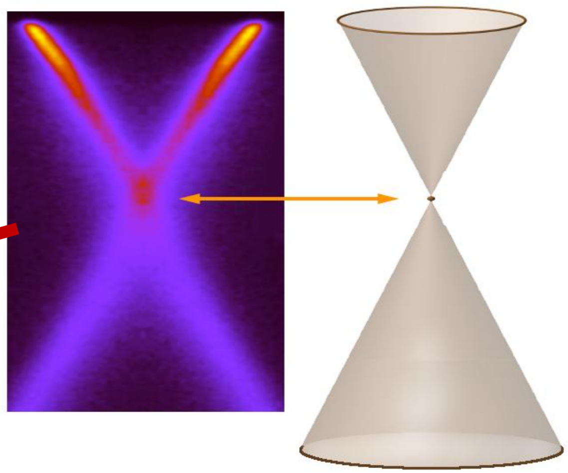
$$E = \sqrt{m^2 c^4 + p^2 c^2}$$

Massless particle

$$E = cp$$

Relativistic particle $E = \sqrt{m^2c^4 + p^2c^2}$

Massless particle $E = cp$



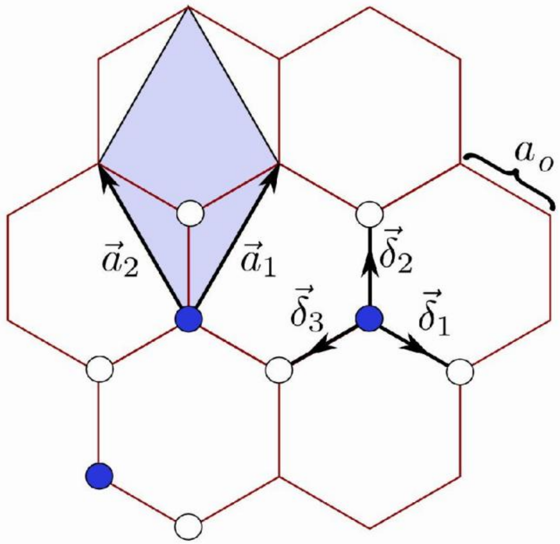
Graphene $E = v_F\, p; \quad v_F = \frac{c}{300};$

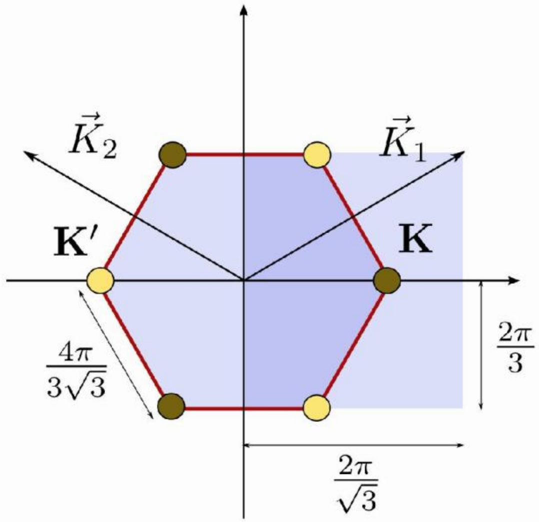
$$\alpha_g = 300\alpha = 2.16 > 1$$

$$\alpha_g > \alpha_g^{crit} = 1.11 \pm 0.06$$

Suspended graphene is the insulator! (???)

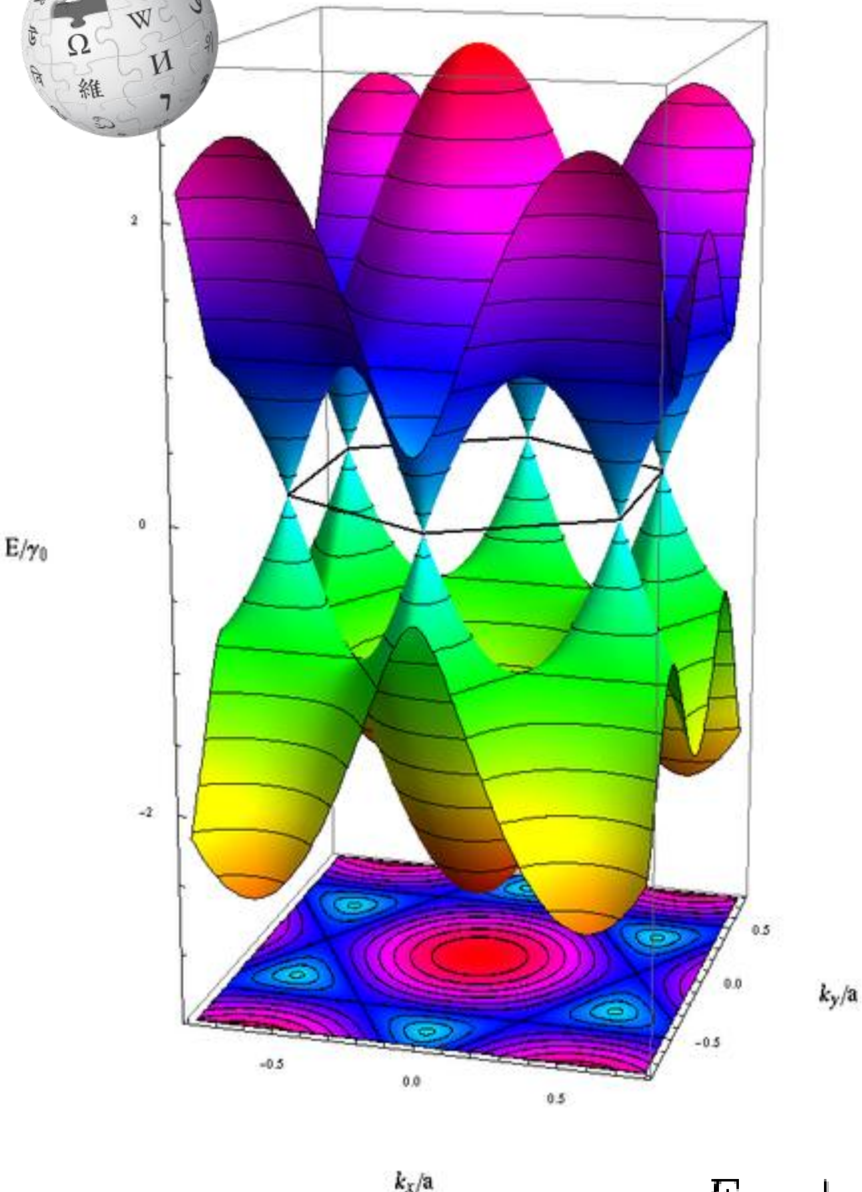
Graphene lattice and Brillouin zone





$$H = -t \sum_{n,\boldsymbol{\delta}_i} |A, \boldsymbol{R}_n\rangle\langle \boldsymbol{R}_n + \boldsymbol{\delta}_i, B| + \mathrm{H.c.}\,,$$

$$E(\boldsymbol{k}) = \pm t|1 + e^{i\boldsymbol{k}\cdot\boldsymbol{a}_1} + e^{i\boldsymbol{k}\cdot\boldsymbol{a}_2}|$$



Wallace, P. R. (1947). "The Band Theory of Graphite". Physical Review 71 (9): 622.

Semenoff, G. W. (*1984*). "Condensed-Matter Simulation of a Three-Dimensional Anomaly". Physical Review Letters 53 (26): 2449.

$$E(\boldsymbol{k}) = \pm t|1 + e^{i\boldsymbol{k}\cdot\boldsymbol{a}_1} + e^{i\boldsymbol{k}\cdot\boldsymbol{a}_2}|$$

$$E = \pm\sqrt{\gamma_0^2\left(1 + 4\cos^2\frac{k_y a}{2} + 4\cos\frac{k_y a}{2}\cdot\cos\frac{k_x\sqrt{3}a}{2}\right)}$$

Fermi velocity, v_F, (velocity at Fermi point)

$$E(q) = v_F \left| \vec{q} \right|$$

$$v_F = \frac{3}{2} \kappa a \approx c/300$$

$a \approx 0.142\, nm$ $\kappa \approx 2.7\, eV$

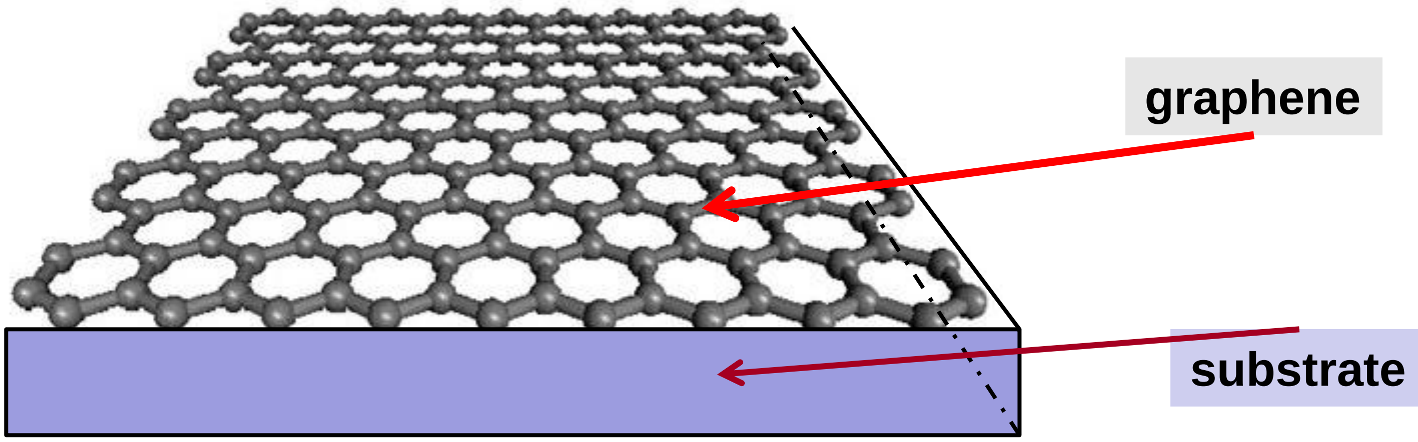
nonrelativistic electrons are “equivalent” to *massless four component Dirac fermions (G. Semenoff 1984)*

We can vary the effective coupling in graphene!

Graphene in the dielectric media $$\alpha_g \to \frac{\alpha_g}{\varepsilon}$$

dielectric permittivity → ε

Graphene on substrate $$\alpha_g \to \frac{2}{1+\varepsilon}\alpha_g$$



$$\text{if} \quad \frac{2}{1+\varepsilon}\alpha_g < \alpha_g^{crit} (\approx 1.11) \quad \text{graphene is the conductor (?)}$$

Effective theory of charge carriers in graphene

1. "Massless" four component Dirac fermions

2. Fermi velocity is $$v_F = c/300$$

3. The effective charge is $$\alpha_g \approx 300\alpha \approx 2.16 > 1$$

4. We can vary the effective charge if we vary the dielectric permittivity of the substrate

$$\alpha_g \to \frac{2}{1+\varepsilon}\alpha_g$$

Vacuum ε=1, silicon dioxide SiO_2 ε ~ 3.9, silicon carbide SiC ε ~ 10

Effective field theory for graphene

$$D[A_0] = \gamma_0(\partial_0 + iA_0) + v_F \gamma_i \partial_i, \quad i = 1,2$$

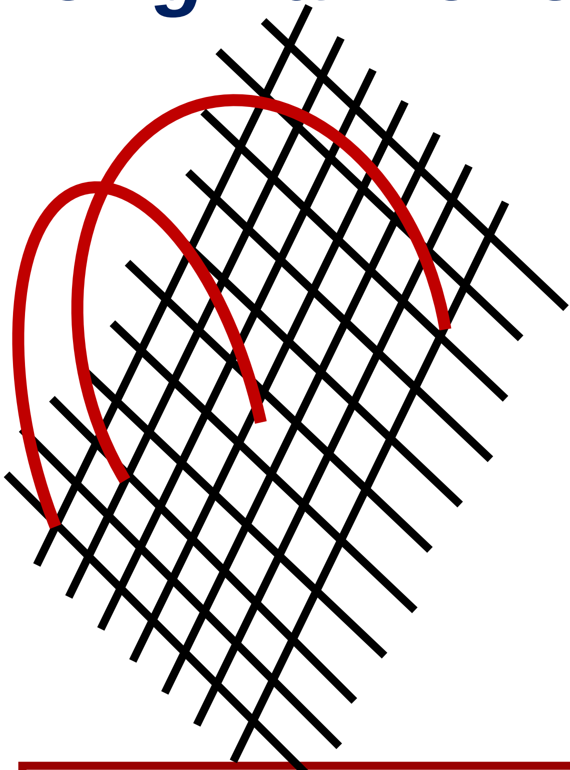
After transformation $t' = v_F t, \quad A'_0 = A_0 / v_F.$

we can neglect A_i, **and**

$$\frac{1}{137} = \alpha \rightarrow \frac{\alpha}{v_F} \approx 300\alpha = \alpha_g \approx 2.2$$

$$S_E \equiv \frac{1}{2g^2} \int d^3x\, dt\, (\partial_i A_0)^2 - \sum_{a=1}^{N_f} \int d^2x\, dt\, \bar{\psi}_a D[A_0] \psi_a,$$

<u>Approach 1,</u> *simulation of the effective theory on hypercubic lattice (forget about original honeycomb lattice)*



J.E. Drut, T.A. Lahde (2009-2012)
P.V. Buividovich et al. (ITEP group) (2012-2013)

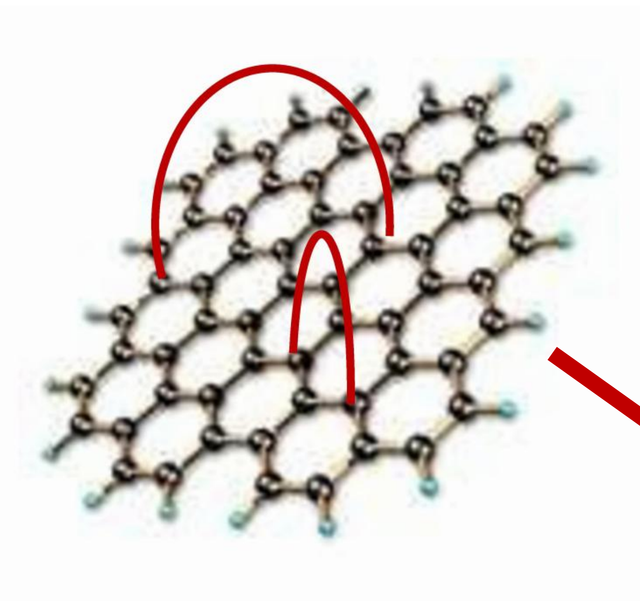
(2+1)D staggered fermions

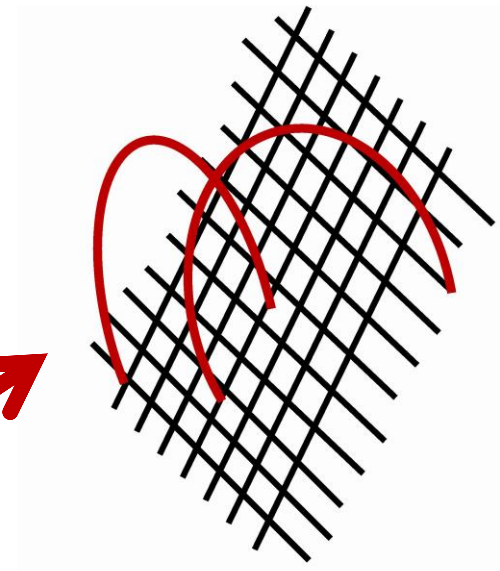
(3+1)D Coulomb

$$S_E \equiv \frac{1}{2g^2} \int d^3x\, dt\, (\partial_i A_0)^2 - \sum_{a=1}^{N_f} \int d^2x\, dt\, \bar{\psi}_a D[A_0] \psi_a,$$

honeycomb lattice – continuum theory - hypercubic lattice

little bit eclectic approach





$$S_E \equiv \frac{1}{2g^2}\int d^3x\,dt\,(\partial_i A_0)^2 - \sum_{a=1}^{N_f}\int d^2x\,dt\,\bar{\psi}_a D[A_0]\psi_a,$$

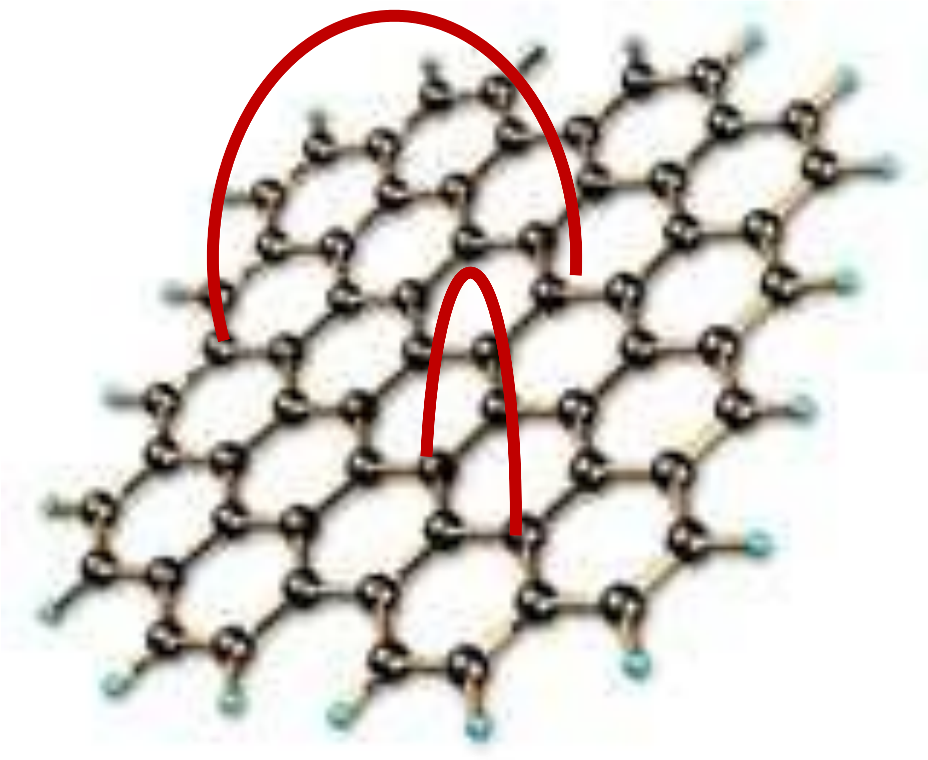
honeycomb lattice – continuum theory - hypercubic lattice

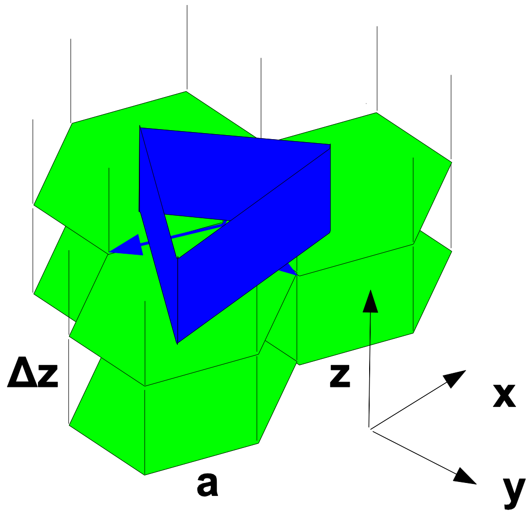
little bit eclectic approach

Elliott Erwitt

Approach 2, 2D honeycomb lattice and rectangular lattice in Z and time dimensions

R. Brower, C. Rebbi, and D. Schaich (2009-2013)
P.V. Buividovich, M.I. Katsnelson, M.V. Ulybyshev, M.I.P. (2012-2013)





Approach 2, 2D hexagonal lattice, Hamiltonian

$$\hat{H} = \hat{H}_{tb} + \hat{H}_I$$

$$\hat{H} = -\kappa \sum_{\sigma=\uparrow,\downarrow} \sum_{<XY>} \left(\hat{\psi}^{\dagger}_{\sigma,X} \exp\left(\pm i\hat{\theta}_{XY}\right) \hat{\psi}_{\sigma,Y} + \right.$$

$$\left. + \hat{\psi}^{\dagger}_{\sigma,Y} \exp\left(\pm i\hat{\theta}_{YX}\right) \hat{\psi}_{\sigma,X} \right) +$$

$$+ \sum_{\sigma=\uparrow,\downarrow} \sum_{X_1} m\, \hat{\psi}^{\dagger}_{\sigma,X_1} \hat{\psi}_{\sigma,X_1} - \sum_{\sigma=\uparrow,\downarrow} \sum_{X_2} m\, \hat{\psi}^{\dagger}_{\sigma,X_2} \hat{\psi}_{\sigma,X_2}$$

2D hexagonal lattice, from Hamiltonian to partition function, see Appendix A,

$$\hat{H} = \hat{H}_{tb} + \hat{H}_{I}$$

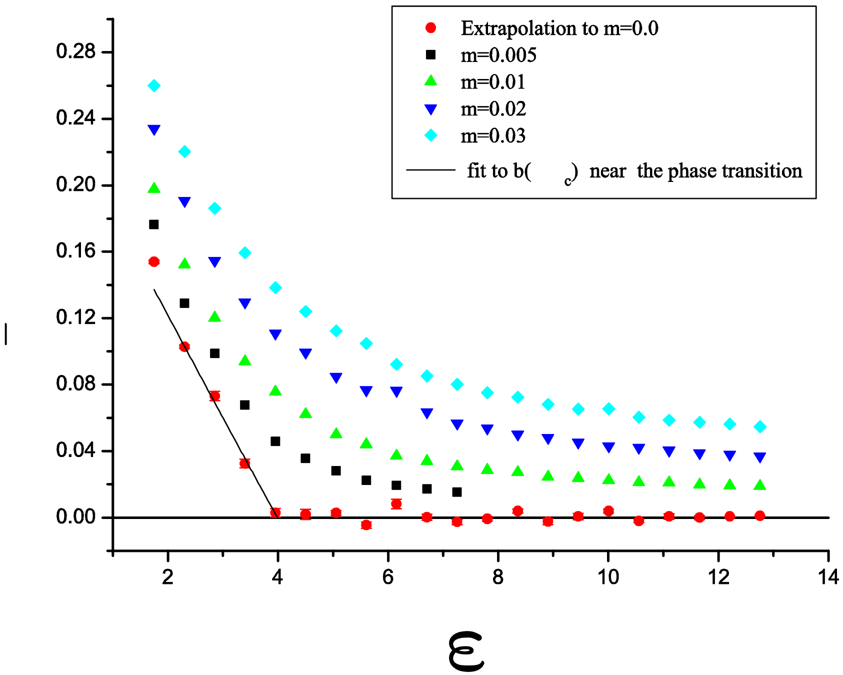
$$\Downarrow$$

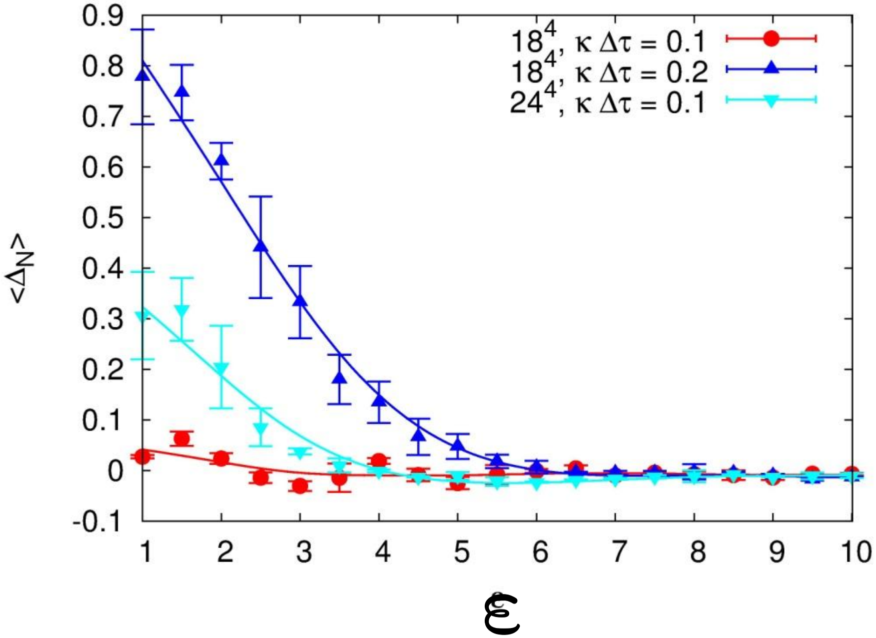
$$Z = Tr\, e^{-\frac{\hat{H}}{kT}}$$

Numerical results
(Monte Carlo for fermions)

ArXiv:1204.0921;
ArXiv:1206.0619
Phys.Rev. B

Fermion condensate as the function of substrate dielectric permittivity



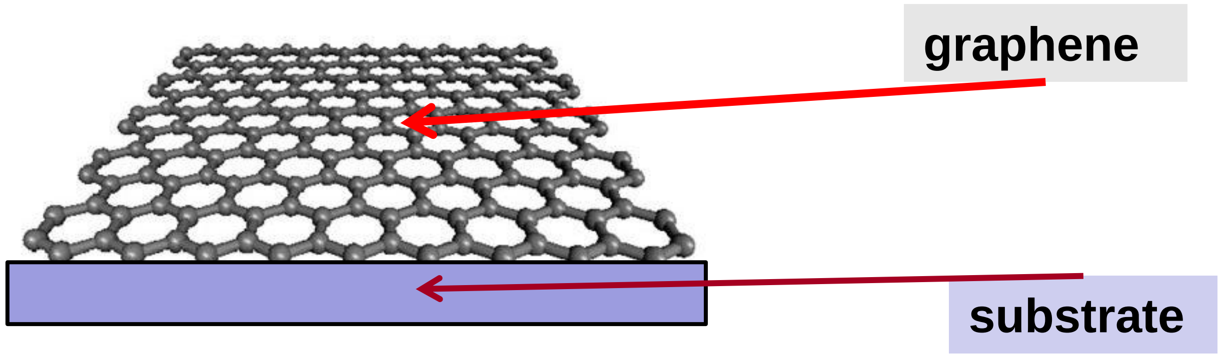


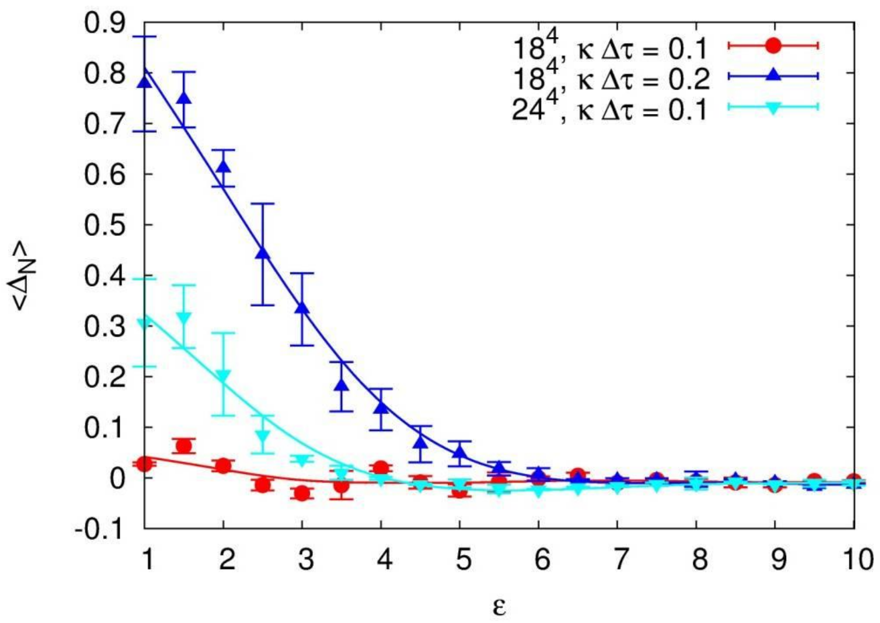
Approach 1

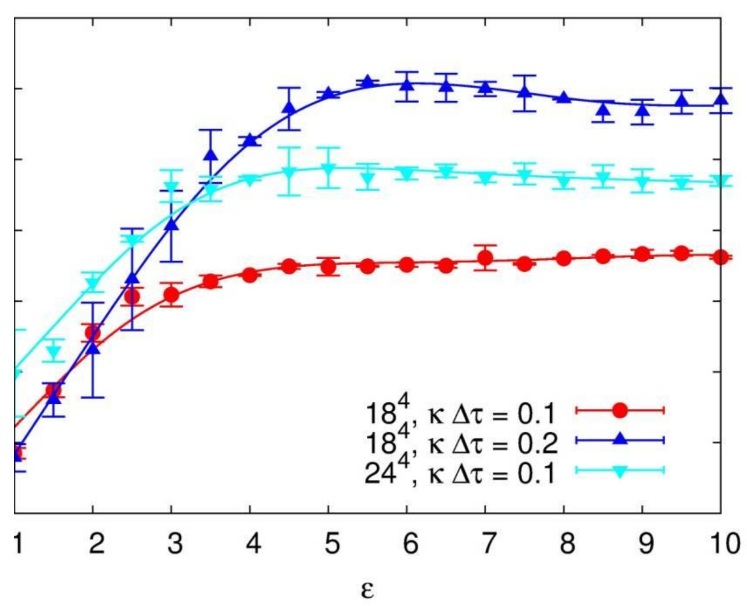
Hypercubic lattice

Approach 2

Hexagonal lattice







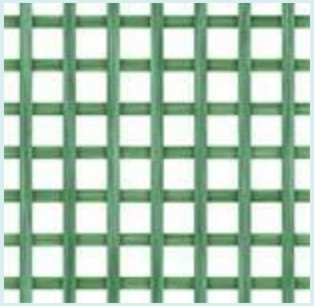
Fermion condensate as a function of substrate dielectric permittivity

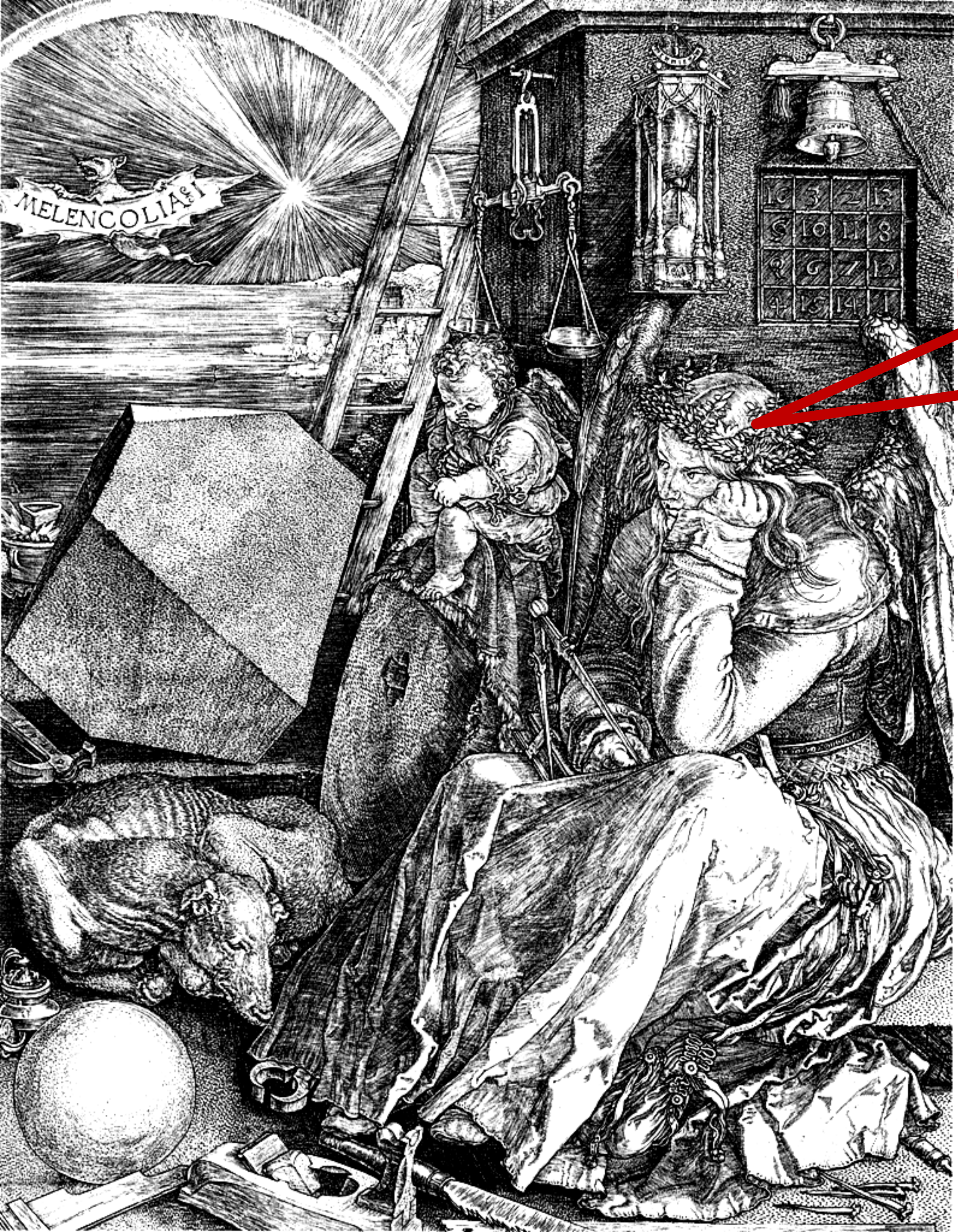
Conductivity as a function of substrate dielectric permittivity

Main Results for Coulomb interaction

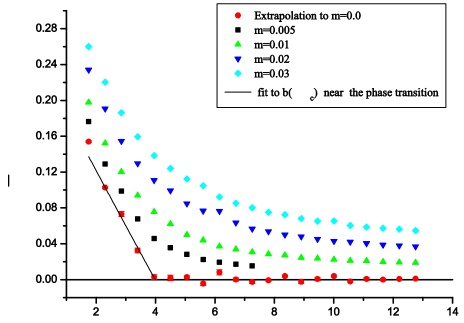
(effective theory and hexagonal lattices)

APPROACH 1	APPROACH 2
HYPERCUBIC LATTICE	HEXAGONAL LATTICE
TRANSITION AT $\varepsilon = 4 \pm 1$	TRANSITION AT $\varepsilon = 4 \pm 1$
SECOND ORDER (?)	CROSSOVER (?)

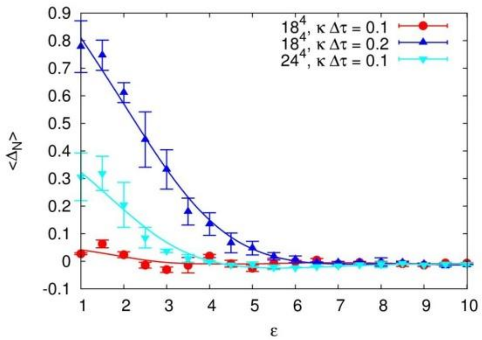



MELENCOLIA I
There exists a very Big problem!

Problem of the phase transition



Approach 1
Hypercubic lattice



Approach 2
Hexagonal lattice

Theory and numerical calculations: Existence of the phase transition at $\varepsilon > 1$

Suspended graphene ($\varepsilon = 1$) is an insulator

Lattice calculations

J. E. Drut, T. A. Lähde, and E. Tölö, PoS **Lattice2010**, 006 (2010), ArXiv:1011.0643.
J. E. Drut and T. A. Lähde, *Signatures of a gap in the conductivity of graphene* (2010), ArXiv:1005.5089.

J. E. Drut and T. A. Lähde, Phys. Rev. Lett. **102**, 026802 (2009), ArXiv:0807.0834.
J. E. Drut and T. A. Lähde, Phys. Rev. B **79**, 165425 (2009), ArXiv:0901.0584.
J. E. Drut and T. A. Lähde, Phys. Rev. B **79**, 241405 (2009), ArXiv:0905.1320.
J. E. Drut, T. A. Lähde, and L. Suoranta, *First-order chiral transition in the compact lattice theory of graphene and the case for improved actions* (2010), ArXiv:1002.1273.
J. E. Drut and T. A. Lähde, PoS **Lattice2011**, 074 (2011), ArXiv:1111.0929.

Solution of the gap equation

H. Leal and D. V. Khveshchenko, Nucl. Phys. B **687**, 323 (2004), ArXiv:cond-mat/0302164.
O. V. Gamayun, E. V. Gorbar, and V. P. Gusynin, Phys. Rev. B **81**, 075429 (2010), ArXiv:0911.4878.

Strong coupling expansion

Y. Araki and T. Hatsuda, Phys. Rev. B **82**, 121403 (2010), ArXiv:1003.1769.
Y. Araki, Ann.Phys. **326**, 1408 (2011), ArXiv:1010.0847.
Y. Araki, Phys. Rev. B **85**, 125436 (2012), ArXiv:1201.1737.

Experiment: Absence of the phase transition

D. C. Elias, R. V. Gorbachev, A. S. Mayorov, S. V. Morozov, A. A. Zhukov, P. Blake, L. A. Ponomarenko, I. V. Grigorieva, K. S. Novoselov, F. Guinea, et al., Nature Phys. **7**, 701 (2011), ArXiv:1104.1396.

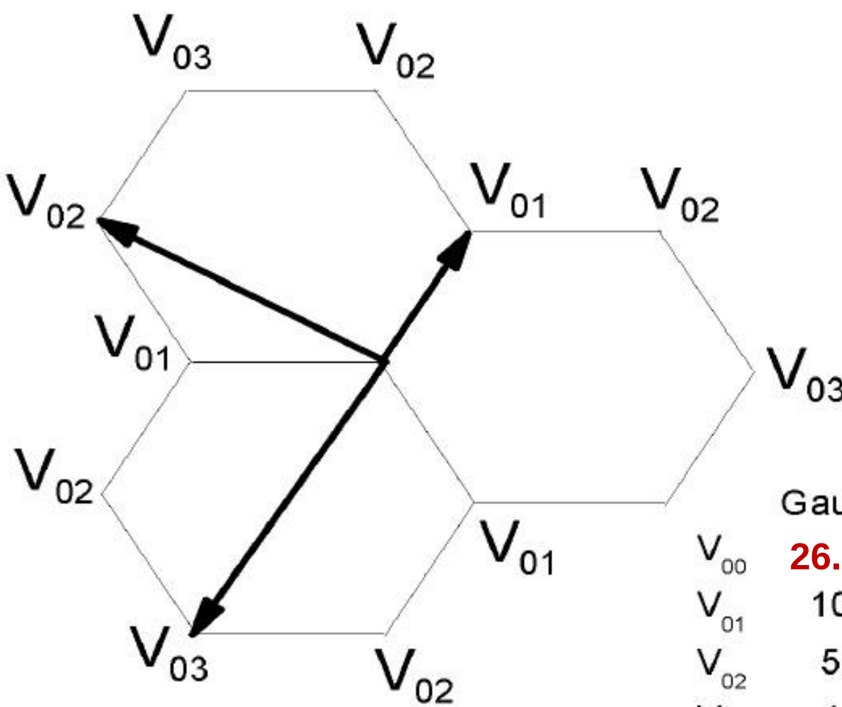
A. S. Mayorov, D. C. Elias, I. S. Mukhin, S. V. Morozov, L. A. Ponomarenko, K. S. Novoselov, A. K. Geim, and R. V. Gorbachev, *How close can one approach the dirac point in graphene experimentally?* (2012), ArXiv:1206.3848.

Suspended graphene ($\varepsilon=1$) is in the conducting phase

Solution of the problem of the phase transition

ArXiv:1304.3660

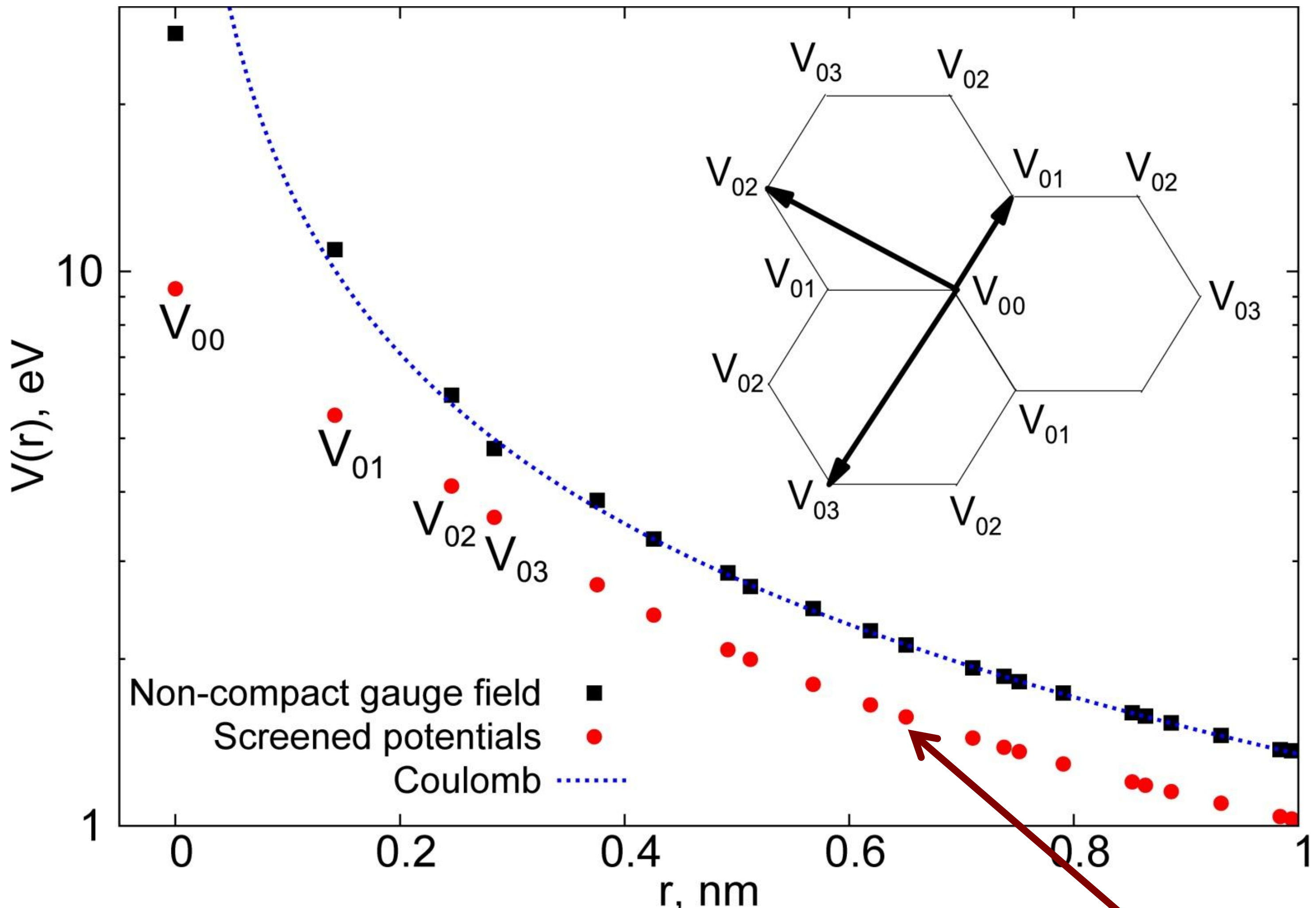
Modification of electrostatic interaction, taking into account the screening of Coulomb potential by electrons on σ-orbitals



arXiv 1101.4007
M.I. Katsnelson et al.

	Gauge field	Phenomenology
V_{00}	**26.2** eV	9.3 eV
V_{01}	10.2 eV	5.5 eV
V_{02}	5.3 eV	4.1 eV
V_{03}	4.1 eV	3.6 eV

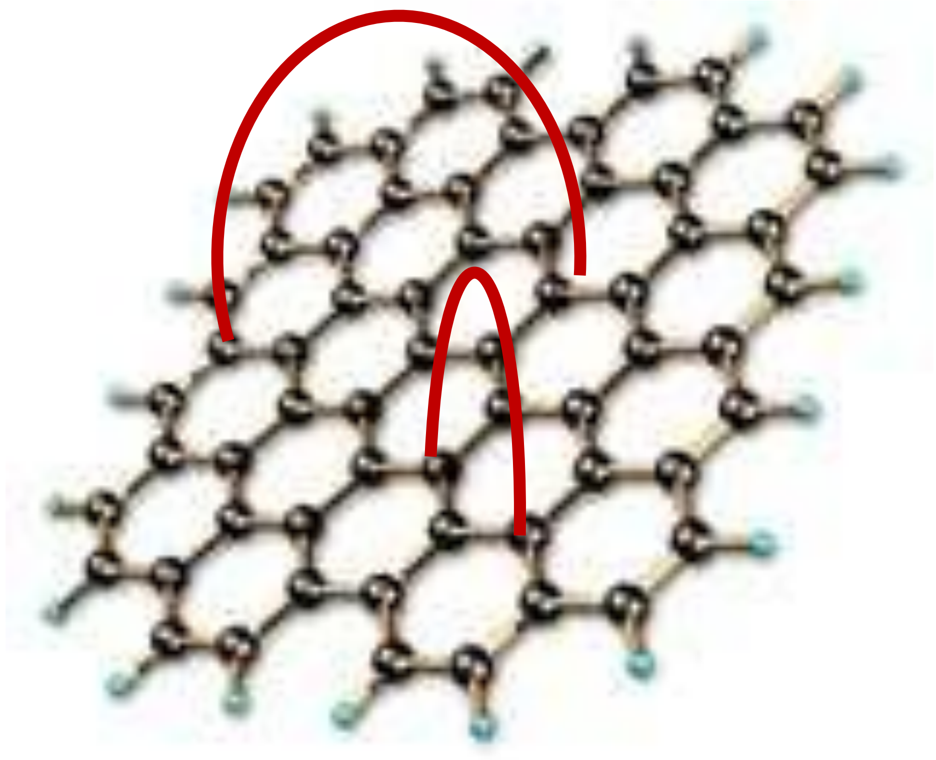
Screening of the Coulomb potential due to electrons on σ-orbitals

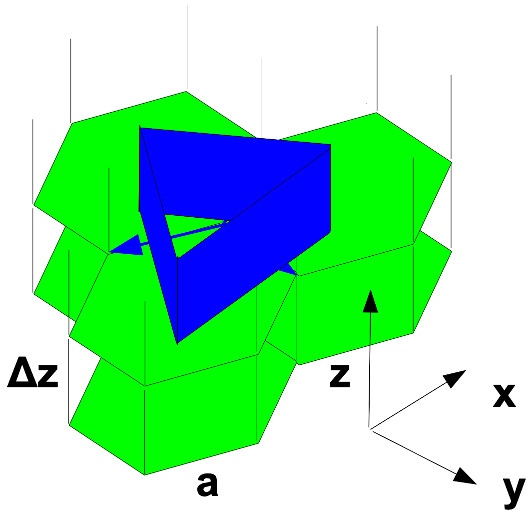


arXiv 1101.4007
M.I. Katsnelson et al.

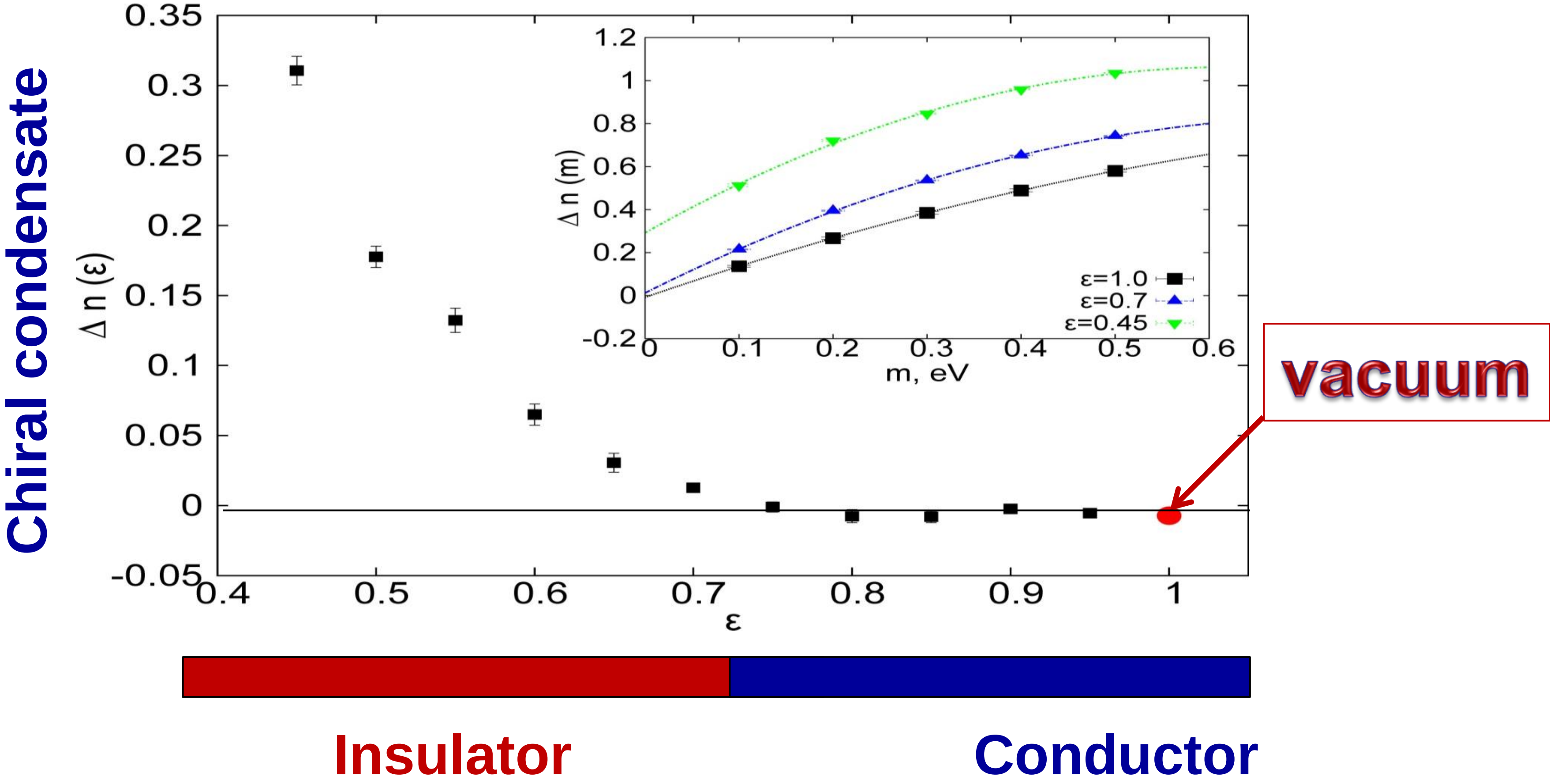
Approach 3, 2D honeycomb lattice, rectangular lattice in Z and time dimensions, screened Coulomb, Hubbard-Stratonovich transformation, see Appendix B

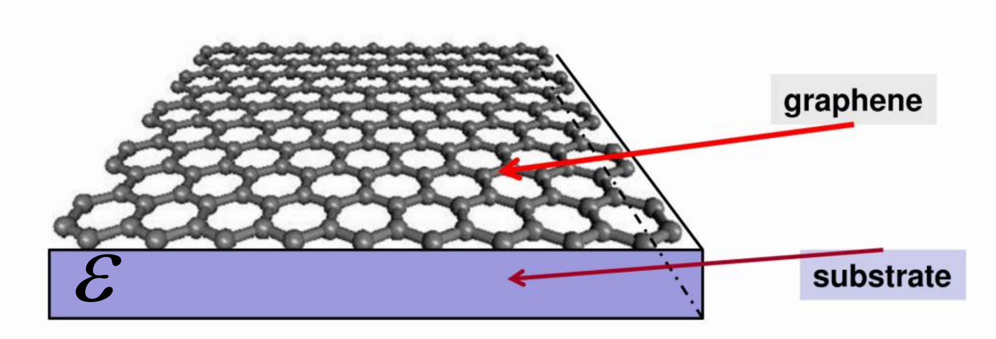
P.V. Buividovich, M.I. Katsnelson, M.V. Ulybyshev, M.I.P. arXiv:1304.3660





Deformed Coulomb potential (Monte Carlo results)

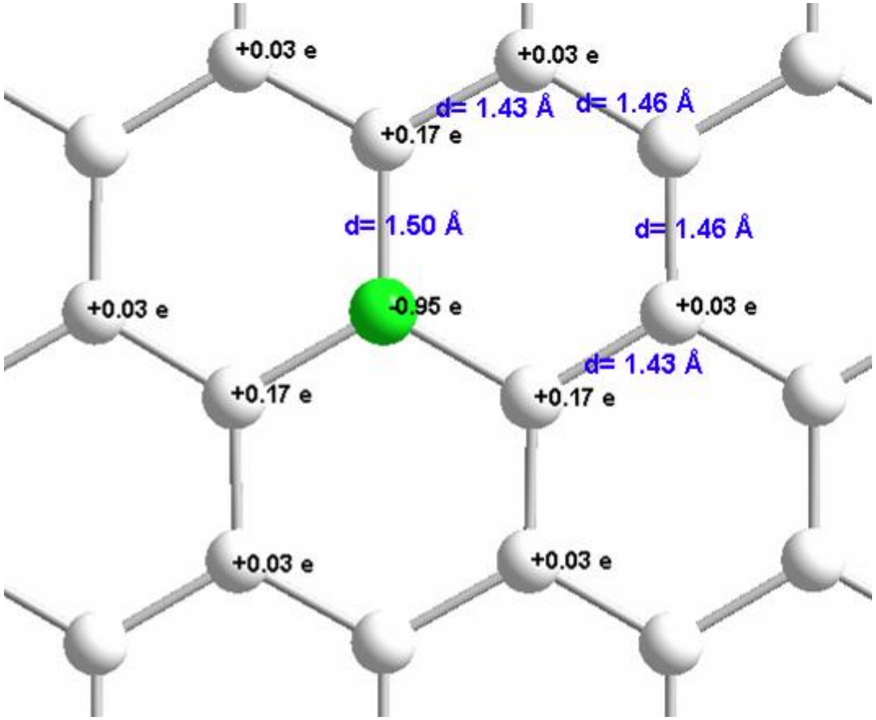




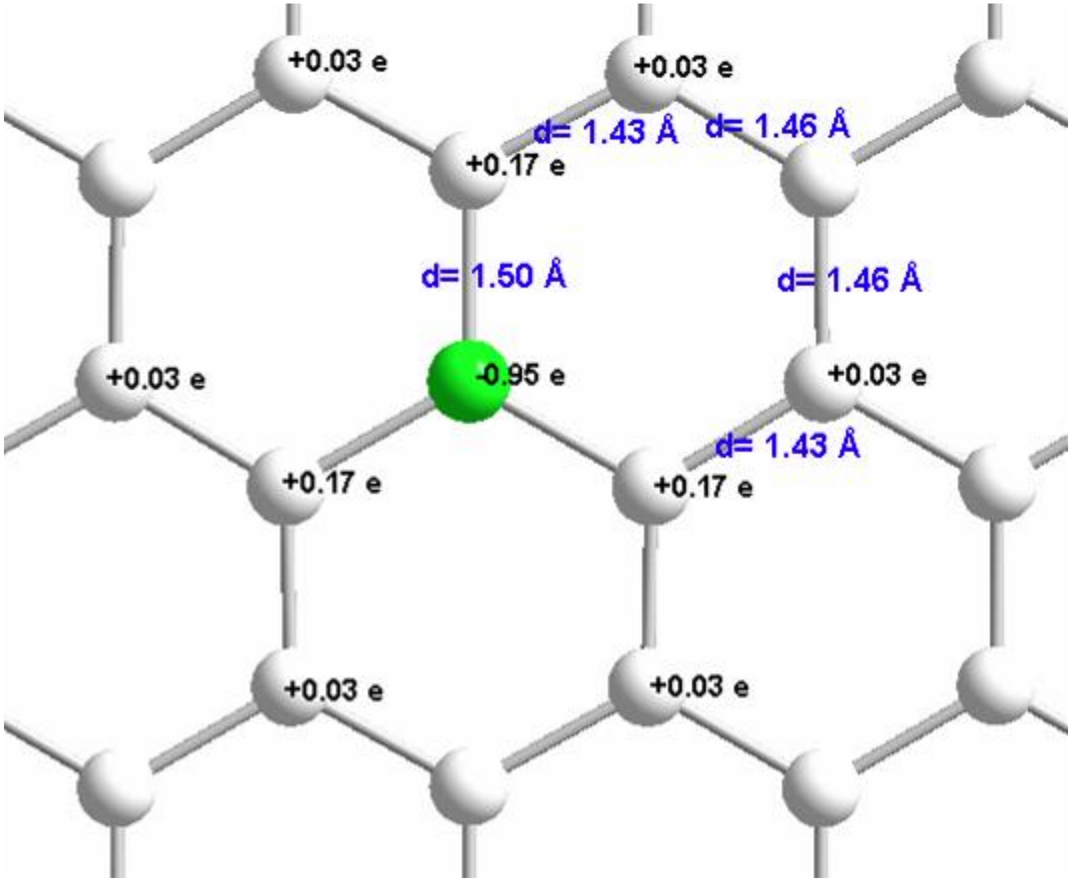
Suspended graphene (graphene in the vacuum) is the conductor but the phase transition is very close.

Question: How to obtain semiconductor, insulator?

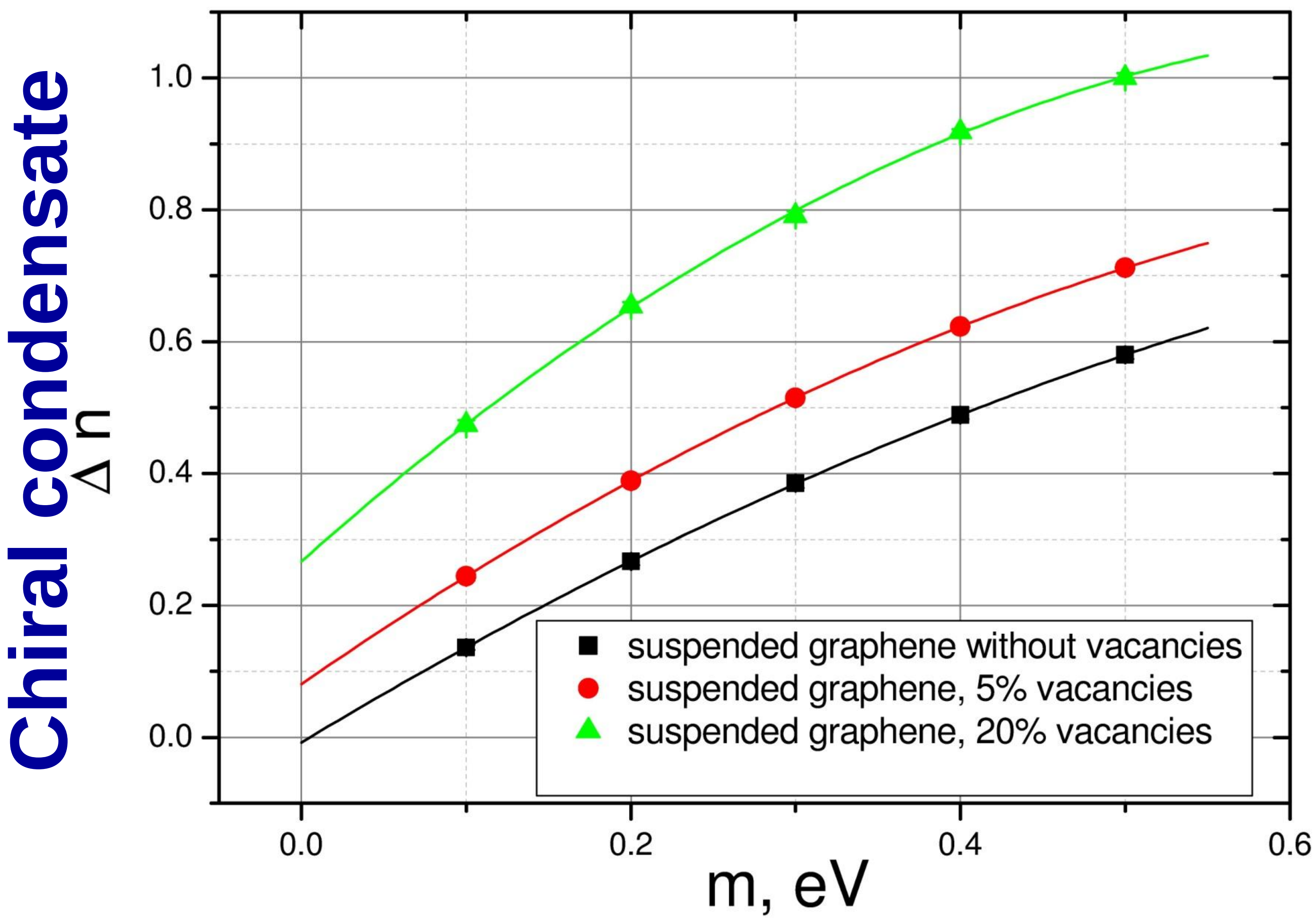
Answer: Introduce defects or vacancies!



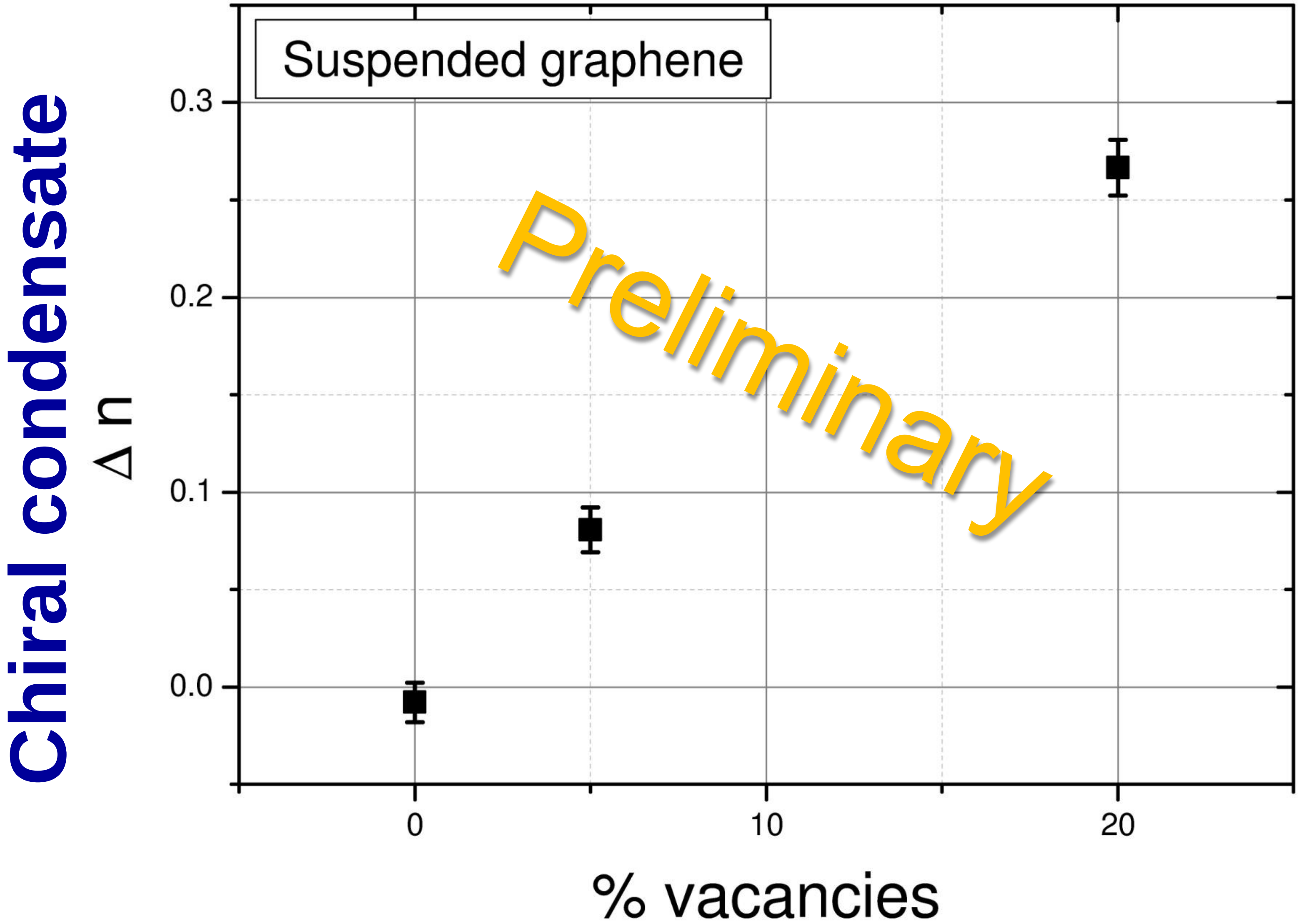
Forbid the hopping of electrons into some percentage of randomly chosen sites (create vacancies)



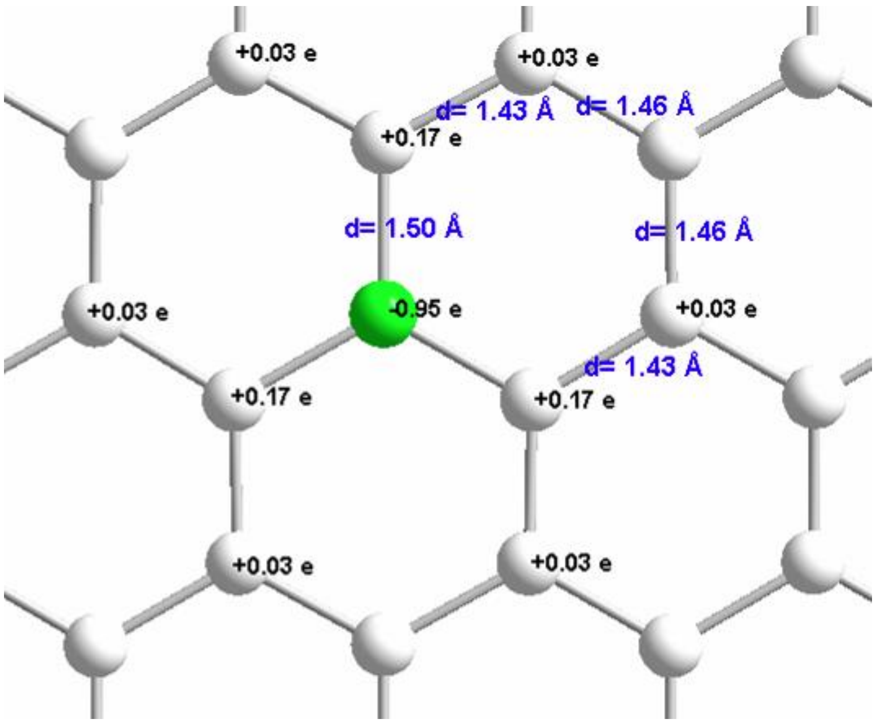
Chiral condensate vs mass for various percentage of vacancies for suspended graphene (preliminary results)



Chiral condensate for various percentage of vacancies for suspended graphene (preliminary Monte Carlo results)



Even small percentage of vacancies produce chiral condensate



From semimetal we can get Semiconductor (?) Insulator

Results

1. **Results of the calculation of graphene conductivity in effective model and on honeycomb lattice contradict experiment**

Results

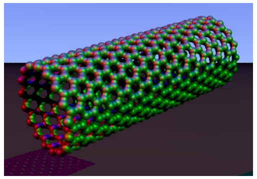
1. Results of the calculation of graphene conductivity in effective model and on honeycomb lattice contradict experiment
2. Modification of Coulomb potential leads to results which do not contradict experimental facts

Results

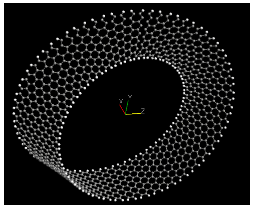
1. Results of the calculation of graphene conductivity in effective model and on honeycomb lattice contradict experiment
2. Modification of Coulomb potential leads to results which do not contradict experimental facts
3. Introduction of defects (vacancies) can shift graphene from conducting phase to semiconducting phase

Problems which can be studied inside MC approach

- Magnetic field
- Finite temperature
- Impurities, vacancies
- 2-3-4 layers
- Nanotubes



- Deformed graphene => 2+1gravity
- Moebius carbon

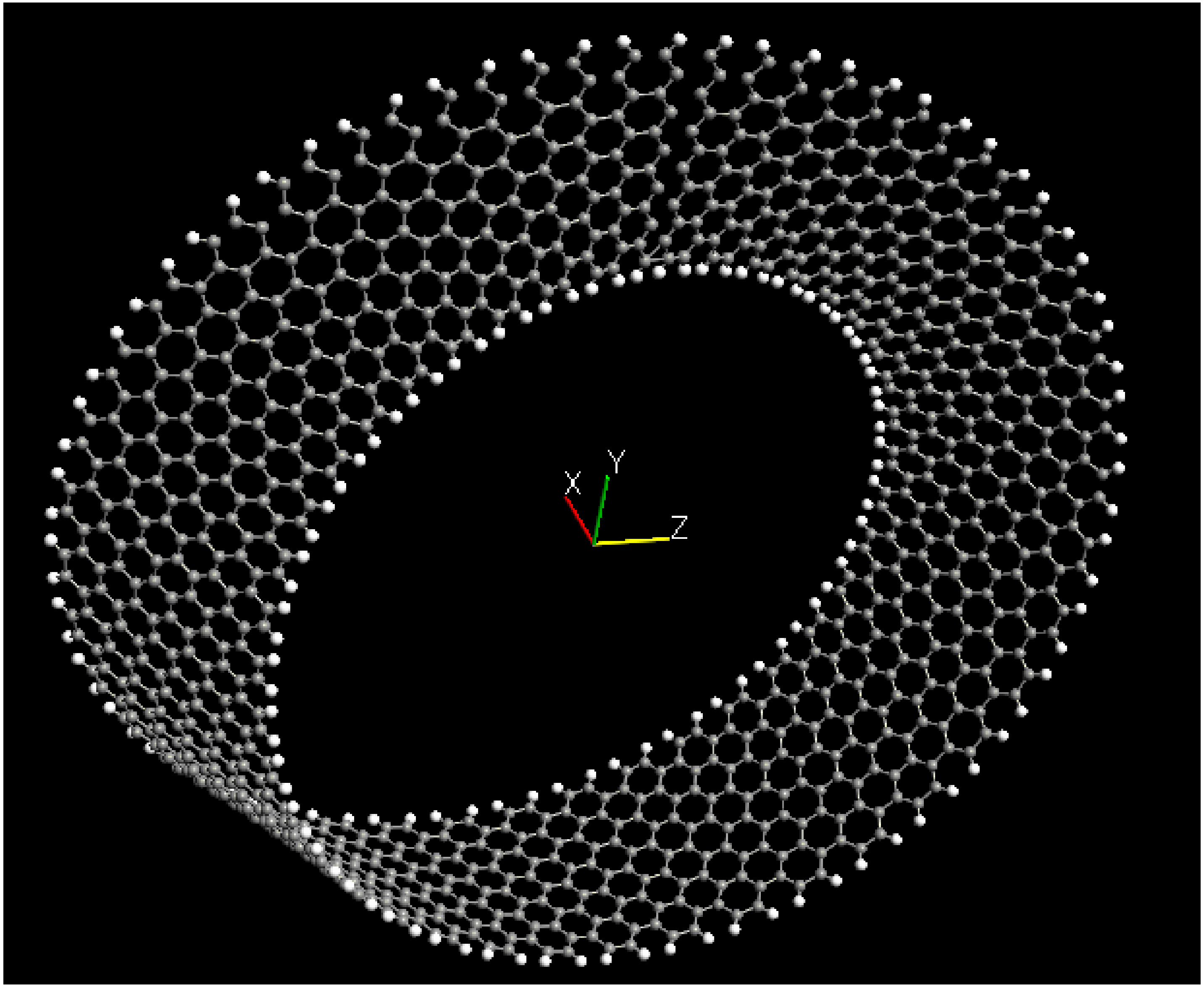


...

http://www.aist.go.jp/aist_j/press_release/pr2012/pr20120925_2/pr20120925_2.html

Mobius carbon is a topological insulator?

ArXiv: 0906.1634



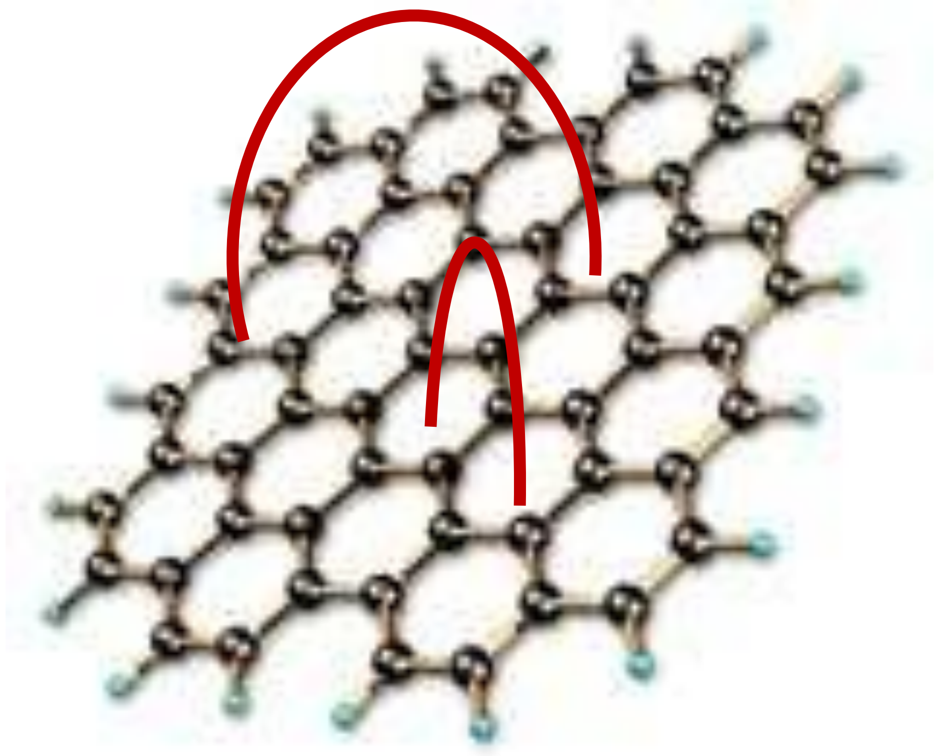
Appendices

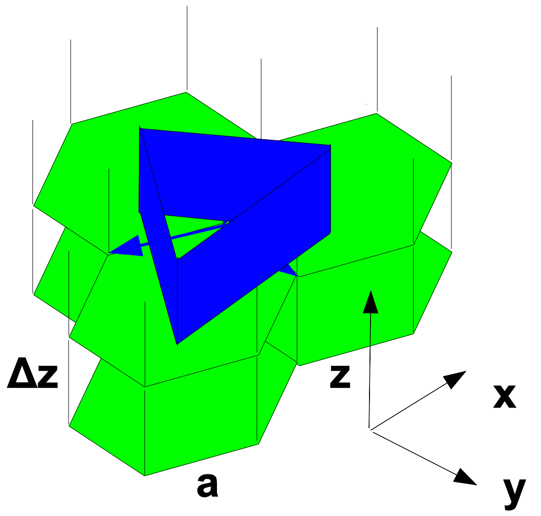
Appendix A

2D hexagonal lattice and rectangular lattice in Z and time dimensions

R. Brower, C. Rebbi, and D. Schaich (2011-2012)

P.V. Buividovich, M.I.P. (2012)





2D hexagonal lattice, from Hamiltonian to partition function

$$\hat{H} = \hat{H}_{tb} + \hat{H}_{I}$$

$$Z = Tr\, e^{-\frac{\hat{H}}{kT}}$$

<u>Approach 2</u>, 2D hexagonal lattice, Hamiltonian

$$\hat{H} = \hat{H}_{tb} + \hat{H}_{I}$$

Approach 2, 2D hexagonal lattice, Hamiltonian

Lattice geometry

$$\hat{H} = \hat{H}_{tb} + \hat{H}_{I}$$

Coulomb interaction

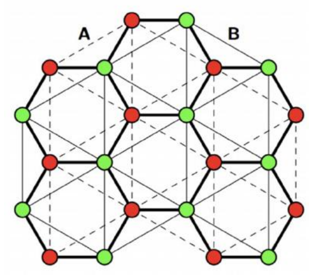
Approach 2, 2D hexagonal lattice, Hamiltonian

Lattice geometry

$$\hat{H} = \hat{H}_{tb} + \hat{H}_{I}$$

Coulomb interaction

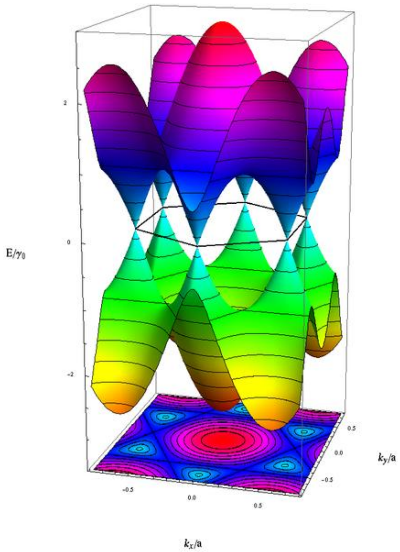
$$\hat{H}_{tb} = -\kappa \sum_{\sigma=\uparrow,\downarrow} \sum_{<XY>} \left(\hat{a}^{\dagger}_{\sigma,X} \hat{a}_{\sigma,Y} + \hat{a}^{\dagger}_{\sigma,Y} \hat{a}_{\sigma,X} \right)$$



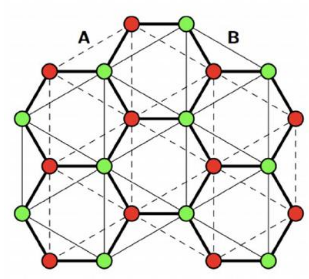
<u>Approach 2</u>, 2D hexagonal lattice, Hamiltonian

$$\hat{H} = \hat{H}_{tb} + \hat{H}_{I}$$

$$\hat{H}_{tb} = -\kappa \sum_{\sigma=\uparrow,\downarrow} \sum_{<XY>} \left(\hat{a}^{\dagger}_{\sigma,X}\, \hat{a}_{\sigma,Y} + \hat{a}^{\dagger}_{\sigma,Y}\, \hat{a}_{\sigma,X} \right)$$



$$v_F = \frac{c}{300}$$



$$\{\hat{a}^{+}_{\sigma,X}, \hat{a}_{\sigma',Y}\} = \delta_{\sigma\sigma'}\delta_{X,Y}$$

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

Approach 2, 2D hexagonal lattice, Hamiltonian

$$\hat{H} = \hat{H}_{tb} + \hat{H}_I$$

Coulomb interaction

$$\hat{H}_I = \sum_{X,Y} e^2/r\,(X,Y)\;\hat{q}_X\,\hat{q}_Y\,,$$

$$\hat{q}_X = \hat{\psi}^\dagger_{\uparrow,X}\,\hat{\psi}_{\uparrow,X} - \hat{\psi}^\dagger_{\downarrow,X}\,\hat{\psi}_{\downarrow,X}. \quad \hat{\psi}_{\uparrow,X} = \hat{a}_{\uparrow,X}\,, \quad \hat{\psi}_{\downarrow,X} = \pm\hat{a}^\dagger_{\downarrow,X}$$

$$\hat{\psi}_{\uparrow,X}\,|0\rangle = 0,\; \hat{\psi}_{\downarrow,X}\,|0\rangle = 0 \qquad \hat{a}_{\uparrow,X}\,|0\rangle = 0, \quad \hat{a}^\dagger_{\downarrow,X}\,|0\rangle = 0.$$

Approach 2, 2D hexagonal lattice, Hamiltonian

$$\hat{H} = \hat{H}_{tb} + \hat{H}_{I}$$

$$\hat{H} = -\kappa \sum_{\sigma=\uparrow,\downarrow} \sum_{<XY>} \left(\hat{\psi}^{\dagger}_{\sigma,X} \exp\left(\pm i\hat{\theta}_{XY}\right) \hat{\psi}_{\sigma,Y} + \right.$$

$$\left. + \hat{\psi}^{\dagger}_{\sigma,Y} \exp\left(\pm i\hat{\theta}_{YX}\right) \hat{\psi}_{\sigma,X} \right) +$$

$$+ \sum_{\sigma=\uparrow,\downarrow} \sum_{X_1} m\, \hat{\psi}^{\dagger}_{\sigma,X_1} \hat{\psi}_{\sigma,X_1} - \sum_{\sigma=\uparrow,\downarrow} \sum_{X_2} m\, \hat{\psi}^{\dagger}_{\sigma,X_2} \hat{\psi}_{\sigma,X_2}$$

Approach 2, 2D hexagonal lattice, partition function

$$\mathcal{Z} = \int \mathcal{D}\bar{\eta}_\sigma(s,\xi,\tau)\,\mathcal{D}\eta_\sigma(s,\xi,\tau)\,\mathcal{D}\phi(s,\xi,\tau,z)\,\exp\left(-\sum_\sigma \bar{\eta}_\sigma M_\sigma\left[\phi(s,\xi,\tau,z=0)\right]\eta_\sigma - S_{em}\left[\phi(s,\xi,\tau,z)\right]\right) =$$

$$= \int \mathcal{D}\phi(s,\xi,\tau,z)\,\left|\det\left(M_\uparrow\left[\phi(s,\xi,z=0,\tau)\right]\right)\right|^2 \exp\left(-S_{em}\left[\phi(s,\xi,\tau,z)\right]\right)$$

$$S_{em}\left[\phi(s,\xi,\tau,z)\right] = \frac{\beta_{hex}}{2}\sum_{b,\xi,\tau,z}\left(\phi(\alpha,\xi,\tau,z) - \phi(\beta,\xi+\rho_b,\tau,z)\right)^2 + \\ + \frac{\beta_z}{2}\sum_{s,\xi,\tau,z}\left(\phi(s,\xi,\tau,z) - \phi(s,\xi,\tau,z+\Delta z)\right)^2$$

$$\beta_{hex} = \frac{\sqrt{3}\,\Delta z}{4\pi e^2 \Delta\tau}\,\frac{\epsilon+1}{2} = \frac{\sqrt{3}}{4\pi e^2}\left(\frac{\Delta z}{a}\right)\frac{(\kappa a)}{(\kappa\Delta\tau)}\,\frac{\epsilon+1}{2}$$

$$\beta_z = \frac{3\sqrt{3}a^2}{16\pi\, e^2\,\Delta z\,\Delta\tau}\,\frac{\epsilon+1}{2} = \frac{3\sqrt{3}}{16\pi\, e^2}\left(\frac{\Delta z}{a}\right)^{-1}\frac{(\kappa a)}{(\kappa\Delta\tau)}\,\frac{\epsilon+1}{2}.$$

Approach 2, 2D hexagonal lattice, partition function

$$\mathcal{Z} = \int \mathcal{D}\bar{\eta}_\sigma(s,\xi,\tau)\,\mathcal{D}\eta_\sigma(s,\xi,\tau)\,\mathcal{D}\phi(s,\xi,\tau,z)\,\exp\left(-\sum_\sigma \bar{\eta}_\sigma \underline{M_\sigma[\phi(s,\xi,\tau,z=0)]}\,\eta_\sigma - S_{em}[\phi(s,\xi,\tau,z)]\right) =$$

$$= \int \mathcal{D}\phi(s,\xi,\tau,z)\,\left|\det\left(\underline{M_\uparrow[\phi(s,\xi,z=0,\tau)]}\right)\right|^2 \exp\left(-S_{em}[\phi(s,\xi,\tau,z)]\right)$$

$$S_{tb}[\eta_\sigma(s,\xi,\tau)] = \sum_{\sigma,s,\xi,\tau,s',\xi',\tau'} \bar{\eta}_\sigma(s,\xi,\tau)\,\underline{M_\sigma[s,\xi,\tau;s',\xi',\tau']}\,\eta_\sigma(s',\xi',\tau') =$$

$$= \sum_{\sigma,s,\xi,\tau} \bar{\eta}_\sigma(s,\xi,\tau)\left(\eta_\sigma(s,\xi,\tau) - e^{\pm i\phi(s,\xi,\tau,z=0)}\,\eta_\sigma(s,\xi,\tau+\Delta\tau,z=0)\right) -$$

$$-\kappa\Delta\tau \sum_{\sigma,\xi,\tau,b} \bar{\eta}_\sigma(\alpha,\xi,\tau)\,e^{\pm i\phi(\alpha,\xi,\tau,z=0)}\eta_\sigma(\beta,\xi+\rho_b,\tau+\Delta\tau) -$$

$$-\kappa\Delta\tau \sum_{\sigma,\xi,\tau,b} \bar{\eta}_\sigma(\beta,\xi,\tau)\,e^{\pm i\phi(\beta,\xi,\tau,z=0)}\eta_\sigma(\alpha,\xi-\rho_b,\tau+\Delta\tau) +$$

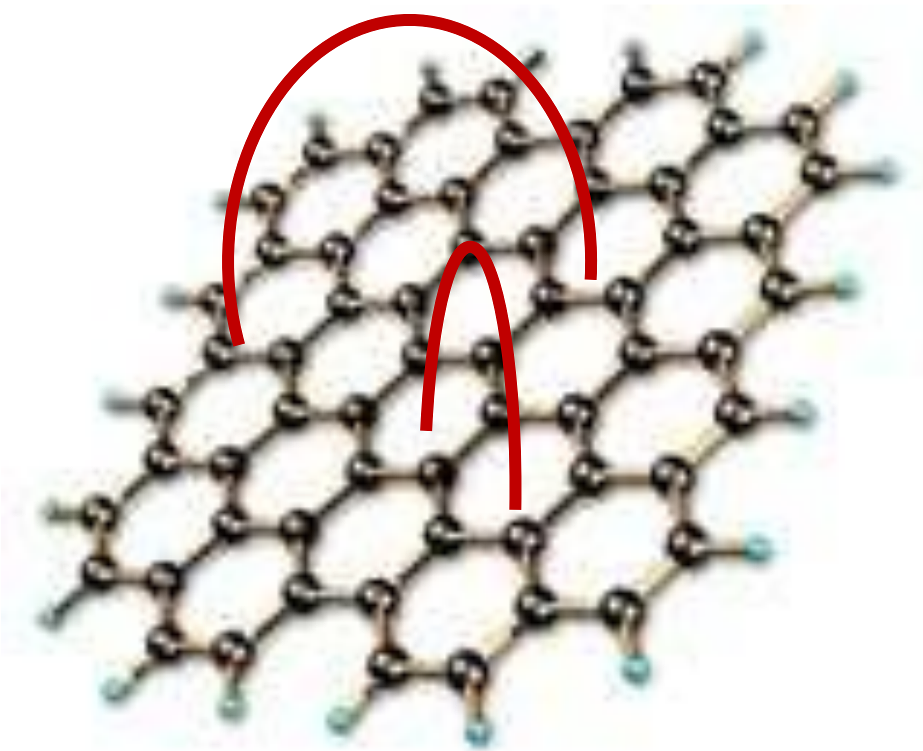
$$+m\,\Delta\tau \sum_{\sigma,\xi,\tau} \bar{\eta}_\sigma(\alpha,\xi,\tau)\,e^{\pm i\phi(\alpha,\xi,\tau,z=0)}\eta_\sigma(\alpha,\xi,\tau+\Delta\tau) -$$

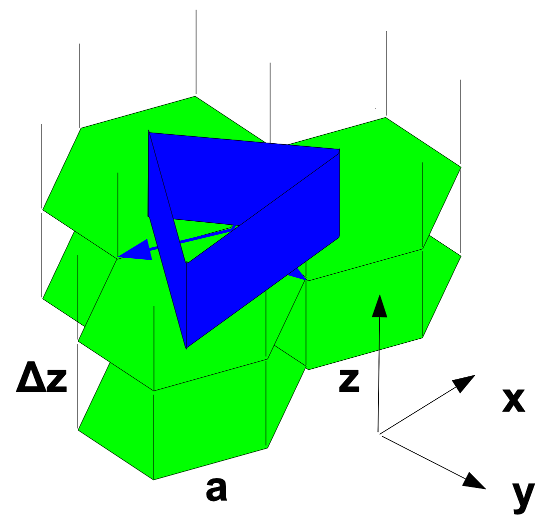
$$+m\,\Delta\tau \sum_{\sigma,\xi,\tau} \bar{\eta}_\sigma(\beta,\xi,\tau)\,e^{\pm i\phi(\beta,\xi,\tau,z=0)}\eta_\sigma(\beta,\xi,\tau+\Delta\tau)\,.$$

Appendix B

2D honeycomb lattice, rectangular lattice in z and time dimensions, screened Coulomb, Hubbard-Stratonovich transformation

P.V. Buividovich, M.I. Katsnelson, M.V. Ulybyshev, M.I.P. arXiv:1304.3660





2D hexagonal lattice, screened Coulomb, from Hamiltonian to partition function

$$\hat{H} = \hat{H}_{tb} + \hat{H}_{C}$$

$$\Downarrow$$

$$Z = Tr\, e^{-\frac{\hat{H}}{kT}}$$

Electric charge at site x:

$$\hat{q}_x = \hat{a}^+_{x,1}\hat{a}_{x,1} + \hat{a}^+_{x,-1}\hat{a}_{x,-1} - 1$$

Introduction of «electrons» and «holes»:

$$\hat{H}_{tb} = -\kappa \sum_{<x,y>} \left(\hat{a}^+_y \hat{a}_x + \hat{b}^+_y \hat{b}_x + h.c.\right)_x = \begin{cases} \hat{a}^+_{x,-1}, x \in \text{sublattice } 0 \\ -\hat{a}^-_{x,-1}, x \in \text{sublattice } 1 \end{cases}$$

$$\hat{H}_C = \frac{1}{2}\sum_{x \neq y} V_{x,y}\hat{q}_x\hat{q}_y + \sum_x V_{xx}\hat{q}^2$$

$$\hat{H} = \hat{H}_C + \hat{H}_{tb}$$

Partition function

$$Z = \mathrm{Tr}(e^{-(H_{tb}+H_C)\beta}) \approx \mathrm{Tr}(e^{-H_{tb}\delta} I e^{-H_C\delta} I e^{-H_{tb}\delta} I e^{-H_C\delta} I \ldots\ldots)$$

Coherent state

$$|\psi,\eta\rangle = e^{-\sum_x \psi_x a_x^+ + \eta_x b_x^+}|\Omega\rangle$$

Some algebra

$$\int d\psi d\eta d\psi^+ d\eta^+ e^{-\sum_x \psi_x^+ \psi_x} |\psi,\eta\rangle\langle\psi^+,\eta^+| = I$$

$$\langle\psi|F(a^+,a)|\psi\rangle = F(\psi^+,\psi)e^{\psi^+\psi}$$

$$\langle\eta|\,\exp\left(\sum_{i,j} A_{ij}\hat{\psi}_i^\dagger\hat{\psi}_j\right)|\eta'\rangle = \exp\left(\sum_{i,j}\left(e^{A}\right)_{ij}\bar{\eta}_i\,\eta'_j\right)$$

And Hubbard-Stratonovich transformation:

$$\int \prod d\varphi_x \exp\left(-\frac{1}{2}\sum_{x,y}\varphi_x V^{-1}_{x,y}\varphi_y - i\sum_x \varphi_x Q_x\right) \cong \exp\left(-\frac{1}{2}\sum_{x,y} Q_x V_{x,y} Q_y\right)$$

The partition function now has the form:

$$\mathrm{Tr}(e^{-H\beta}) = \int D\psi D\eta D\psi^+ D\eta^+ \exp\left(-\sum_{x,y,t,t'} \eta^+_{x,t} M^*_{x,y,t,t'} \eta_{y,t'} - \sum_{x,y,t,t'} \psi^+_{x,t} M_{x,y,t,t'} \psi_{y,t'} - S_{Hubbard}\right)$$

Where the action for Hubbard field is:

$$S_{Hubbard} = \frac{\delta}{2}\sum_{x,y,t} \varphi_{x,t} V^{-1}_{x,y} \varphi_{y,t} \qquad \delta = \frac{\beta}{N_t}$$

Finally

$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}} = \int \mathcal{D}\varphi_{x,n} \mathcal{D}\psi_{x,n} \mathcal{D}\eta_{x,n} \mathcal{D}\bar{\psi}_{x,n} \mathcal{D}\eta_{x,n}$$

$$e^{-S[\varphi_{x,n}] - \sum\limits_{x,y,n,n'} \left(\bar{\eta}_{x,n} \bar{M}_{x,y,n,n'} \eta_{y,n'} + \bar{\psi}_{x,n} M_{x,y,n,n'} \psi_{y,n'} \right)},$$

$$S[\varphi_{x,n}] = \frac{\delta}{2} \sum_{x,y,n} \varphi_{x,n} V_{xy}^{-1} \varphi_{y,n}$$

$$\sum_{x,y,t,t'} \psi^{+}_{x,t} M_{x,y,t,t'} \psi_{y,t'} = \sum_{n=0}^{N_t-1} \Bigg[\sum_{x} \psi^{+}_{x,2n} (\psi_{x,2n} - \psi_{x,2n-1}) +$$

$$+ \sum_{x} \psi^{+}_{x,2n+1} \psi_{x,2n+1} - \delta\kappa \sum_{<x,y>} \left(\psi^{+}_{x,2n} \psi_{y,2n+1} + \psi^{+}_{y,2n} \psi_{x,2n+1} \right) +$$

$$+ m\delta \sum_{1st\ subLat} \psi^{+}_{x,2n} \psi_{x,2n+1} - m\delta \sum_{2d\ subLat} \psi^{+}_{x,2n} \psi_{x,2n-1} - \sum_{x} e^{-i\delta\phi_{x,2n+1}} \psi^{+}_{x,2n+1} \psi_{x,2n+2} \Bigg]$$