INSULATING PHASE TRANSITION IN GRAPHENE

M.E. Carrington, Brandon University, Manitoba, Canada

outline

1. introduction: low energy effective theory
   - look for metalic to insulator phase transition
   - calculate gap / condensate / mass of fermionic quasi-particle
2. calculation set-up: schwinger dyson equations
3. approximations in solid state physics
4. numerical method
5. results
6. conclusions

collaborators:
C.S. Fischer, L. von Smekal, M.H. Thoma, Justus-Liebig-Universität, Giessen

1: INTRODUCTION

graphene is a 2d crystal (hexagonal lattice) of carbon

there are many technological applications . . .

interest for physicists:

lower dimensional condensed matter analogue of many problems studied in high energy physics using relativistic QFT

- topological phase transitions
- chiral symmetry breaking
- strong coupling dynamics

reviews:

A. Castro Neto, F. Geinea, N. Peres, K. Novoselov and A. Geim, Rev. Mod. Phys **81**, *109 (2009);*

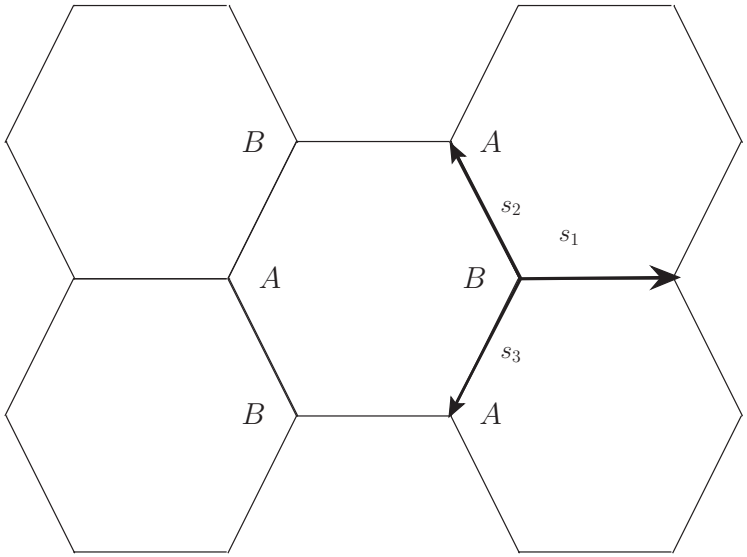
V.N. Kotov, B. Uchoa, V.M. Pereira, A Castro Neto and F. Guinea, Rev. Mod. Phys **84**, *1067 (2012).*

simplest system: monolayer suspended graphene at half filling

low energy effective dynamics are described by a continuum QFT

hexagonal lattice is represented as two interwoven triangular sublattices

- each carbon atom has 3 nearest neighbours on the opposite sublattice



6 electrons per carbon atom – 2 are buried in the $1s^2$ level

3 (of remaining 4) form valance bonds with 3 nearest neighbours (σ bonds)

the last is called the π orbital – gives metalic behaviour

tight binding hamiltonian (kinetic term in the hubbard model)

kinetic energy of the electrons hopping between nn sites

$$H = -t \sum_{\vec{r},i,\sigma} (b^{\dagger}_{\vec{r}+\vec{s}_i;\sigma} a_{\vec{r};\sigma} + b_{\vec{r}+\vec{s}_i;\sigma} a^{\dagger}_{\vec{r};\sigma})$$

$a^{\dagger}_{\vec{r};\sigma}$ creates an electron on sublattice A at position $\vec{r}$ with spin σ, etc

$\vec{s}_i$ with $i \in \{1, 2, 3\}$ gives the positions of the nn's

t is the hopping parameter ~ 2.8 eV

fourier transform to momentum space (discrete FT on the lattice)

$\rightarrow$ solutions for energy as a function of the inverse lattice vectors

there are 2 inequivalent 'dirac points' where the energy goes to zero

expand around these points - energy is linear

$\rightarrow$ electronic quasiparticles have a linear dispersion relation $E = \pm v_F k$

$v_F = \sqrt{\frac{3}{2}}\, a\, t$ is the velocity of a massless electron in graphene =c/300

(lattice separation $a \sim 1.4$ Å)

$\Rightarrow$ kinetic term in the (Eucledian) action:

$$S = i \int d^3x \sum_{a=1}^{N_f} \bar{\psi}_a \, \gamma_\mu \, M_{\mu\nu} \, \partial_\nu \psi_a$$

$$M = \begin{bmatrix} 1 & 0 & 0 \\ 0 & v_F & 0 \\ 0 & 0 & v_F \end{bmatrix} . \qquad (1)$$

Lorentz invariance is explicitly broken by $v_F \neq 1$.

ψ =4 component spinor (2 dirac points $\times$ 2 triangular sub lattices)
the matrices γ_μ satisfy the Eucledian Clifford algebra $\{\gamma_\mu, \gamma_\nu\} = \delta_{\mu\nu}$

the true spin of the electron $\rightarrow$ additional 'flavour' quantum number

P.R. Wallace, Phys. Rev. **71**, *622 (1947);*
G.W. Semenoff, Phys. Rev. Lett **53**, *2449 (1984).*

now include interactions

so far it looks like qed in (1+2) dimensions

but the photon can propagate out of the plane of the graphene sheet

we integrate out the photon modes in the 3rd spatial dimension

$\rightarrow$ a 'brane' action

$$S = \int d^3x \sum_a \bar{\psi}_a \left(i\partial_\mu - eA_\mu\right) M_{\mu\nu}\gamma_\nu\psi_a$$
$$- \frac{1}{4}\int d^3x F_{\mu\nu}\frac{1}{2\sqrt{-\partial^2}}F_{\mu\nu} \quad + \quad \text{gauge fixing}$$

E.V. Gorbar, V.P. Gusynin, V.A. Miransky and I.A. Shovkovy, Phys. Rev. B 66 045108 (2002).

effective coupling $= \frac{c}{v_F}\,\alpha_{\rm qed} \sim 2.2$

$\rightarrow$ (dimensionless) strong coupling

$\alpha_{\max} = 2.2$ is the maximum possible value of the physical coupling

several factors we have ignored could decrease α:

(1) additional screening from the electrons in the σ bands

(2) finite thickness of the graphene sheet

'monolayer' graphene means we ignore this

(2) controllable experimental factors

- immerse sample in a dielectric medium

- attach it to a substrate

'suspended' graphene means assume no medium induced screening

(3) thermal fluctuations or impurities (?)

Questions of physical interest

- is there a transition to a mott-insulating state at some critical coupling?

a mott insulator is caused by electron-electron interactions

- not part of the usual fermi-liquid picture

- the band gap is dynamically generated

analogue in high energy physics is a chiral condensate

results indicate $\alpha_c \gtrsim \alpha_{\max}$

there is other evidence that the transition is close (v_F renormalization)

maybe magnetic fields or some mechanical/physical transformation could drive the system to transition?

- how important are frequency dependencies ?

- frequency dependence of fermionic Green functions

- retardation effects

$\rightarrow$ vertex corrections and magnetic contributions

2: CALCULATIONAL SET-UP

goal: calculate dynamically generated gap function (fermion 'mass' term)

$$\lim_{\alpha \to \alpha_c} \Delta(0,0) \to 0$$

strong coupling $\rightarrow$ nonperturbative methods

options:

1. functional renormalization group
2. nPI
3. schwinger dyson equations
4. lattice simulations

lattice calculations - issues with continuum and infinite volume limits

continuum methods - some kind of truncation is needed

Schwinger Dyson equations

include non-perturbative effects by introducing dressing functions

$\rightarrow$ infinite coupled hierarchy

introduce an ansatz for the 3-vertex that satisfies gauge invariance

- this truncates the coupled set of sd equations

fermion propagator

lorentz invariance is broken $\rightarrow$ has 3 dressing functions

$$S^{-1}(p_0, \vec{p}) = i[Z(p_0, \vec{p})\gamma_0 p_0 + v_F\, A(p_0, \vec{p})\vec{\gamma}\cdot\vec{p}] + \Delta(p_0, \vec{p})$$

photon propagator

use a 1-loop approximation for the photon polarization tensor

- this is motivated by - density of states at the dirac points vanishes

photon propagator (Landau gauge)

$$P^1_{\mu\nu} = \delta_{\mu\nu} - \frac{Q_\mu Q_\nu}{Q^2}\,, \quad P^3_{\mu\nu} = \frac{n_\mu n_\nu}{n^2}\,, \quad n_\mu = \delta_{\mu 0} - \frac{q_0 Q_\mu}{Q^2}$$

$$\Pi_{\mu\nu} = \alpha P^1_{\mu\nu} + \gamma P^3_{\mu\nu}$$

$$G^{-1}_{\mu\nu} = (G^0_{\mu\nu})^{-1} + \Pi_{\mu\nu}$$

$$G_{\mu\nu} = \frac{P^1_{\mu\nu}}{G_T(q_0,\vec{q})} + P^3_{\mu\nu}\left(\frac{1}{G_L(q_0,\vec{q})} - \frac{1}{G_T(q_0,\vec{q})}\right)$$

$$G_T(q_0,\vec{q}) = 2\sqrt{Q^2} + \alpha$$

$$G_L(q_0,\vec{q}) = 2\sqrt{Q^2} + \alpha + \gamma$$

$$\Pi_{00} = \frac{q^2}{Q^2}(\alpha+\gamma)\,, \qquad \mathrm{Tr}\,\Pi = 2\alpha + \gamma$$

$$\Pi_{00} = \frac{\pi\alpha q^2 v_F}{\sqrt{q^2 v_F^2 + q_0^2}}$$

$$\mathrm{Tr}\,\Pi = \frac{\pi\alpha v_F\left(2\left(q^2 v_F^2 + q_0^2\right) + q^2\left(1 - v_F^2\right)\right)}{\sqrt{q^2 v_F^2 + q_0^2}}$$

vertex ansatz

modified Ball-Chiu vertex:

J.S. Ball and T.W Chiu, Phys Rev. D **22**, *2542 (1980).*

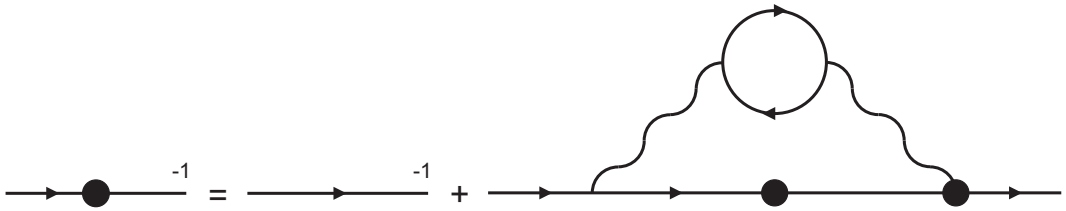
$$\begin{aligned}\Gamma_\mu(P,K) &= \frac{1}{2}(\mathbf{A}_{\mu\nu}(p_0,\vec{p}) + \mathbf{A}_{\mu\nu}(k_0,\vec{k}))\gamma_\nu \\ &+[\frac{1}{2}(P_\sigma + K_\sigma)(\mathbf{A}_{\sigma\nu}(p_0,\vec{p}) - \mathbf{A}_{\sigma\nu}(k_0,\vec{k}))\gamma_\nu \\ &+i(\Delta(p_0,\vec{p}) - \Delta(k_0,\vec{k}))]\frac{(P_\mu + K_\mu)}{P^2 - K^2}\end{aligned}$$

$$\mathbf{A}(p_0,\vec{p}) = \begin{bmatrix} Z(p_0,\vec{p}) & 0 & 0 \\ 0 & A(p_0,\vec{p}) & 0 \\ 0 & 0 & A(p_0,\vec{p}) \end{bmatrix}$$

satisfies the Ward identity

$$-iQ_\mu\Gamma_\mu = S^{-1}(p_0,\vec{p}) - S^{-1}(k_0,\vec{k})$$

summary of the strategy



solve self consistently coupled set of integral eqns for fermion dressing fcns

if we start with some large α will find $\Delta(0,0) \neq 0$

reduce α until we find α_c for which $\Delta(0,0) \to 0$

3. connection to the standard solid state calculations

electrons interact through a long range Coulomb interaction

photons that mediate the Coulomb interaction faster than electrons

$\Rightarrow$ assume Coulomb interaction is 'instantaneous'

$G_{\mu\nu} = \delta_{\mu 0}\delta_{\nu 0} G_{00}$

$\{q_0, v_F\} \sim \delta$ and expand in δ

$$\rightarrow G_{00}(q_0, q) = \frac{1}{2q + \Pi_{00}}, \quad \Pi_{00}(q_0, \vec{q}) = \frac{\pi\alpha q^2 v_F}{\sqrt{q^2 v_F^2 + q_0^2}} \tag{2}$$

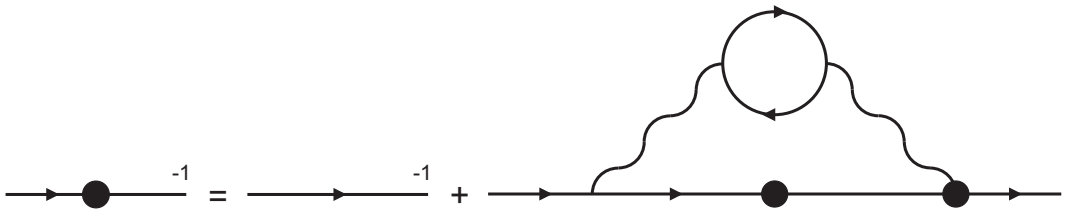
Π_{00} represents screening due to particle-hole pair production

will show: instantaneous coulomb approx decreases screening

$\rightarrow$ decreases α_c (about 5%)

comment: $\Pi_{00}(0, \vec{q})$ (static screening) gives $\alpha_c \rightarrow \infty$

4. NUMERICAL PROCEDURE



k integral: ultra-violet cut-off Λ

use a logarithmic scale to increase sensitivity to infra-red

k_0 integral: ultra-violet cut-off Λ_0 and log scale

checked that results are insensitive to the ratio $\Lambda_0/\Lambda \;\rightarrow\;$ choose $\Lambda_0 = \Lambda$

dimensionless variables $\hat{k} = k/\Lambda$, $\hat{k}_0 = k_0/\Lambda$, $\hat{\Delta} = \Delta/\Lambda$

– all hats suppressed

solve the coupled set of equations using an iterative relaxation method

comment: can also do the calculation using a bifurcation analysis

- set $\Delta(p_0, p) = 0$ and solve for $Z(p_0, p)$ and $A(p_0, p)$

use these solutions and try to solve Δ eqn starting from initial value of 10^{-12}.

if $\alpha > \alpha_c$ the solution moves away from zero

reduce α and look for the largest value for which the zero solution is stable

- no information about the momentum dependence of the dressing functions

advantage: calculation is much faster

– total number of iterations $\sim N^2 + N$ (instead of N^3)

– no 'critical slowing down' (stuck between 2 solns that are close together)

5. RESULTS

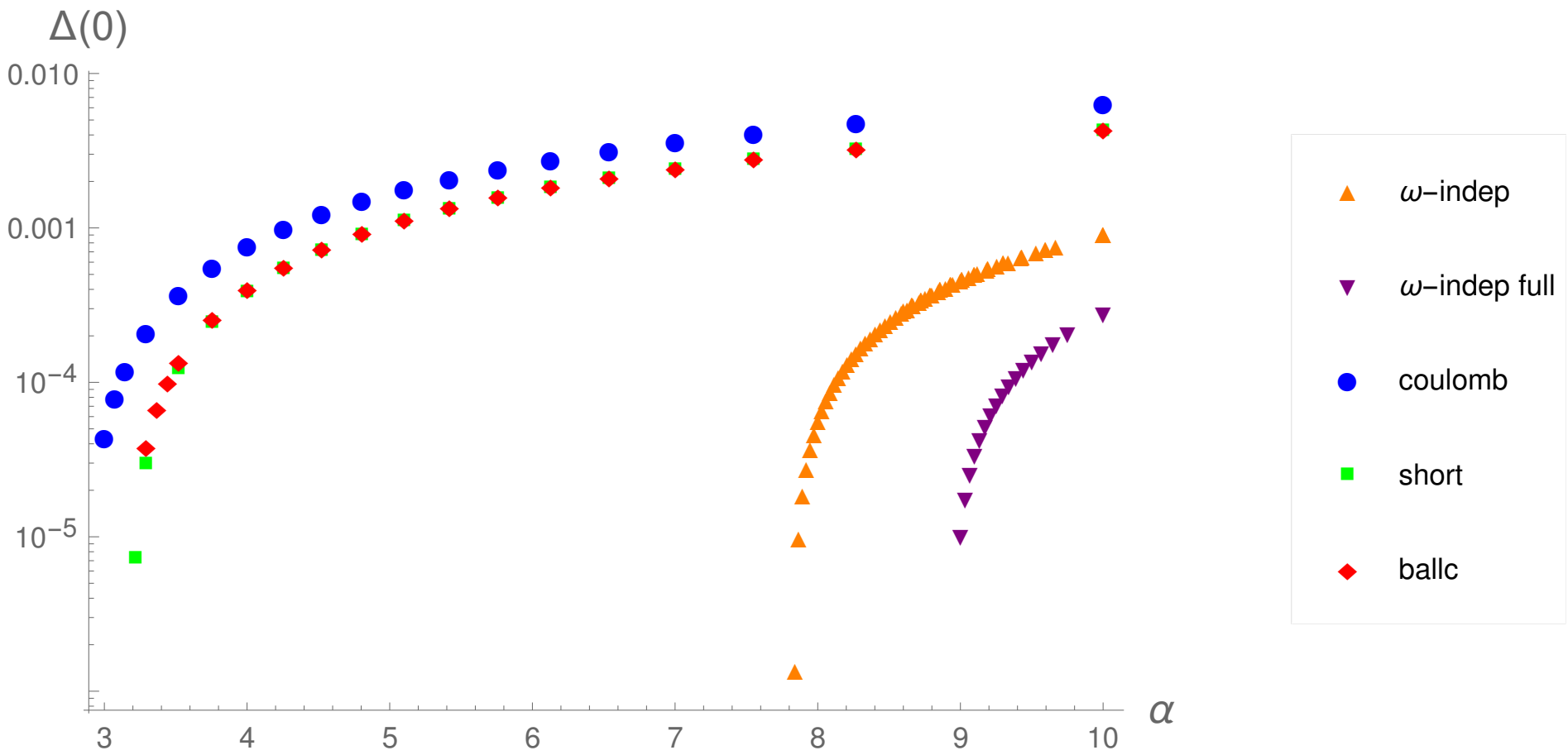
1. BALL-CHIU: the full calculation described above
2. SHORT: take only the first term in the Ball-Chiu vertex
3. COULOMB: Coulomb approximation applied to the SHORT calculation

   Jing-Rong Wang and Guo-Zhu Liu, New J. Phys. **14**, *043036 (2012).*

4. ω-independent: freq independent dressing functions and Coulomb approx

   C. Popovici, C.S. Fischer and L. von Smekal, Phys. Rev. B **88**, *205429 (2013).*

Results


Δ(0)
0.010
0.001
10^−4
10^−5
3
4
5
6
7
8
9
10
α
ω−indep
ω−indep full
coulomb
short
ballc

calculation	α_c	bifurcation range
ω-independent	7.80	7.776-7.777
ω-independent-full	8.955	
COULOMB	2.906	2.900 - 2.899
SHORT	3.190	3.190 - 3.191
BALL-CHIU	3.178	

fermi velocity renormalization

recall the dressed fermion propagator

$$S^{-1}(p_0, \vec{p}) = i[Z(p_0, \vec{p})\gamma_0 p_0 + v_F\, A(p_0, \vec{p})\vec{\gamma}\cdot\vec{p}] + \Delta(p_0, \vec{p})$$

the fermi velocity renormalization is defined as $A(p_0, \vec{p})/Z(p_0, \vec{p})$

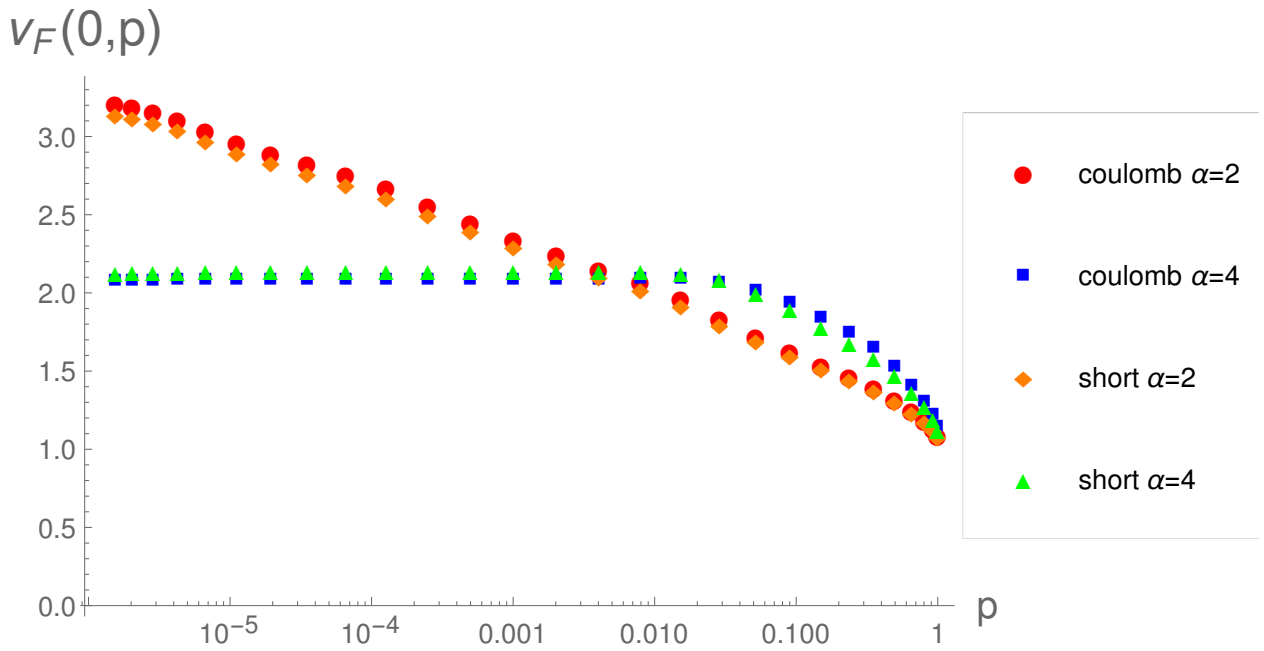
important quantity experimentally - enters many graphene observables

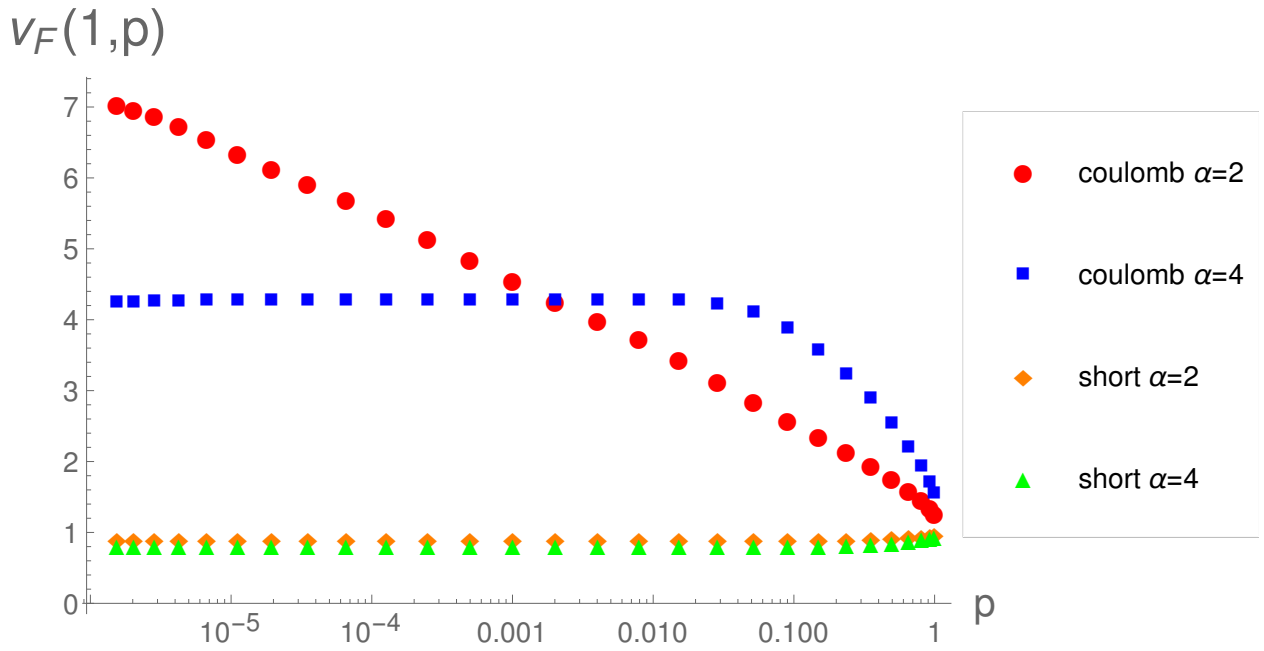
measurements: scales like $\log(1/p)$ close to the transition

physics: comes from the vanishing density of states at the dirac points

$\rightarrow$ produces unconventional behaviour in many observables

like specific heat, compressibility . . .


$v_F(0,p)$
3.0
2.5
2.0
1.5
1.0
0.5
0.0
10^{-5}
10^{-4}
0.001
0.010
0.100
1
p
coulomb α=2
coulomb α=4
short α=2
short α=4


$v_F(1,p)$
7
6
5
4
3
2
1
0
10^{-5}
10^{-4}
0.001
0.010
0.100
1
p
coulomb α=2
coulomb α=4
short α=2
short α=4

assessment of the coulomb approximation:

pretty good in the infra-red

far off in the ultra-violet

as shown previously a change in α_c of about 5 percent

6. CONCLUSIONS

calculation of dynamically generated gap in mono-layer suspended graphene system described with a low energy effective field theory

used a non-perturbative continuum Schwinger Dyson approach
$\rightarrow$ solved a set of three coupled self-consistent integral equations
– determined the fermion dressing functions

three effects that have not previously been included:

1. magnetic effects (contributions from transverse parts of photon propagator)
2. vertex corrections using an ansatz that preserves gauge invariance
3. full frequency dependence in dressing functions and loop integrals

Ball-Chiu and Short calculations are almost identical

note: QED_{2+1} the Ball-Chiu vertex does effect the condensate

$\rightarrow$ surprising (?) that reduced QED_{3+1} with a 2-brane is so different

Coulomb result for α_c differs by about 5%

perturbative Lindhard-type screening function in photon propagator

complete calculation: self-consistently determined photon dressing functions

- Π is determined from a fermion loop
- fermion velocity renormalization is large

$\rightarrow$ self-consistent caln of photon screening could have significant effect

this calculation is currently in progress $\cdots$