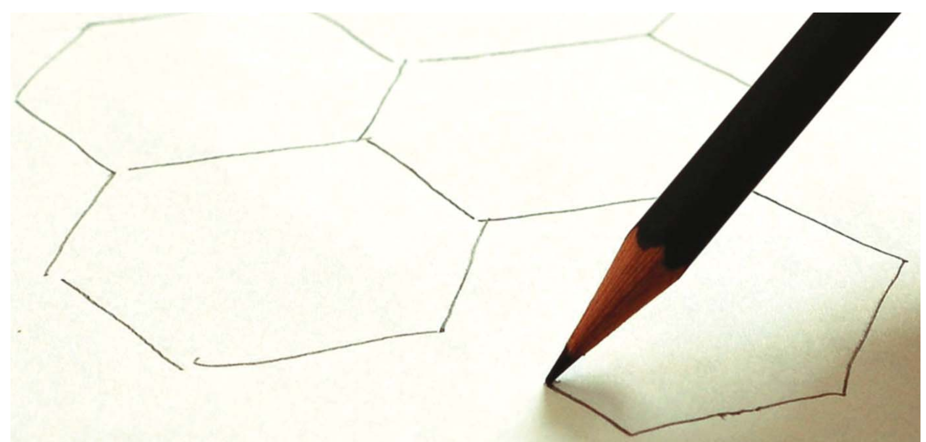
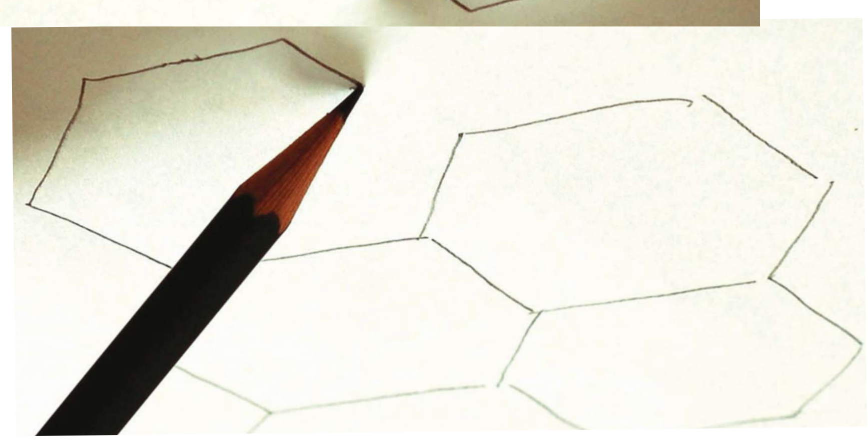
# Monte Carlo Simulation of a Quantum Critical Point in Graphene

Simon Hands (Swansea University)





Collaborators:
Wes Armour (Oxford)
Costas Strouthos
(European U. Cyprus)

*Holography and Condensed Matter Physics*, Perugia, 25th September 2015

# In this talk I will

- introduce a relativistic field theory for low-energy electron excitations in graphene

- argue that at strong coupling there is a phase transition to a **Mott insulator** described by a quantum critical point (**QCP**)

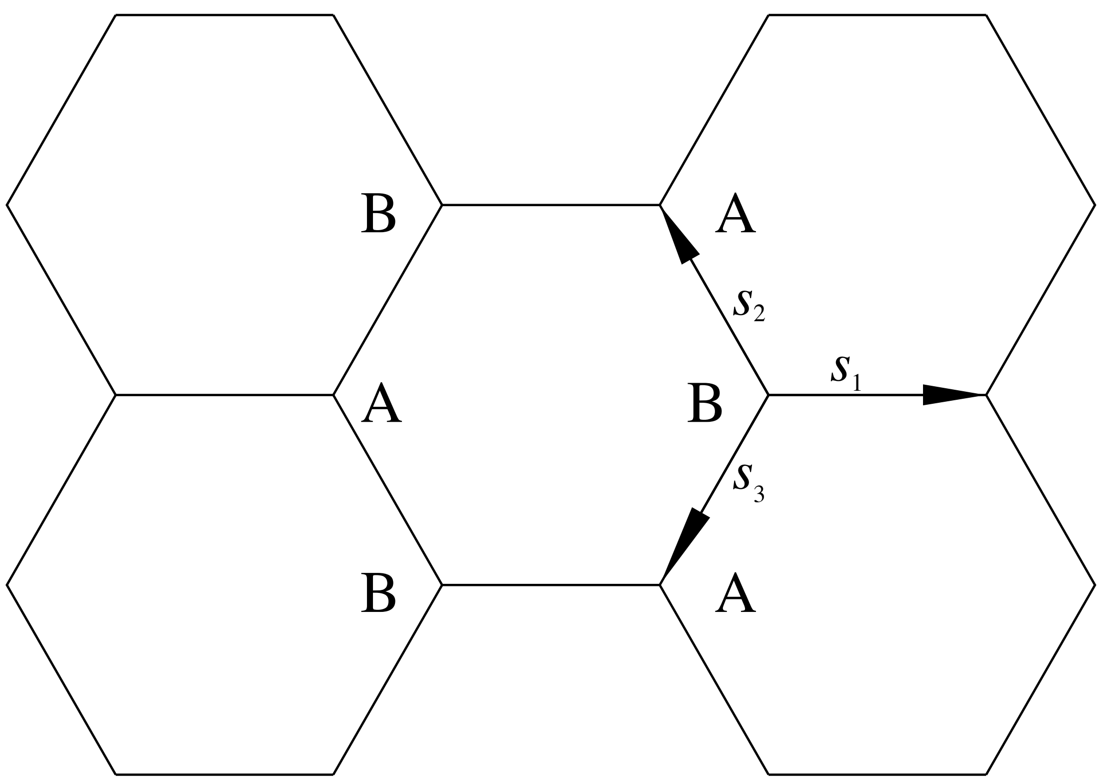
- generalise to bilayer graphene with an inter-layer bias voltage

- present simulation results probing **degenerate matter** with strong interactions

# Relativity in Graphene

The electronic properties of graphene were first studied theoretically almost 70 years ago

P.R. Wallace, Phys. Rev. **71** (1947) 622




$$H = -t \sum_{\mathbf{r}\in\mathbf{B}} \sum_{i=1}^{3} b^\dagger(\mathbf{r})a(\mathbf{r}+\mathbf{s}_i) + a^\dagger(\mathbf{r}+\mathbf{s}_i)b(\mathbf{r})$$

"tight -binding" Hamiltonian

describes hopping of electrons in π-orbitals from A to B sublattices and *vice versa*

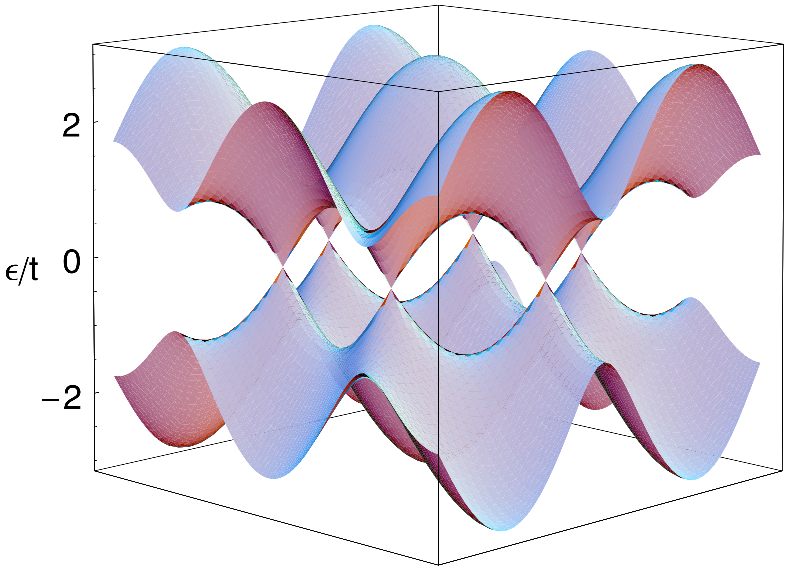
In momentum space

$$H = \sum_{\vec{k}} \left( \Phi(\vec{k})a^\dagger(\vec{k})b(\vec{k}) + \Phi^*(\vec{k})b^\dagger(\vec{k})a(\vec{k}) \right)$$

with $\Phi(\vec{k}) = -t\left[ e^{ik_x l} + 2\cos\left(\frac{\sqrt{3}k_y l}{2}\right) e^{-i\frac{k_x l}{2}} \right]$

Define states $|\vec{k}_{\pm}\rangle = (\sqrt{2})^{-1}[a^{\dagger}(\vec{k}) \pm b^{\dagger}(\vec{k})]|0\rangle$

$$\Rightarrow \quad \langle\vec{k}_{\pm}|H|\vec{k}_{\pm}\rangle = \pm(\Phi(\vec{k}) + \Phi^{*}(\vec{k})) \equiv \pm E(\vec{k})$$




Energy spectrum is symmetric about $E = 0$

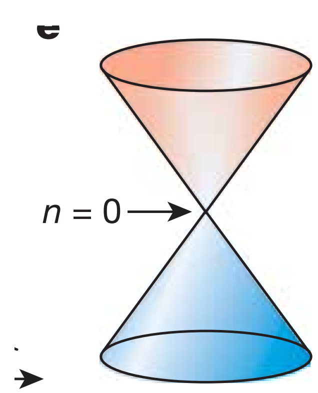
Half-filling (neutral or "undoped" graphene) has zero energy at "Dirac points" at corners of first Brillouin Zone:

There are two independent Dirac points in BZ1

$$\Phi(\vec{k}) = 0 \;\Rightarrow\; \vec{k} = \vec{K}_{\pm} = (0, \pm\frac{4\pi}{3\sqrt{3}l})$$

Taylor expand @ Dirac point

$$\Phi(\vec{K}_{\pm} + \vec{p}) = \pm v_F[p_y \mp i p_x] + O(p^2)$$




with "Fermi velocity" $v_F = \frac{3}{2}tl$

Define modified operators $a_\pm(\vec{p}) = a(\vec{K}_\pm + \vec{p})$ etc.

Now combine them into a "4-spinor" $\Psi = (\, b_+, a_+, a_-, b_-)^{tr}$

$$\Rightarrow \quad H \simeq v_F \sum_{\vec{p}} \Psi^\dagger(\vec{p}) \begin{pmatrix} & p_y + ip_x & & \\ p_y - ip_x & & & \\ & & & -p_y - ip_x \\ & & -p_y + ip_x & \end{pmatrix} \Psi(\vec{p})$$

$$= v_F \sum_{\vec{p}} \Psi^\dagger(\vec{p}) \vec{\alpha}.\vec{p}\, \Psi(\vec{p})$$

Dirac Hamiltonian

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}$$

ie. low-energy excitations are relativistic massless fermions with velocity $v_F = \frac{3}{2} tl \approx \frac{1}{300} c$

For monolayer graphene the number of flavors $N_f = 2$
(2 C atoms/cell x 2 Dirac points/zone x 2 spins)

# Interactions between electrons: an effective field theory

(Son, Khveshchenko,...)

fermions live on two-dimensional "braneworld" interact with photons living in the 3*d* bulk

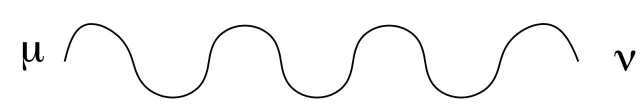
$$S = \sum_{a=1}^{N_f} \int dx_0 d^2x(\bar{\psi}_a \gamma_0 \partial_0 \psi_a + v_F \bar{\psi}_a \vec{\gamma}.\vec{\nabla}\psi_a + iV\bar{\psi}_a\gamma_0\psi_a)$$
$$+ \frac{1}{2e^2}\int dx_0 d^3x(\partial_i V)^2,$$

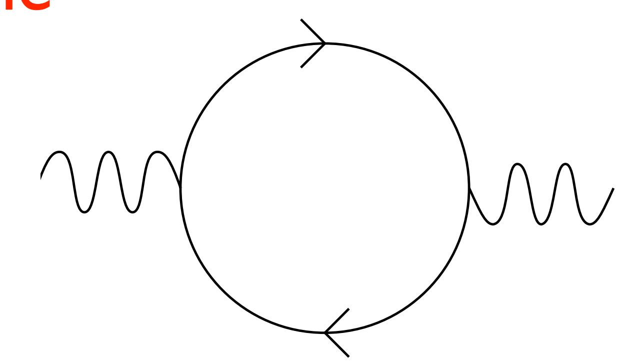
"instantaneous" Coulomb potential

since $v_F \ll c$ - unscreened since $\varrho(E=0)=0$

ie. this is *not* $QED_3$

Number of "flavors" $N_f$ = 2 for monolayer graphene



classical 3d Coulomb $\propto r^{-1}$

V-propagator (large-$N_f$): $$D(p) = \left(\frac{2|\vec{p}|}{e^2} + \frac{N_f}{8}\frac{|\vec{p}|^2}{(p_0^2 + v_F^2|\vec{p}|^2)^{\frac{1}{2}}}\right)^{-1}$$

quantum screening due to virtual electron-hole pairs $\propto r^{-1}$

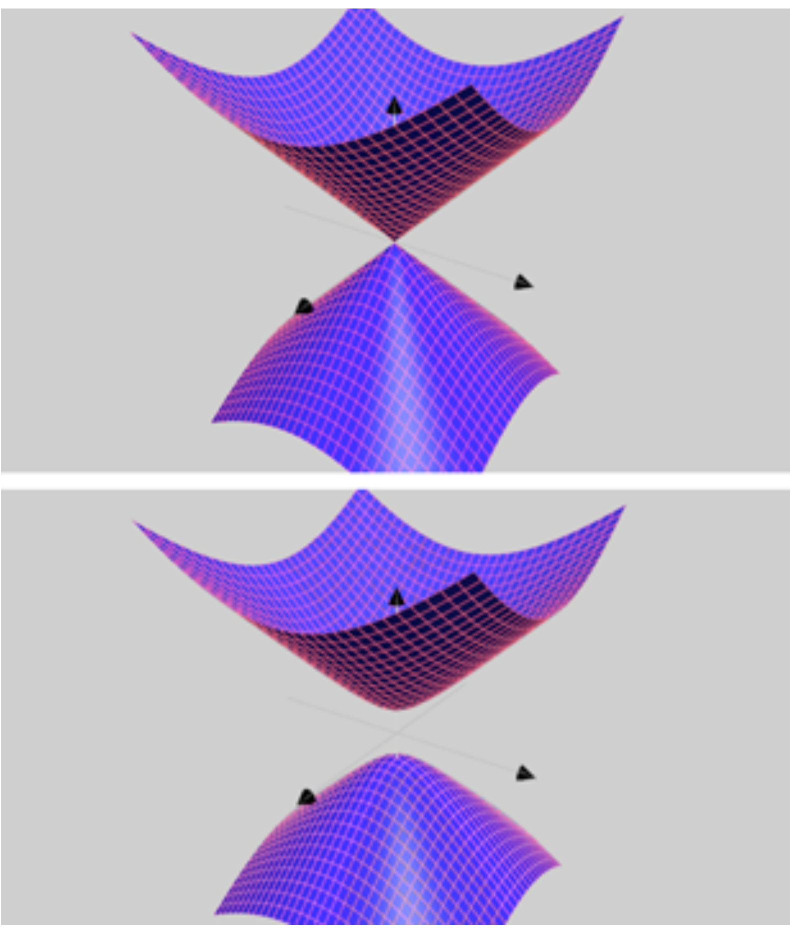
$$\lambda = \frac{e^2 N_f}{16\varepsilon\varepsilon_0\hbar v_F} \simeq \frac{1.4N_f}{\varepsilon}$$

(i) parametrises quantum vs. classical

(ii) depends on dielectric properties of substrate

For sufficiently large $e^2$, or sufficiently small $N_f$, the Fock vacuum may be disrupted by a particle-hole "excitonic" condensate $\langle\bar{\psi}\psi\rangle \neq 0$

spontaneously breaks $\mathrm{U(2N_f)} \rightarrow \mathrm{U(N_f)} \otimes \mathrm{U(N_f)}$



In particle physics this is "chiral symmetry breaking" (χSB) leading to dynamical mass (gap) generation

In condensed matter physics this phase is a Mott insulator

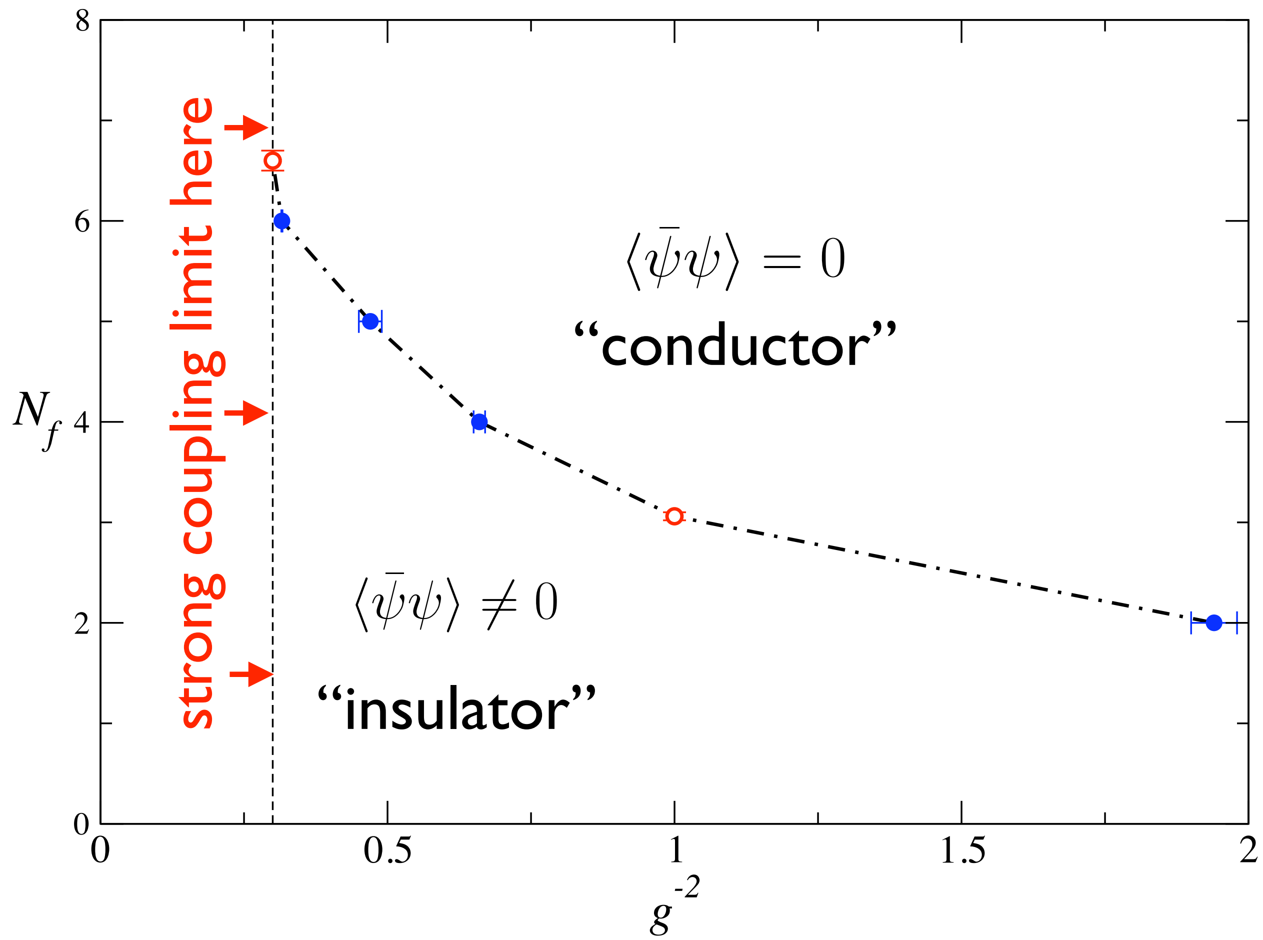
Hypothesis: the χSB transition at $e^2(N_f)$ defines a **Quantum Critical Point** (QCP) whose universal properties characterise the low-energy excitations of graphene

D.T. Son, Phys. Rev. B**75** (2007) 235423

QCP characterised by anomalous scaling e.g. $\langle\bar{\psi}\psi\rangle|_{e^2=e_c^2} \propto m^{\frac{1}{\delta}}$

Physically corresponds to a metal-insulator transition

of technological importance?




The proposed phase diagram resembles that of another 2+1d QFT, the Thirring Model

Phase diagram determined by lattice Monte Carlo simulations

## Consider "Thirring-like" model for graphene (units $v_F = 1$)

$$S = \sum_{a=1}^{N_f} \int dx_0 d^2x \left[ \bar\psi_a \gamma_\mu \partial_\mu \psi_a + iV\bar\psi_a\gamma_0\psi_a + \frac{1}{2g^2}V^2 \right]$$

**local**, non-covariant field theory in $d$=2+1

V-propagator: $D(p) = \left( \frac{1}{g^2} + \frac{N_f}{8} \frac{|\vec p|^2}{(p_0^2 + v_F^2|\vec p|^2)^{\frac{1}{2}}} \right)^{-1}$

coincides with Coulombic model as $N_f \to \infty$, or $e^2, g^2 \to \infty$

but long-range interaction is **screened** for $g^2 < \infty$

# Numerical Lattice Approach

$$S_{latt} = \frac{1}{2}\sum_{x\mu i} \bar{\chi}_x^i \eta_{\mu x}(1 + i\delta_{\mu 0}V_x)\chi_{x+\hat{\mu}}^i - \bar{\chi}_x^i \eta_{\mu x}(1 - i\delta_{\mu 0}V_{x-\hat{0}})\chi_{x-\hat{\mu}}^i$$

$$+ \, m\sum_{xi} \bar{\chi}_x^i \chi_x^i + \frac{N}{4g^2}\sum_x V_x^2$$

$i = 1, \ldots, N$

explicit mass gap

$\chi_x^i, \; \bar{\chi}_x^i$ single spin-component fermion fields defined at sites of a ***cubic*** lattice

$V_x$ bosonic auxiliary field defined on link between $x$ and $x+0$

$$\eta_{\mu x} \equiv (-1)^{x_0 + \cdots + x_{\mu-1}}$$

Kawamoto-Smit phases ensure covariant continuum limit for $g^2=0$

Relation between coupling $g^2$ and $e^2$, $\lambda$ not known *a priori*

**Chiral symmetry:** $U(N)\otimes U(N) \to U(N)$ (if $m \neq 0$)

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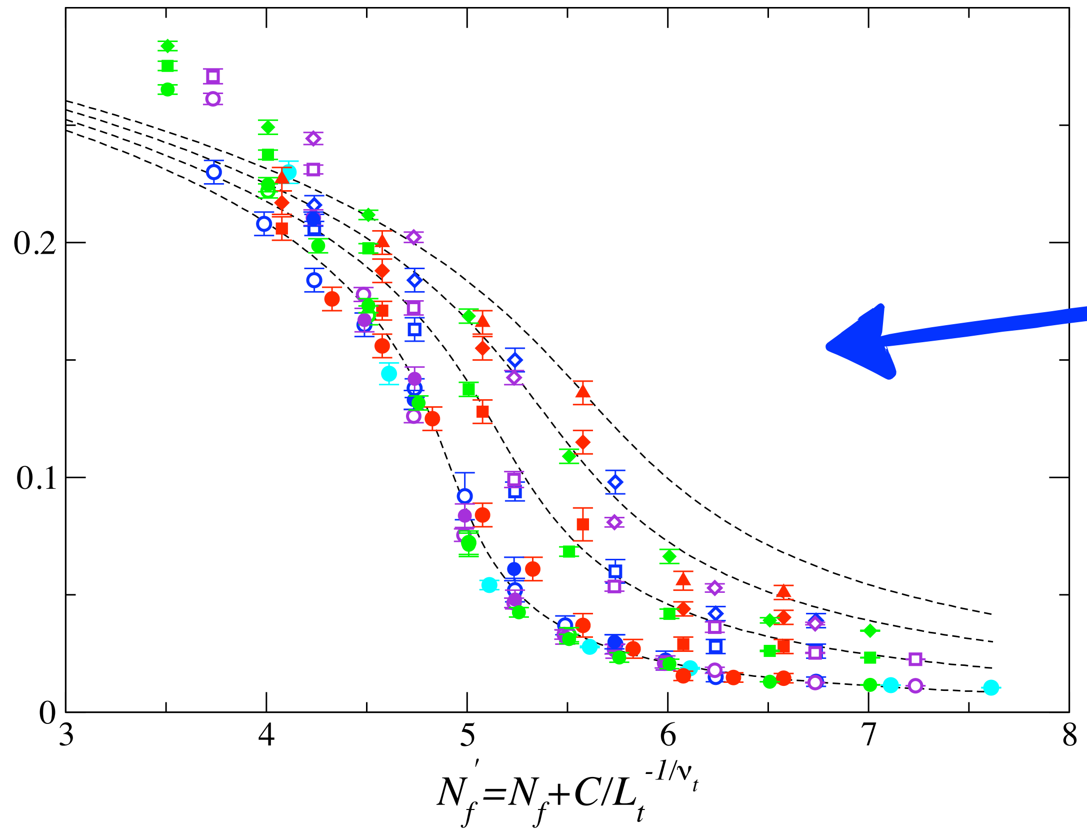
In **weak coupling** continuum limit, can show $U(2N_f)$ and Lorentz symmetries are recovered, with $N_f = 2N$

What happens at a **QCP** is anyone's guess!

# EoS results

SJH & C.G. Strouthos, Phys. Rev. B78(2008) 165423
W. Armour, SJH & C.G. Strouthos, Phys. Rev. B81(2010) 125105




## Strong coupling limit

$N_{fc} = 4.8(2) > 2$

$\delta(N_{fc}) = 5.5(3)$

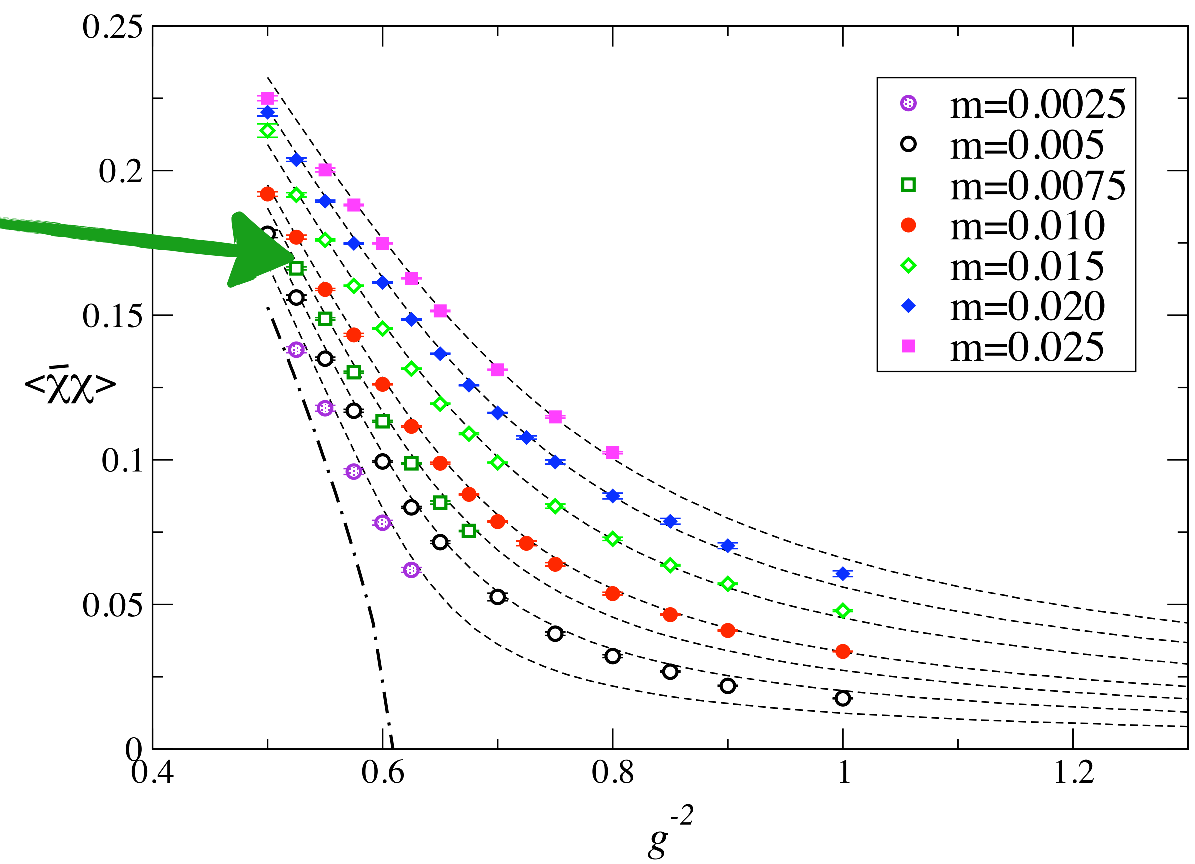
⇒ graphene *is* an insulator for sufficiently strong coupling

⇒ QCP potentially relevant for $N_f = 2$

## Monolayer graphene: $N_f = 2$

$g_c^{-2} = 0.609(2)$

$\delta(N_f{=}2) = 2.66(3)$ so $\delta$ depends on $N_f$




Cf braneworld simulation

Drut & Lähde Phys. Rev. B79(2009) 241405(R)

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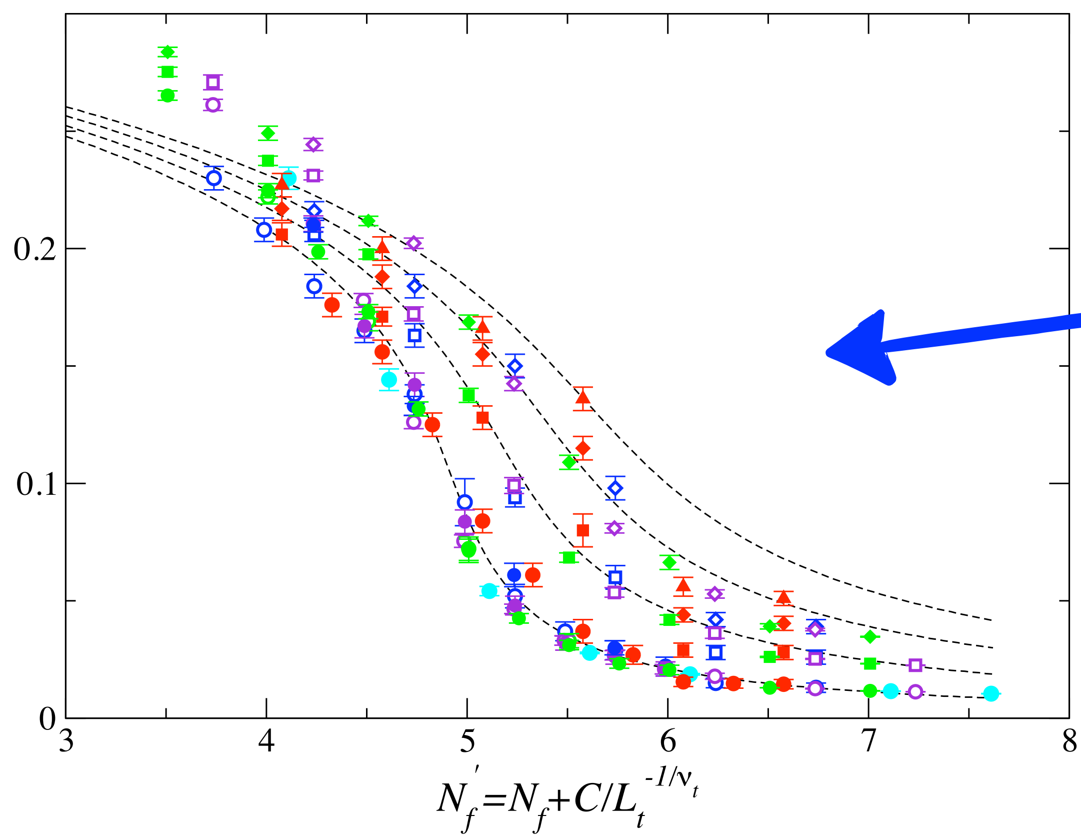


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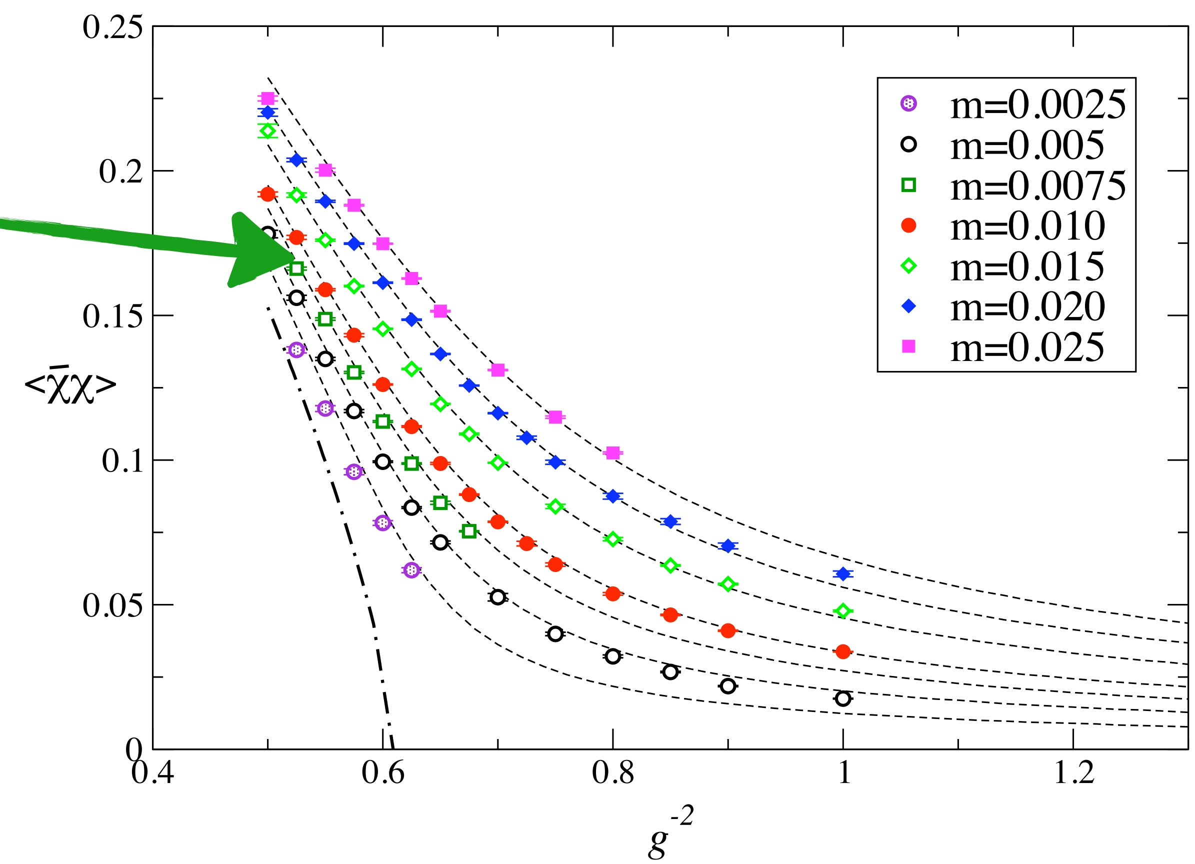


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Cf. honeycomb lattice with “realistic” interaction:

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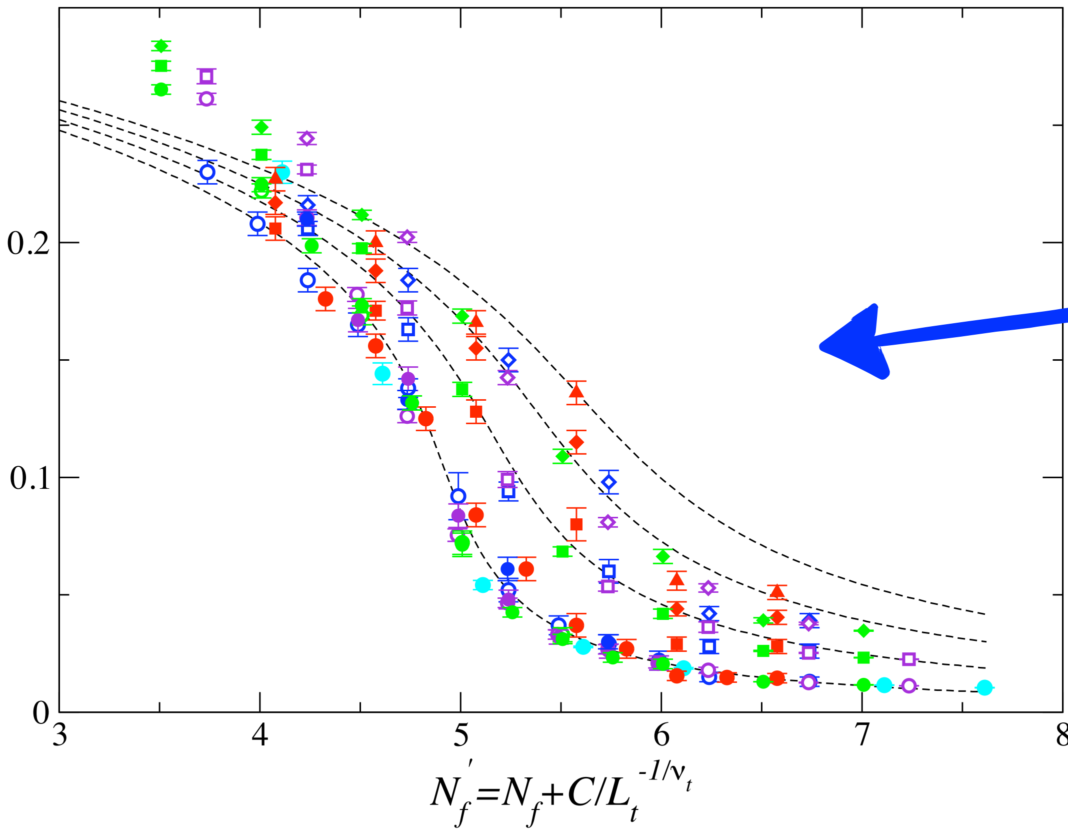


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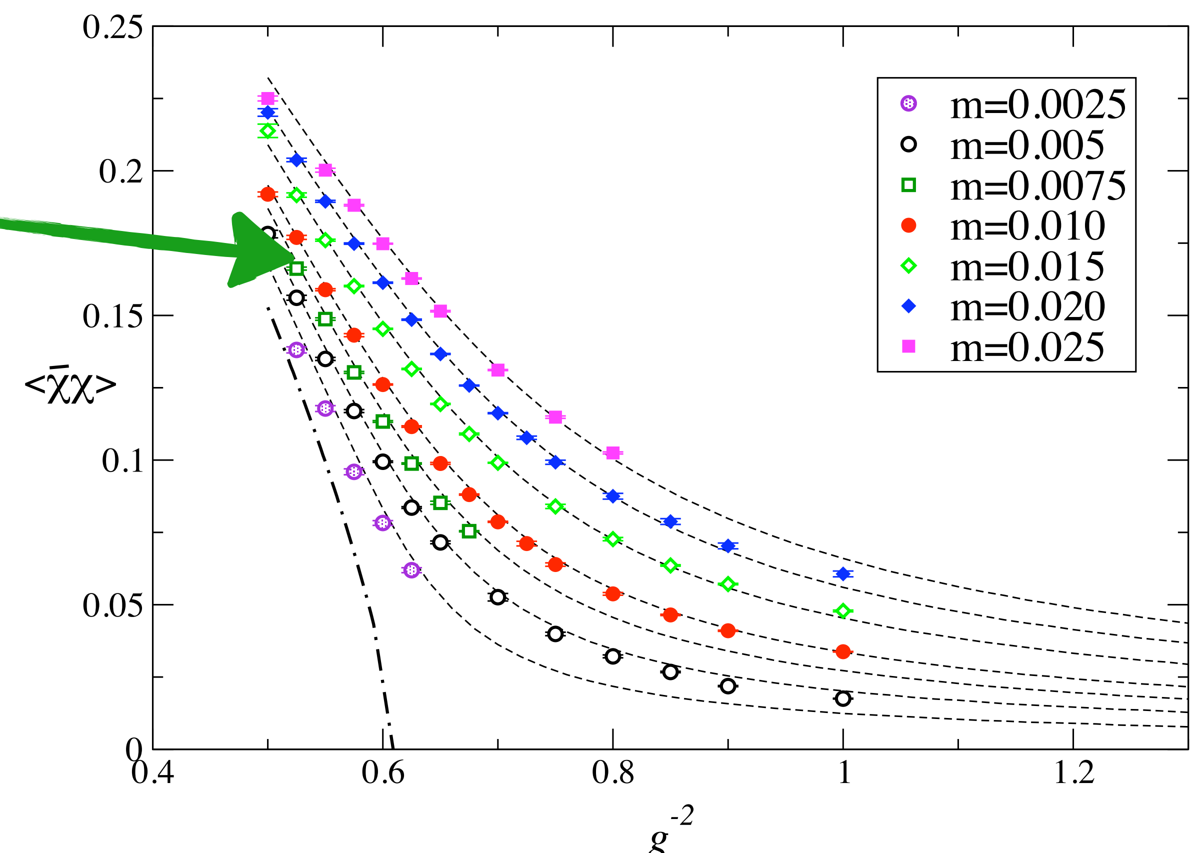



Cf braneworld simulation

Drut & Lähde Phys. Rev. B79(2009) 241405(R)

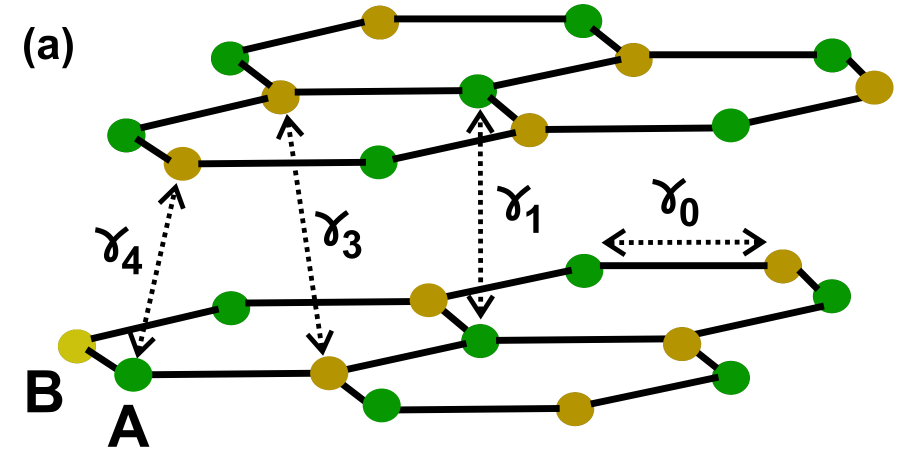
Cf. honeycomb lattice with "realistic" interaction: suspended graphene (ε=1) lies in metallic phase

Ulybyshev, Buividovich, Katsnelson & Polikarpov Phys. Rev. Lett. 111(2013) 056801)

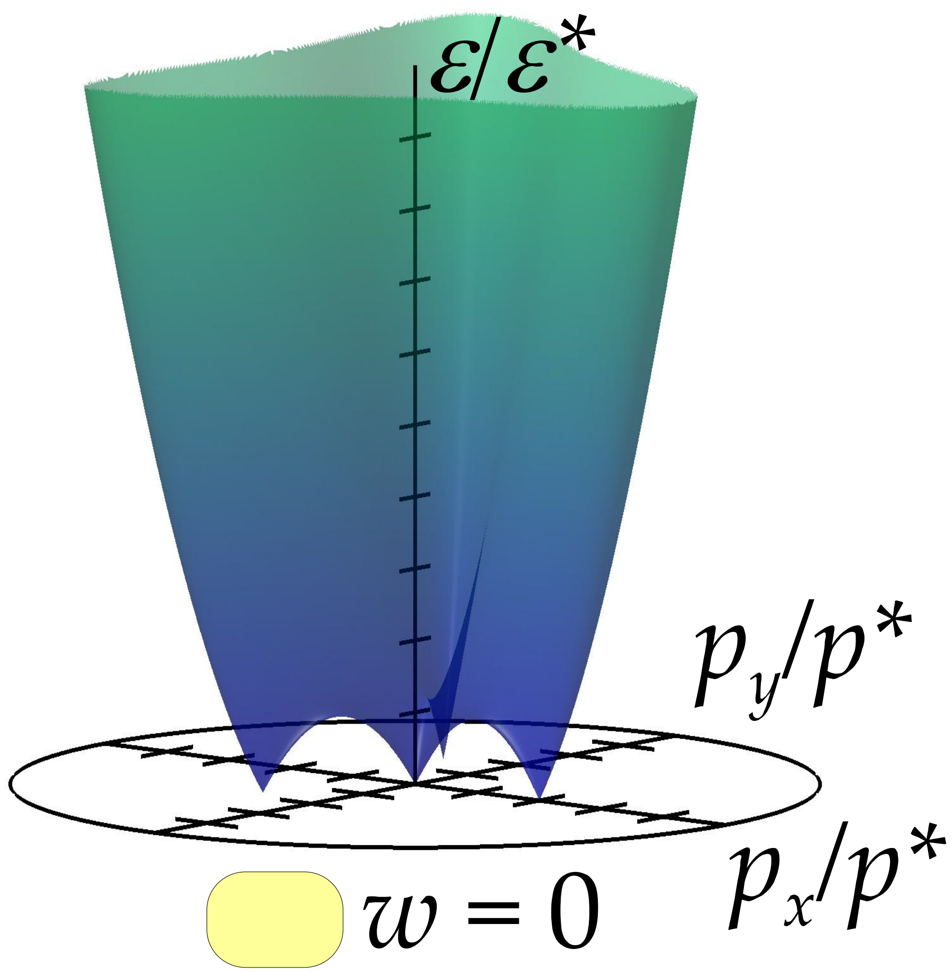
# Bilayer graphene

Coupling $\gamma_3 \neq 0$ results in trigonal distortion of band and doubles number of Dirac points

(Mucha-Kruczynski *et al*, PRB**84**(2011)041404




$N_f = 4$ EFT description plausible for $ka \lesssim \gamma_1\gamma_3/\gamma_0^2$




Introduction of a bias voltage $\mu$ between the layers induces electrons on one, holes on the other.

Inter-layer exciton condensation driven by enhanced density of (e,h) states at Fermi surface leads to gap formation?

# Bilayer effective theory ($N$=2 staggered flavors)

$$\mathcal{L} = (\bar{\psi}, \bar{\phi}) \begin{pmatrix} D[A;\mu] + m & ij \\ -ij & D[A;-\mu] - m \end{pmatrix} \begin{pmatrix} \psi \\ \phi \end{pmatrix} + \frac{1}{2g^2} A^2$$

$$\equiv \bar{\Psi} \mathcal{M} \Psi. + \frac{1}{2g^2} A^2$$

Bias voltage $\mu$ couples to layer fields $\psi$, $\varphi$ with opposite sign

(Cf. isospin chemical potential in QCD)

Intra-layer $(\psi\psi)$ and inter-layer $(\psi\varphi)$ interactions have same strength

"Gap parameters" $m, j$ are IR regulators

$D^\dagger[A;\mu] = -D[A;-\mu]$. inherited from gauge theory

☞ $\det\mathcal{M} = \det[(D+m)^\dagger (D+m) + j^2] > 0$

**No sign problem!**

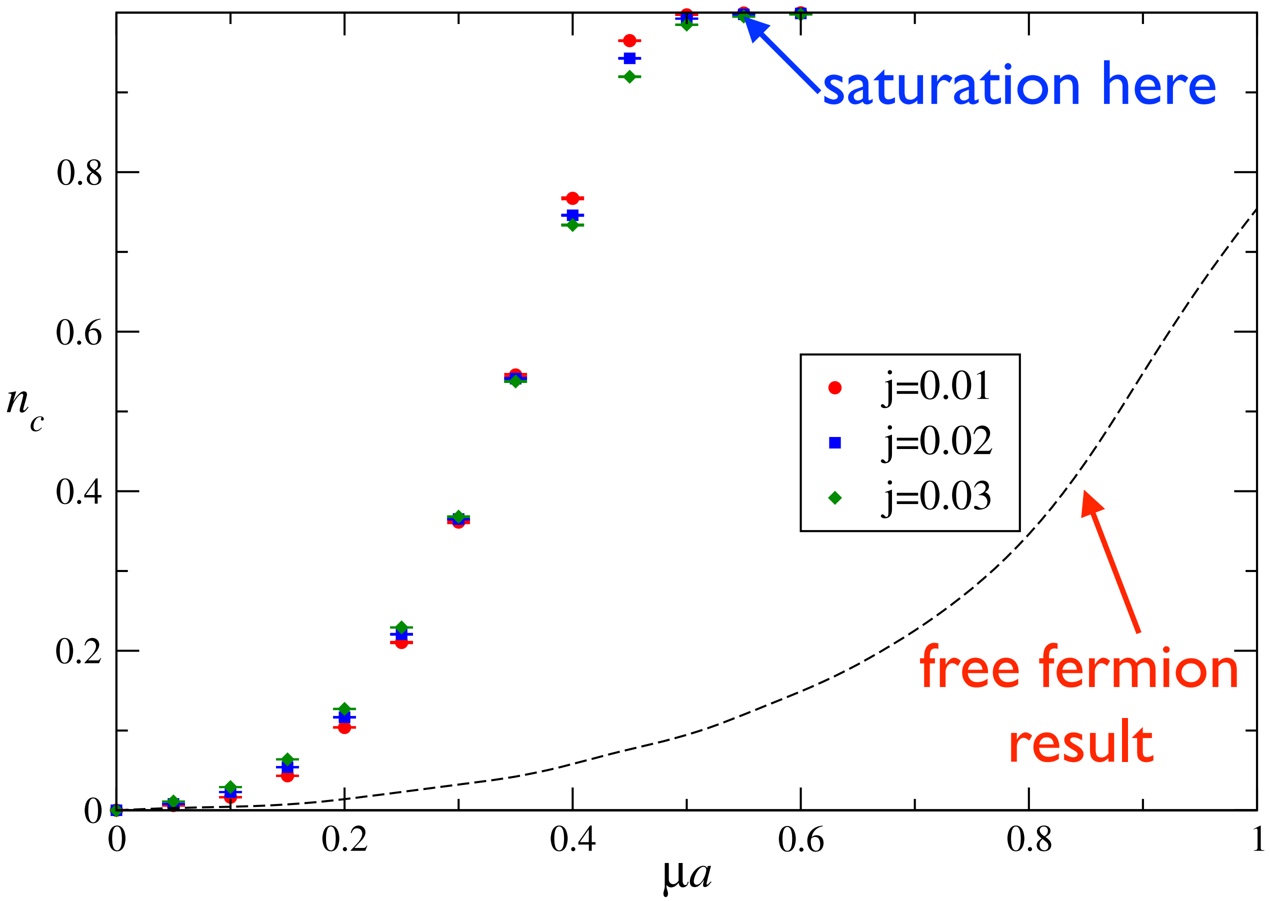
In practice no problem with setting $m$=0

# Simulation observables:

W. Armour, SJH & C.G. Strouthos
PRD87 (2013) 065010

- carrier density $$n_c \equiv \frac{\partial \ln Z}{\partial \mu} = \langle \bar{\psi} D_0 \psi \rangle - \langle \bar{\phi} D_0 \phi \rangle.$$
- exciton condensate (interlayer) $$\langle \Psi\Psi \rangle \equiv \frac{\partial \ln Z}{\partial j} = i\langle \bar{\psi}\phi - \bar{\phi}\psi \rangle$$
- chiral condensate (intralayer) $$\langle \bar{\Psi}\Psi \rangle \equiv \frac{\partial \ln Z}{\partial m} = \langle \bar{\psi}\psi \rangle - \langle \bar{\phi}\phi \rangle$$

# Carrier Density




Observe premature saturation at $\mu a \approx 0.5$ (other lattice models typically saturate at $\mu a \gtrsim 1$)

$\Rightarrow$ $\mu a_t \approx E_F a_t < k_F a_s$

$n_c^{free}(\mu) << n_c^{free}(k_F) \approx n_c(\mu)$

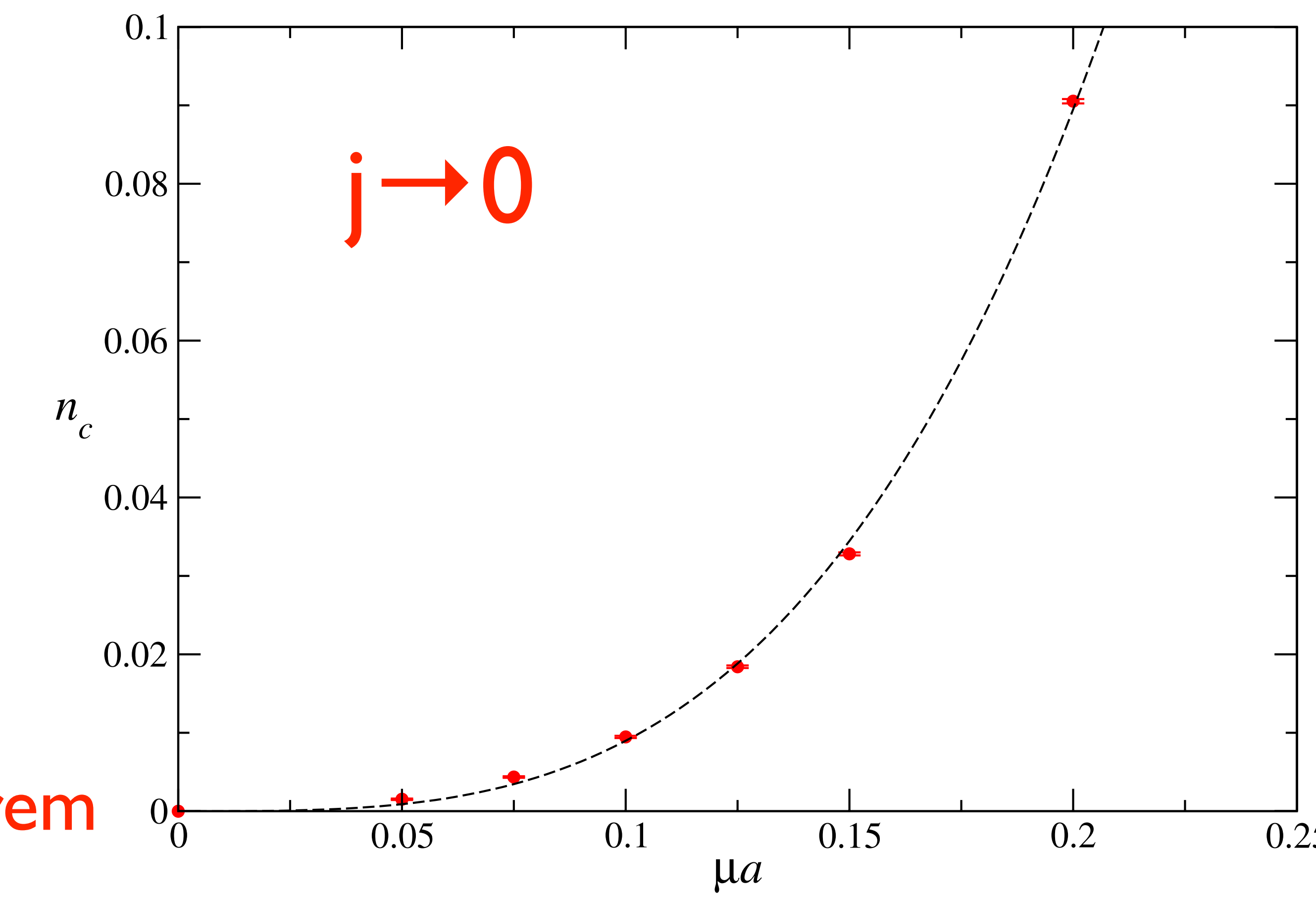
no discernable onset $\mu_o > 0$

Fit small-μ data:

$n_c(j=0) \propto \mu^{3.32(1)}$

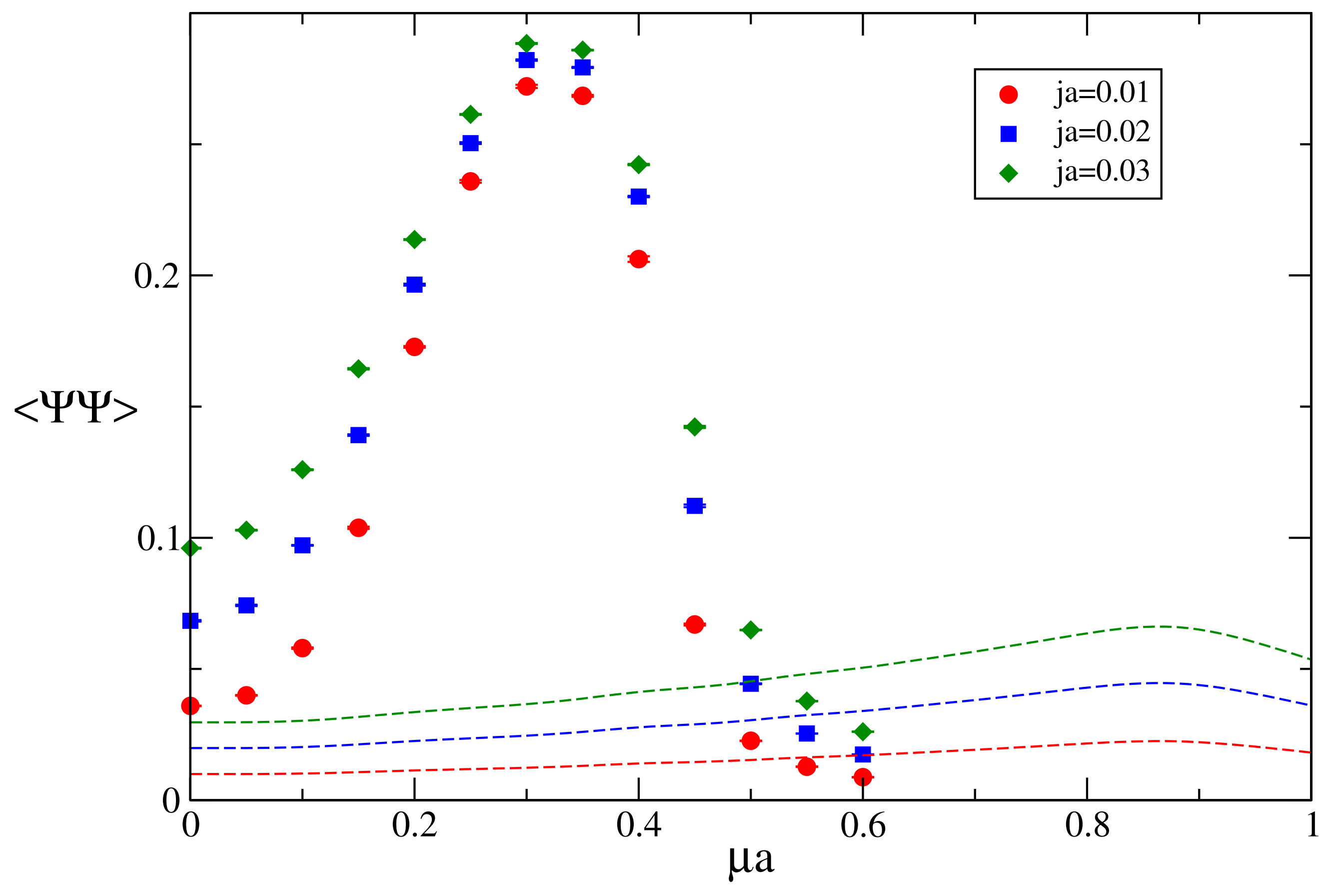
Cf. free-field

$n_c^{free} \propto \mu^d \propto \mu^2$




NB $n_c \propto k_F^2$ Luttinger's theorem

# Exciton Condensate

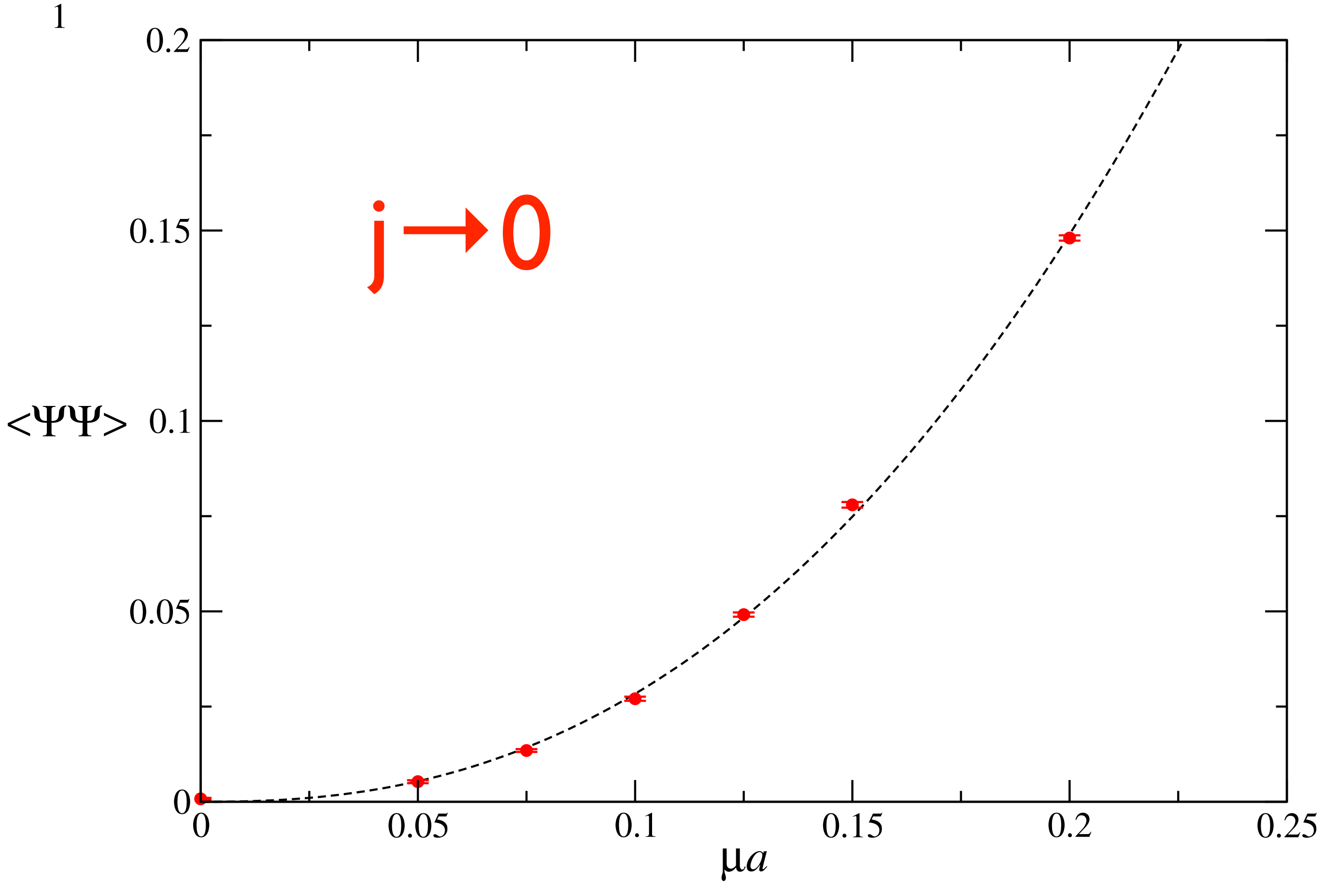



rapid rise with $\mu$ to exceed free-field value, peak at $\mu a \approx 0.3$, then fall to zero in saturation region

Exciton condensation, with no discernable onset $\mu_o > 0$

**Fit small-$\mu$ data:**

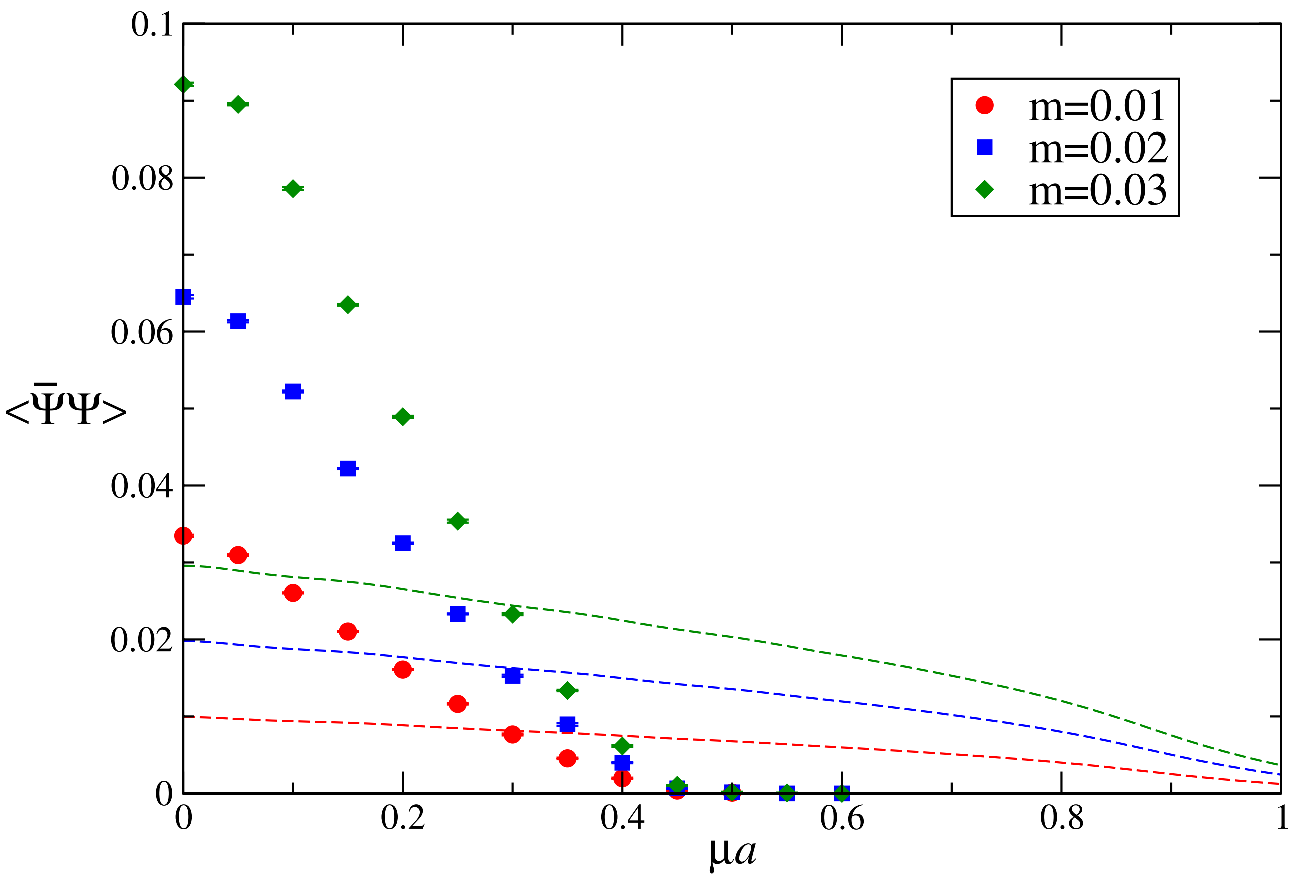
$$\langle \Psi\Psi(j=0) \rangle \propto \mu^{2.39(2)}$$




**Cf. weak BCS pairing**

$$\langle \Psi\Psi \rangle \propto \Delta\mu^{d-1} \propto \mu \ ?$$

# Chiral Condensate




exceeds free-field value for small $\mu$, indicative of nearby QCP, then rapidly falls to zero as $\mu$ increases.

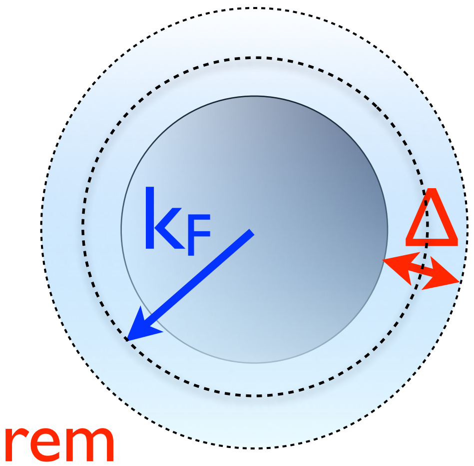
Interlayer pairing suppressed as $E_F$ grows

$$|\langle\bar{\Psi}\Psi\rangle| \approx \tfrac{1}{3}\, |\langle\Psi\Psi\rangle|_{peak}$$

ie. particle-hole pairing is promoted by the large Fermi surface induced by $\mu\neq0$

the two condensates **compete**:
$\langle\bar{\Psi}\Psi\rangle < \langle\bar{\Psi}\Psi\rangle_{free}$ when $\langle\Psi\Psi\rangle$ peaks

For a BCS-style condensation - ie. pairing at Fermi surface leading to gap generation $\Delta>0$

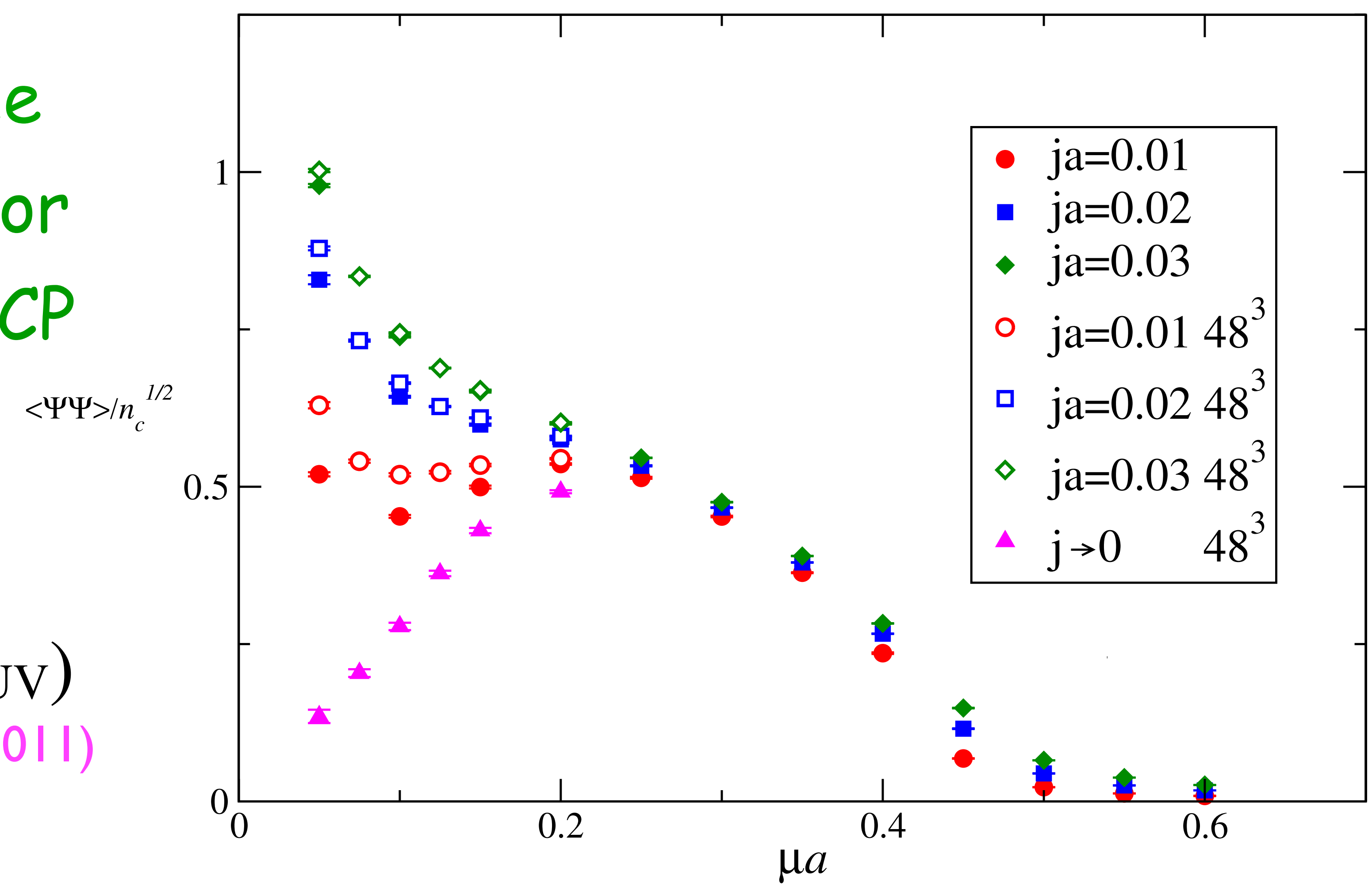



expect $\langle\Psi\Psi\rangle \propto \Delta k_F^{d-1} \propto \Delta n_c^{\frac{d-1}{d}}$

where last step follows from Luttinger's theorem

Thus $\Delta(\mu)\propto \langle\Psi\Psi\rangle/\sqrt{n_c}\propto\mu^{1.44}$ ?

Find near-linear dependence $\Delta\propto\mu$ at small $\mu$: expected for conformal behaviour near QCP




Cf. NJL model: $\Delta=O(\Lambda_{UV})$

(SJH & D.N. Walters PRD69 (2004) 076011)

$QC_2D$: $\Delta=O(\Lambda_{QCD})$

(S. Cotter et al PRD87 (2013) 034507)

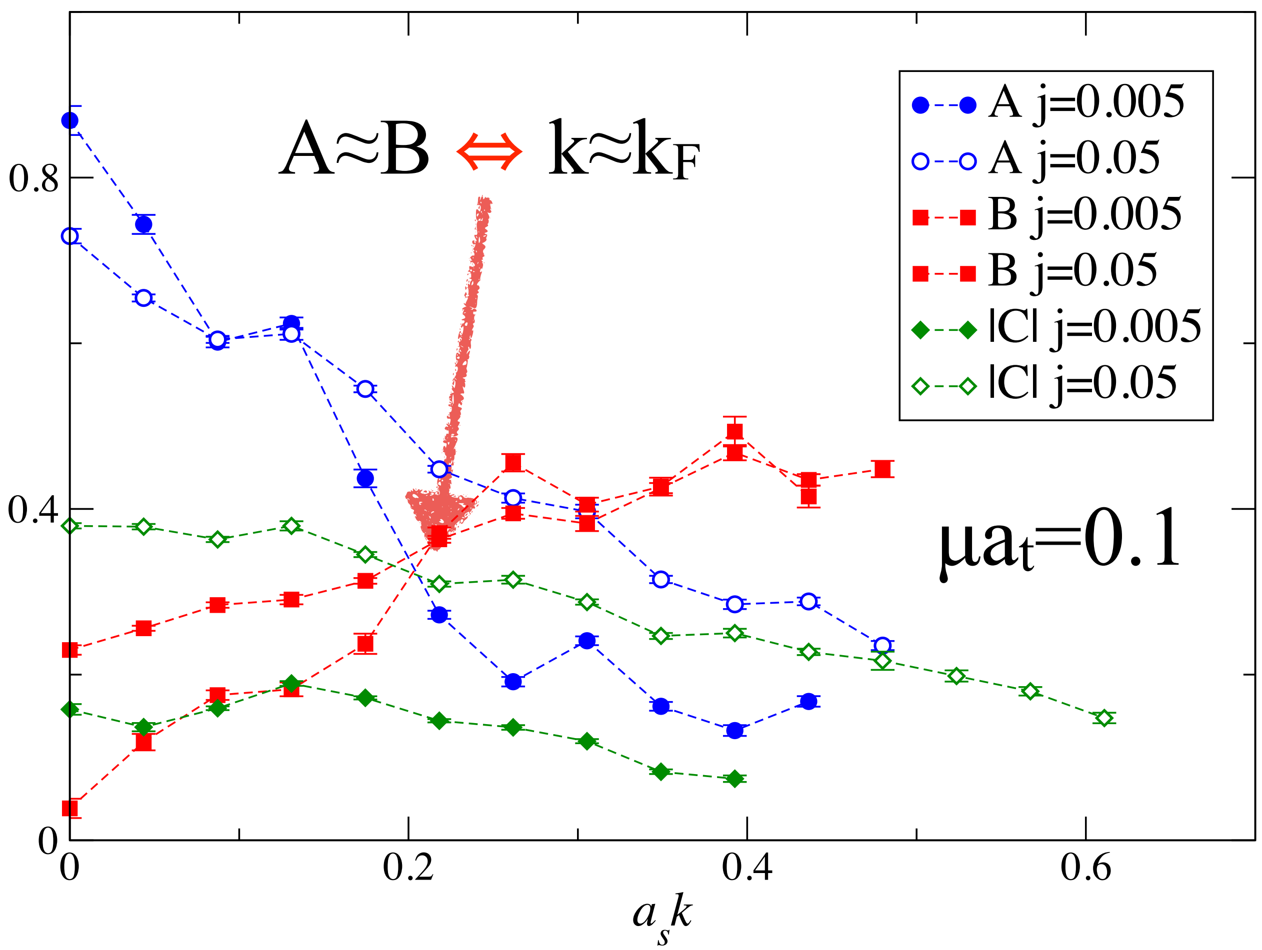
in both cases (roughly) $\mu$-independent

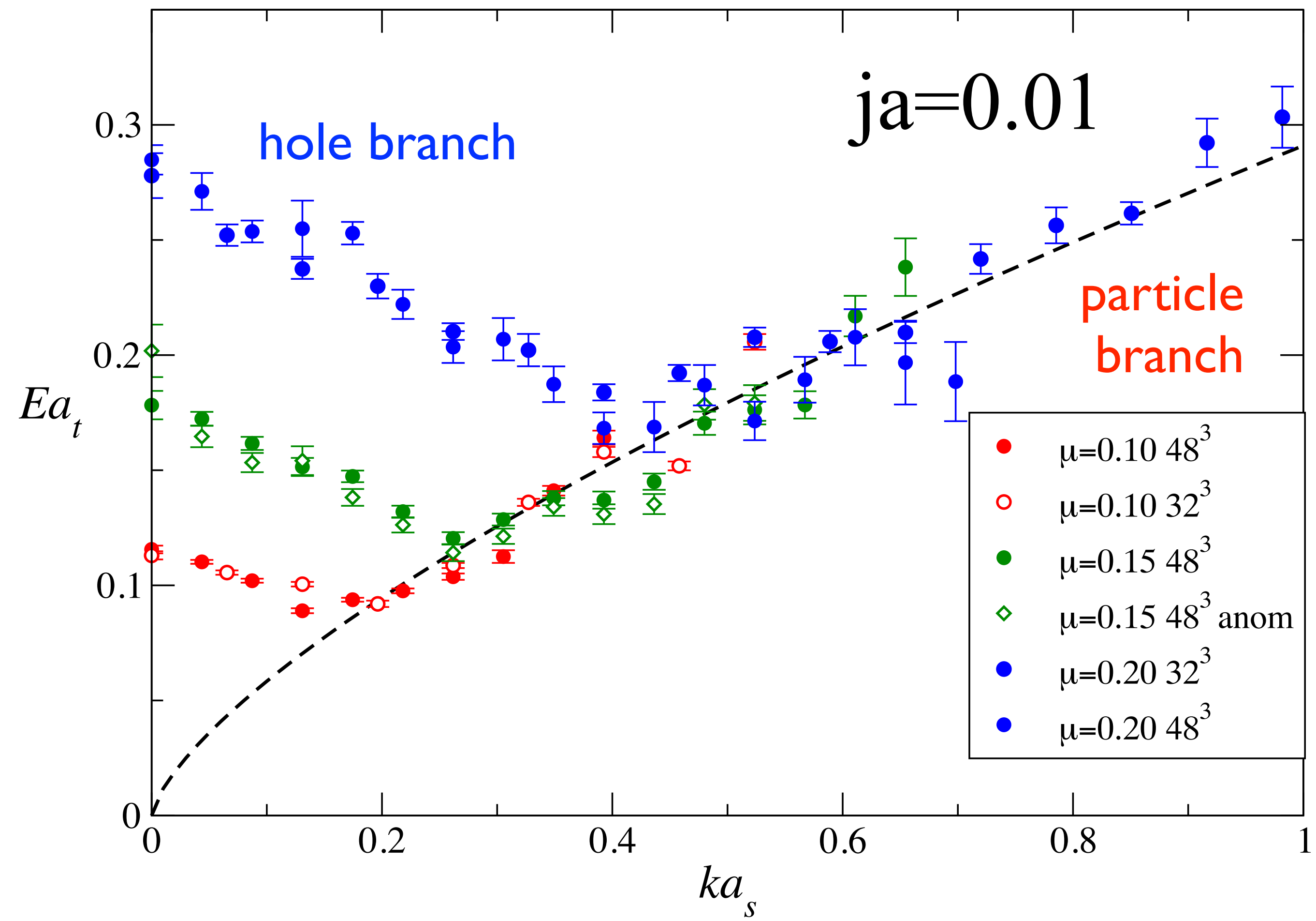
# Quasiparticle Dispersion

W. Armour, SJH & C.G. Strouthos
arXiv: 1509.03401

$<\Psi(k)\overline{\Psi}(k)> \sim e^{-E(k)t}$

partially twisted spatial b.c. improve momentum resolution - no gauge fixing needed!




Normal $C_N(\vec{k},t) = \langle\psi(\vec{k},t)\bar{\psi}(\vec{k},t)\rangle = Ae^{-E_N t} + Be^{-E_N(L_t-t)};$

Anomalous $C_A(\vec{k},t) = \langle\psi(\vec{k},t)\bar{\phi}(\vec{k},t)\rangle = C[e^{-E_A t} - e^{-E_A(L_t-t)}].$

Amplitudes A, B, C show crossover from holes to particles

Dispersions E(k) show $k_F$ varying with μ with $k_F a_s > \mu a_t$

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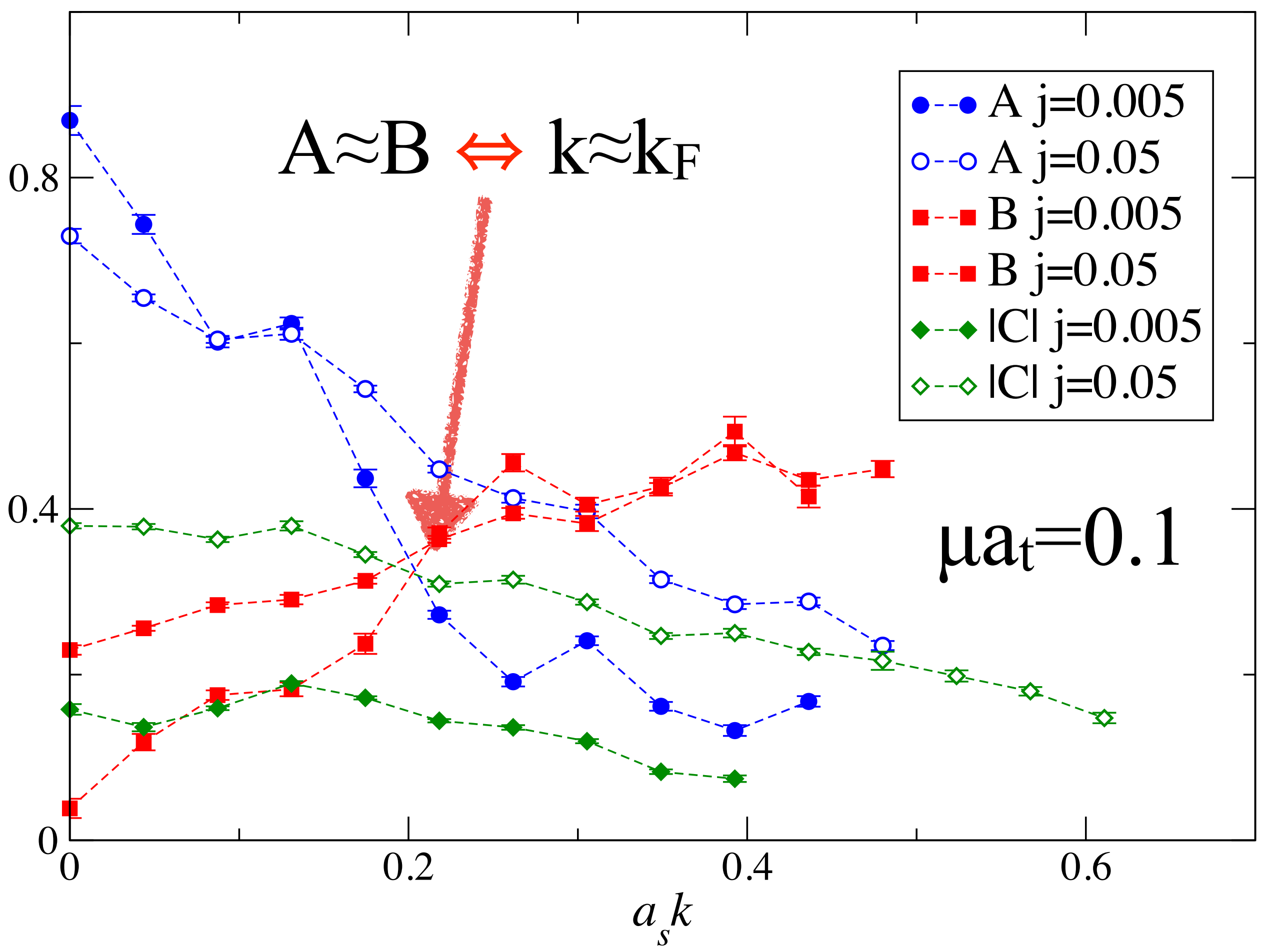


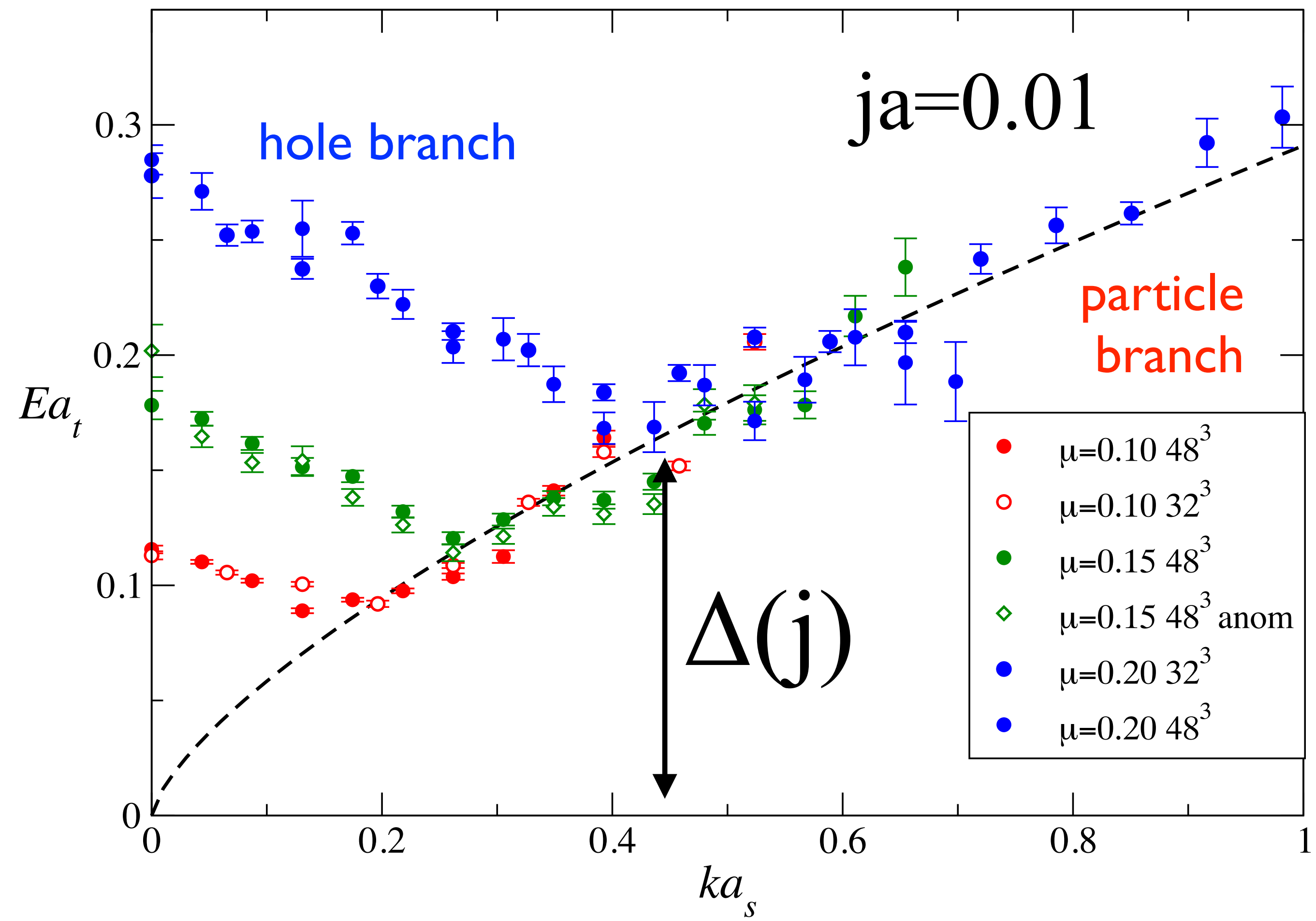


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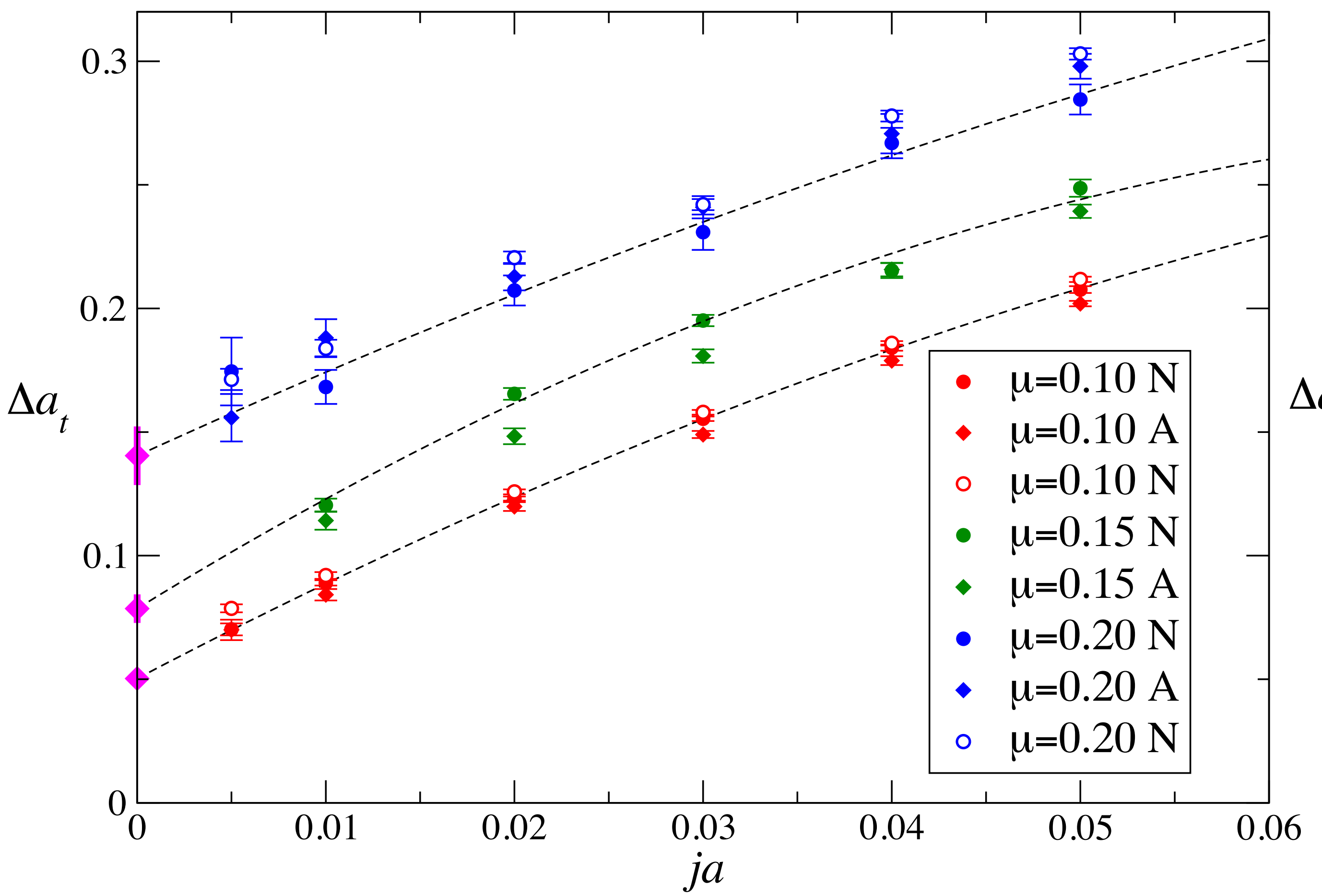
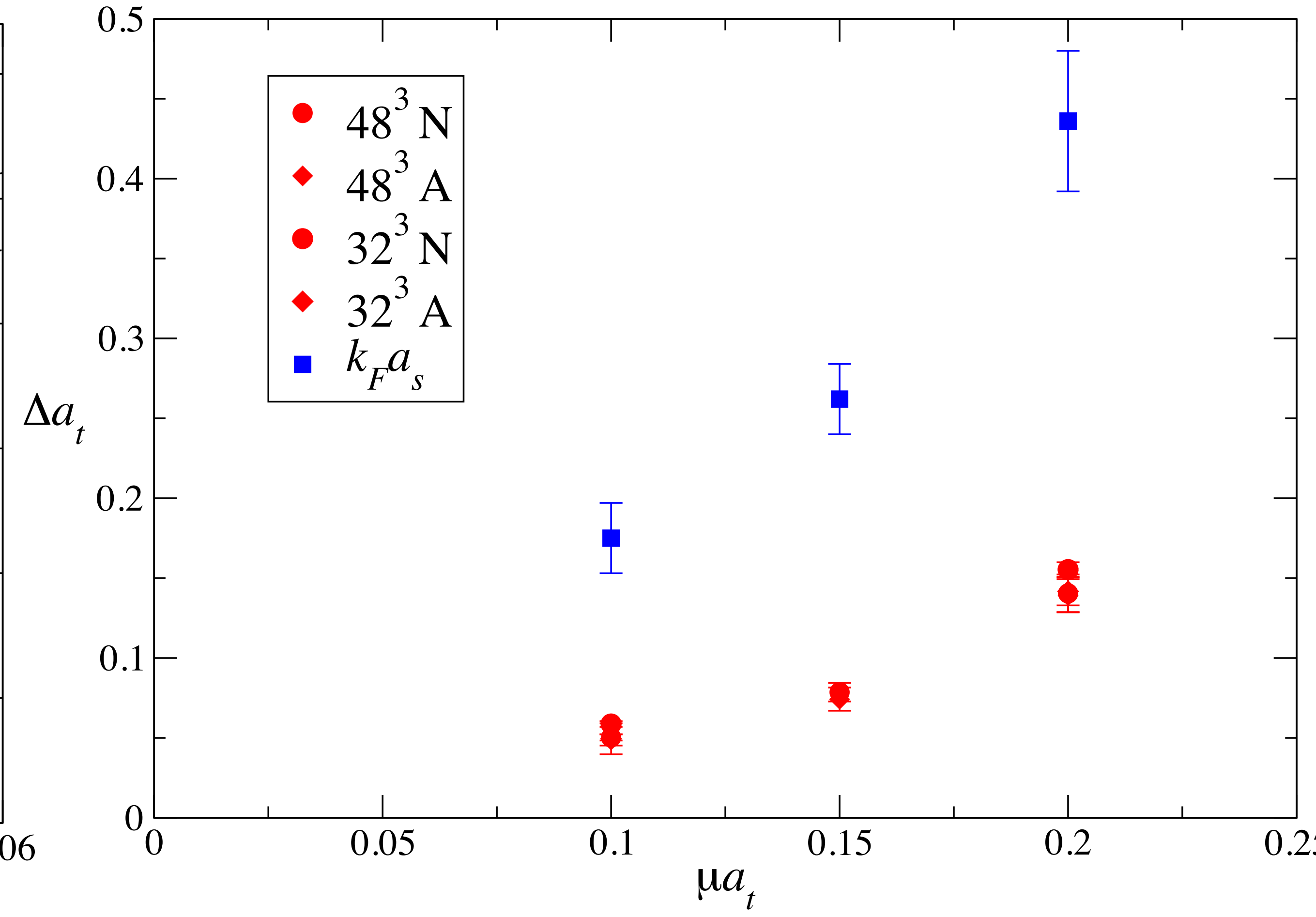
Dispersions E(k) show $k_F$ varying with μ with $k_F a_s > \mu a_t$

# And the gap Δ ?....




Again, consistent with a gapped Fermi surface with $\Delta/\mu = O(1)$

Cf. $\Delta/\mu \sim 10^{-7}$ found in diagrammatic approach

Kharitonov & Efetov Semicond. Sci. Technol. **25** 034004 (2010)

$\Delta/\mu \sim O(1)$ found if screening treated self-consistently

Sodemann, Pesin & MacDonald PRB **85** 195136 (2012)

Both Δ and $k_F$ scale superlinearly with μ

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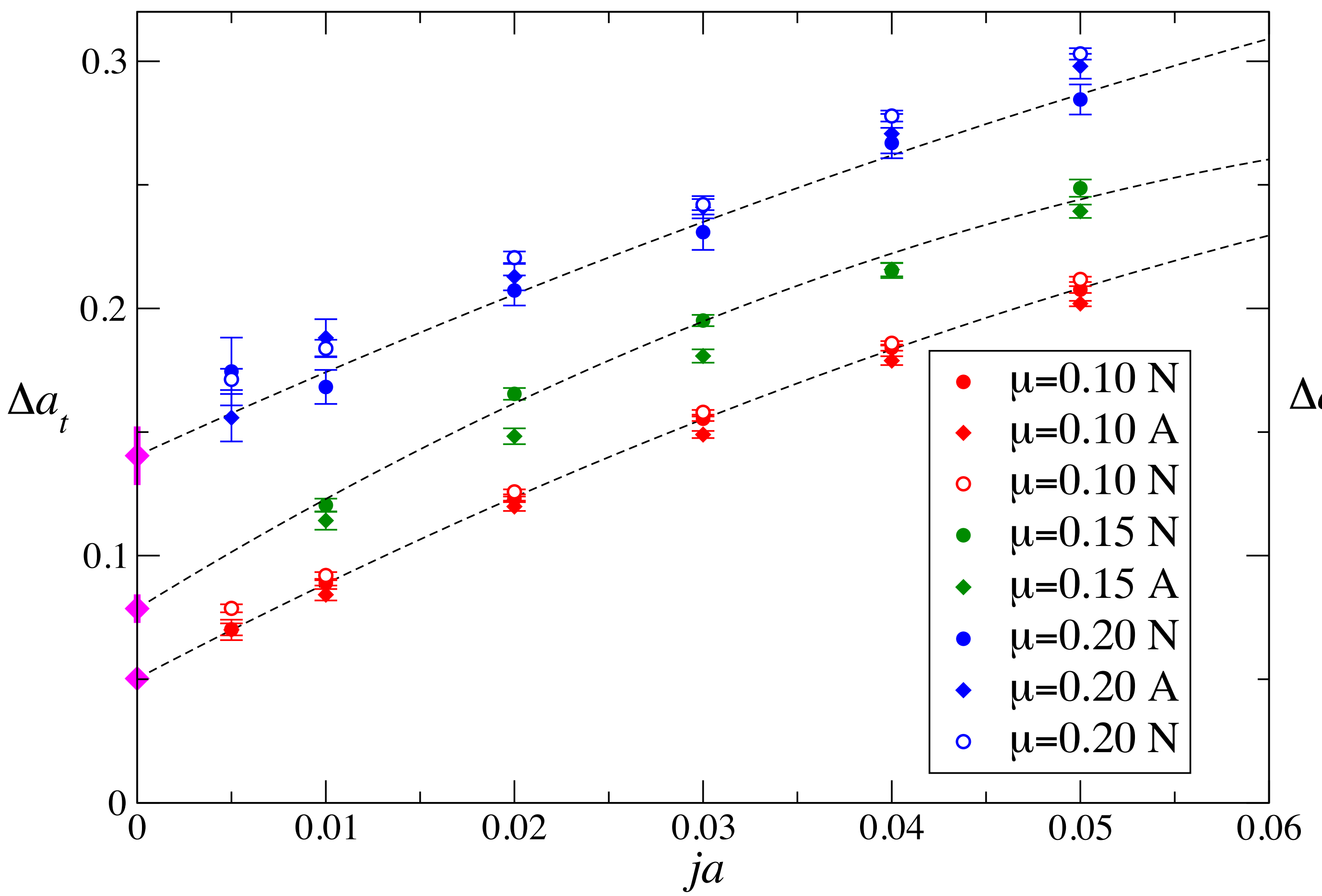


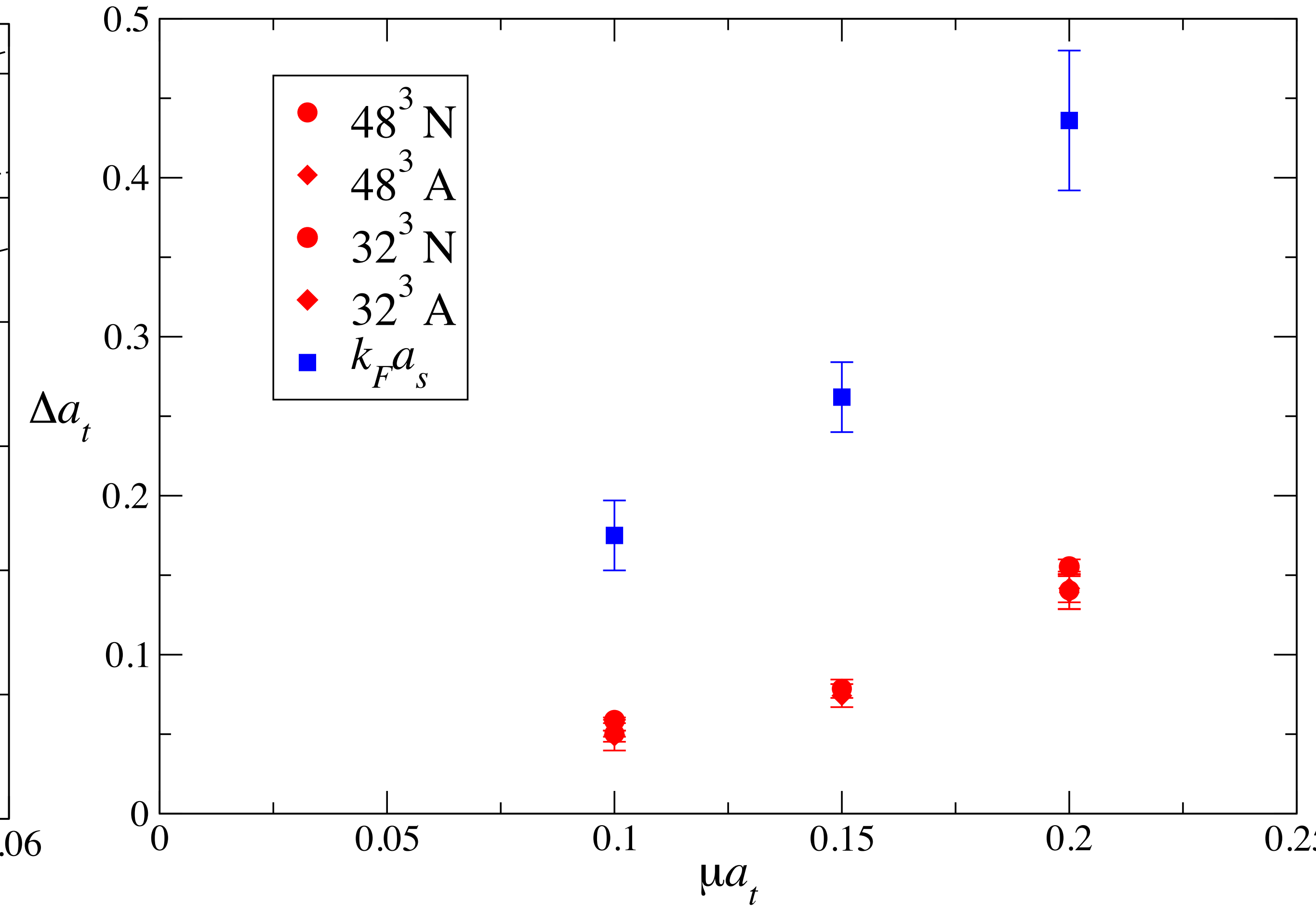


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Both Δ and $k_F$ scale superlinearly with μ

consistent with $\Delta(\mu) \propto \mu^{1.44}$ ?

# Summary

- A new, interesting member of the small class of models permitting MC study with $\mu \neq 0$
- Behaviour very different from previous ($QC_2D$, NJL) ⇔ residual interactions at Fermi surface are **strong**

  Densities and condensates scale anomalously with $\mu$
  Quasiparticle dispersion $E(k)$ exposes Fermi surface disrupted by pair condensation
- Strongly-interacting QCP ⇔ $\Delta=\Delta(\mu)$, $\Delta/\mu=O(1)$
- $\Delta \propto \mu^\sigma$ with $\sigma > 1$?
- Next move: **domain wall lattice fermions** to better reproduce global symmetries of 2+1d

$$U(8) \underset{\mu\neq 0}{\longrightarrow} U(4)\otimes U(4) \underset{j\neq 0}{\longrightarrow} U(4)$$

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