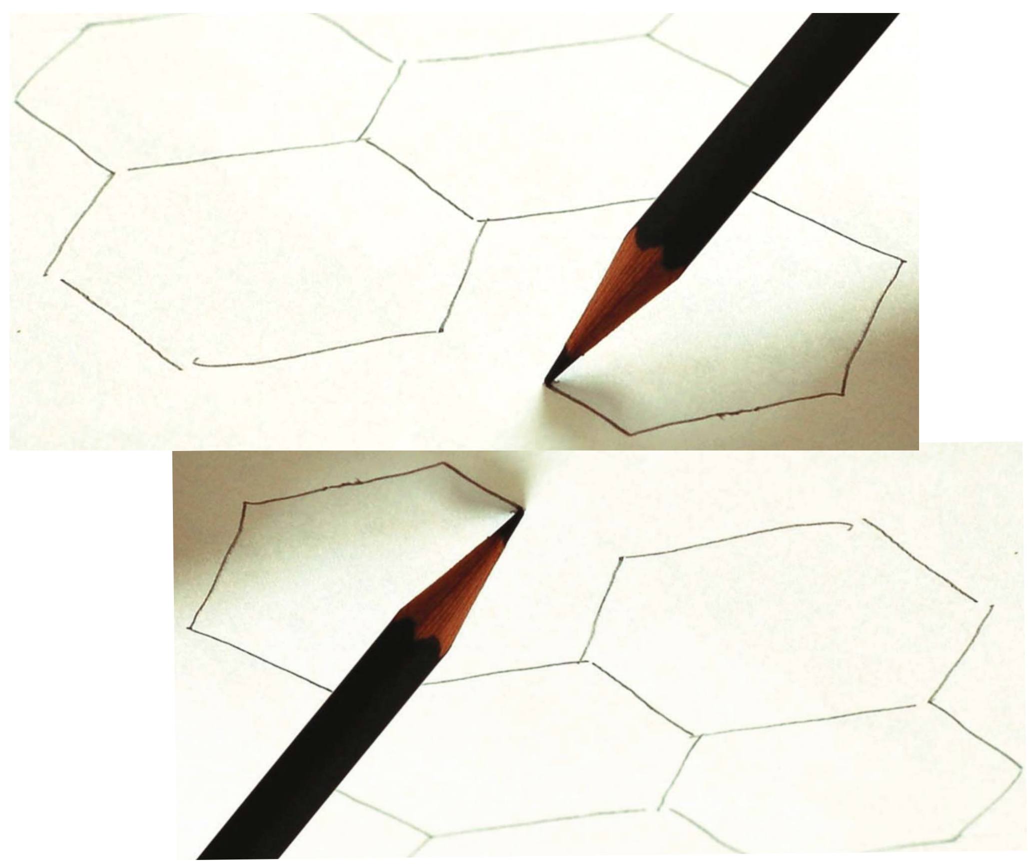
Graphene as a lattice gauge theory

Simon Hands (Swansea U.)



with Wes Armour & Costas Strouthos,
Phys. Rev. D87 (2013) 065010

PPCM Boston 8th May 2014

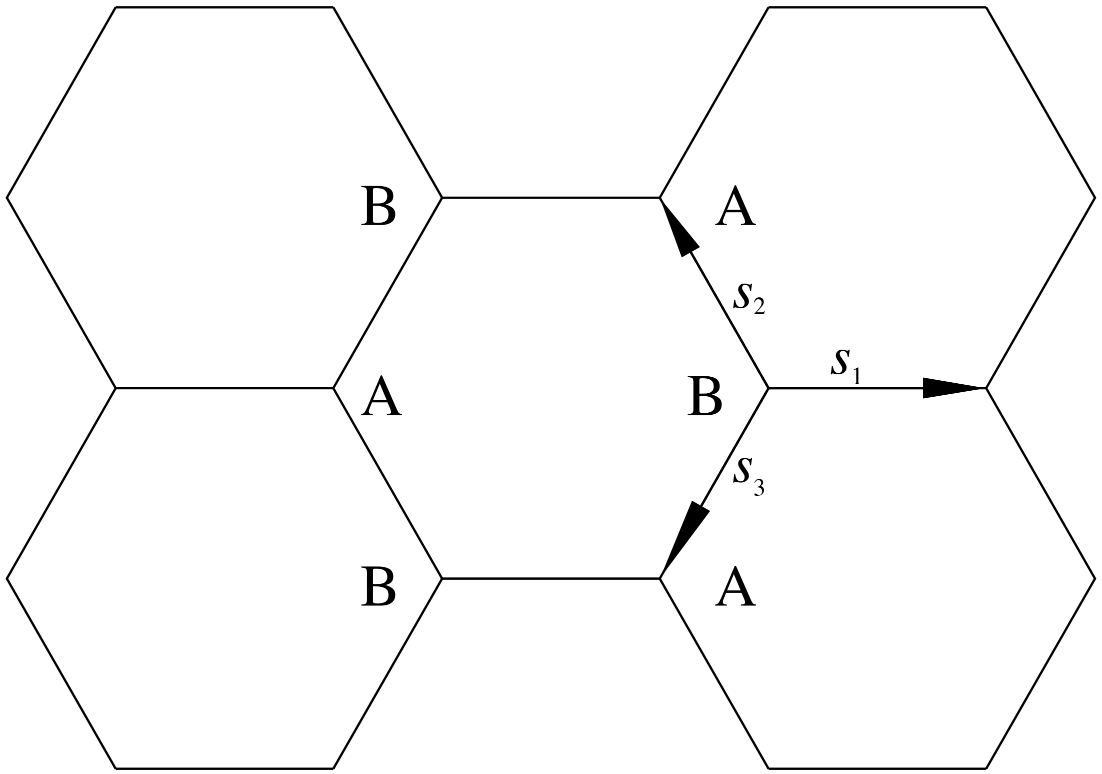
In this talk I will

- 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 a non-zero inter-layer bias voltage (aka isopsin chemical potential).
- present simulation results probing degenerate matter in the presence of strong interactions

Relativity in Graphene

The electronic properties of graphene were first studied theoretically over 60 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*

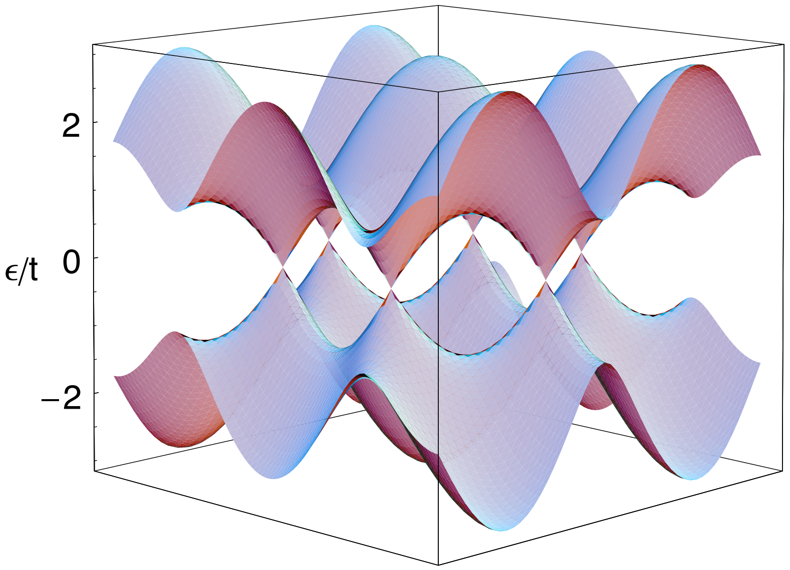
In momentum space

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

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 $E = 0$

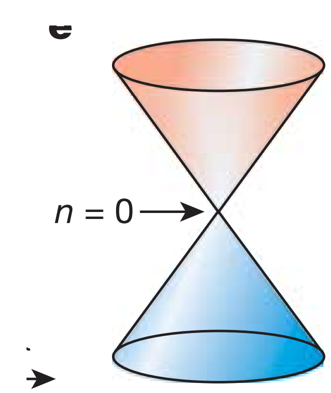
Half-filling (neutral or "undoped" graphene) has zero energy at "Dirac points" at corners of first Brillouin Zone:

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" $v_F = \frac{3}{2} t l$

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

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 $v_F = \frac{3}{2} t l \approx \frac{1}{300} c$

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

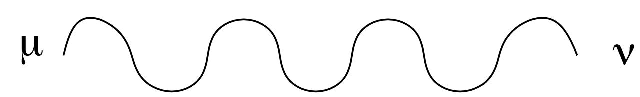
$$S = \sum_{a=1}^{N_f} \int dx_0 d^2x (\bar{\psi}_a \gamma_0 \partial_0 \psi_a + v_F \bar{\psi}_a \vec{\gamma}.\vec{\nabla}\psi_a + iV\bar{\psi}_a\gamma_0\psi_a) + \frac{1}{2e^2}\int dx_0 d^3x (\partial_i V)^2,$$

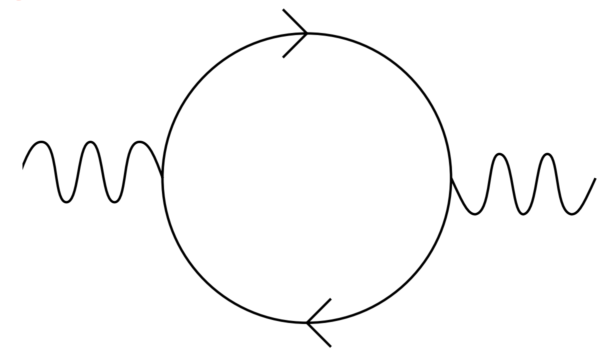
"instantaneous" Coulomb potential

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

$\propto r^{-1}$

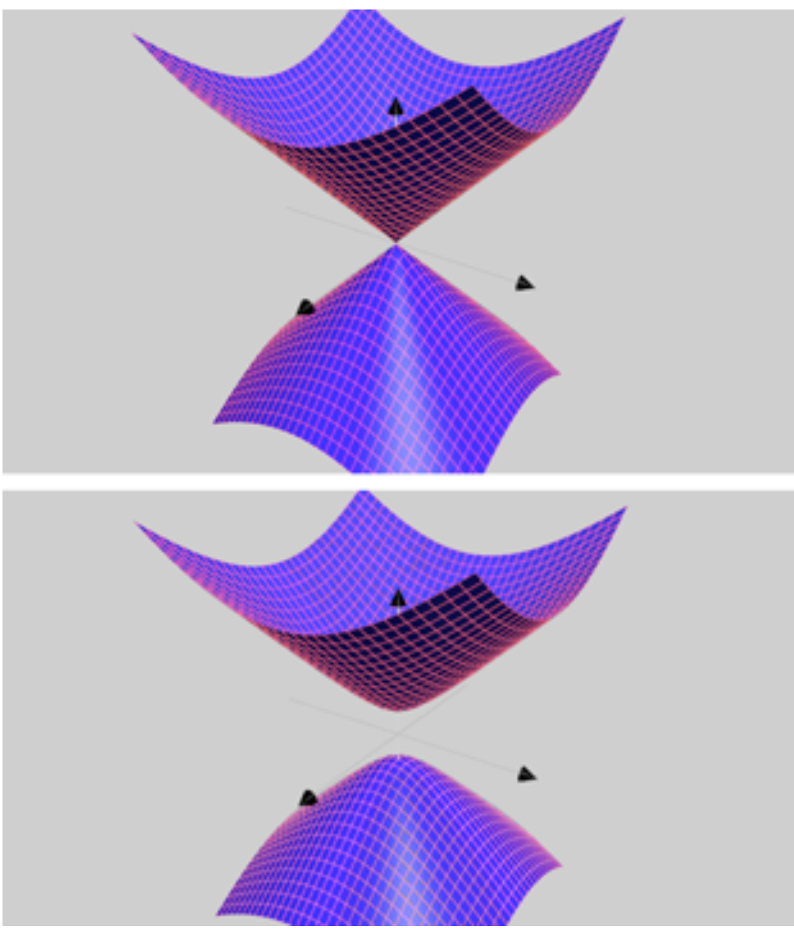
$$\lambda = \frac{e^2 N_f}{16 \varepsilon \varepsilon_0 \hbar v_F} \simeq \frac{1.4 N_f}{\varepsilon}$$

(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 U(2N$_f$) → U(N$_f$)⊗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?

Numerical Lattice Approach

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

$$+ \; m\sum_{xi}\bar{\chi}_x^i\chi_x^i + \frac{N}{4g^2}\sum_x V_x^2 \qquad\qquad i = 1,\ldots,N$$

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, λ not known a priori

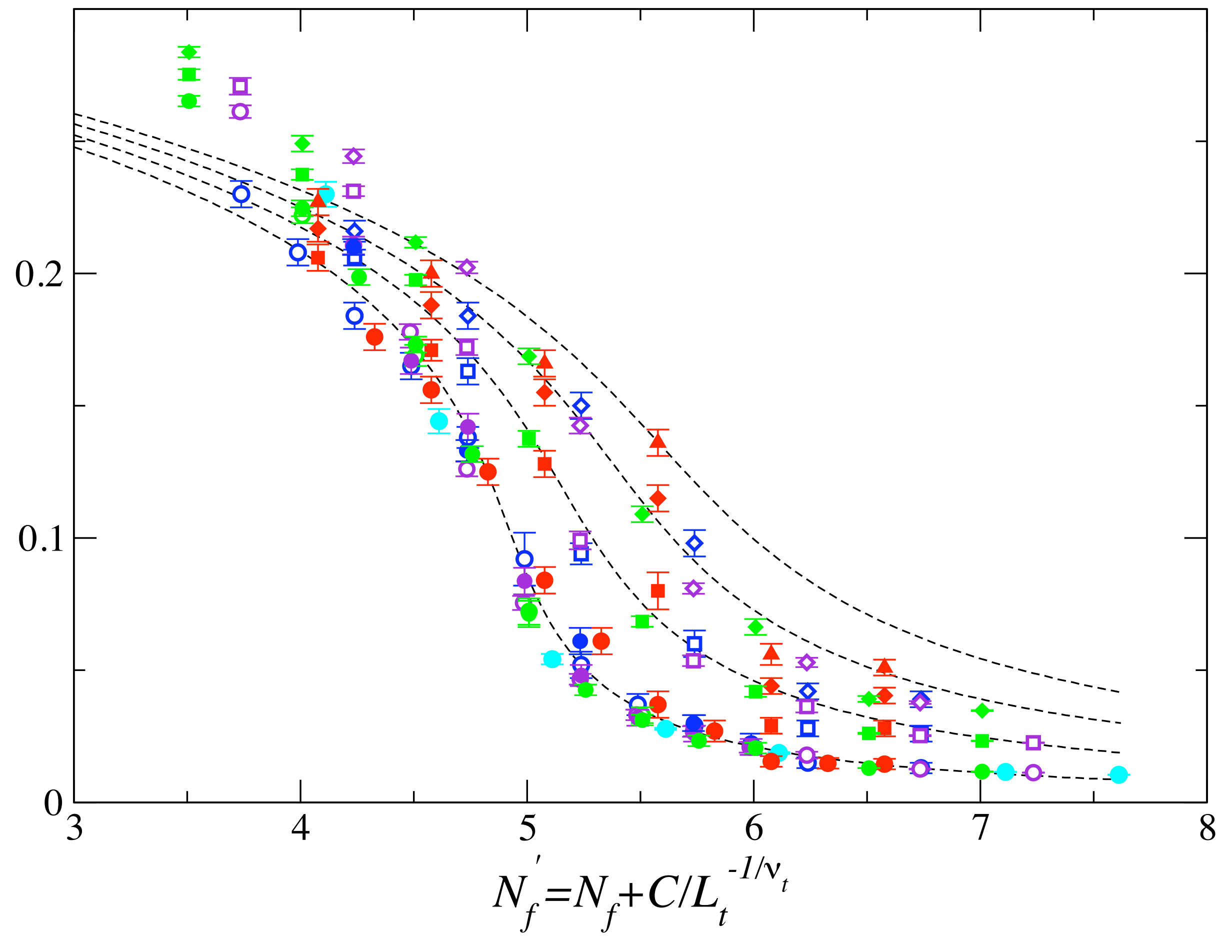
Chiral symmetry: $U(N)\otimes U(N) \to U(N)$ (if $m \neq 0$)

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

"taste symmetry restoration"

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

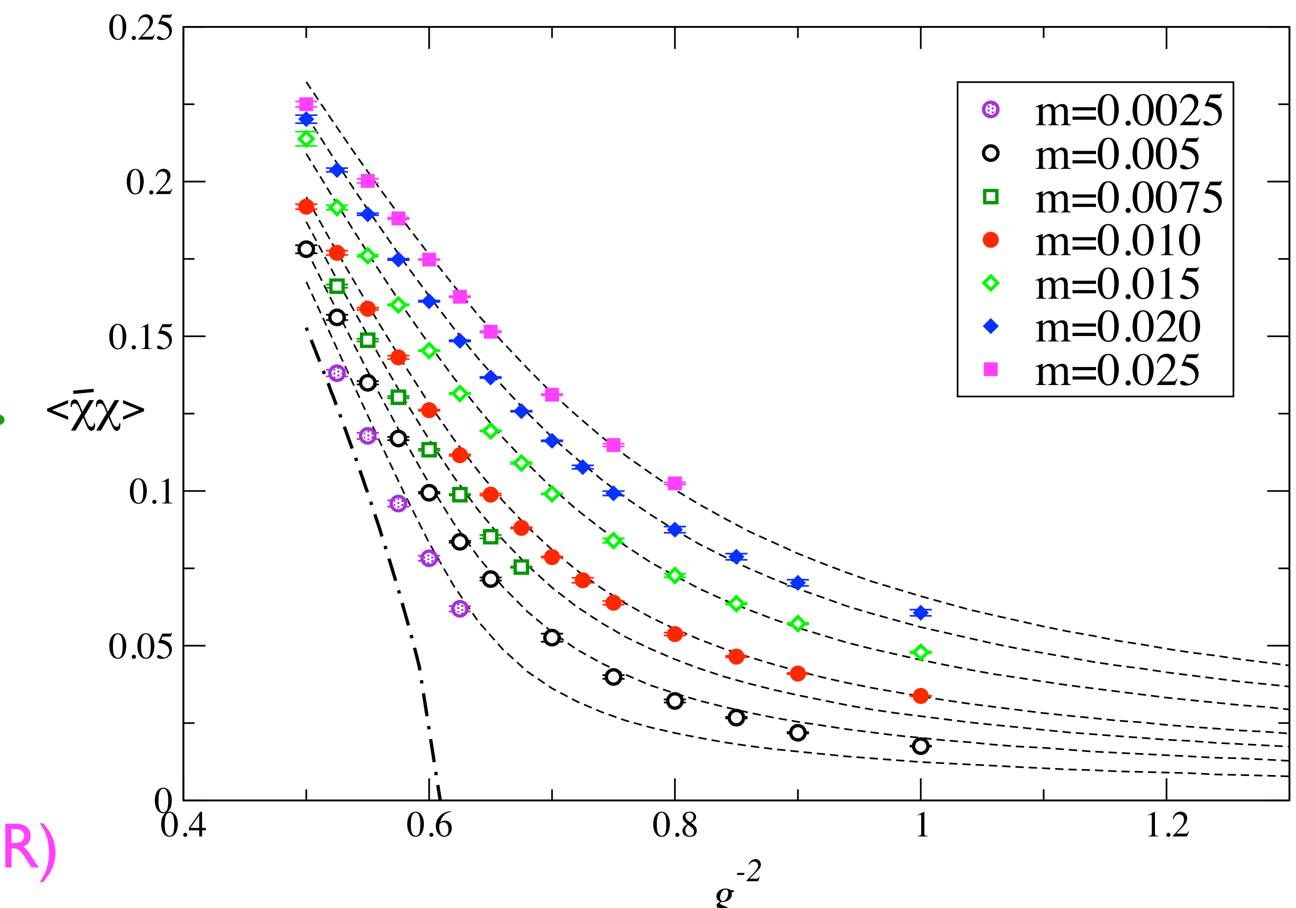
⇒ QCP potentially relevant for N_f = 2

Physical graphene N_f=2

g_c^{-2} = 0.609(2)

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

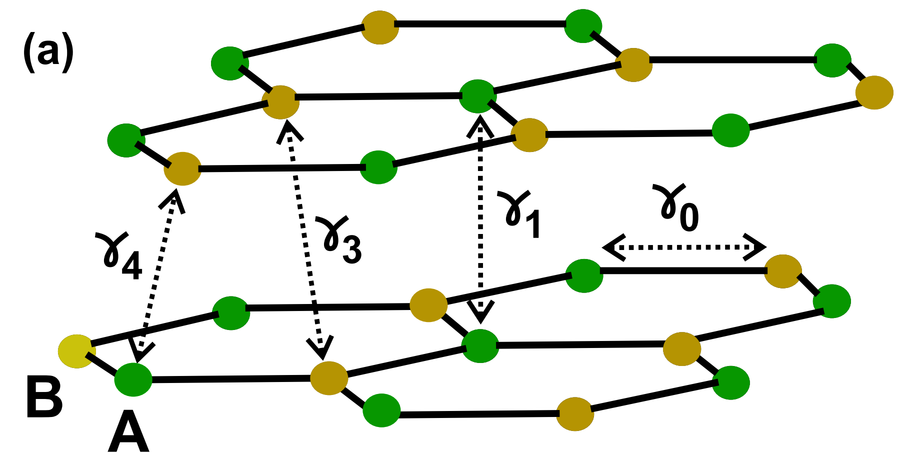
So δ depends on N_f



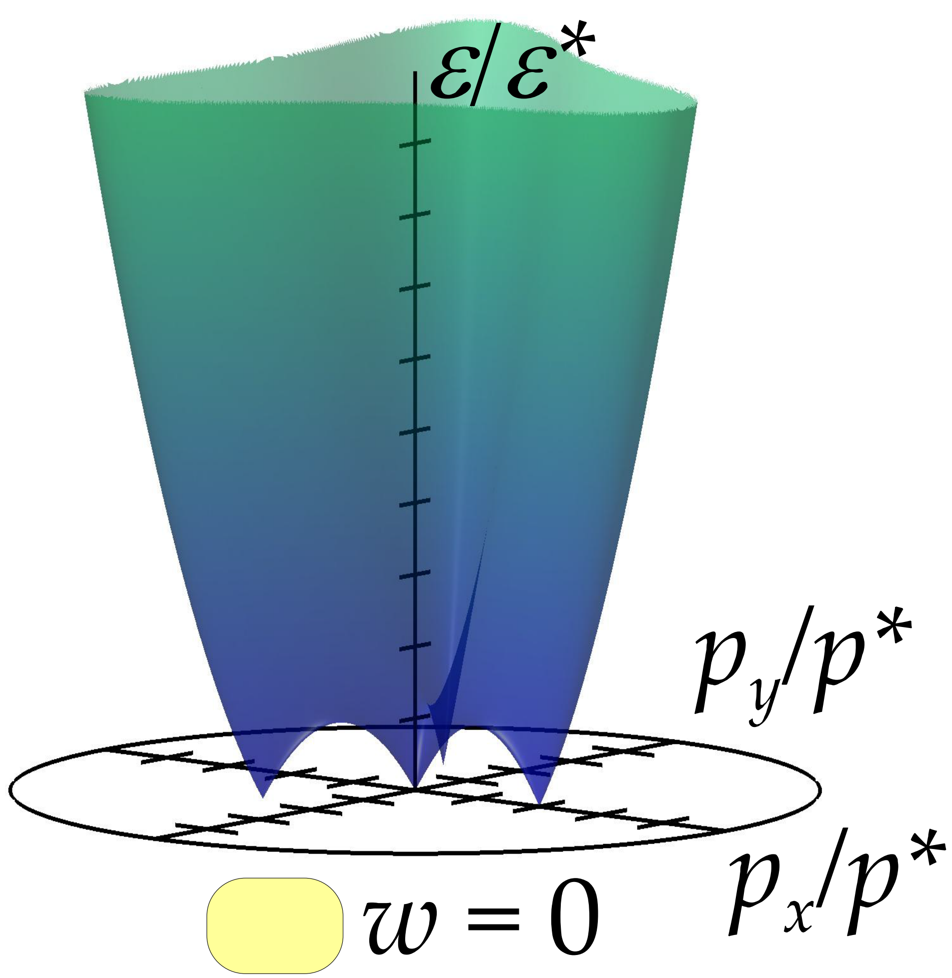
Cf Drut & Lähde Phys. Rev. B79(2009) 241405(R)

Bilayer graphene

Coupling $\gamma_3 \neq 0$ results in trigonal distortion of band
and doubles number of Dirac points
(McCann & Fal'ko PRL96(2006)086805)



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



Introduction of a bias voltage μ 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 μ couples to layer fields ψ, φ 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

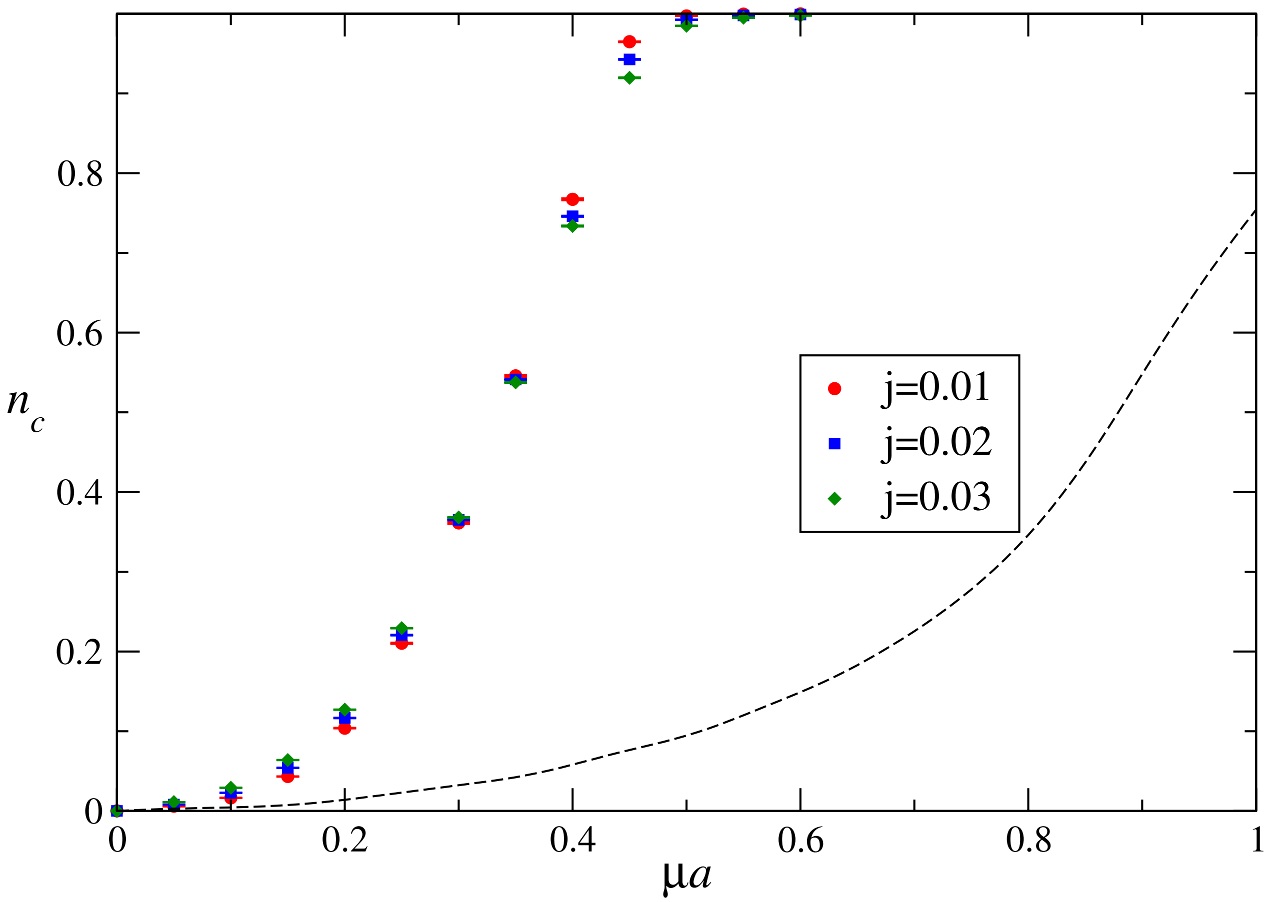
Details of the simulation

- Simulate using hybrid Monte Carlo (HMC) algorithm
- no sign problem even with $\mu\neq 0$
- lattice sizes 32^3, 48^3
- $1/g^2a = 0.4$ throughout - close to QCP on chirally symmetric side
- $ja = 0.01, \ldots, 0.07$ enables polynomial extrapolation to $j=0$
- $\mu a = 0.0, \ldots, 0.6$

Main observables:

- 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 $\mu a \gtrsim 1$)

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

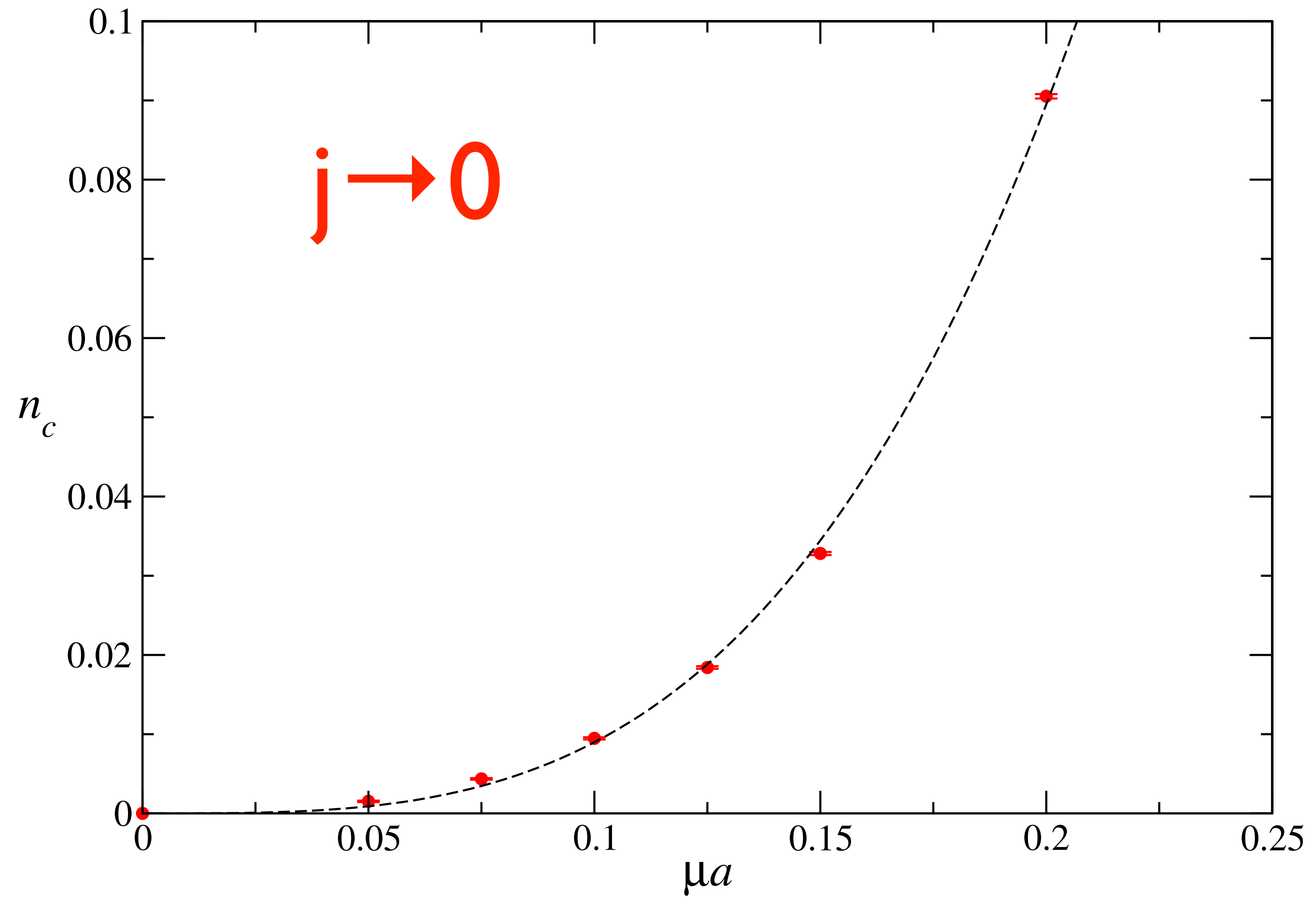
system is strongly self-bound, no discernable onset $\mu_o > 0$

Fit small-μ data:

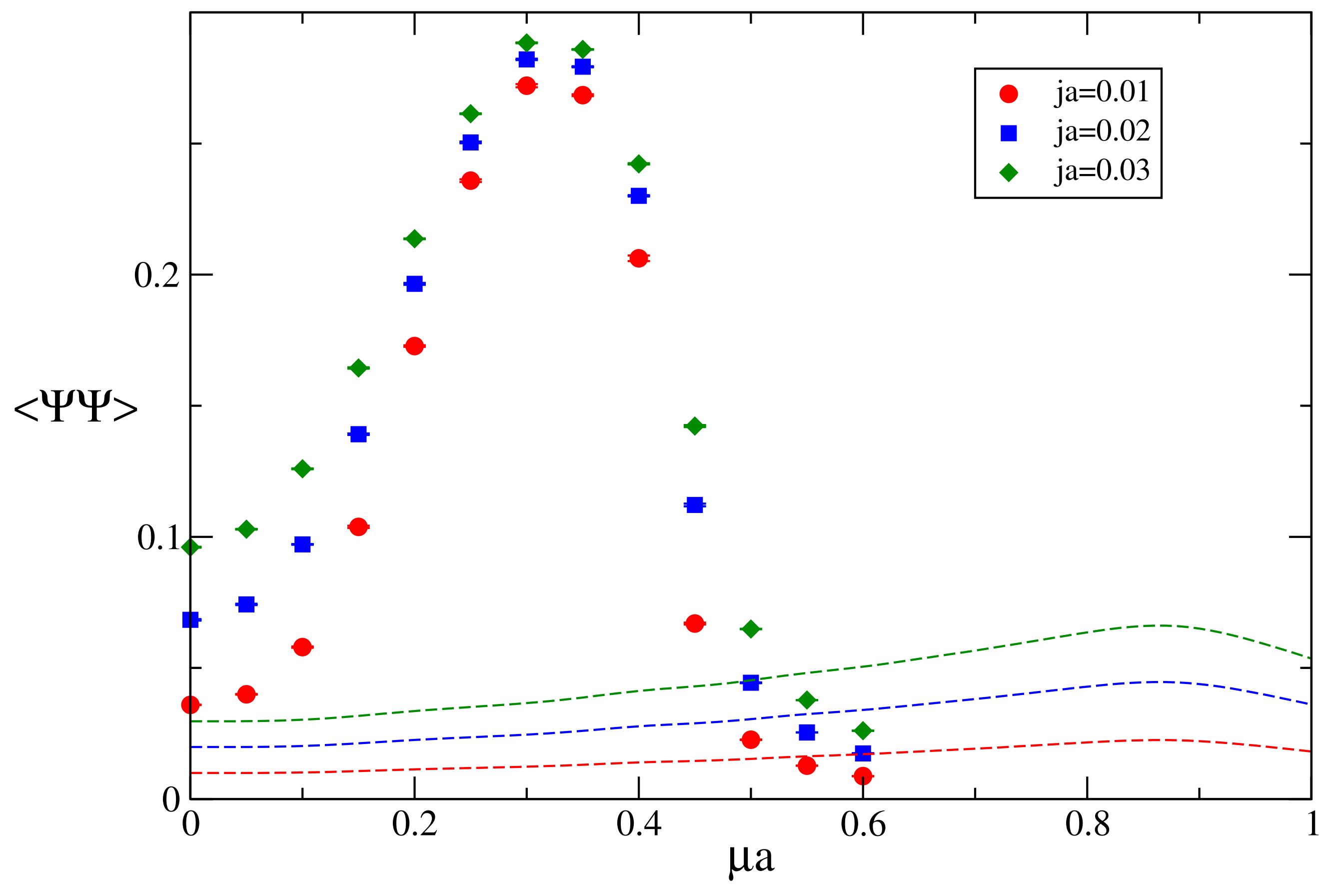
$n_c(j=0) \propto \mu^{3.32(1)}$

Cf. free-field

$n_c \propto \mu^d \propto \mu^2$



Exciton Condensate



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

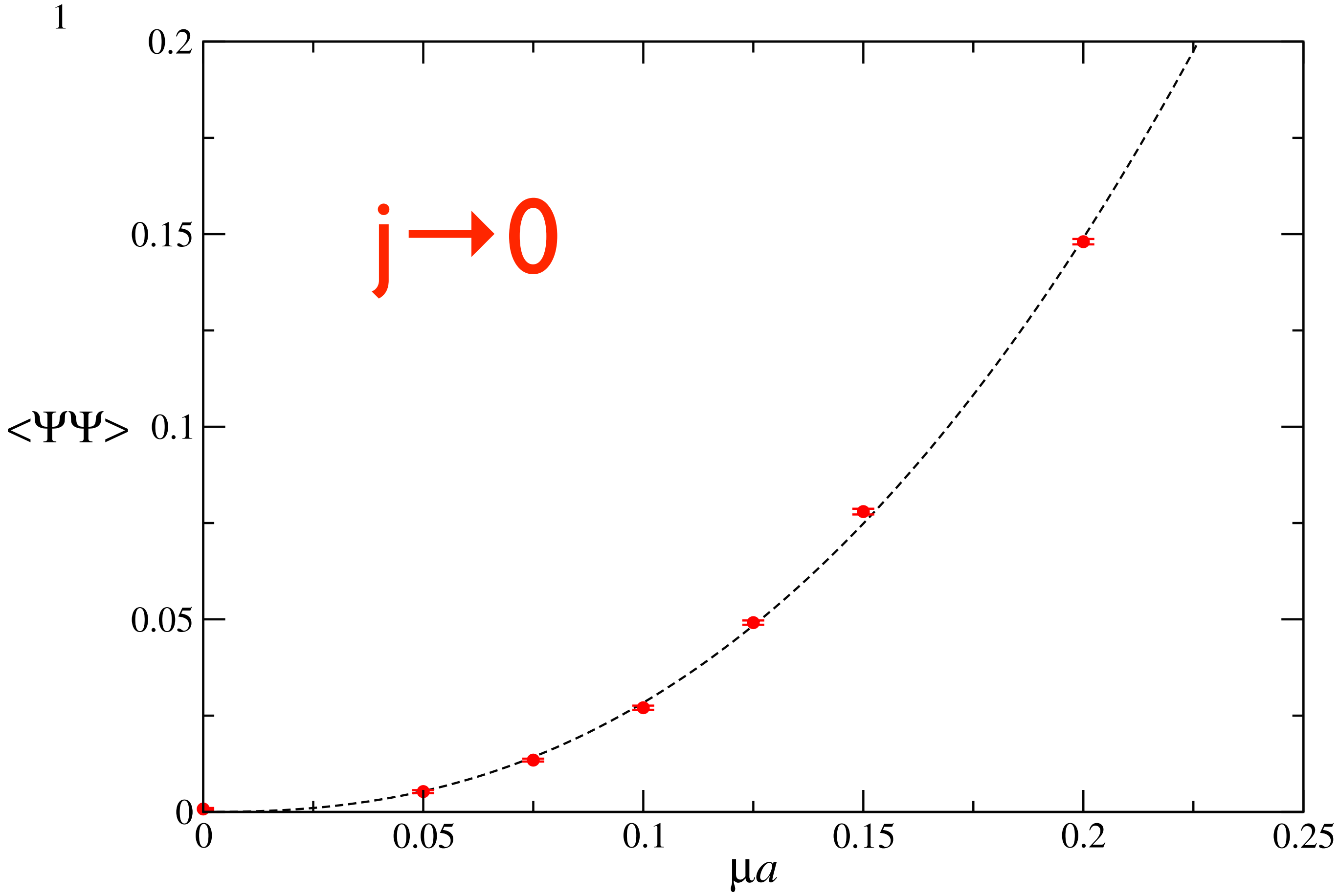
Exciton condensation, with no discernable onset $\mu_o > 0$

Fit small-μ data:

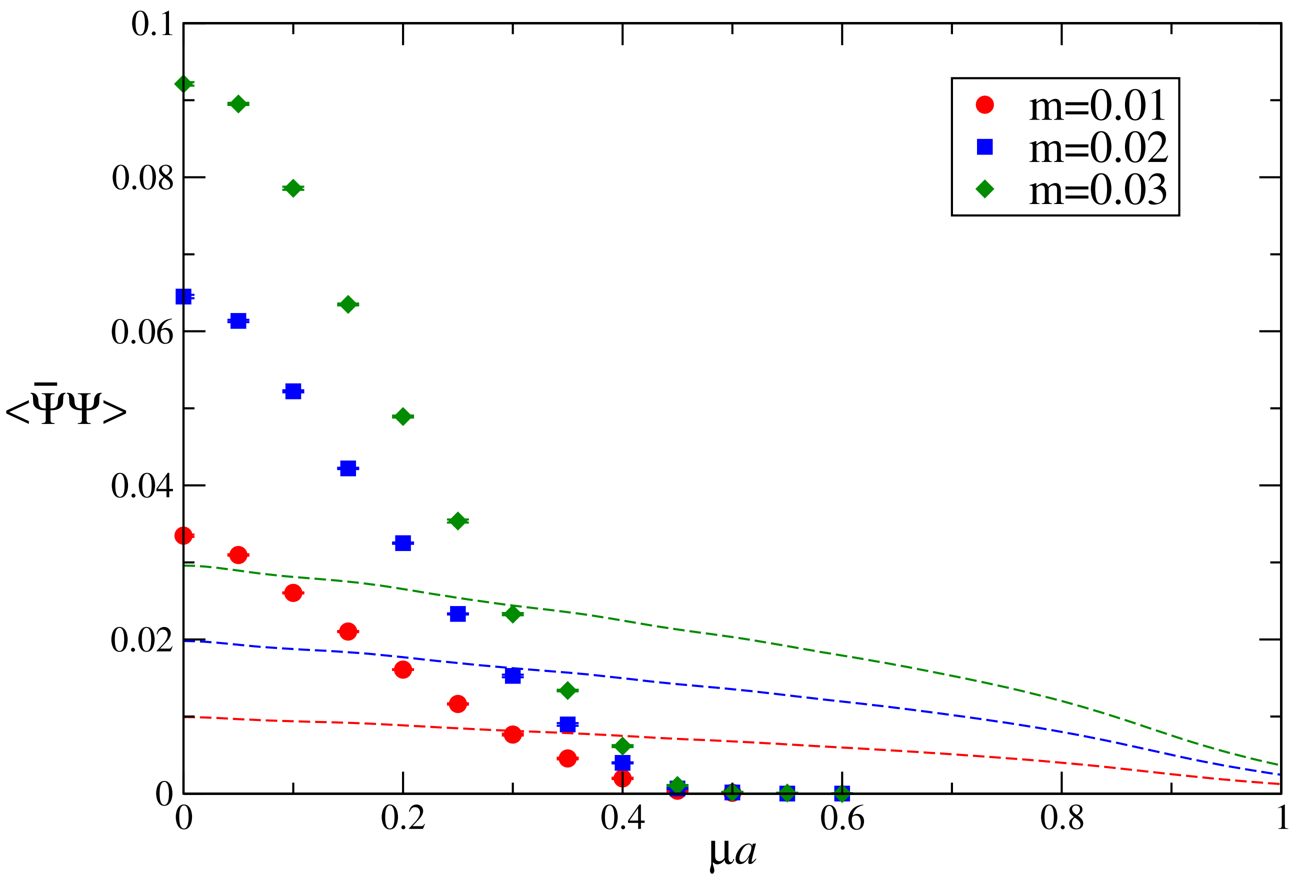
$$\langle \Psi\Psi(j=0) \rangle \propto \mu^{2.39(2)}$$

Cf. weak BCS pairing

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



Chiral Condensate



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

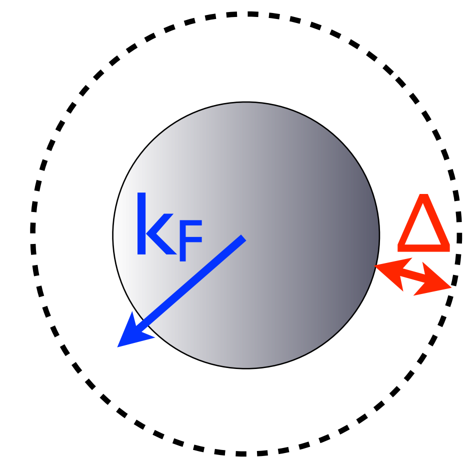
Interlayer pairing suppressed as E_F grows

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

ie. particle-hole pairing is promoted by the large Fermi surface induced by $\mu\neq 0$

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 $\Delta>0$

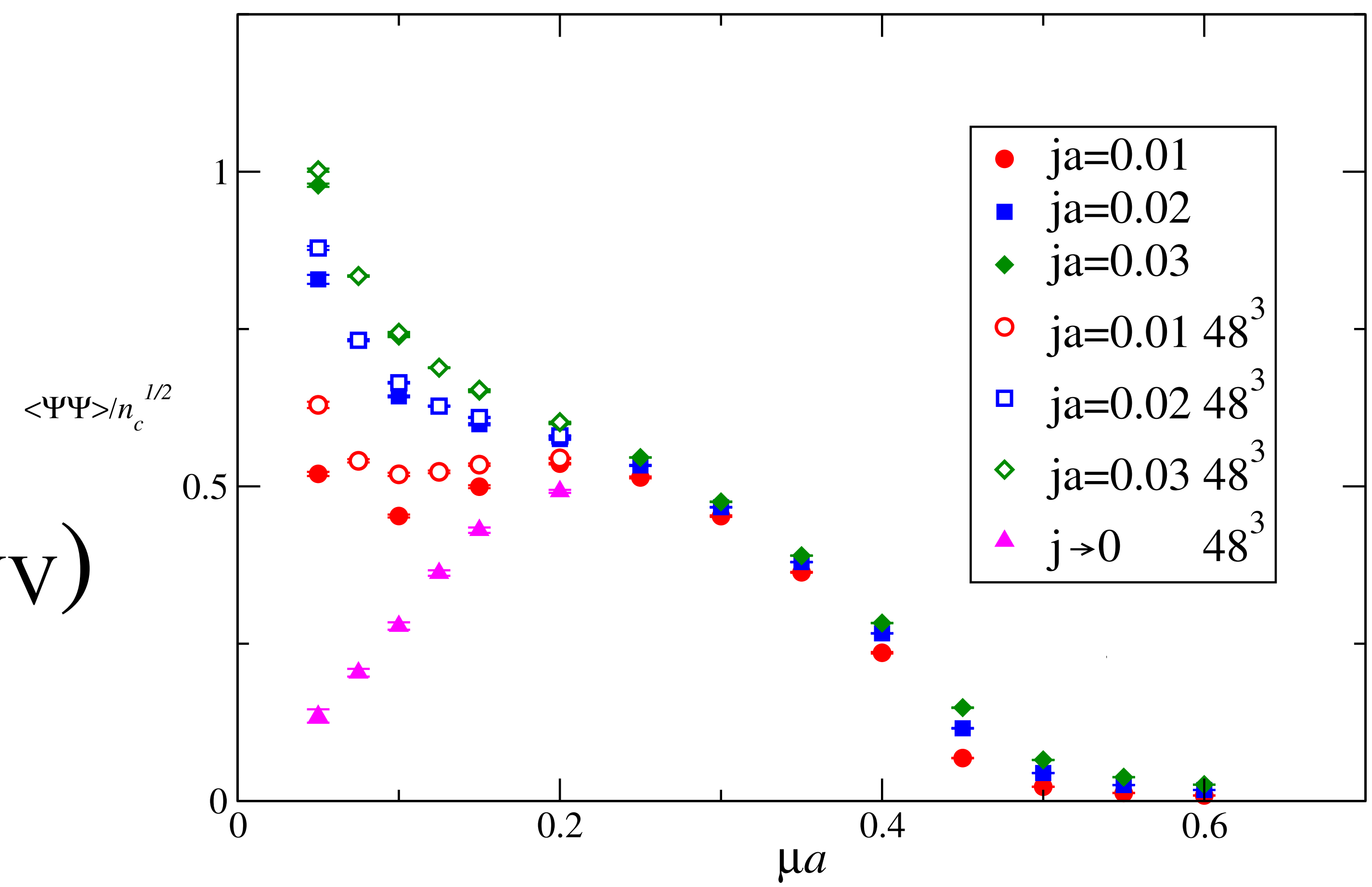


expect $$\langle\Psi\Psi\rangle \propto \Delta k_F^{d-1} \propto \Delta n_c^{\frac{d-1}{d}}$$

where last step follows from Luttinger's theorem

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

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



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

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

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

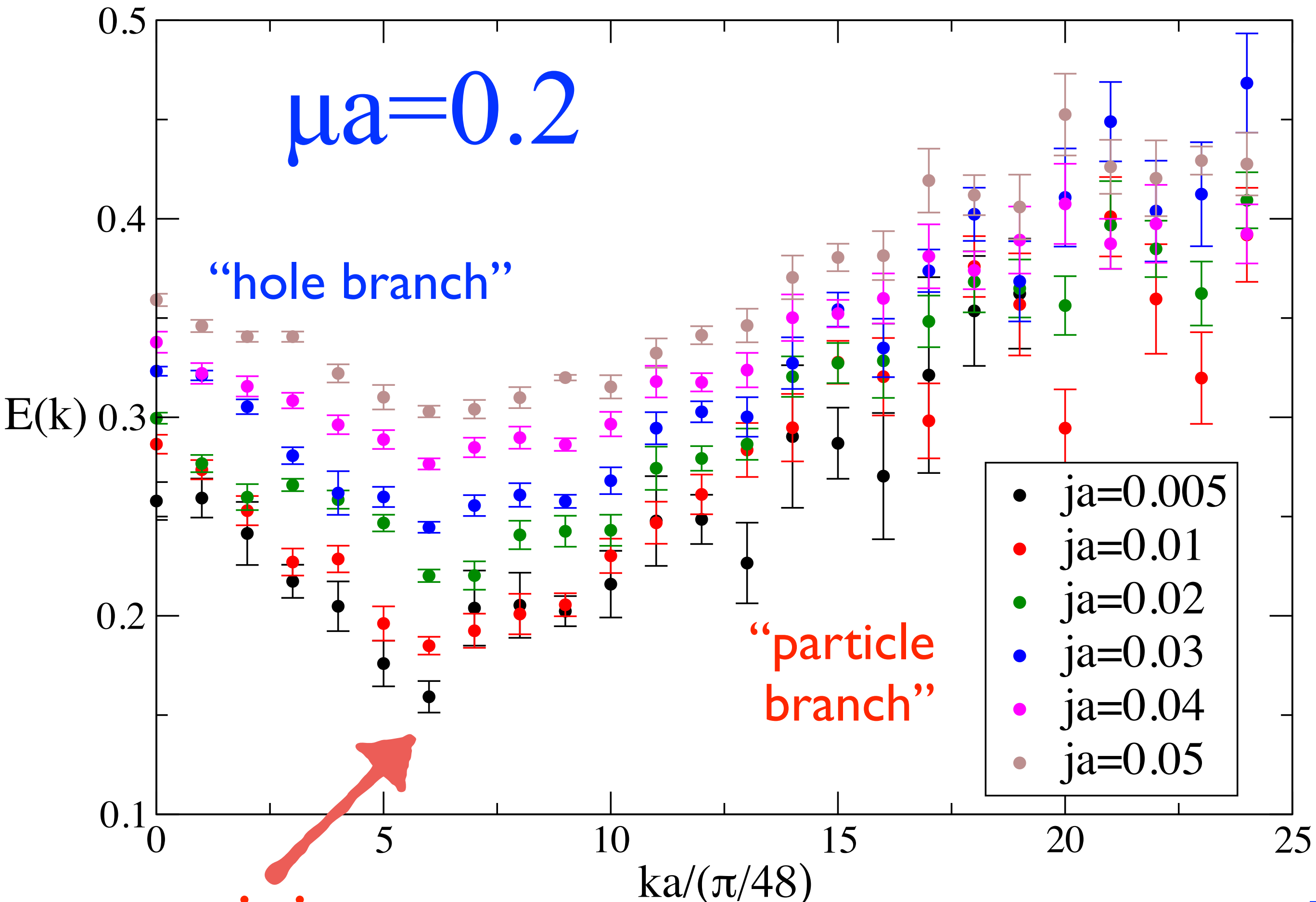
(S. Cotter et al PRD87 (2013) 034507)

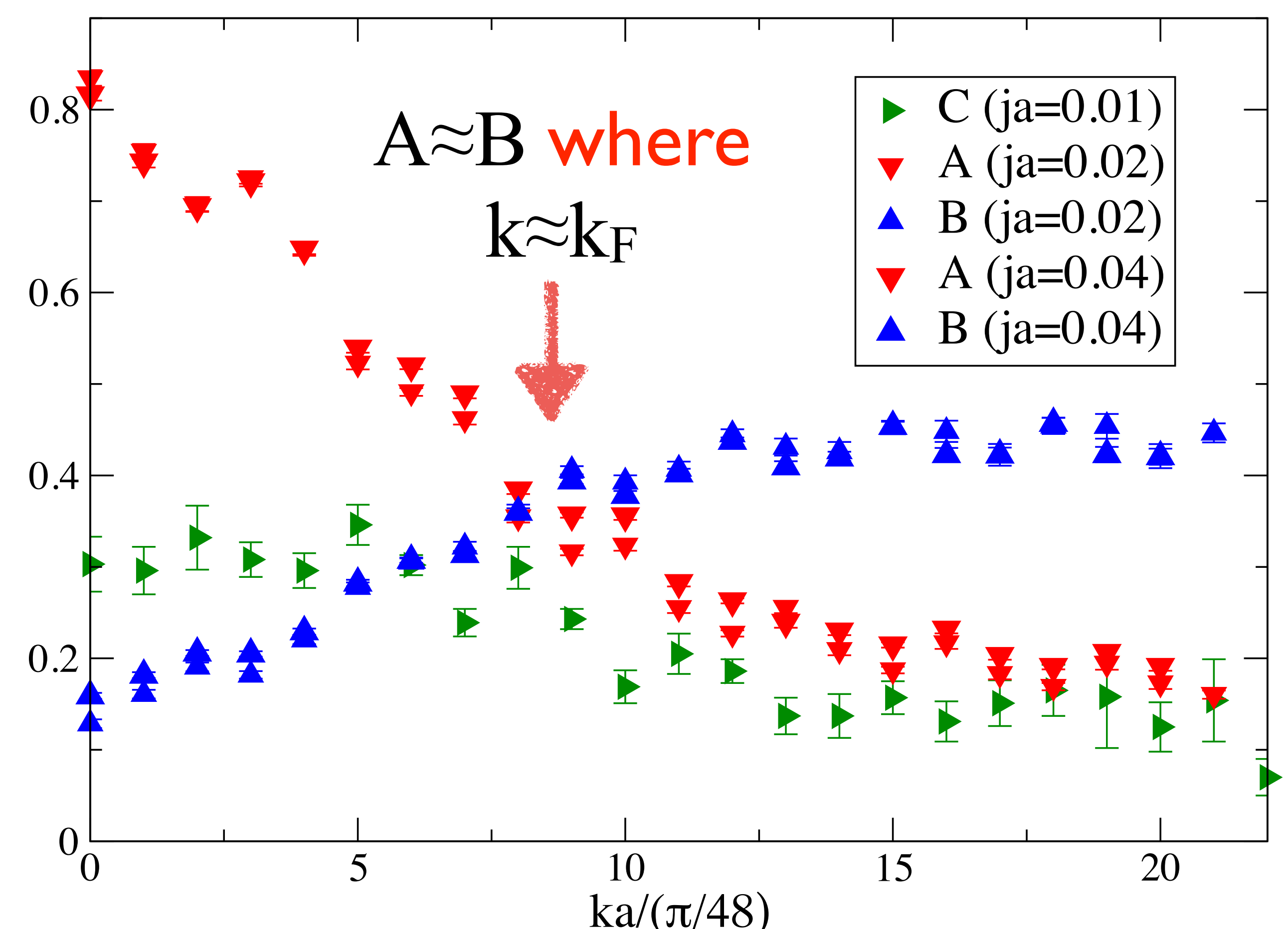
in both cases (roughly) μ-independent

Quasiparticle Dispersion for $\mu a = 0.2$ (preliminary)

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

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





minimum at

$k_F a \approx \pi/8 \approx 0.4 > \mu a$

$\Rightarrow \quad n_c a^2 = k_F^2/2\pi \approx 0.063$

Cf. directly measured value 0.09

Fit functions:

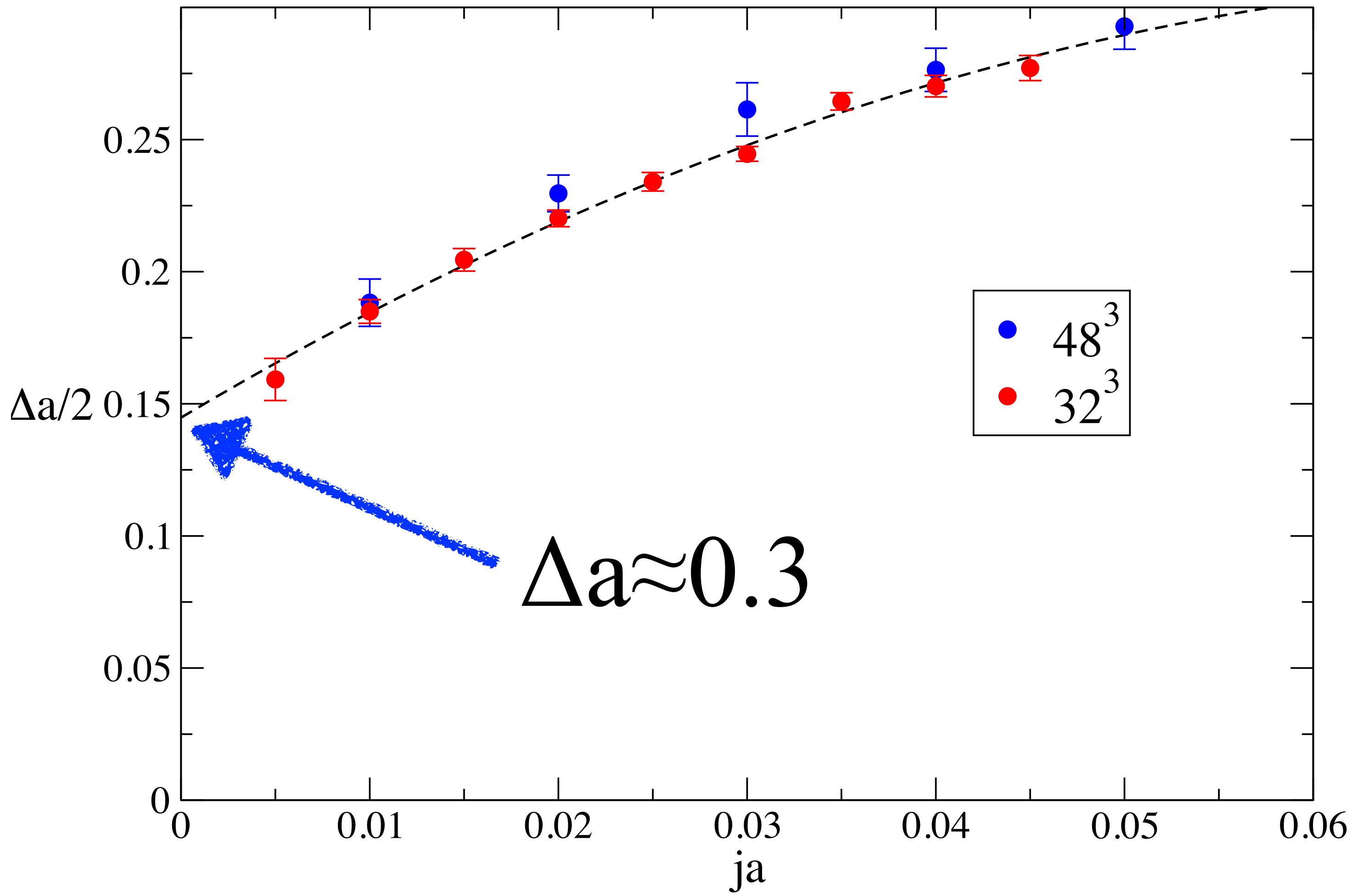
"Normal" $\mathrm{Re}(C_N(\vec{k}, t)) = Ae^{-Et} + Be^{-E(L_t - t)}$,

"Anomalous" $\mathrm{Im}(C_A(\vec{k}, t)) = C(e^{-Et} - e^{-E(L_t - t)})$,

Amplitudes show crossover from holes to particles

Note $\mu = E_F < k_F$ consistent with a self-bound system

And the gap?....



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)

Summary

- A new, interesting member of the small class of models permitting MC study with $\mu\neq0$
- Behaviour very different from previous (QC_2D, NJL) $\Leftrightarrow$ residual interactions at Fermi surface are **strong**

  Densities and condensates scale anomalously with μ
  Quasiparticle dispersion $E(k)$ exposes Fermi surface

- Strongly-interacting QCP $\Leftrightarrow$ $\Delta=\Delta(\mu)$, $\Delta/\mu=O(1)$

- Future: Examine helicity modulus Υ to compare with
  $$\Upsilon_{GMOR} = 4j\langle\Psi\Psi\rangle/M_{Goldstone}$$
- Move to overlap fermions to better reproduce global symmetry pattern?
  $$U(8) \xrightarrow{\mu\neq0} U(4)\otimes U(4) \xrightarrow{j\neq0} U(4)$$