Is the semimetal-insulator transition in graphene a conformal transition? [ArXiv:1812.06435]

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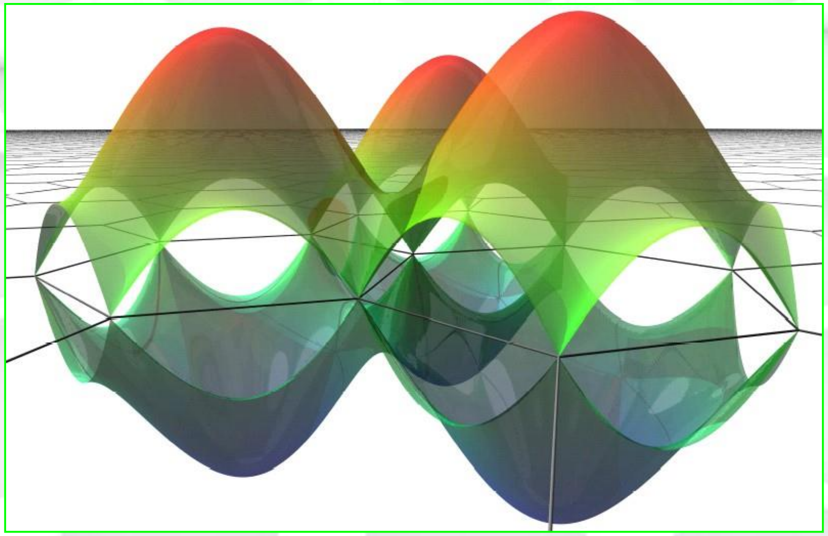
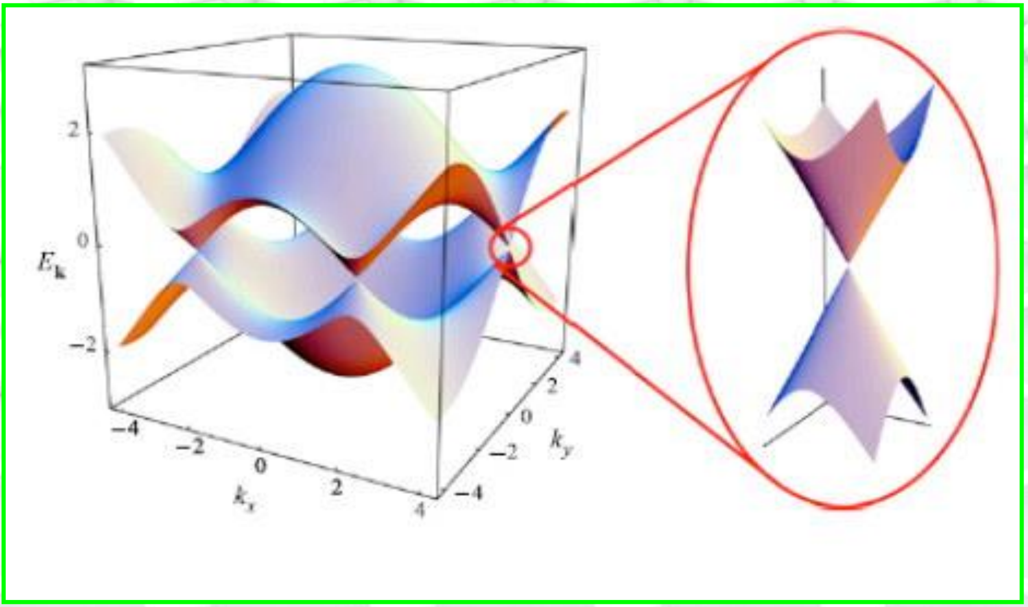
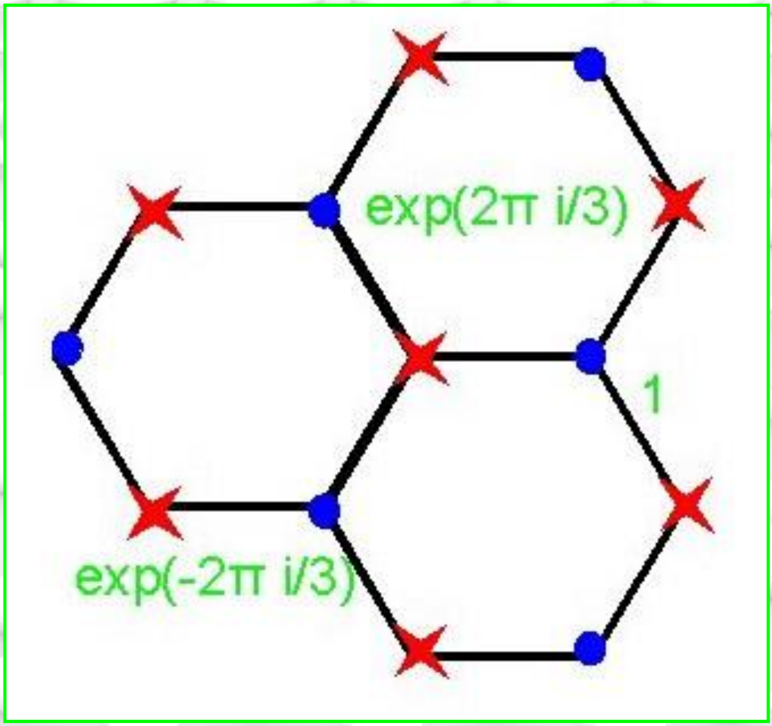


Spectrum of quasiparticles in graphene





Close to the «Dirac points»:

$$E = \sqrt{v_F^2 k^2 + m^2}$$

"Staggered potential" m = Dirac mass

Lattice QFT of Graphene

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

$$\hat{\psi}_{\uparrow,X} = \hat{a}_{\uparrow,X}, \quad \hat{\psi}_{\downarrow,X} = \pm \hat{a}^{\dagger}_{\downarrow,X},$$

Redefined creation/annihilation operators

$$\hat{q}_X = \hat{\psi}^{\dagger}_{\uparrow,X} \hat{\psi}_{\uparrow,X} - \hat{\psi}^{\dagger}_{\downarrow,X} \hat{\psi}_{\downarrow,X}.$$

Charge operator

$$\hat{\psi}_{\uparrow,X} |0\rangle = 0, \ \hat{\psi}_{\downarrow,X} |0\rangle = 0$$

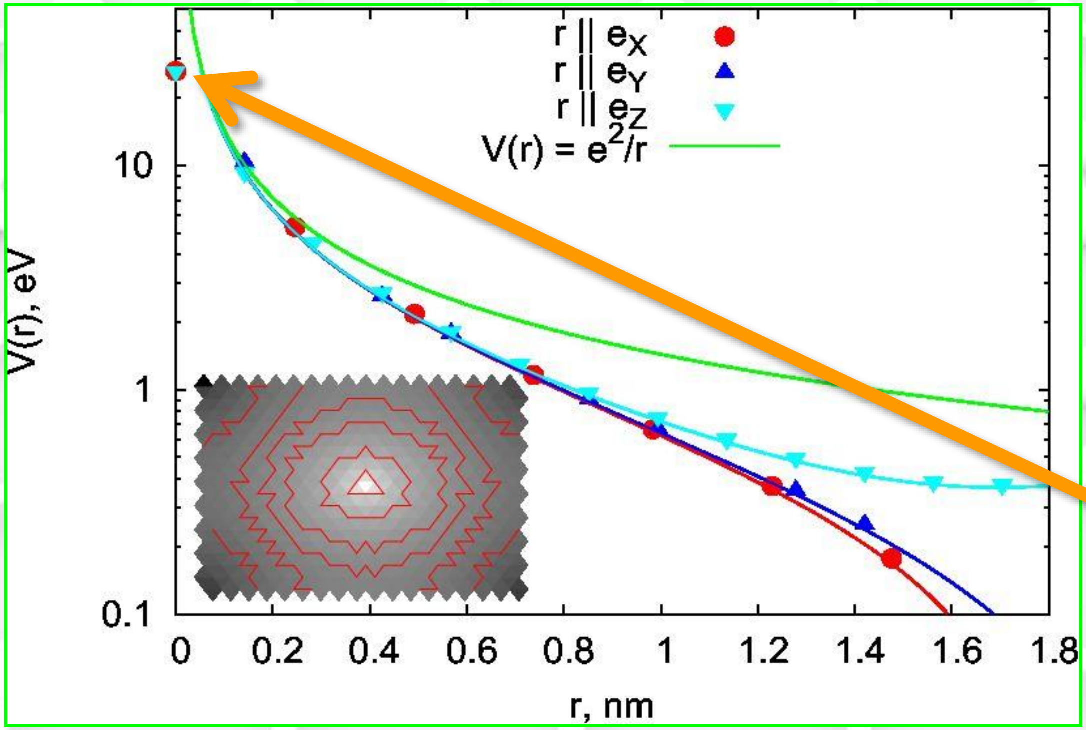
Standard QFT vacuum

Introducing interactions

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

$$\hat{H}_I = \frac{1}{2} \sum_{x,y} \hat{q}_x \, V_{x,y} \, \hat{q}_y$$

Charge operators



On-site potential, additional parameter fixed by discretization

First studies – Coulomb potential on square & hexagonal lattices [Lahde&Drut'0807.0834,PB' 1206.0619]

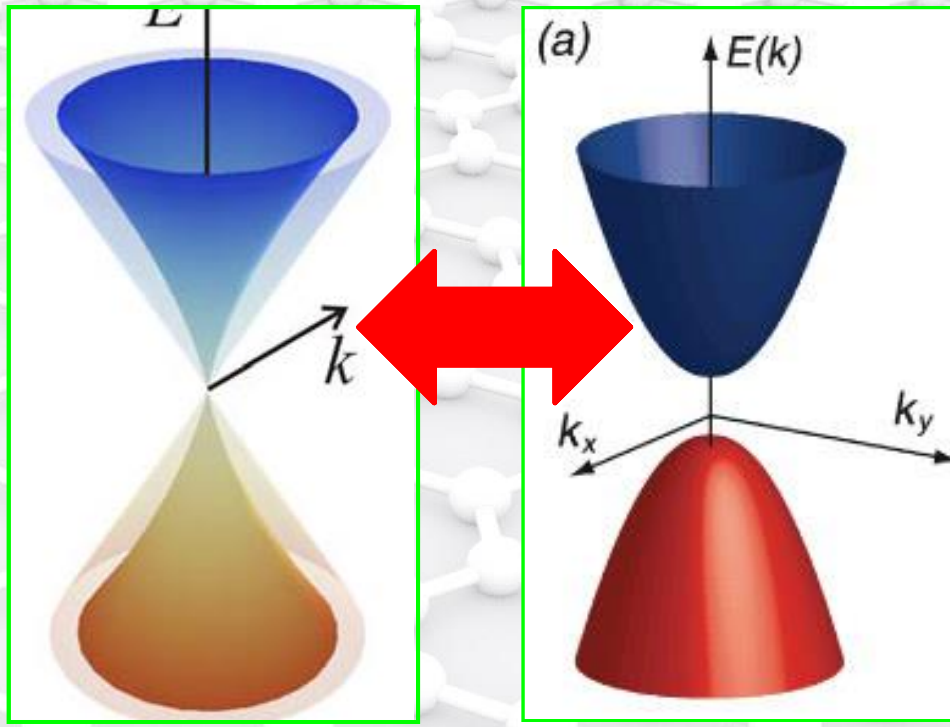
Semimetal-insulator phase transition

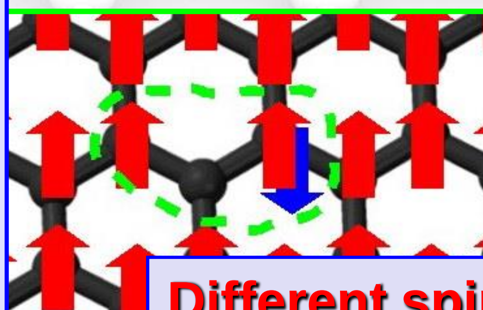
Good gap in graphene + High carrier mobility = Graphene-based semiconductors

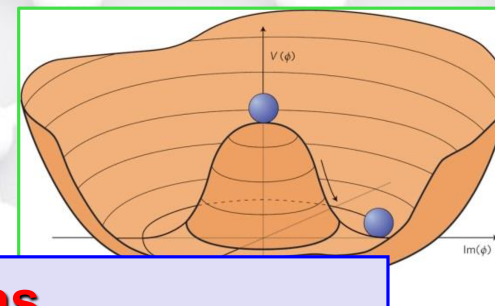
Interesting for theorists: Gap due to interactions?

$$\alpha_{eff} = \alpha_{QED}/v_F \approx \approx \frac{1}{137}/\frac{1}{300} \approx 2.2$$

- **Antiferromagnetic state as the main symmetry breaking channel**
- **AFM order: most natural option for on-site interactions [e.g. Herbut,cond-mat/0606195]**







Different spins of A and B sublattices

$$\Delta_S = S_A - S_B$$

Suspended graphene is a semimetal

Experiments by Manchester group [Elias et al. 2011,2012]:

<u>Gap < 1 meV</u>

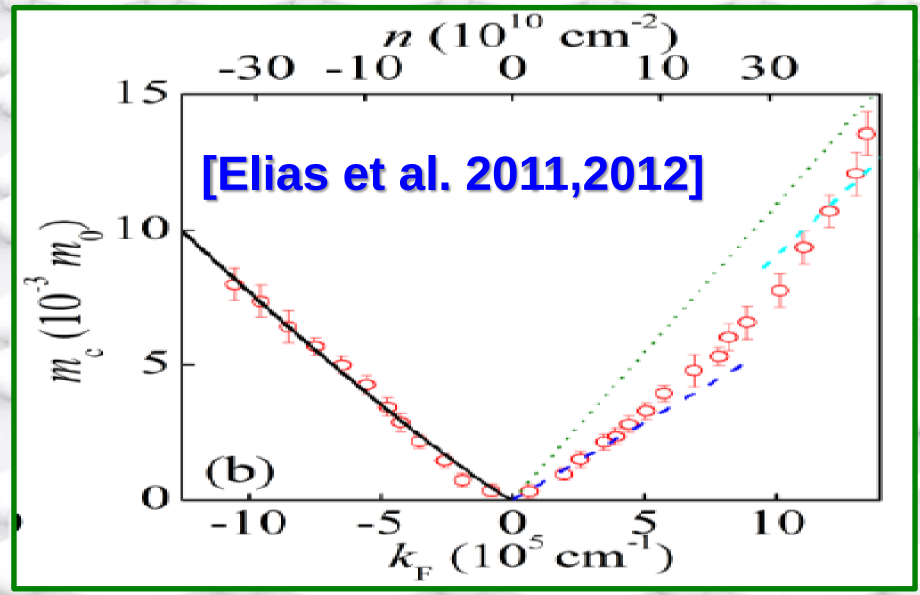
HMC simulations (ITEP, Regensburg and Giessen) [1304.3660,1403.3620]

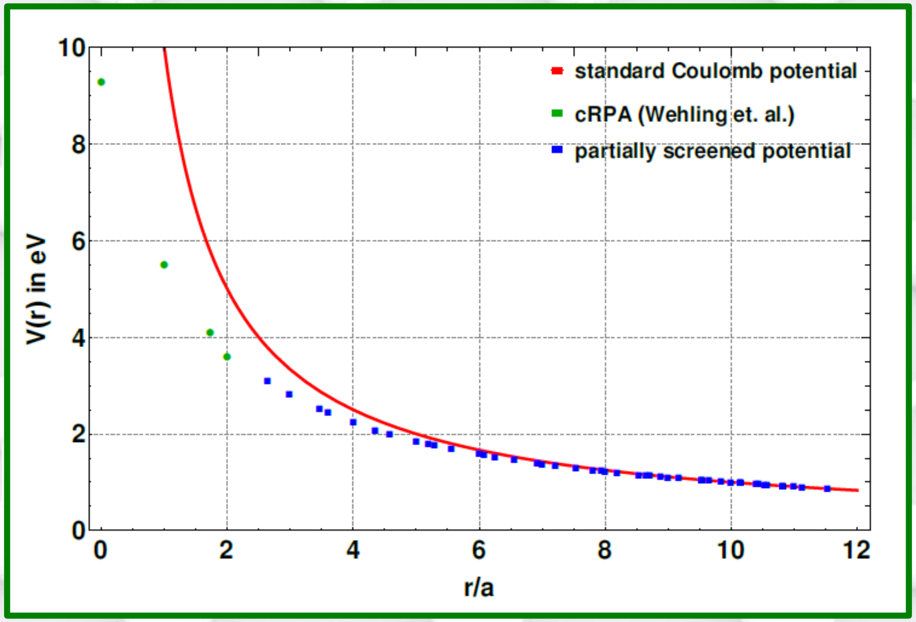
<u>Unphysical $\alpha_c \sim 3 > \alpha_{eff} = 2.2$</u>

Schwinger-Dyson equations [M. Bischoff, 1308.6199]

<u>Unphysical $\alpha_c \sim 5 > \alpha_{eff} = 2.2$</u>

In the meanwhile: <u>Graphene Gets a Good Gap on SiC</u> [M. Nevius et al. 1505.00435] – interactions are not so important…





Phase diagram with nonlocal interactions

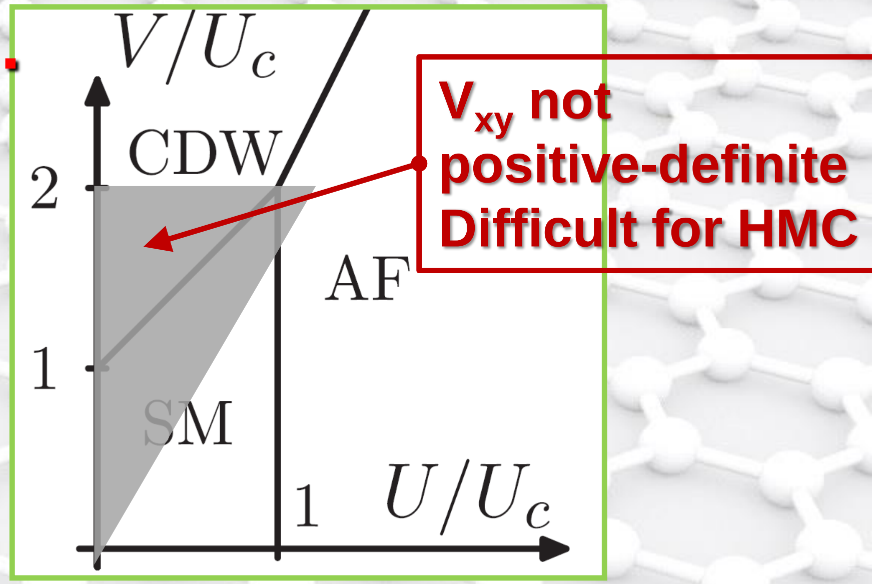
Only AFM order was tested…

Tunable interactions and spontaneous symmetry breaking can be still realized:

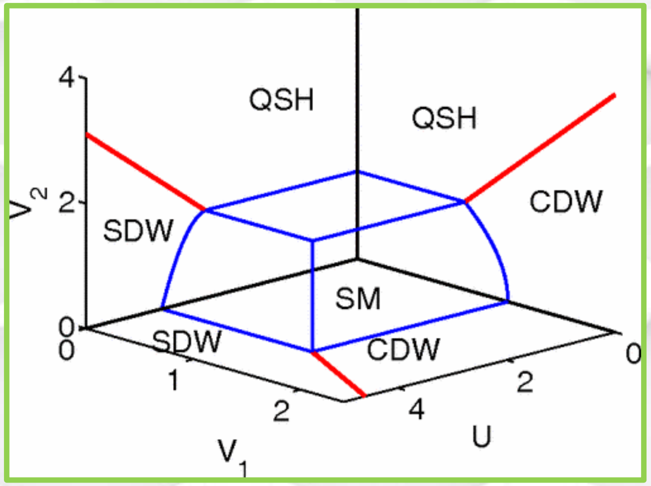
- In artificial graphene
- In strained graphene
- In graphene “superlattices” made with adatoms

Novel phases from tunable interactions:

- Charge density wave
- Quantum Spin Hall state (TI)
- Spin liquid
- Kekule distortion…



[I. Herbut, cond-mat/0606195]



[Raghu, Qi, Honerkamp, Zhang 0710.0030]

Revisiting the phase structure of graphene

- Can it be that we are missing some non-AFM ordered phase, and do not see it because we only look at AFM order parameter?
- If our lattice setup is reproducing the phases of graphene, what are the nontrivial phases that are closest to the "physical point"? [E.g. think of QCD "Columbia plot"]
- Closeness to one or the other phase boundary – useful information for describing non-perturbative features
  - Fluctuations of order parameter
  - Convergence radius of perturbative expansion
  - Most likely channel of symmetry breaking upon small deformations of V_{xy}

Revisiting the phase structure of graphene

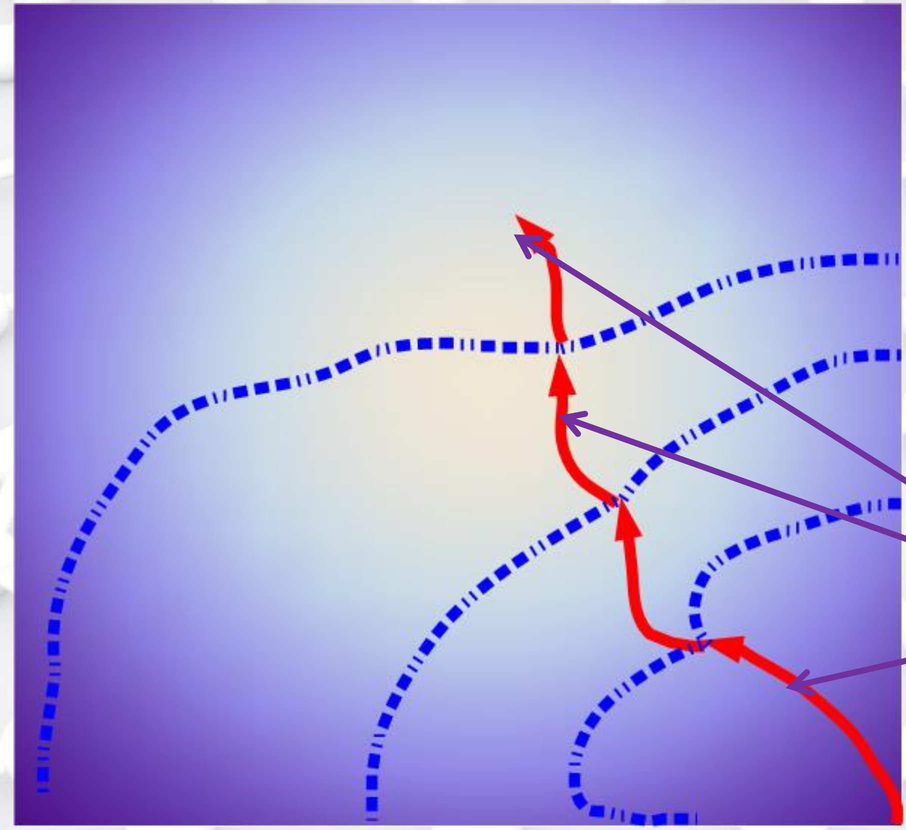
$$\hat{H}_I = \frac{\lambda}{2} \sum_{x,y} \hat{q}_x \, V_{x,y} \, \hat{q}_y$$

- **What is the first phase that we encounter when increasing *λ* ???**
- **Can it be that we are in the CDW phase already at *λ=1* ?**
- **We want to be as unbiased as possible**
- **Avoid any source terms that favor one symmetry breaking channel over another**

Simulations without source terms

Hubbard-Stratonovich + Suzuki-Trotter for partition function

$$\mathcal{Z} = \int \mathcal{D}\phi_x(\tau)\, \det\left(M^{\psi}\right)\, \det\left(M^{\chi}\right)\, \exp\left(-\frac{1}{2}\int_0^{T^{-1}} d\tau \sum_{x,y} \phi_x(\tau)\, V_{xy}^{-1} \phi_y(\tau)\right)$$



- **HMC with real-valued Hubbard field can get stuck at zeros of determinant**

Molecular Dynamics Trajectories

Simulations without source terms: Complex Hubbard-Stratonovich fields

Coupling to both charge & spin

$$\frac{V_{xx}}{2}\hat{q}_x^2 = \eta\frac{V_{xx}}{2}\hat{q}_x^2 - (1-\eta)\frac{V_{xx}}{2}\hat{s}_x^2 + (1-\eta)V_{xx}\,\hat{s}_x$$

$$\hat{q}_x = \hat{\psi}^\dagger_{\uparrow,x}\hat{\psi}_{\uparrow,x} - \hat{\psi}^\dagger_{\downarrow,x}\hat{\psi}_{\downarrow,x},$$

$$\hat{s}_x = \hat{\psi}^\dagger_{\uparrow,x}\hat{\psi}_{\uparrow,x} + \hat{\psi}^\dagger_{\downarrow,x}\hat{\psi}_{\downarrow,x},$$

$$e^{-\frac{\delta\tau}{2}\sum_{x,y} V_{xy}\hat{q}_x\hat{q}_y} \cong \int D\phi\, e^{-\frac{1}{2\delta\tau}\sum_{x,y}\phi_x V^{-1}_{xy}\phi_y}\, e^{i\sum_x \phi_x\,\hat{q}_x}.$$

$$e^{\frac{\delta\tau}{2}(1-\eta)\sum_x V_{xx}\hat{s}_x^2} \cong \int D\chi\, e^{-\frac{1}{2\delta\tau}\sum_x \frac{\chi_x^2}{(1-\eta)V_{xx}}}\, e^{\sum_x \chi_x\hat{s}_x}.$$

Simulations without source terms: Complex Hubbard-Stratonovich fields

$$\mathcal{Z} = \int D\phi\, D\chi\, \det M(\phi + i\chi)\, \det M(\phi - i\chi) e^{-S_\eta(\phi,\chi)},$$

We can go over determinant zeros

$$S_\eta(\phi,\chi) = \frac{1}{2\delta\tau} \sum_{x,y,t} \phi_{x,t} \widetilde{V}^{-1}_{xy} \phi_{y,t} + \\ + \sum_{x,t} \frac{\left(\chi_{x,t} - (1-\eta)\,\delta\tau V_{xx}\right)^2}{2\,(1-\eta)\,\delta\tau\, V_{xx}}.$$

Reducing Trotter discretization effects

$$\det\left(M\left(\phi\right)\right) = \det\left(1 + e^{-\delta\tau\, h} e^{i\phi_1} e^{-\delta\tau\, h} e^{i\phi_2} \ldots\right)$$

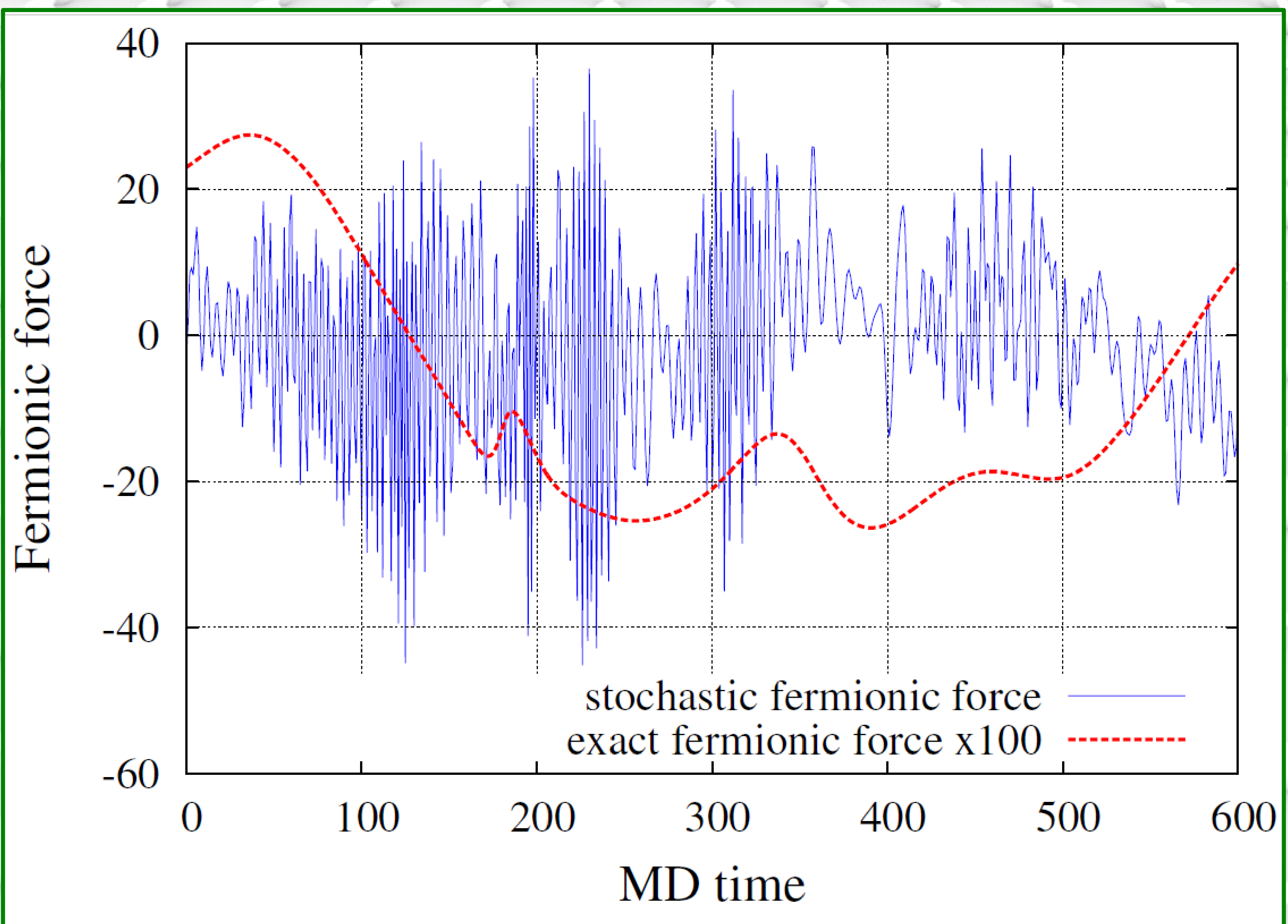
Instead of stochastic estimators, we calculate fermionic forces exactly:

$$\frac{\partial \ln \det M}{\partial \phi_{x,t}} = \mathrm{tr}\left(M^{-1} \frac{\partial M}{\partial \phi_{x,t}} \right)$$

(Re-using some tricks from the BSS-QMC algorithm)

We can increase integrator stepsize by a factor > 50 as compared to HMC !!!

Stochastic force vs exact force



Detecting spin- and charge-ordered phases (SDW and CDW)

- We have no sources, hence no condensates in finite volume
- All observables need to be related to fluctuations of order parameters

$$\langle \hat{q}^2 \rangle = \left\langle \frac{1}{L^4} \left(\sum_{x \in A} \hat{q}_x \right)^2 \right\rangle + \left\langle \frac{1}{L^4} \left(\sum_{x \in B} \hat{q}_x \right)^2 \right\rangle$$

$$\langle \hat{s}^2 \rangle = \left\langle \frac{1}{L^4} \left(\sum_{x \in A} \hat{s}_x \right)^2 \right\rangle + \left\langle \frac{1}{L^4} \left(\sum_{x \in B} \hat{s}_x \right)^2 \right\rangle ,$$

Simulation parameters

- Lattice sizes *6 x 6, 12 x 12, 18 x 18, 24 x 24*, rectangular compactification a-la toric nanotube
- Tips of the Dirac cones covered by discrete lattice momenta
- $N_t = 128$ Trotter steps
- Trotter step size $\kappa\, \delta\tau = 0.168$
- Complexification parameter $\eta = 0.9$
- Several hundreds of configurations per dataset
- Binning to calculate statistical errors

Antiferromagnetic state vs charge-density wave

Leading-order fits for size-dependent order parameters

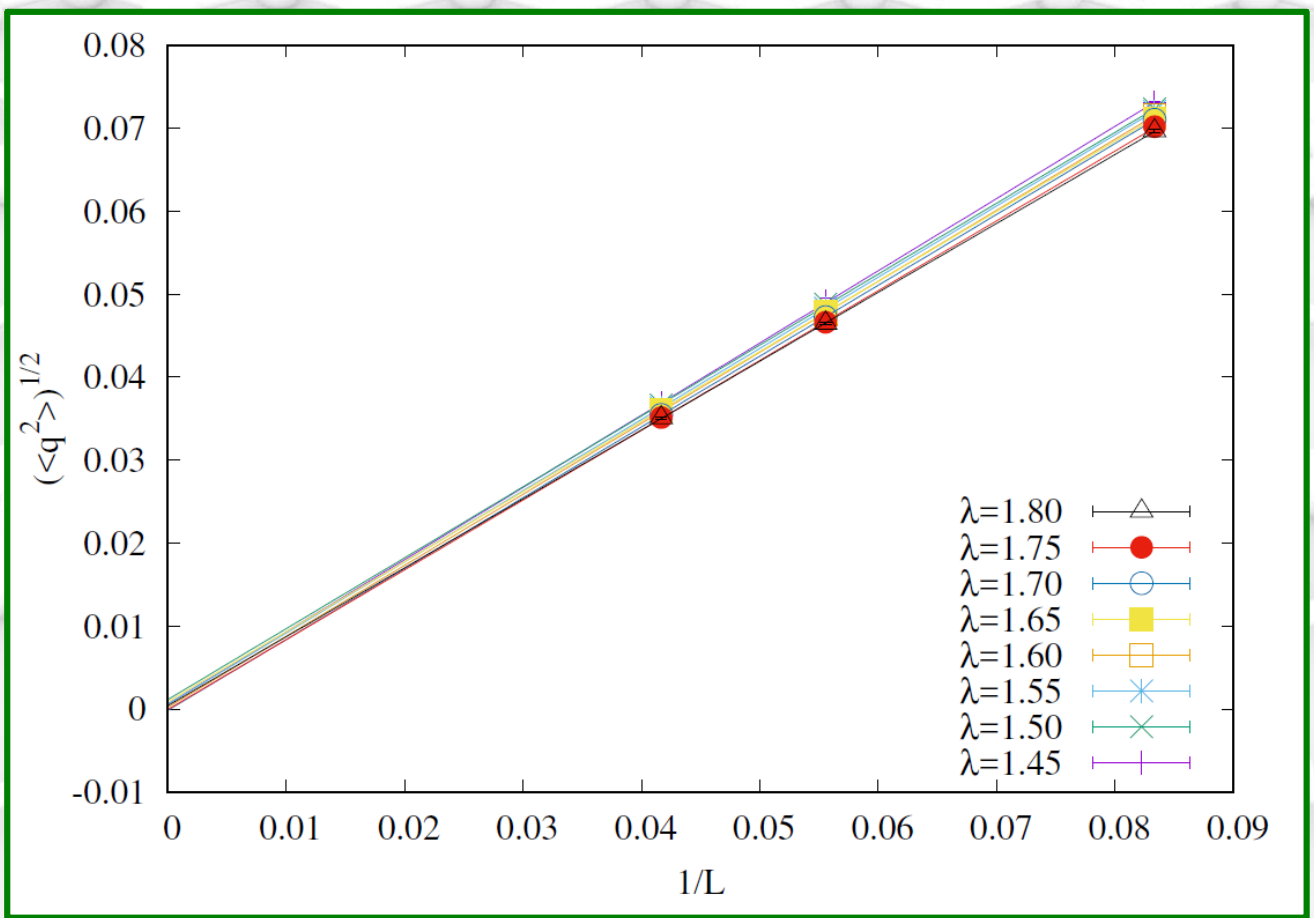
$$f\left(\lambda, 1/L_s\right) = \begin{cases} \sqrt{\langle\, \hat{s}^2 \,\rangle} \\ \sqrt{\langle\, \hat{q}^2 \,\rangle} \end{cases}$$

$$f\left(\lambda, 1/L_s\right) = f_0\left(\lambda\right) + f_1\left(\lambda\right)/L_s$$

Expected to work away from the phase transition

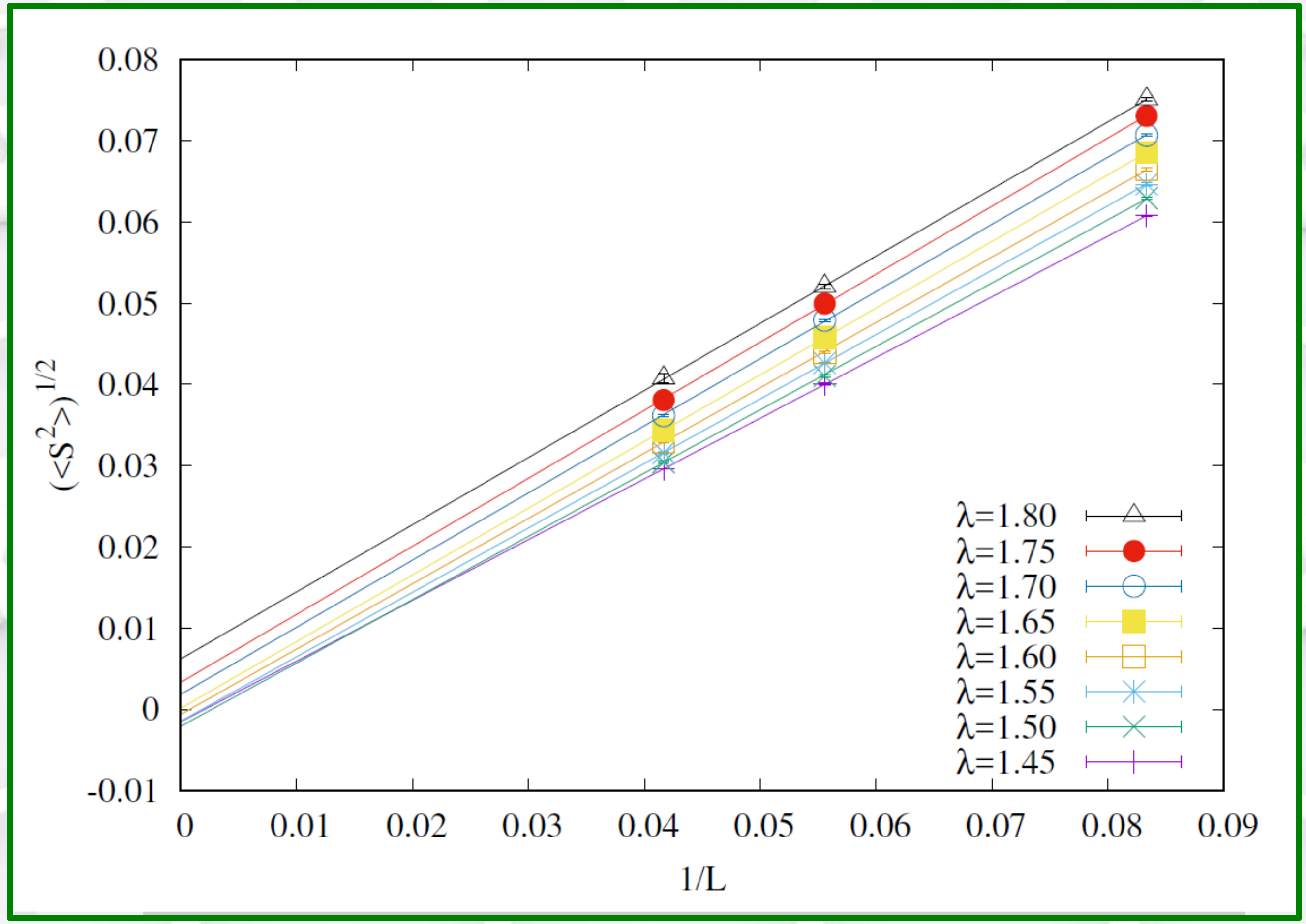
Antiferromagnetic state vs charge-density wave

Charge density wave fluctuations are thermodynamically irrelevant



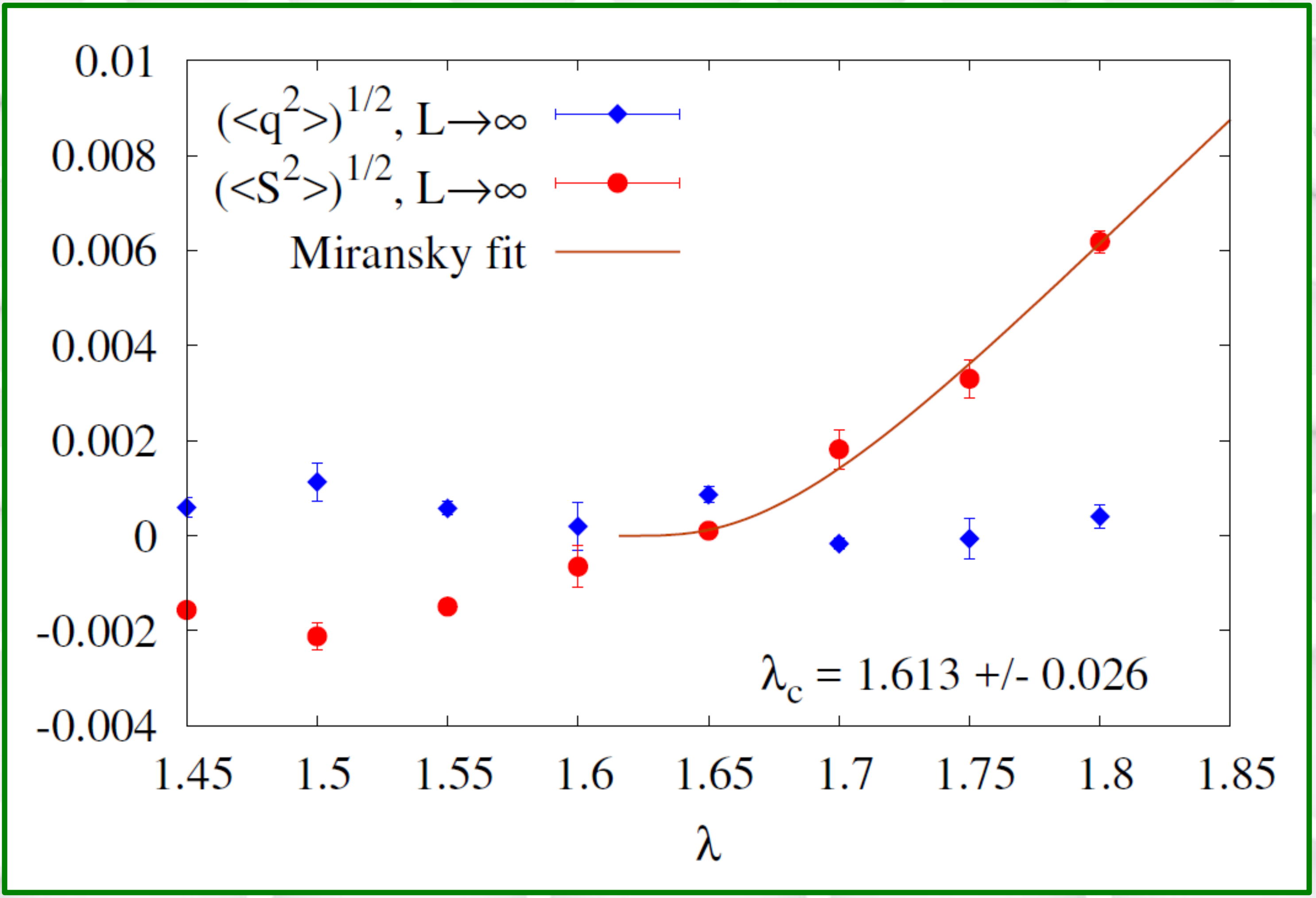
Antiferromagnetic state vs charge-density wave

Nonzero extrapolation at L->∞ for spin-density wave parameter



Antiferromagnetic state vs charge-density wave

Nonzero extrapolation for $\lambda_c \geq 1.61 \pm 0.02$



Critical scaling

Close to a second-order phase transition:

$$\langle \hat{s}^2 \rangle = L^{-\frac{2\beta}{\nu}} \phi\left(L^{1/\nu} \left(\lambda - \lambda_c\right) / \lambda_c\right)$$

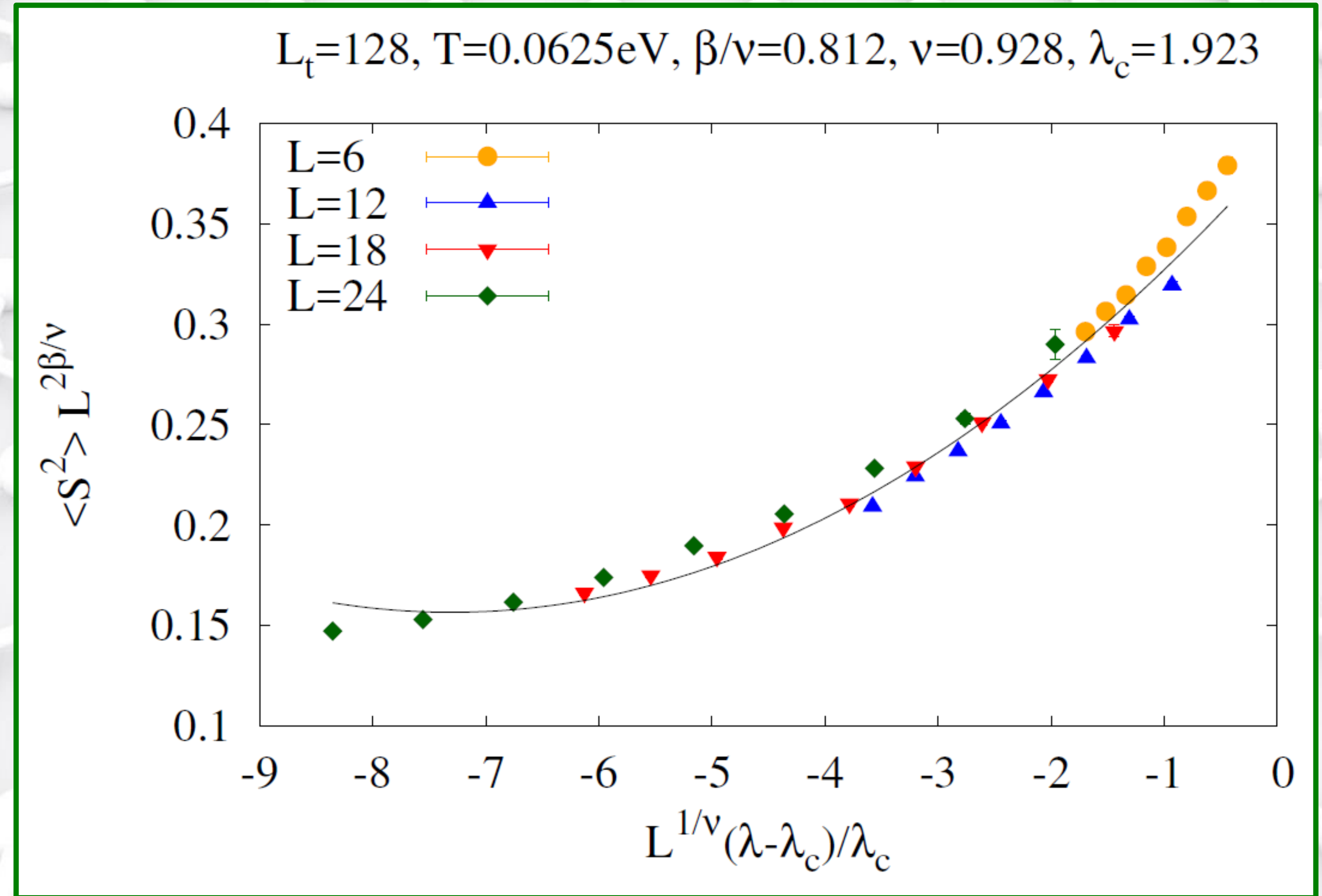
It is most natural to expect the chiral Gross-Neveau universality class

Let's fix *β/ν=0.812, ν=0.928* (our results obtained with BSS on same lattices)

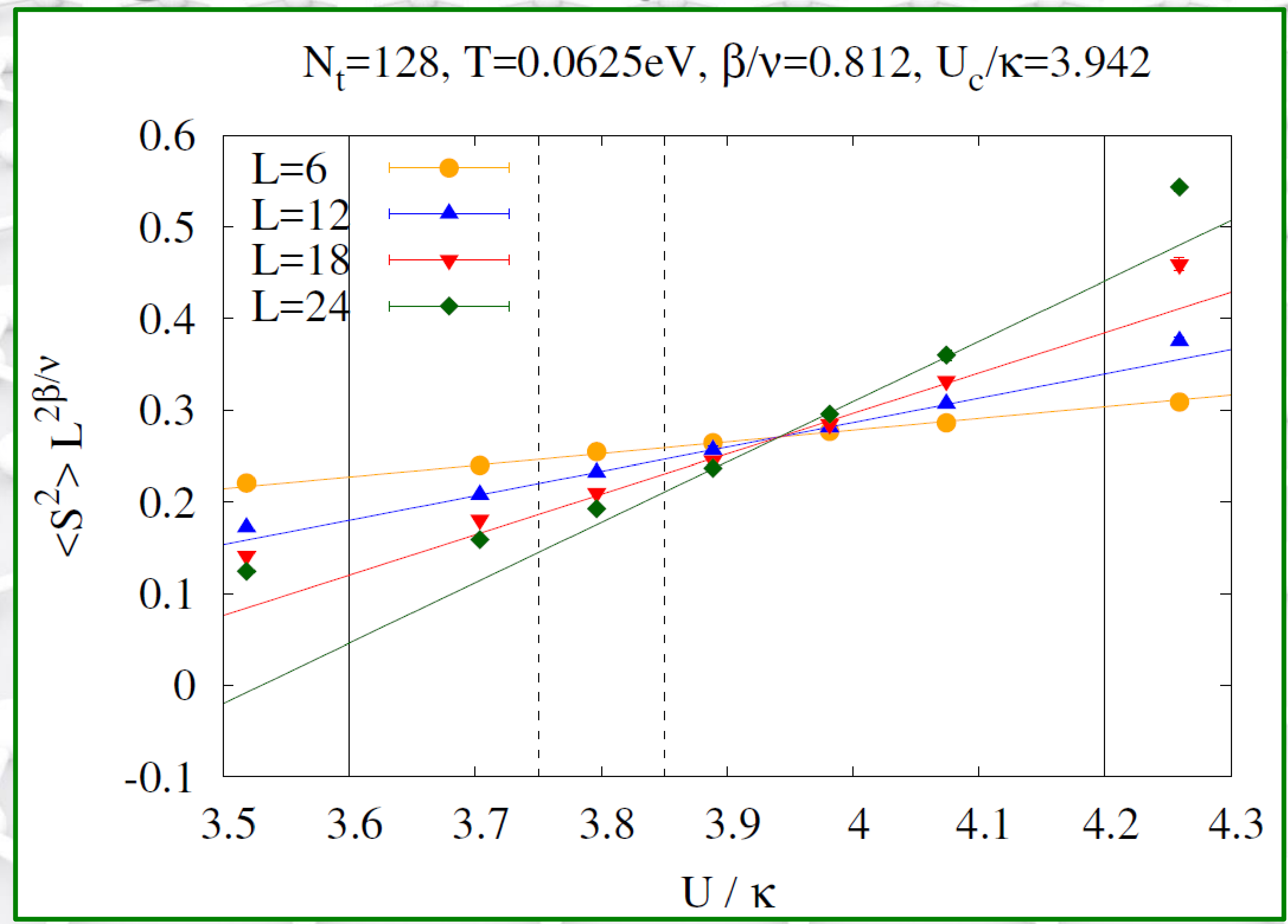
<u>Can we get a nice collapse plot?</u>

Critical scaling

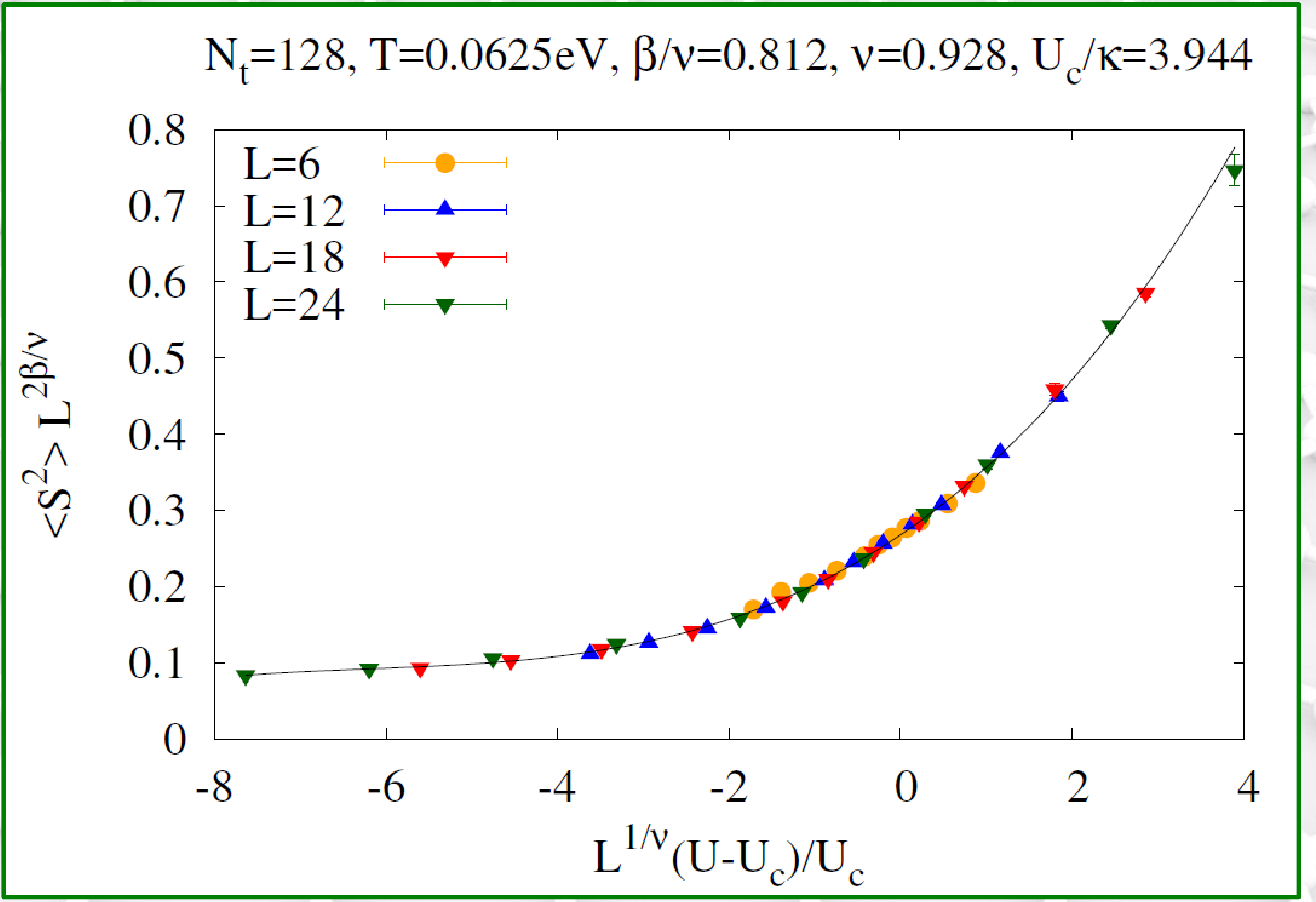
Our best collapse plot for χGN universality (no good intersection plots)



Intersection plot for Hubbard model on hexagonal lattices (same size & action)

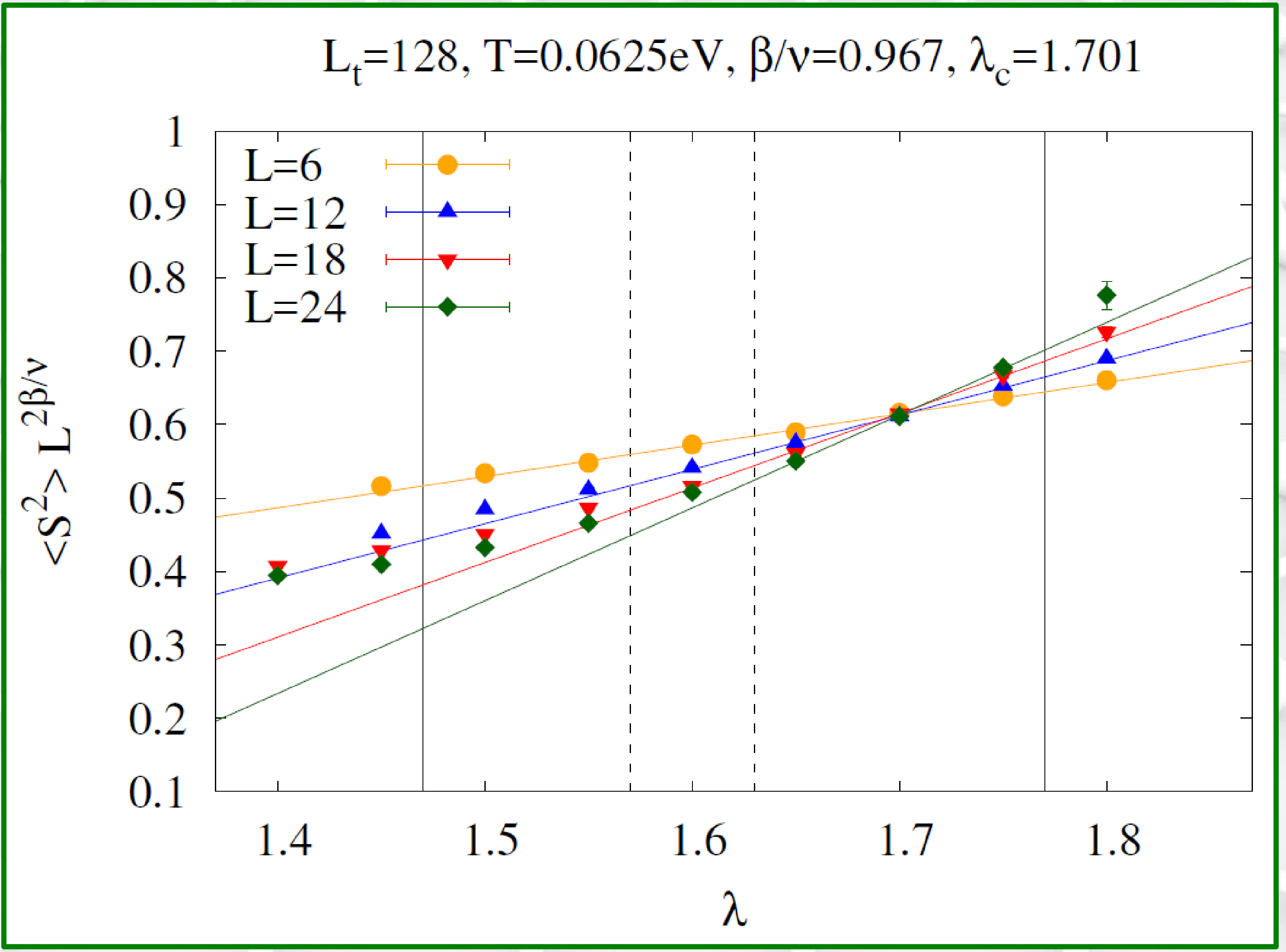


Collapse plot for Hubbard model on hexagonal lattices (same size & action)



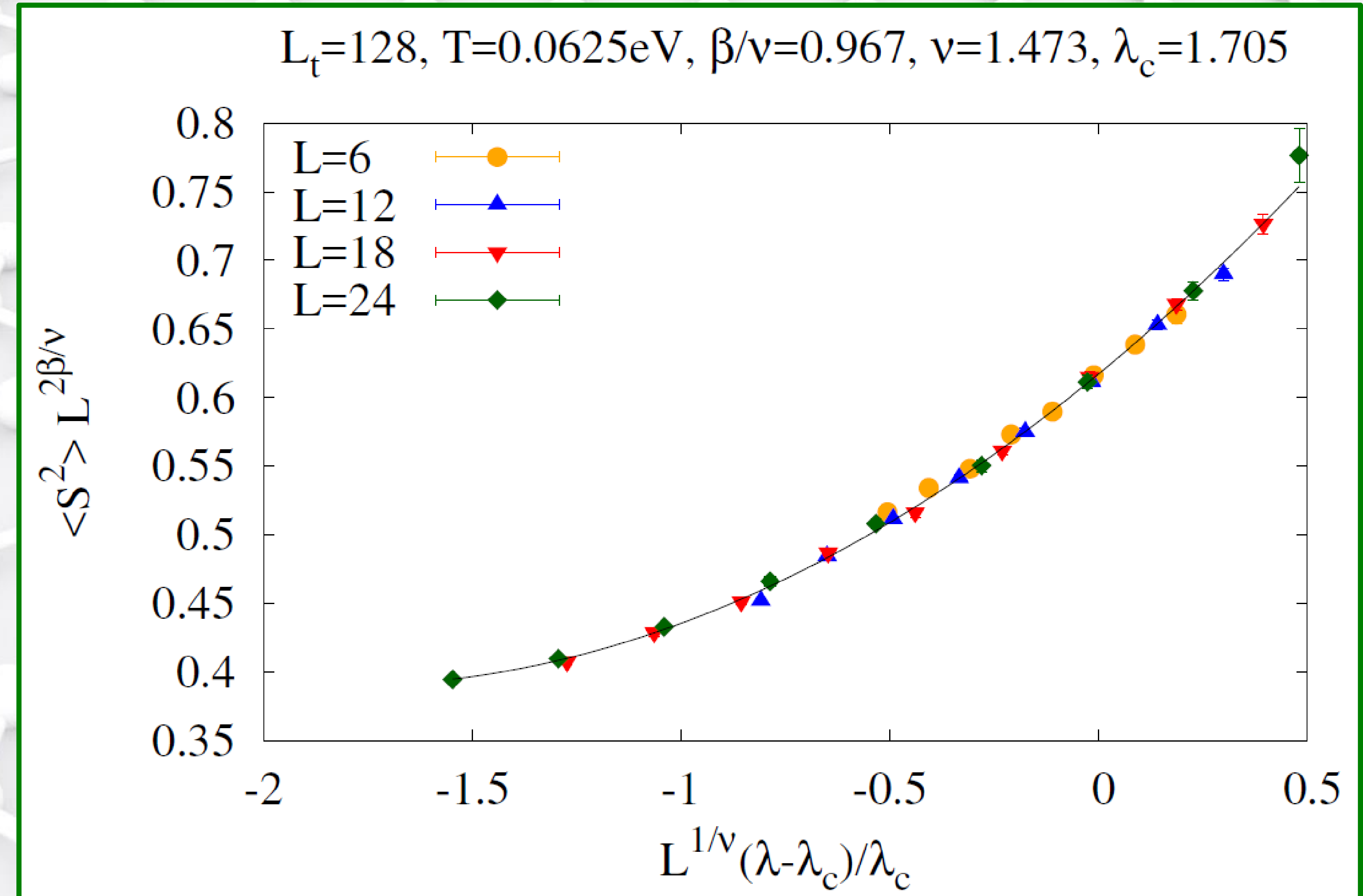
Independent determination of β and ν

Best intersection plot for β/ν=0.967



Independent determination of β and ν

Best collapse plot: β/ν=0.967, cν=1.473

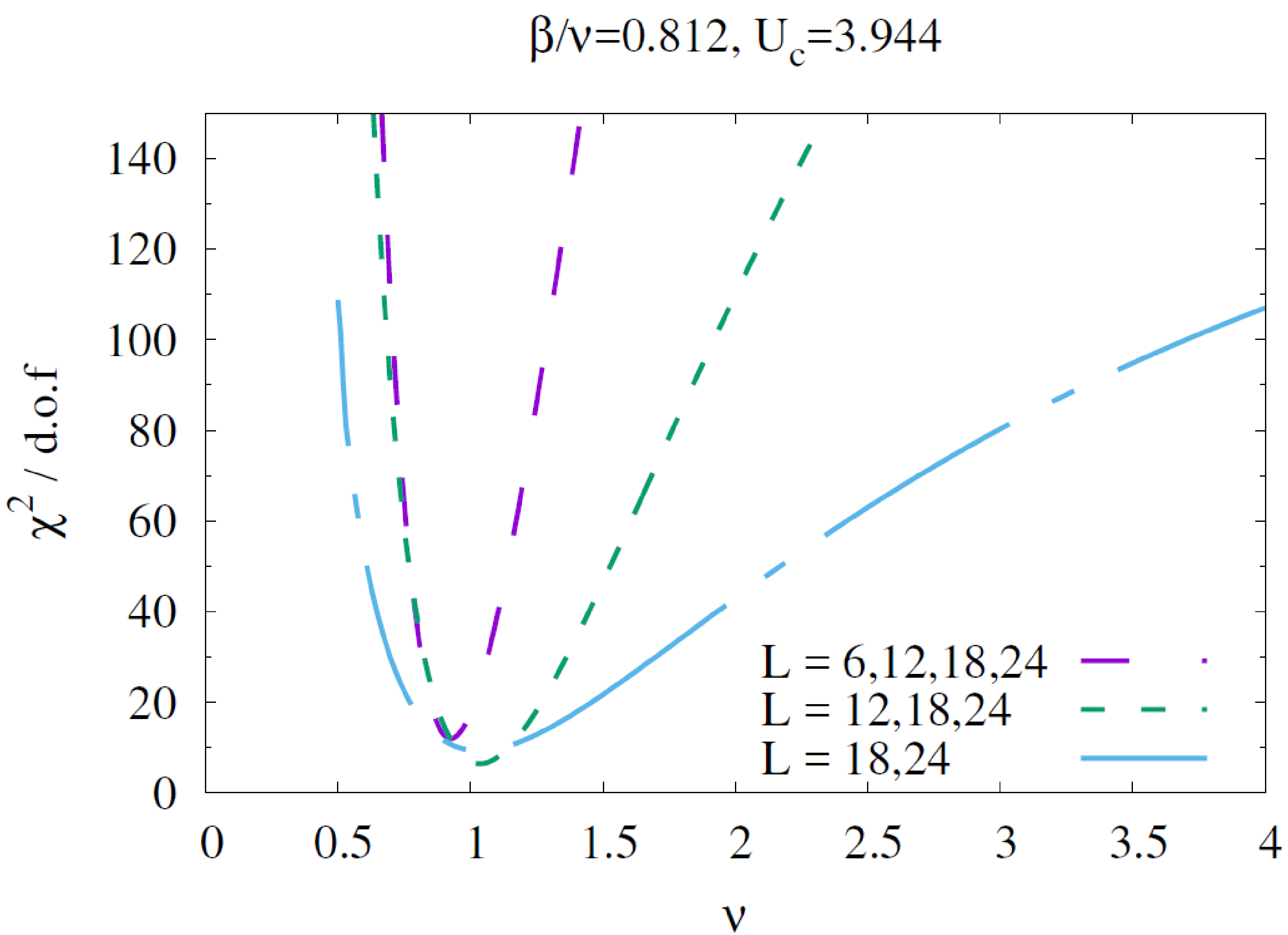


Independent determination of β and ν

- Our value $\beta/\nu=0.967$ is close to the RG prediction $\beta/\nu=1.0$
- Can it be that Hubbard model simply has larger corrections to universal scaling?
- Our result $\nu=1.473$ is still significantly larger than the RG prediction $\nu=1.2$
- Let us check how our data constrains the value of ν

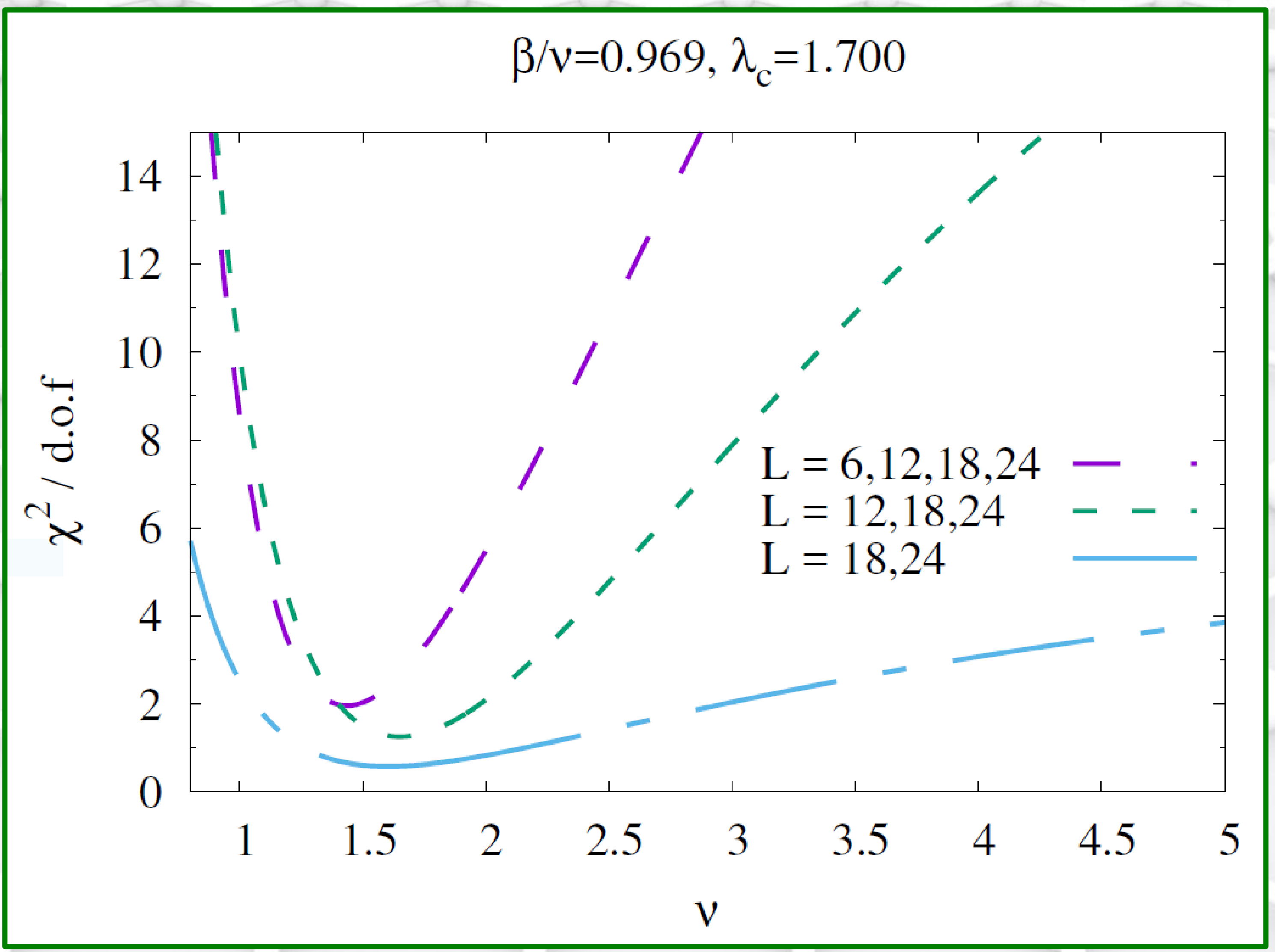
χ2 as a function of ν

Hubbard model results



χ2 as a function of ν

Graphene results – note the scale!



Constraining the value of v

- Graphene data constrains **v** much weaker than the comparable-quality Hubbard model data
- As we remove smaller lattices, **v** becomes practically unconstrained towards larger values
- Smaller values (e.g. $v = 1.2$) are much stronger constrained

Graphene data is very different from Hubbard model data!!!

Could our data hint at a Conformal Phase Transition?

- Conformal phase transition [Miransky,Yamawaki,hep-th/9611142]: Essential singularity in the order parameter

$$\boxed{\langle\, \hat{s}_x^2 \,\rangle = a \exp\left(-\frac{b}{\sqrt{\lambda-\lambda_c}}\right)}$$

- Happens in massless QED in 3+1 and 2+1 dimensions (w.r.t. N_f)

Graphene is in between!

Could our data hint at a Conformal Phase Transition?

- **Correlation length at a CPT:**

$$\boxed{l_c \sim \exp\left(\frac{1}{\sqrt{\lambda - \lambda_c}}\right)}$$

- **For any *ν* grows faster than**

$$\boxed{l_c \sim (\lambda - \lambda_c)^{-\nu}}$$

- **In a finite volume, often looks like second-order phase transition**
  [Braun,Fischer,Gies'1012.4279]

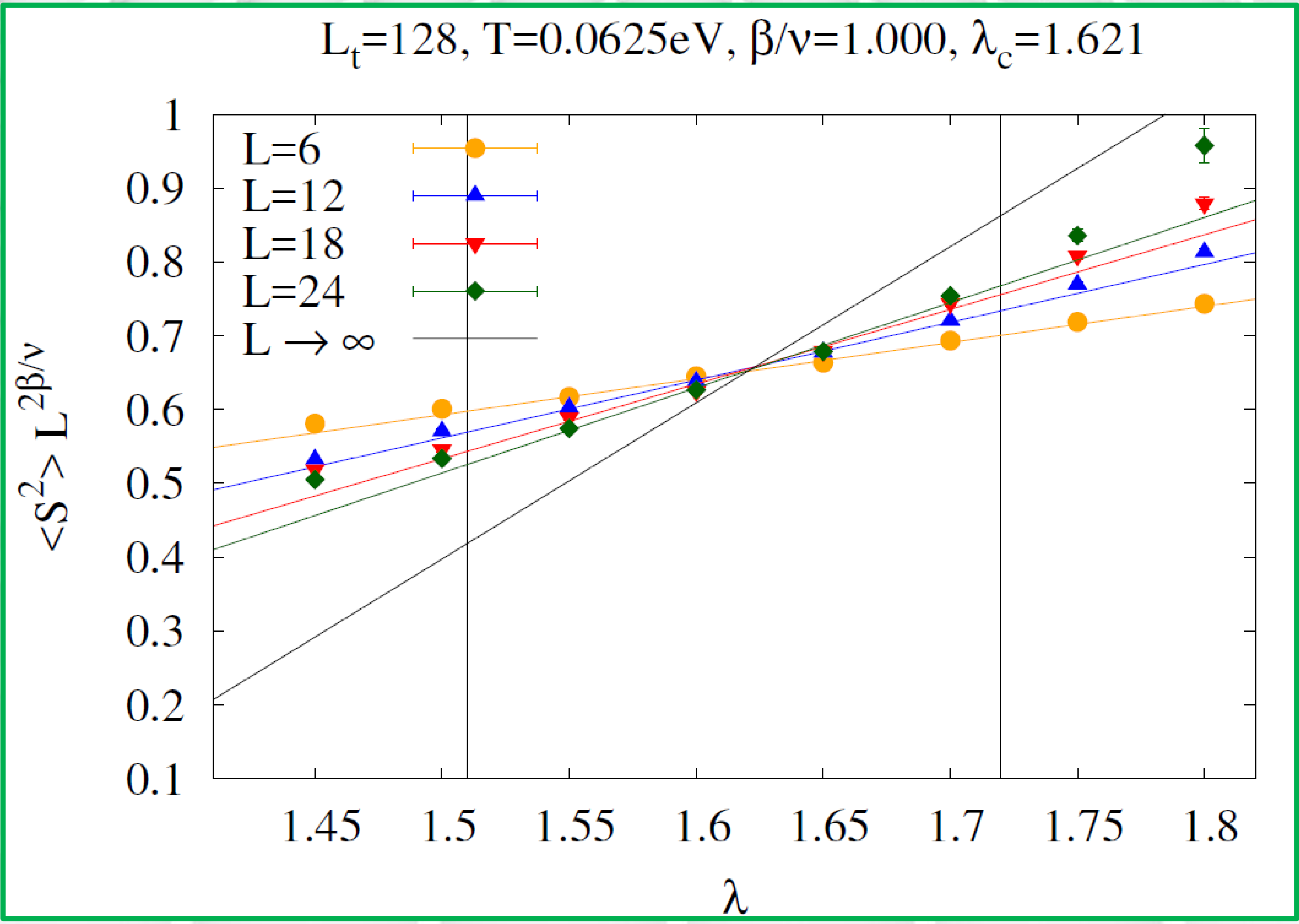
Could our data hint at a Conformal Phase Transition?

- Formally, CPT corresponds to a limit $\beta \to \infty$, $\nu \to \infty$
- Hyperscaling relations may still hold with $\delta=1$ ($d = 2$ in our case) [Gamayun,Gorbar,Gusynin'0911.4878]

$$\boxed{\frac{\beta}{\nu} = \frac{d}{\delta + 1}}$$

- Agrees well with our result $\beta/\nu=0.967$

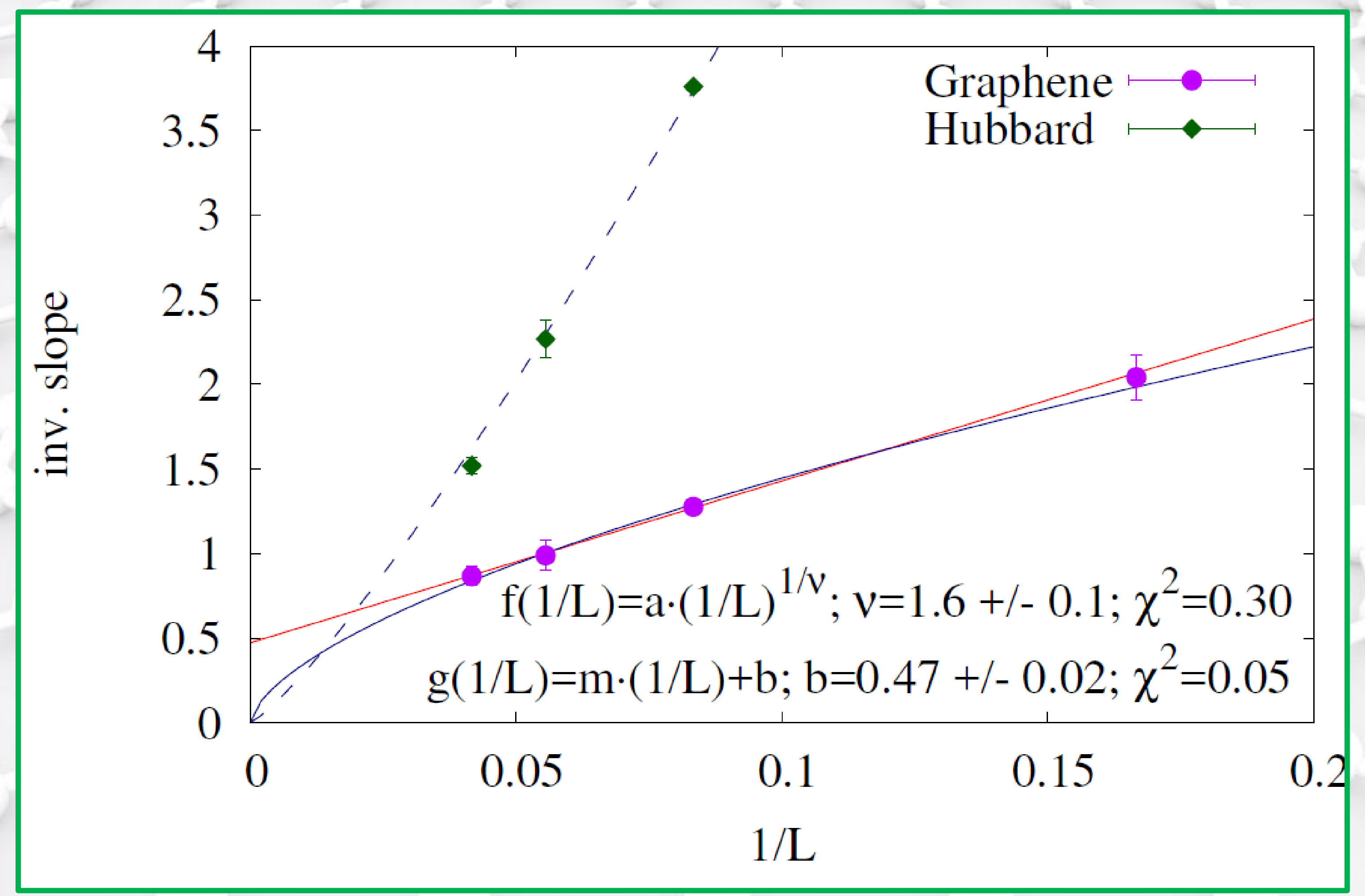
A test of critical scaling at *β/ν=1*



Good-quality intersection plot is obtained

2^{nd} order PT vs CPT

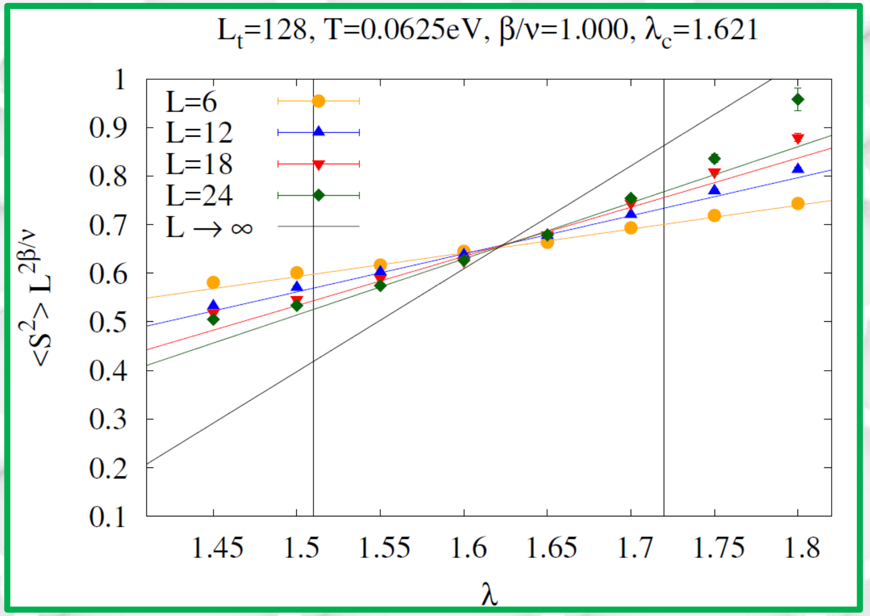
2^{nd} order PT: slope diverges as $L\to\infty$

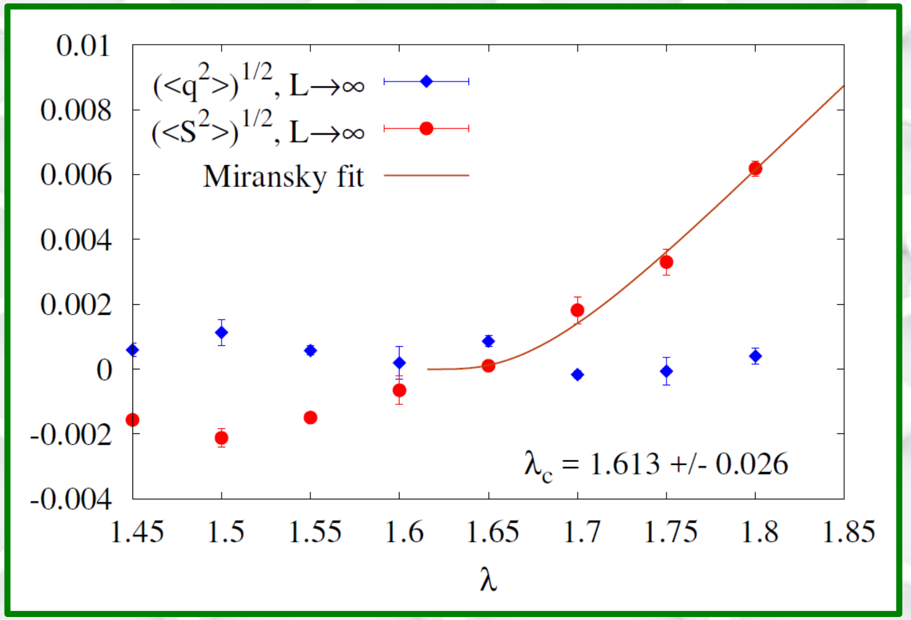


Data consistent with finite slope at $L\to\infty$

2^{nd} order PT vs CPT

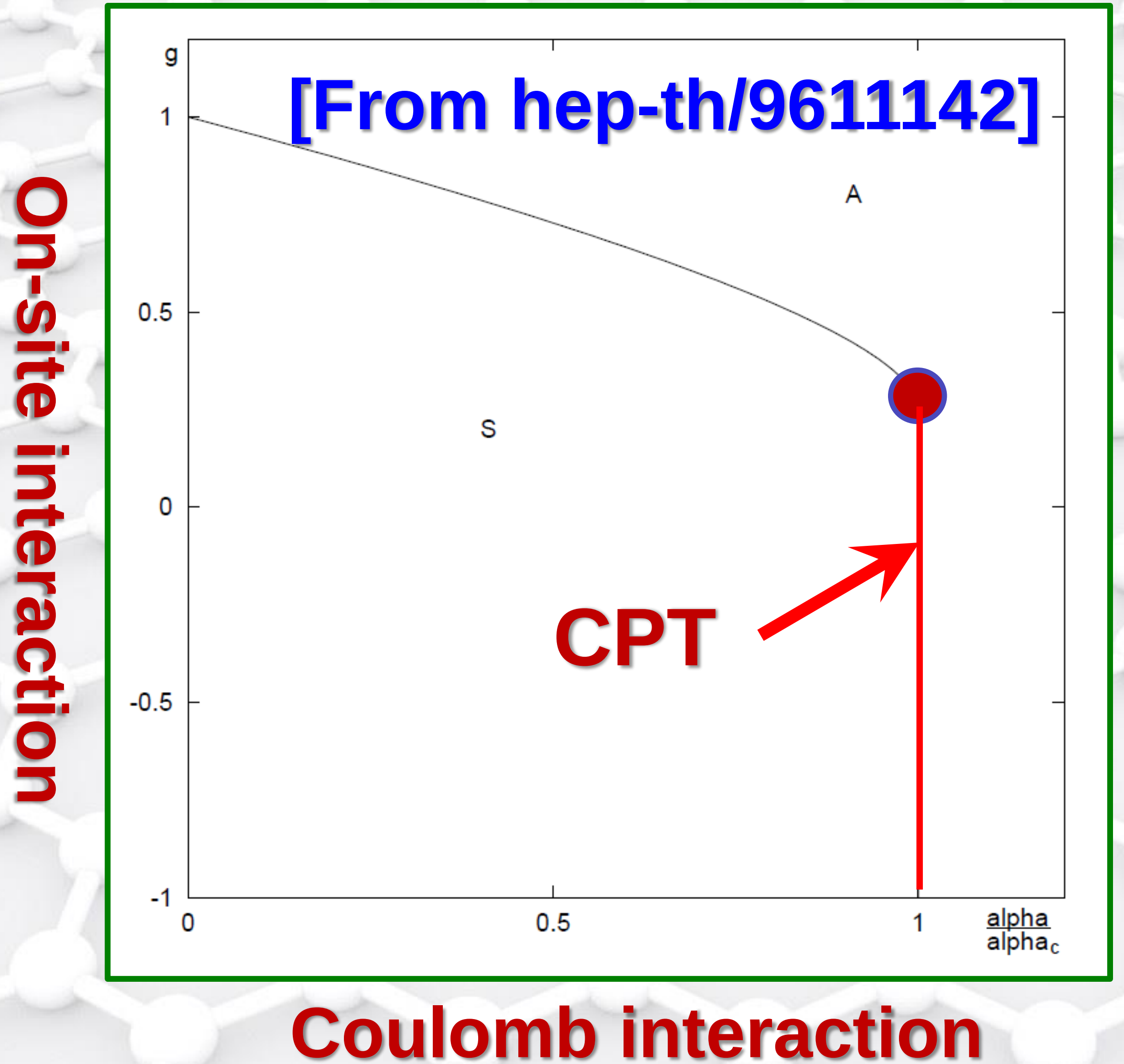
- Intersection plot at $\beta/\nu=1$: $\lambda_c = 1.62$
- Fit to Miransky scaling yields $\lambda_c = 1.61$





All evidence at the border of statistical significance! Expected numerical difficulties with CPT …

Conformal Phase Transition: Hubbard vs Coulomb interactions



Conformal Phase Transition appears to provide a more "natural" description of our data

Input from larger lattices or alternative simulation methods would be highly desirable

Conclusions

- Scaling study of graphene with realistic interactions rescaled by some factor λ
- We find $\lambda_c \approx 1.61$ – far from $\lambda=1$
- No bias towards specific symmetry breaking channel
- Anti-ferromagnetic state and CDW considered as possible options
- Other orders interesting, but usually require $V_2 > V_1 > U$

Outlook

- Interesting to consider "theoretically pure" case of pure Coulomb + on-site interactions and map out the phase diagram

- CPT is often discussed in high-energy physics
- For QCD it is located at $g = 0$
- Walking technicolor (Higgs as technidilaton)
- Phase transitions with respect to N_f