EVAN BERKOWITZ

INSTITUT FÜR KERNPHYSIK

INSTITUTE FOR ADVANCED SIMULATION,
JÜLICH SUPERCOMPUTING CENTRE

FORSCHUNGSZENTRUM JÜLICH

26 JUNE 2023

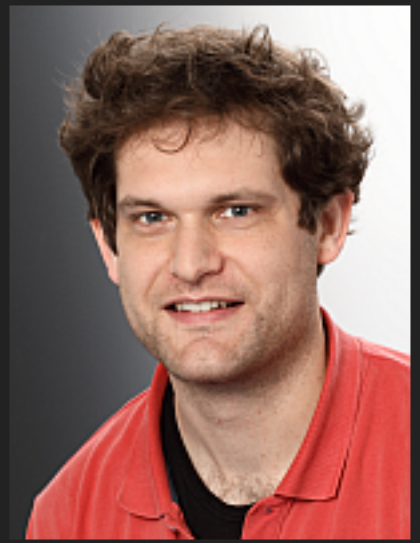
ML FOR LATTICE FIELD THEORY AND BEYOND

LEARNING ABOUT THE HUBBARD MODEL

Saturday Morning Breakfast Cereal

Christopher Körber

Jan-Lukas Wynen



Stefan Krieg

Peter Labus

Timo Lähde

Tom Luu

Johann Ostmeyer

1710.06213 EB, Körber, Krieg, Labus, Lähde, Luu, Lattice 2017 10.1051/epjconf/201817503009

1812.09268 Wynen, EB, Körber, Lähde, Luu, PRB 100:075141 10.1103/PhysRevB.100.075141

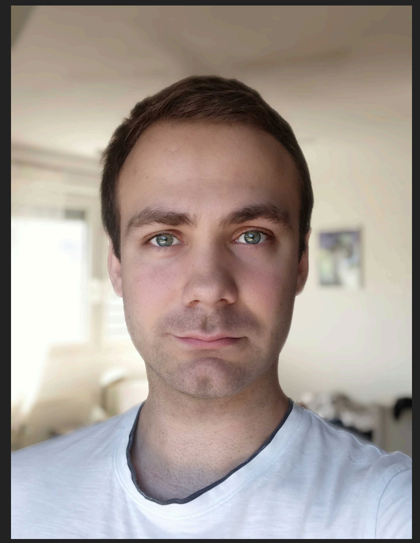
2005.11112 Ostmeyer, EB, Krieg, Lähde, Luu, Urbach, PRB 102:245105 10.1103/PhysRevB.102.245105

2006.11221 Wynen, EB, Krieg, Luu, Ostmeyer, PRB 103:125153 10.1103/PhysRevB.103.125153

2105.06936 Ostmeyer, EB, Krieg, Lähde, Luu, Urbach, PRB 104:155142 10.1103/PhysRevB.104.155142

2203.00390 Rodekamp, EB, Gäntgen, Krieg, Luu, Ostmeyer; PRB 106(12):125139 10.1103/PhysRevB.106.125139

Marcel Rodekamp



Christoph Gäntgen

LEARNING ABOUT THE DOPED HUBBARD MODEL

L. Ron Hubbard House
Washington DC

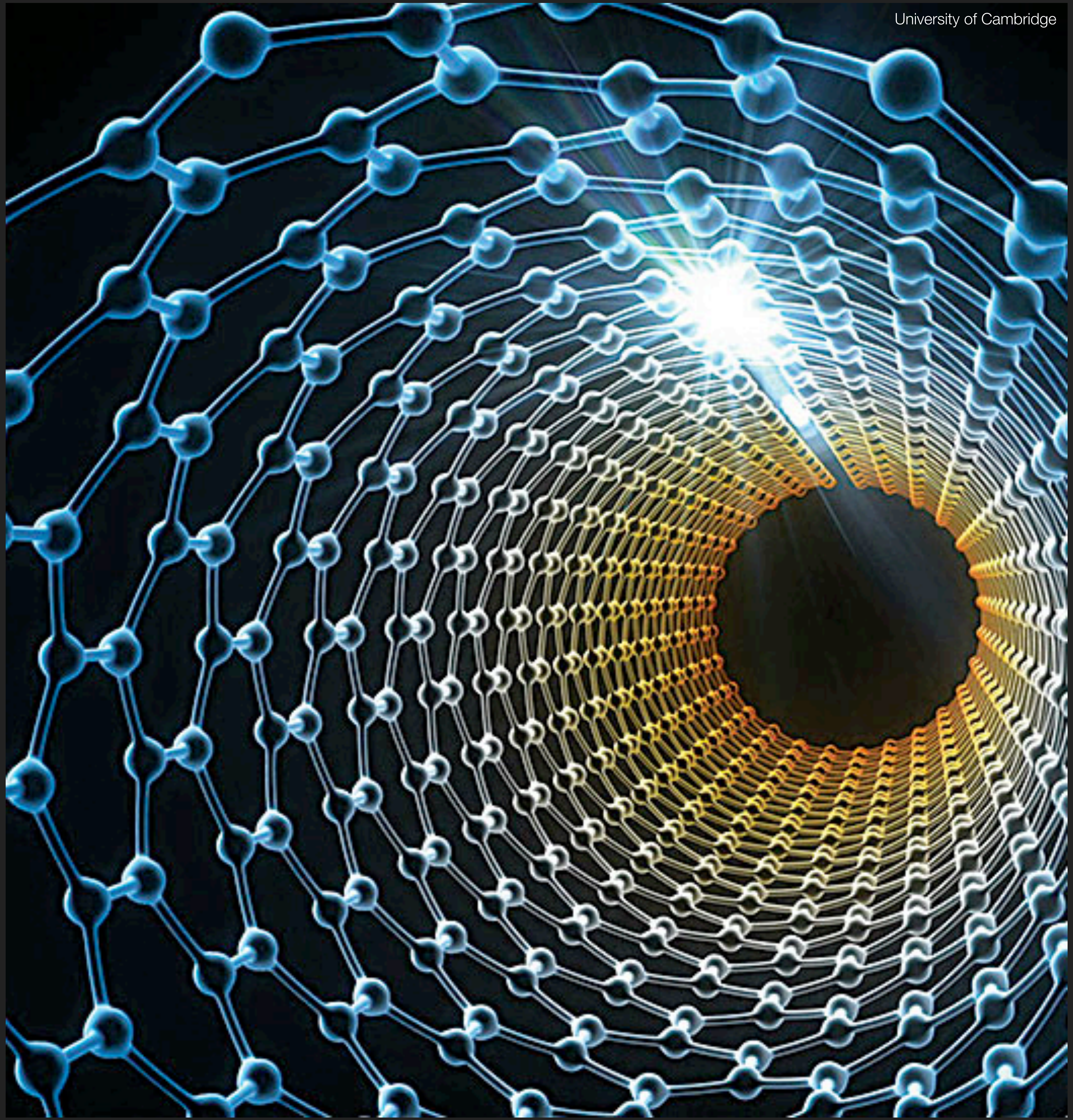
THE HUBBARD MODEL

INTRODUCTION

OVERSIMPLIFIED BUT RICH

WHY THE HUBBARD MODEL?

- simplest possible Hamiltonian with electronic movement and interactions
- captures the Mott transition
- strong interactions render the model intractable
- easy to decorate / enrich to model realistic materials → all sorts of industrial applications
- much simpler than QCD



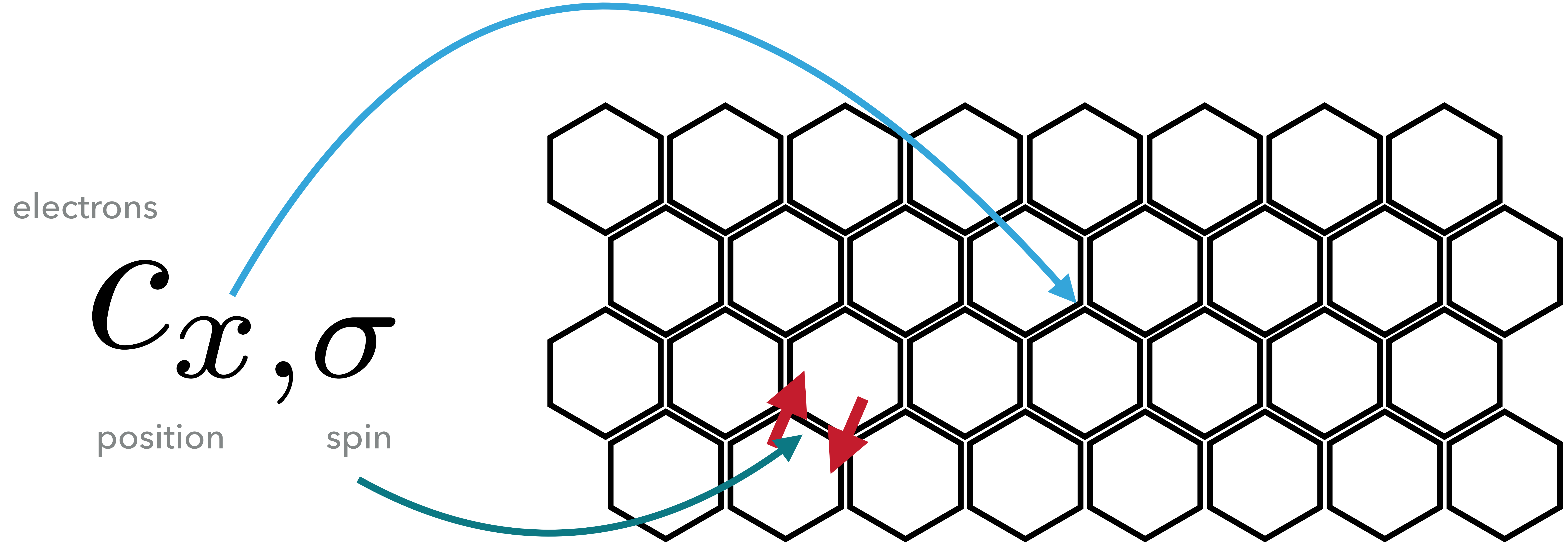
Hubbard Gold Medal of Anne Morrow Lindbergh

THE HUBBARD MODEL

BACKGROUND

THE TIGHT-BINDING MODEL

Bloch Zeit. für Physik 52 555-600 1929



Tight Binding

$$H_0 = -\sum_{x,y,\sigma} c^\dagger_{x,\sigma} h_{xy} c_{y,\sigma}$$

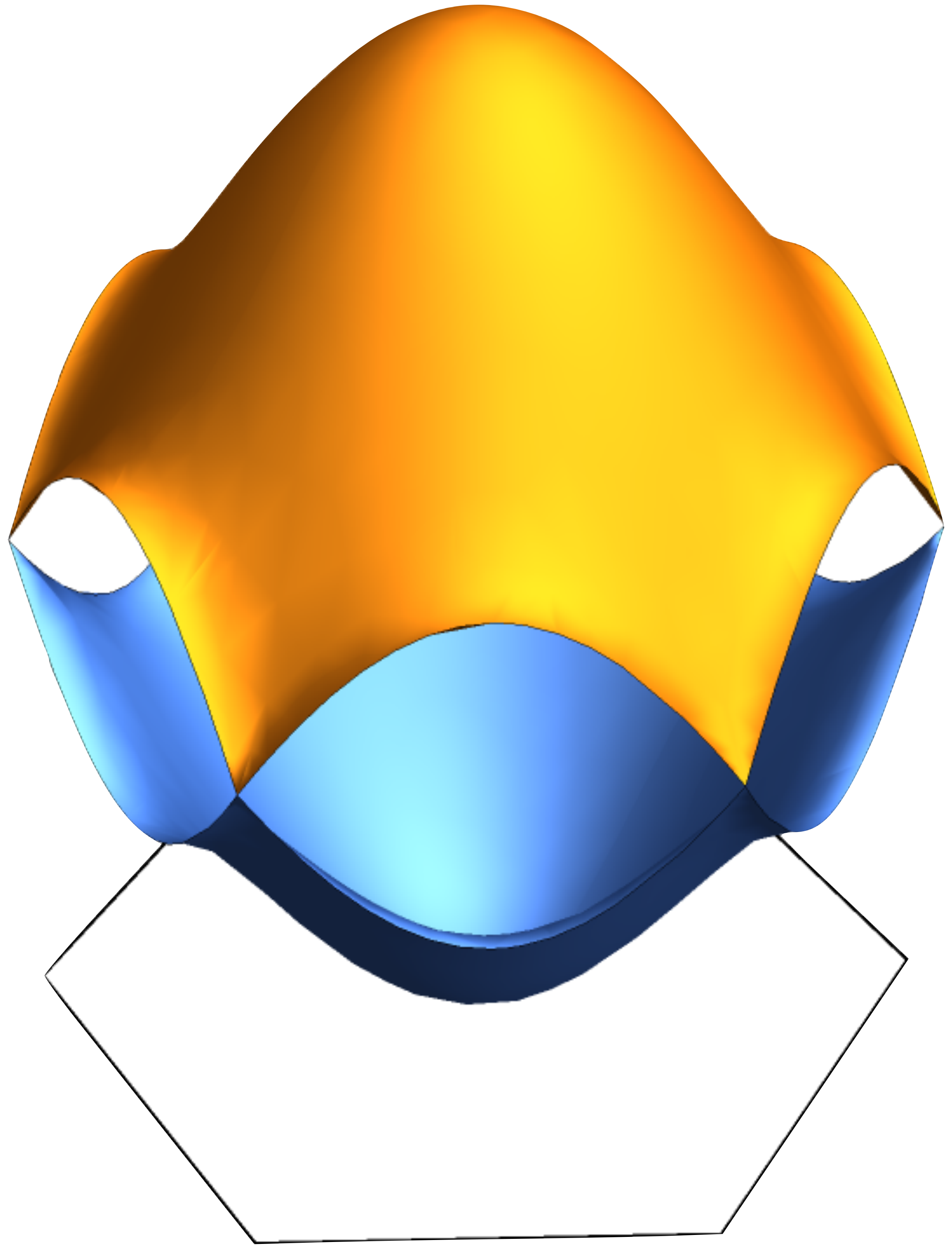
- Honeycomb:
  - triangular Bravais lattice
  - 2 sites per cell

$$h_{xy} = \kappa \delta_{\langle xy \rangle}$$

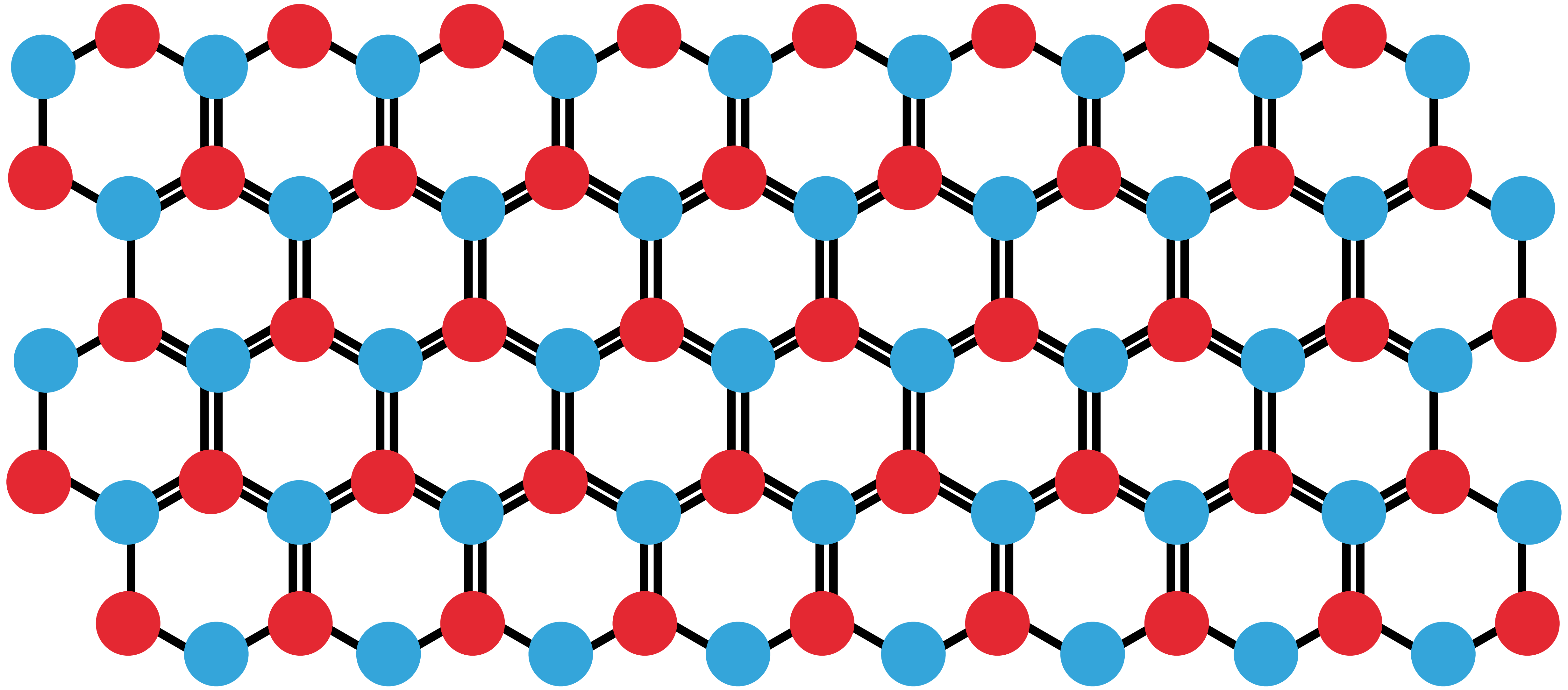
Nearest-neighbor hopping

THE TIGHT-BINDING MODEL

Wallace Phys. Rev. 71 622-634 (9 1947)



Brillouin Zone (BZ)

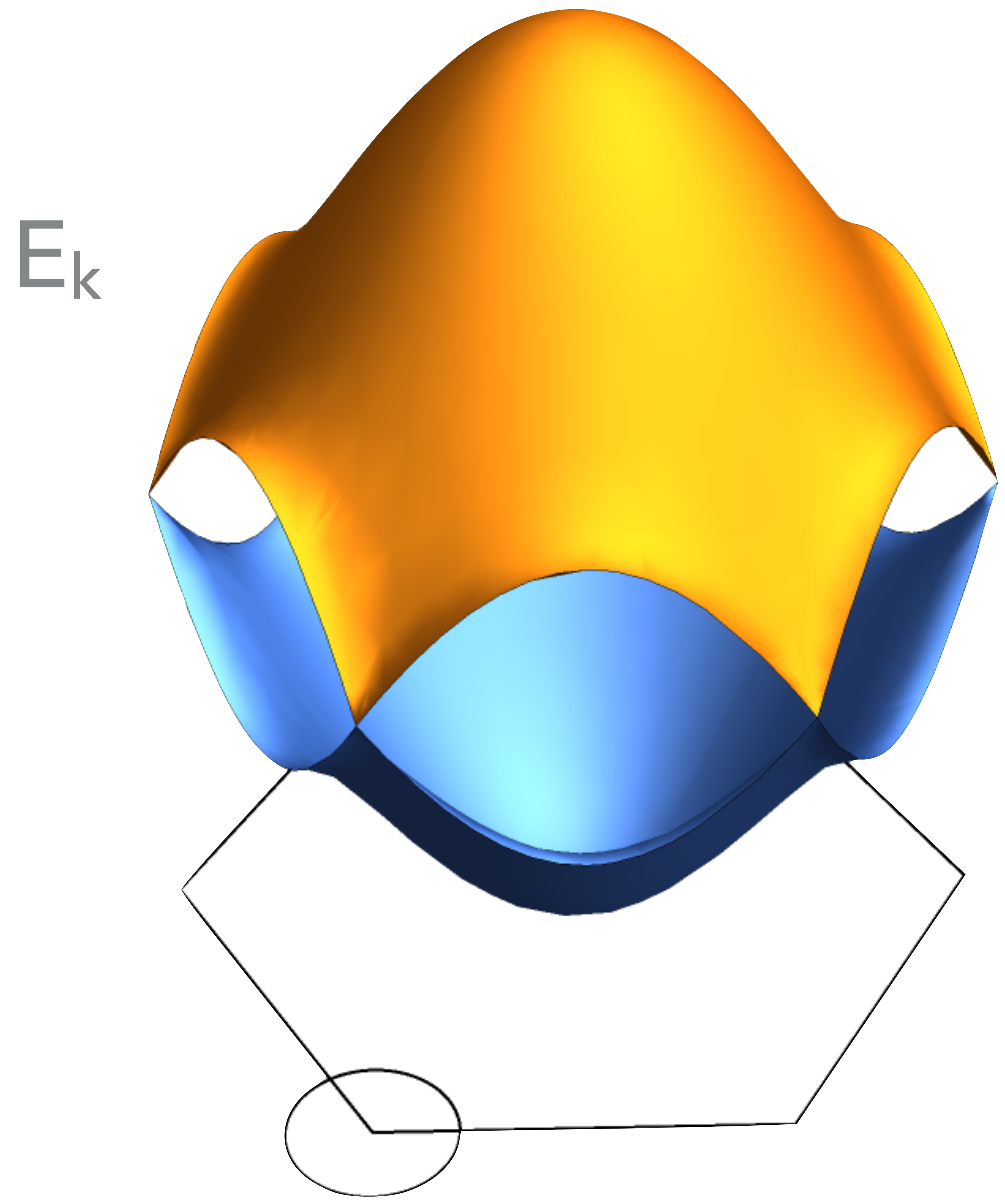


$$H_0 = - \sum_{x,y,\sigma} c^{\dagger}_{x,\sigma} h_{xy} c_{y,\sigma}$$

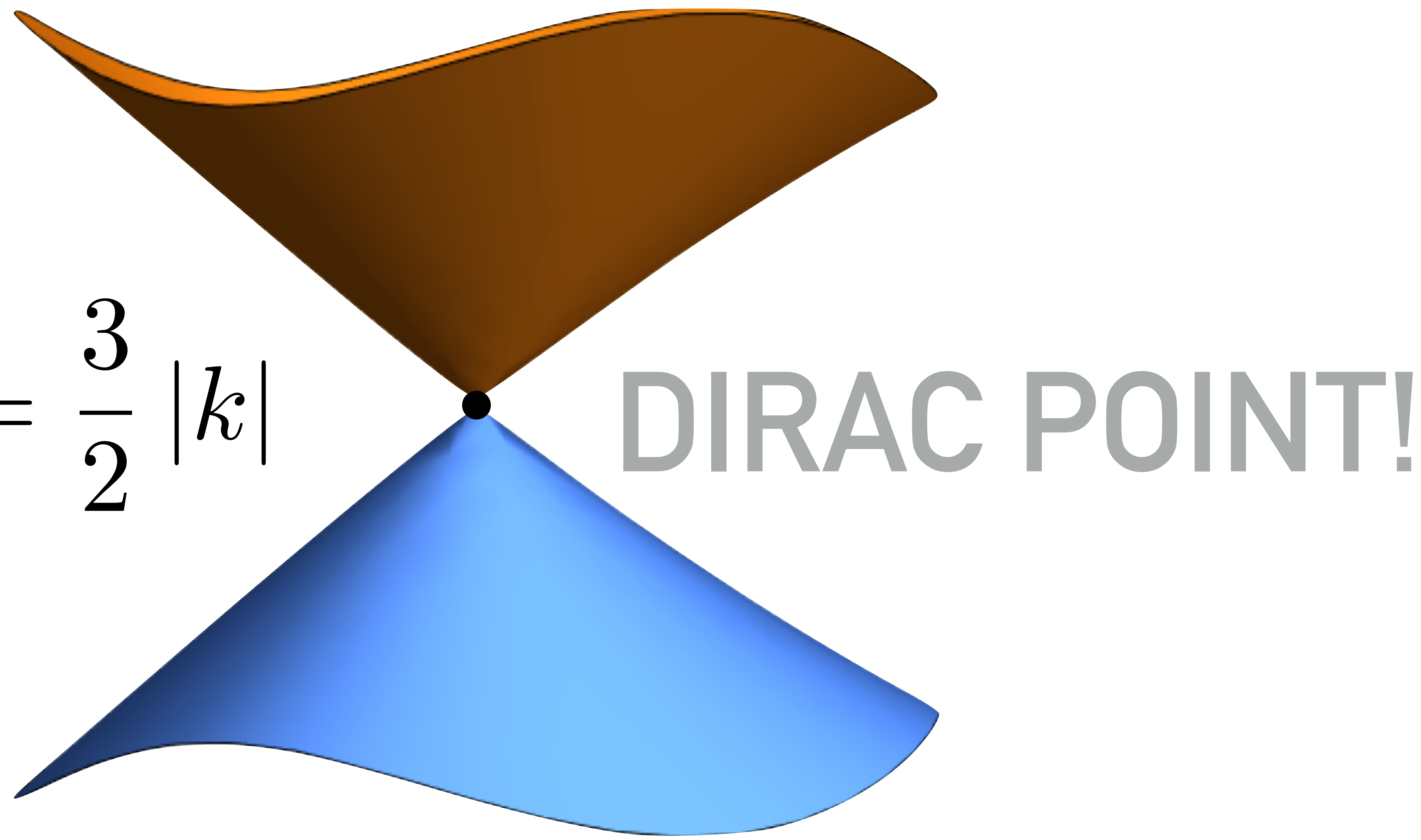
$$E_k/\kappa = \pm\sqrt{3 + 2\left(\cos\left(\frac{3}{2}k_x + \frac{\sqrt{3}}{2}k_y\right) + \cos\left(\frac{3}{2}k_x - \frac{\sqrt{3}}{2}k_y\right) + \cos\left(\sqrt{3}k_y\right)\right)}$$

THE TIGHT-BINDING MODEL

Wallace Phys. Rev. 71 622-634 (9 1947)



$$E_k/\kappa = \frac{3}{2}\,|k|$$



$$E_k/\kappa = \pm\sqrt{3 + 2\left(\cos\left(\frac{3}{2}k_x + \frac{\sqrt{3}}{2}k_y\right) + \cos\left(\frac{3}{2}k_x - \frac{\sqrt{3}}{2}k_y\right) + \cos\left(\sqrt{3}k_y\right)\right)}$$

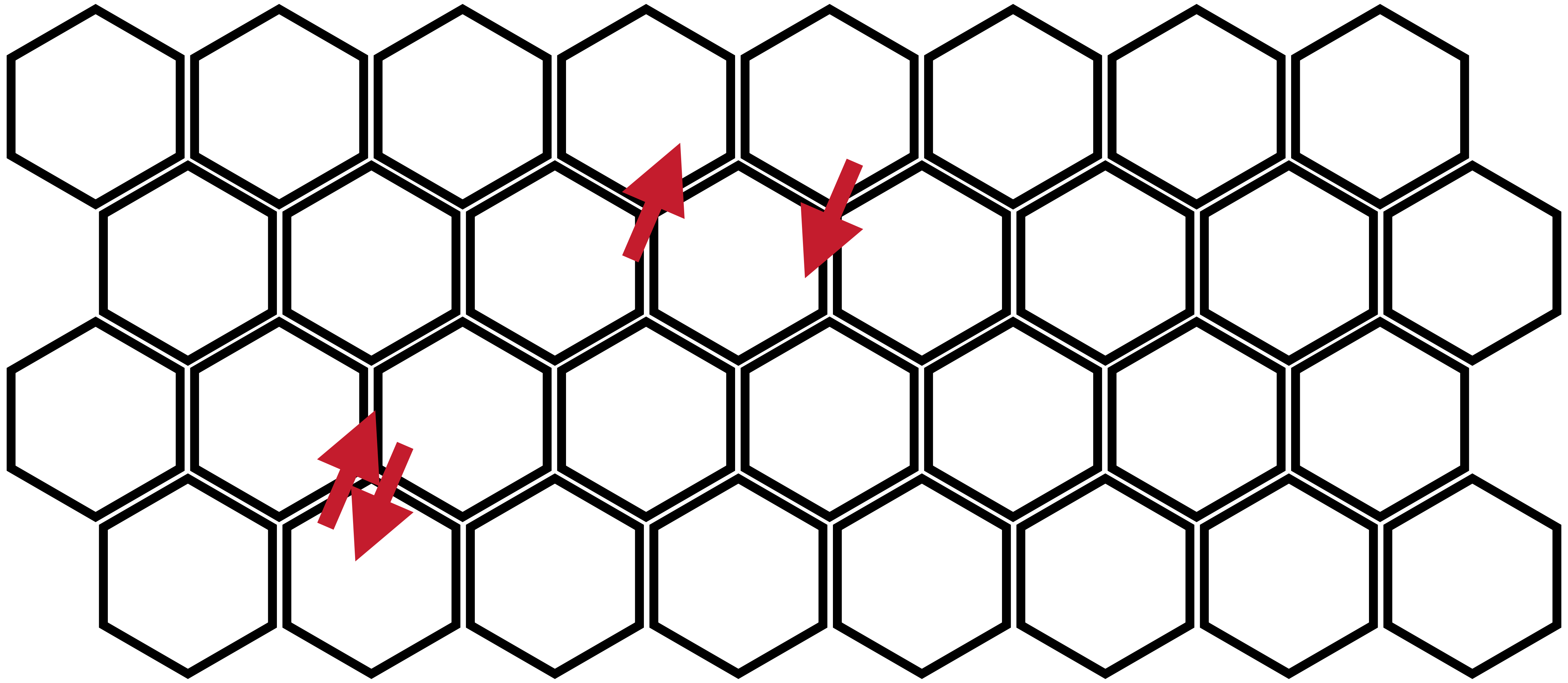
THE HUBBARD MODEL

Hubbard, Proc. Roy. Soc. A 1963 10.1098/rspa.1963.0204

$$n_{x\sigma} = c^{\dagger}_{x,\sigma} c_{x,\sigma}$$

$$H_I = -\frac{U}{2} \sum_x \left(n_{x\uparrow} - n_{x\downarrow}\right)^2$$

U>0 is repulsive



Spin

$$S^i_x = \frac{1}{2} \sum_{ss'} c_{xs} \sigma^i_{ss'} c^{\dagger}_{xs'}$$

$$\left[S^i_x, S^j_y\right] = i\delta_{xy} \epsilon^{ijk} S^k_x$$

Charge

$$\rho_x = 1 - 2S^0_x$$

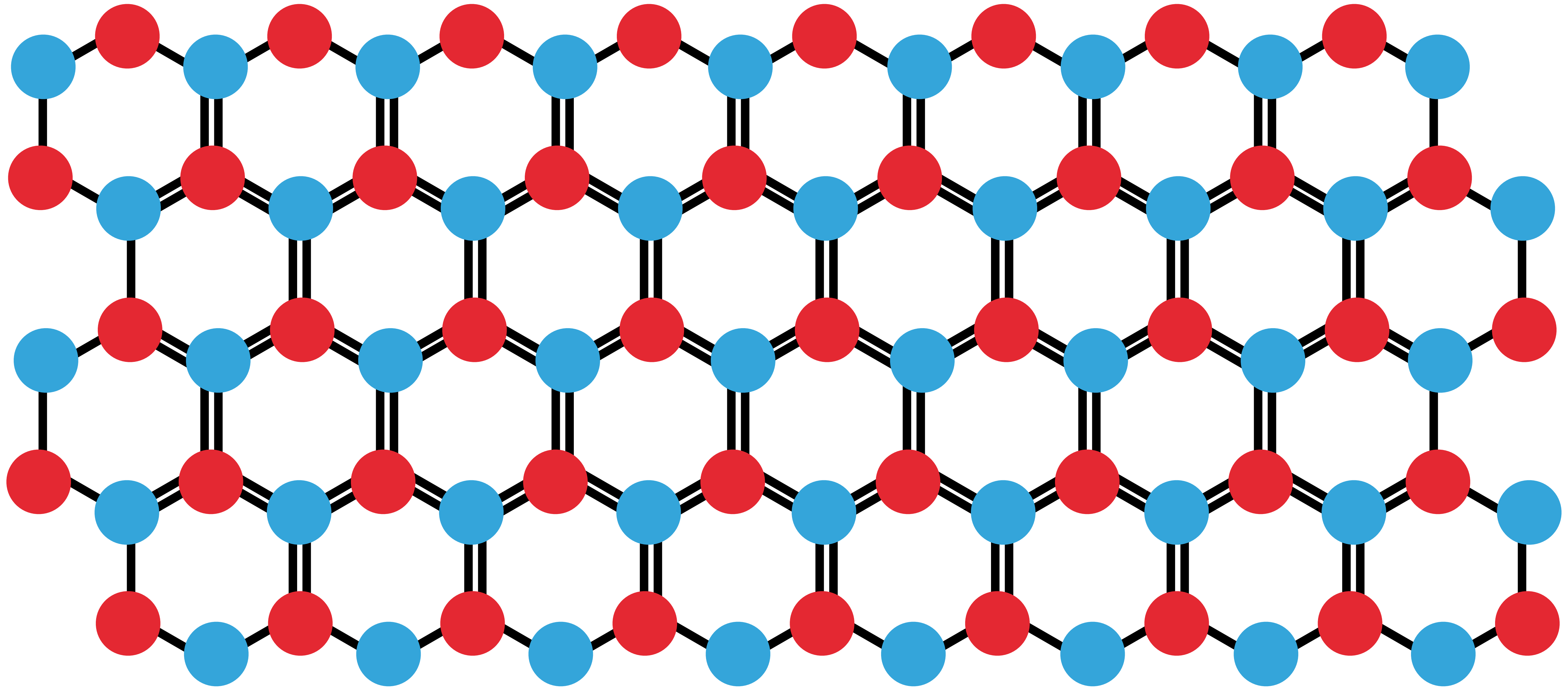
Half-filling: $\mu_\rho = 0$

THE HUBBARD MODEL

Néel Ann. de Phys. 12 (3): 137-198 (1948) 10.1051/anphys/194812030137

$$n_{x\sigma} = c^\dagger_{x,\sigma} c_{x,\sigma}$$

$$H_I = -\frac{U}{2} \sum_x (n_{x\uparrow} - n_{x\downarrow})^2$$



U/κ very large

$$H_{\text{eff}} \sim +\frac{\kappa^2}{U} \sum_{\langle x,y \rangle} \vec{S}_x \cdot \vec{S}_y$$

alternating, checkerboard, or *Néel* order

+1 (red)

−1 (blue)

antiferromagnetic (Mott) insulator! (AFMI)

THE HUBBARD MODEL

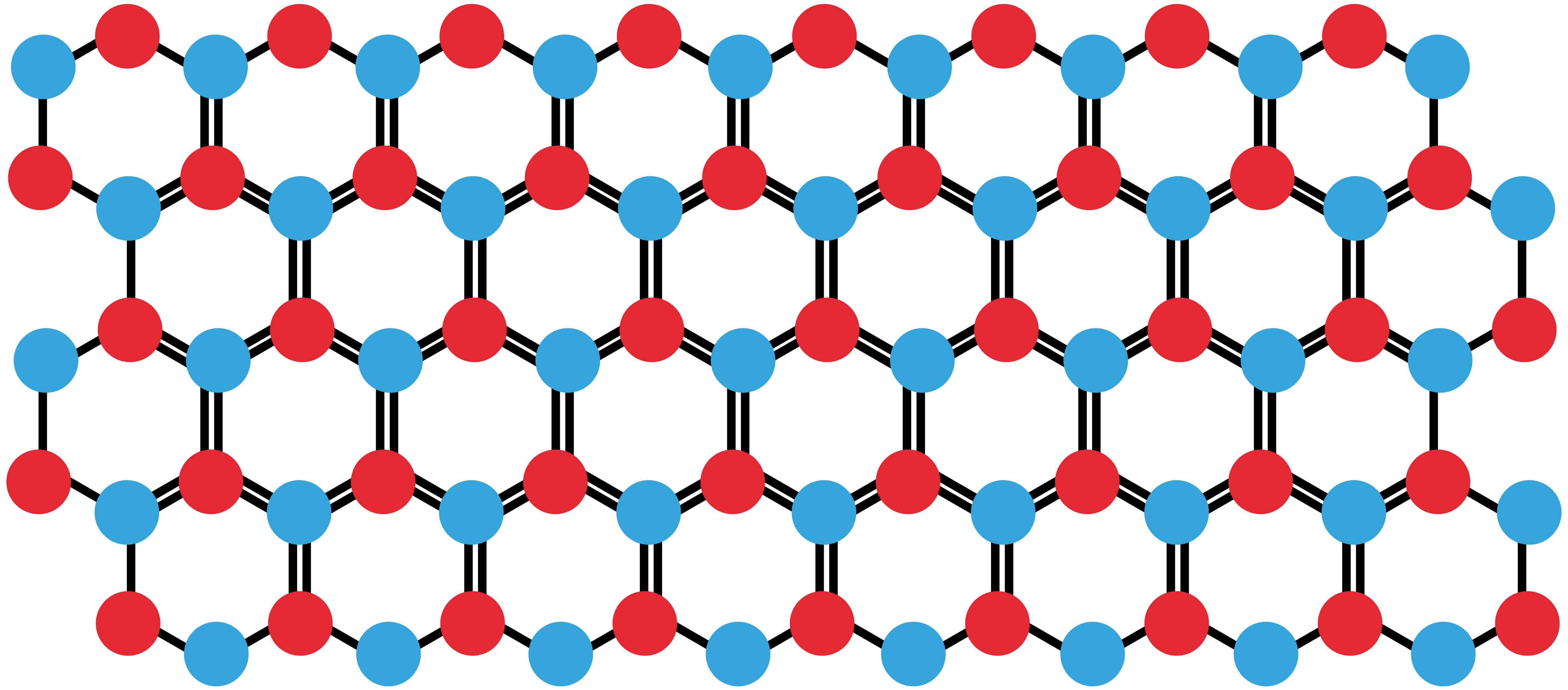
Hubbard, Proc. Roy. Soc. A 1963 10.1098/rspa.1963.0204

Bipartite lattice!

$$a_x = c_{x\uparrow} \qquad a_x^\dagger = c_{x\uparrow}^\dagger$$

$$b_x = (-1)^x c_{x\downarrow}^\dagger \qquad b_x^\dagger = (-1)^x c_{x\downarrow}$$

$$H = \sum_{xy} \left(a_x^\dagger h_{xy} a_y + b_x^\dagger h_{xy} b_y\right) + \frac{U}{2} \sum_x \left(n_x^a - n_x^b\right)^2$$



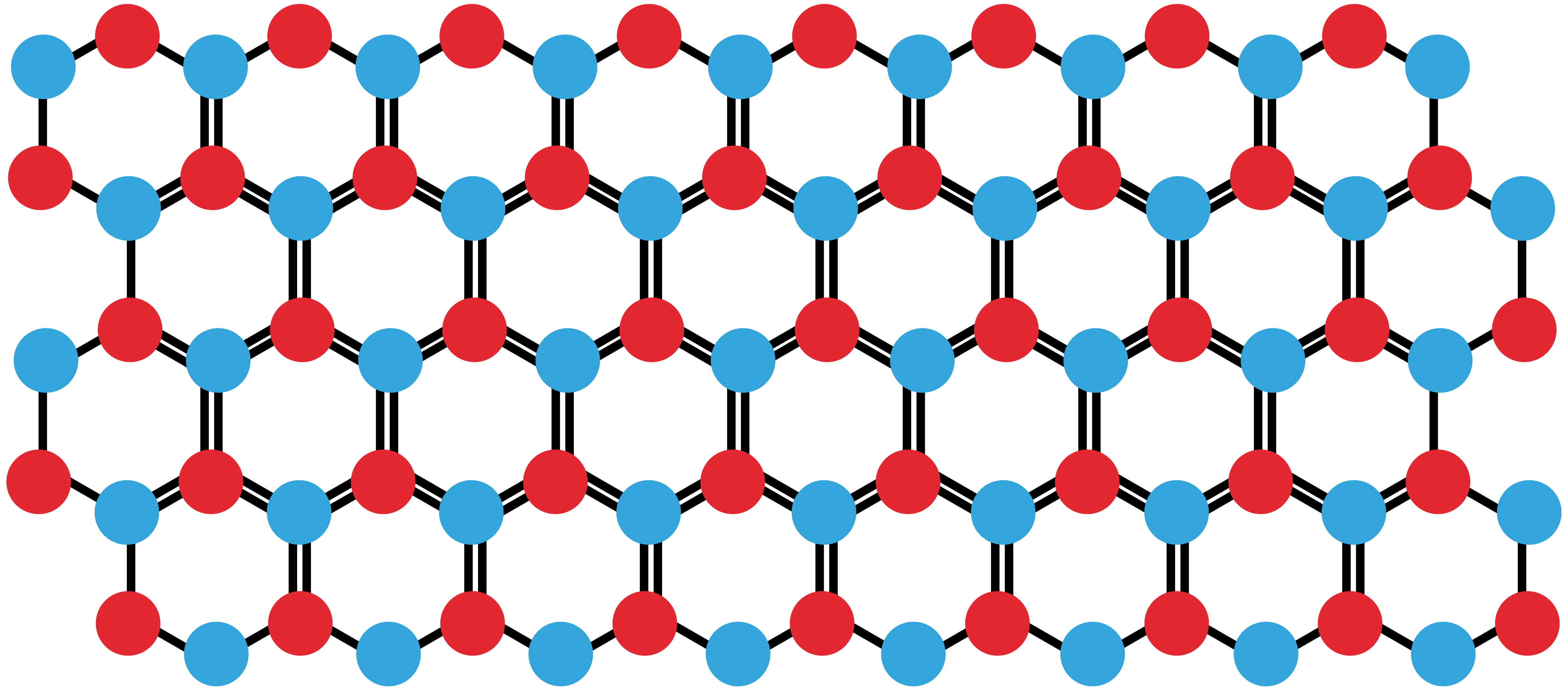
THE HUBBARD MODEL

Hubbard, Proc. Roy. Soc. A 1963 10.1098/rspa.1963.0204

Bipartite lattice!

$$a_x = c_{x\uparrow} \qquad a_x^\dagger = c_{x\uparrow}^\dagger$$

$$b_x = (-1)^x c_{x\downarrow}^\dagger \qquad b_x^\dagger = (-1)^x c_{x\downarrow}$$



$$H = \sum_{xy} \left(a_x^\dagger h_{xy} a_y + b_x^\dagger h_{xy} b_y\right)$$

$$+ \frac{U}{2} \sum_x \left(n_x^a - n_x^b\right)^2$$

$$\left(\frac{1}{2} \sum_{xy} \rho_x V_{xy} \rho_y\right)$$

Half filling: ⟨ρ⟩= 0 $\qquad \rho_x = n_x^a - n_x^b$

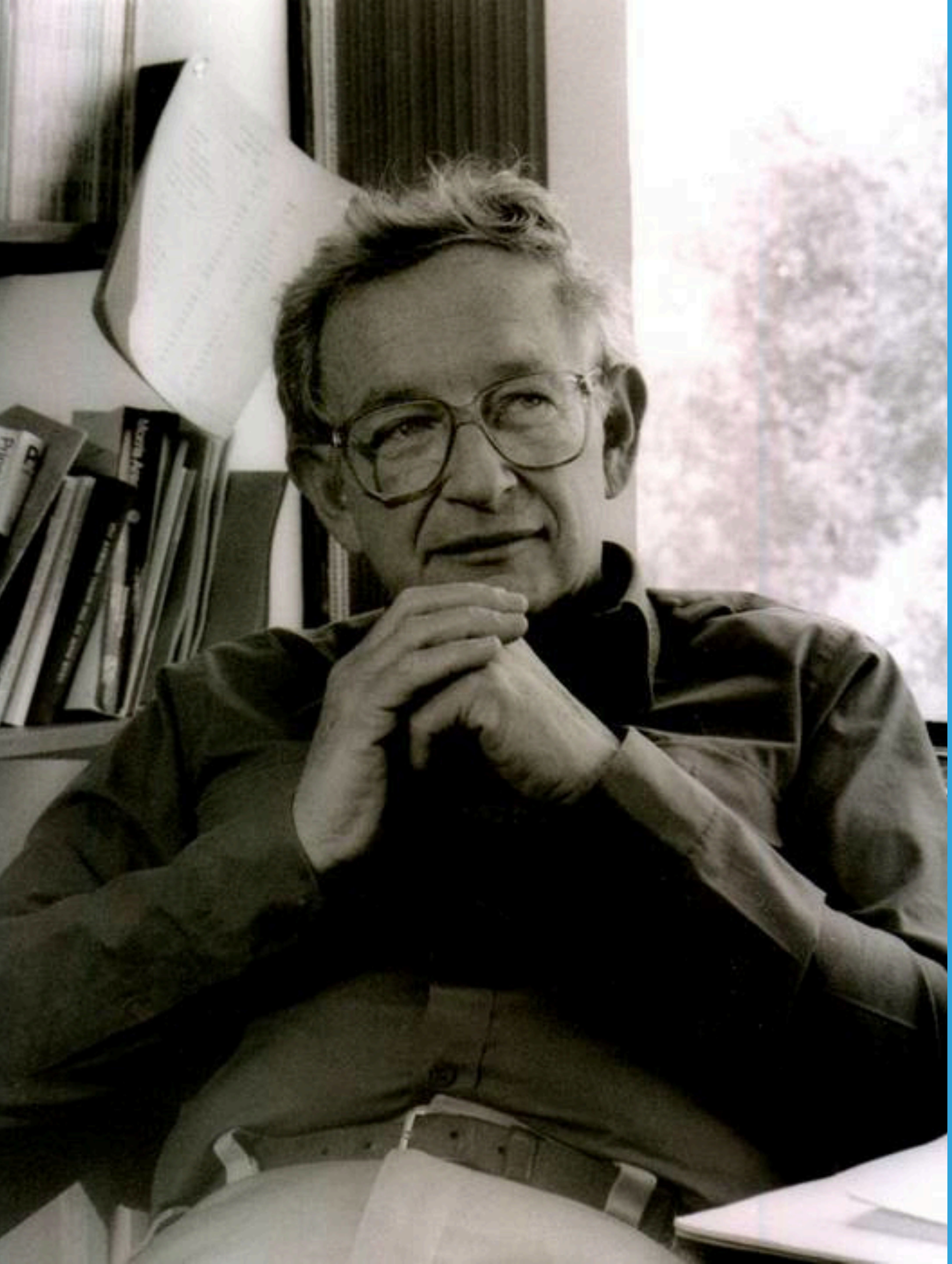
V = screened Coulomb

Ulybyshev, Buividovich, Katsnelson, Polikarpov PRL 111 056801 (2013) 2010.1103/PhysRevLett.111.056801 1403.3620

V = on-site + nearest neighbor

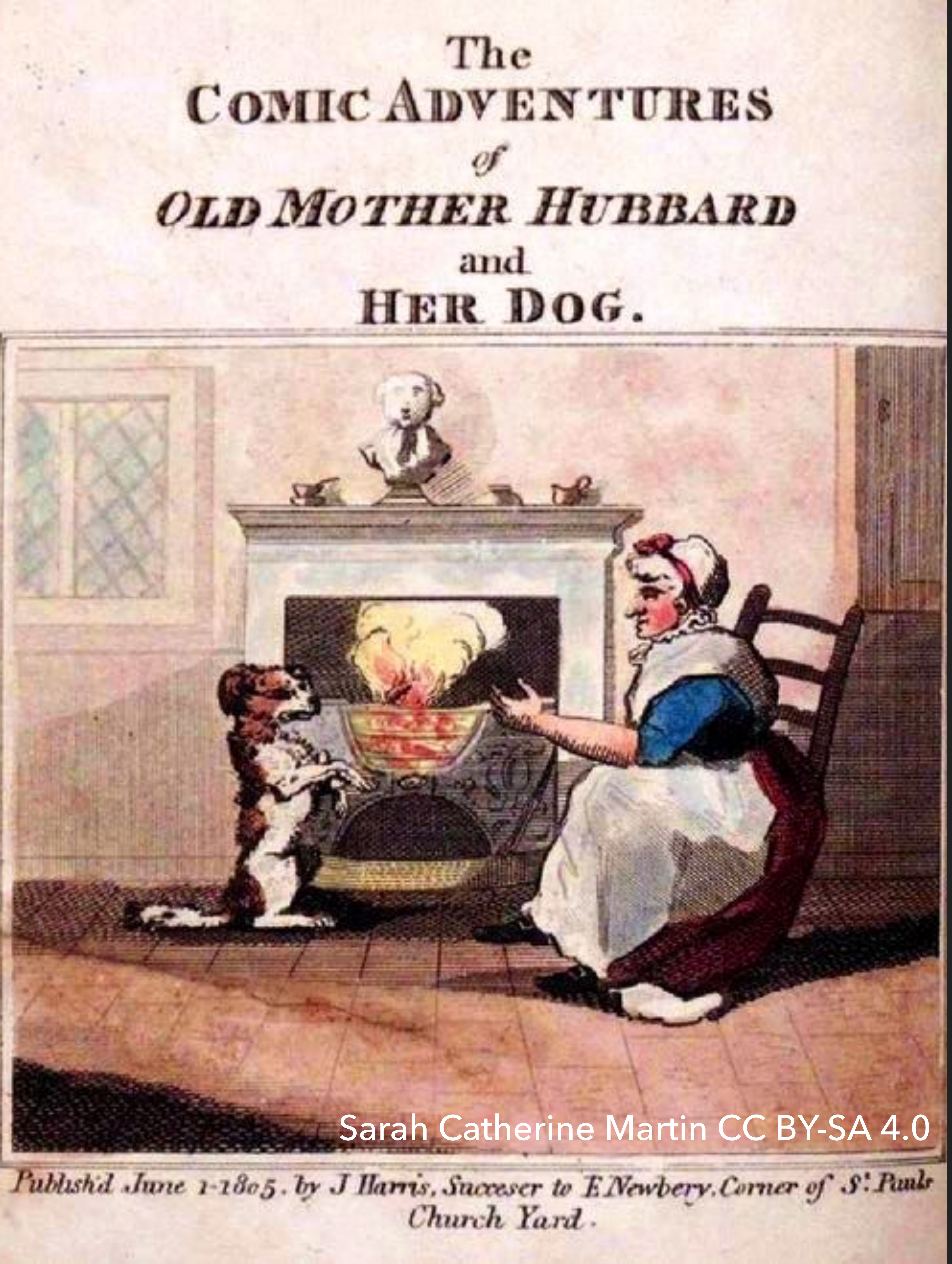
Buividovich, Smith, Ulybyshev, von Smekal LATTICE2016 244 10.22323/1.256.0244 1610.09855

- + staggered mass
- + chemical potential
- + ...



IT HAS YET TO RECEIVE ADEQUATE MATHEMATICAL TREATMENT, AND ONE HAS TO RESORT TO THE INDIGNITY OF NUMERICAL SIMULATIONS TO SETTLE EVEN THE SIMPLEST QUESTIONS ABOUT IT.

Philip W. Anderson
Nobel Lecture
8 December 1977



THE HUBBARD MODEL

SIGN-PROBLEM-FREE RESULTS

PHASE DIAGRAM

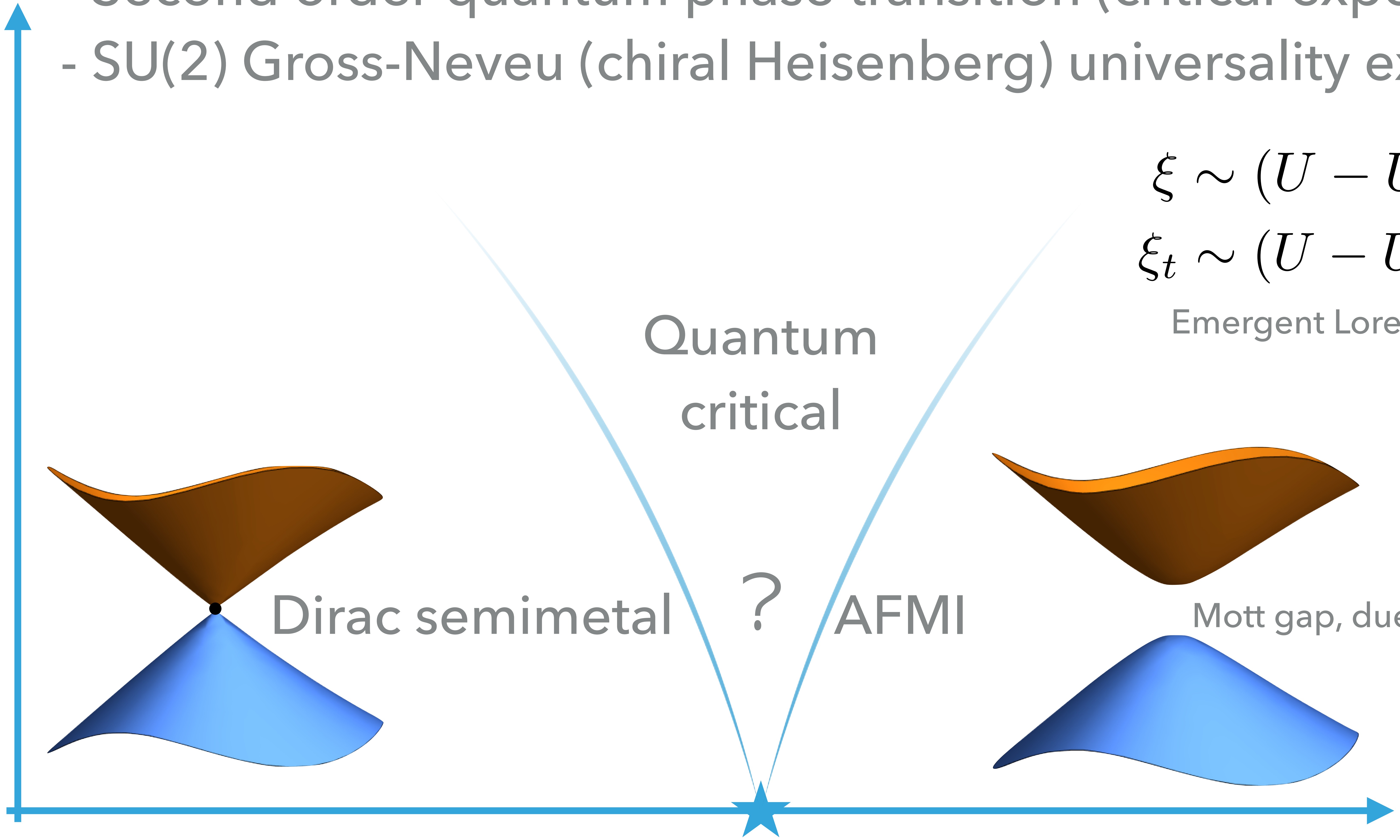
Herbut, Juričić, and Roy, PRB 79 085116 (2009)
0811.0610 10.1103/PhysRevB.79.085116

- Second order quantum phase transition (critical exponents)
- SU(2) Gross-Neveu (chiral Heisenberg) universality expected

$$\xi \sim (U - U_c)^{-\nu}$$

$$\xi_t \sim (U - U_c)^{-z\nu} \sim \xi^z$$

Emergent Lorentz symmetry: z=1

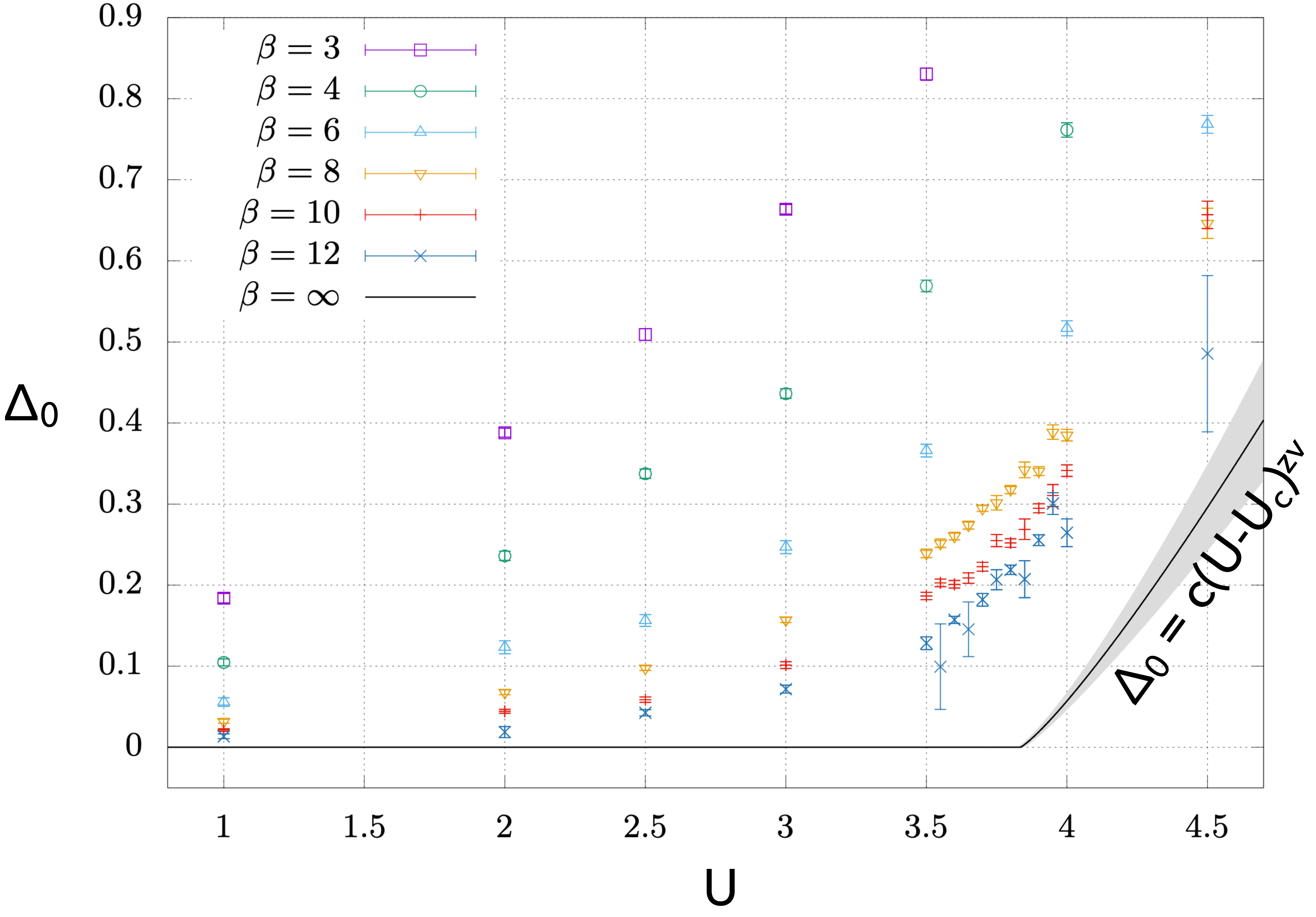


Mott gap, due to interactions only!

pressure

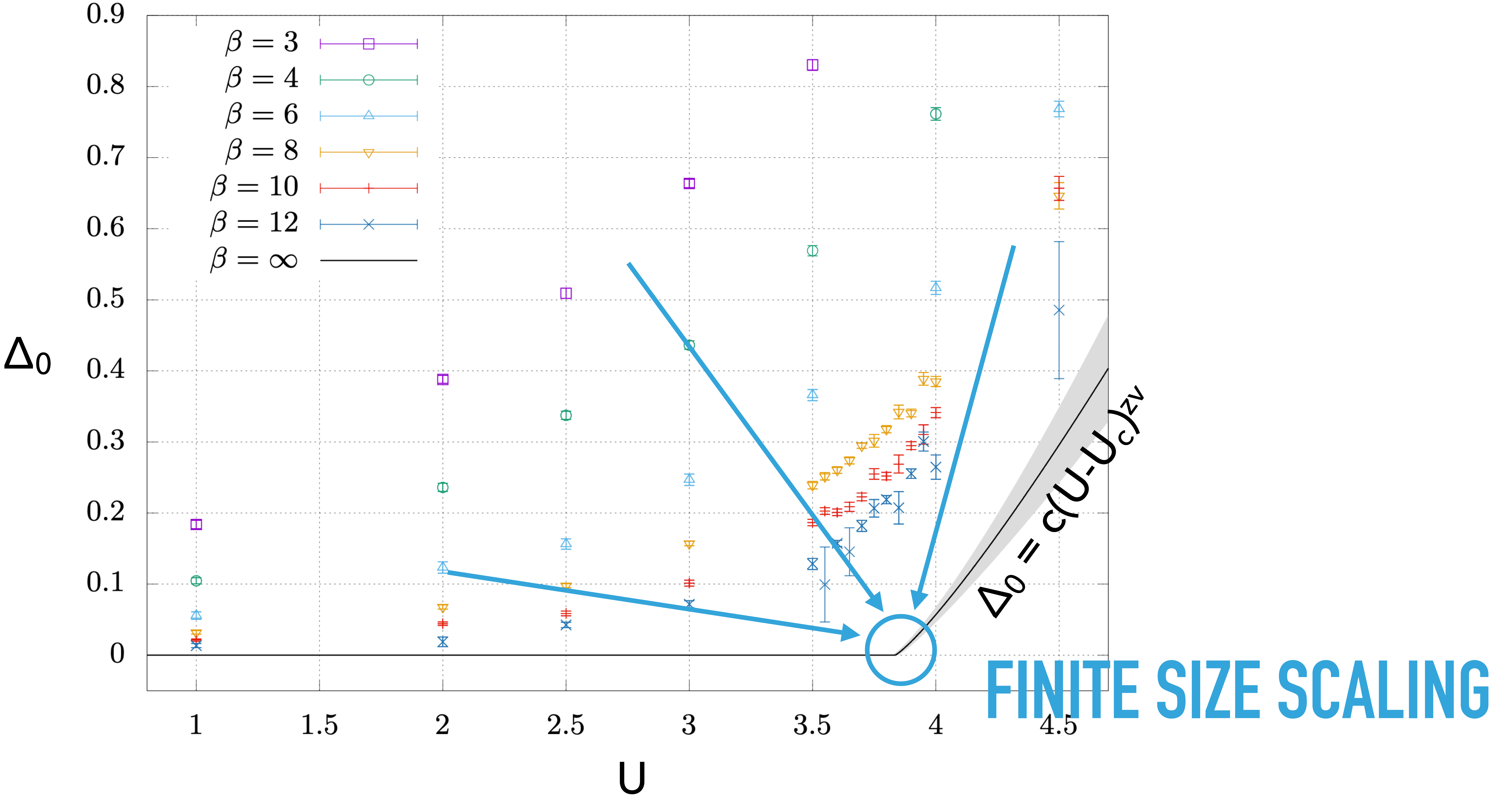
SEMIMETAL / AFMI TRANSITION

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112



SEMIMETAL / AFMI TRANSITION

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112

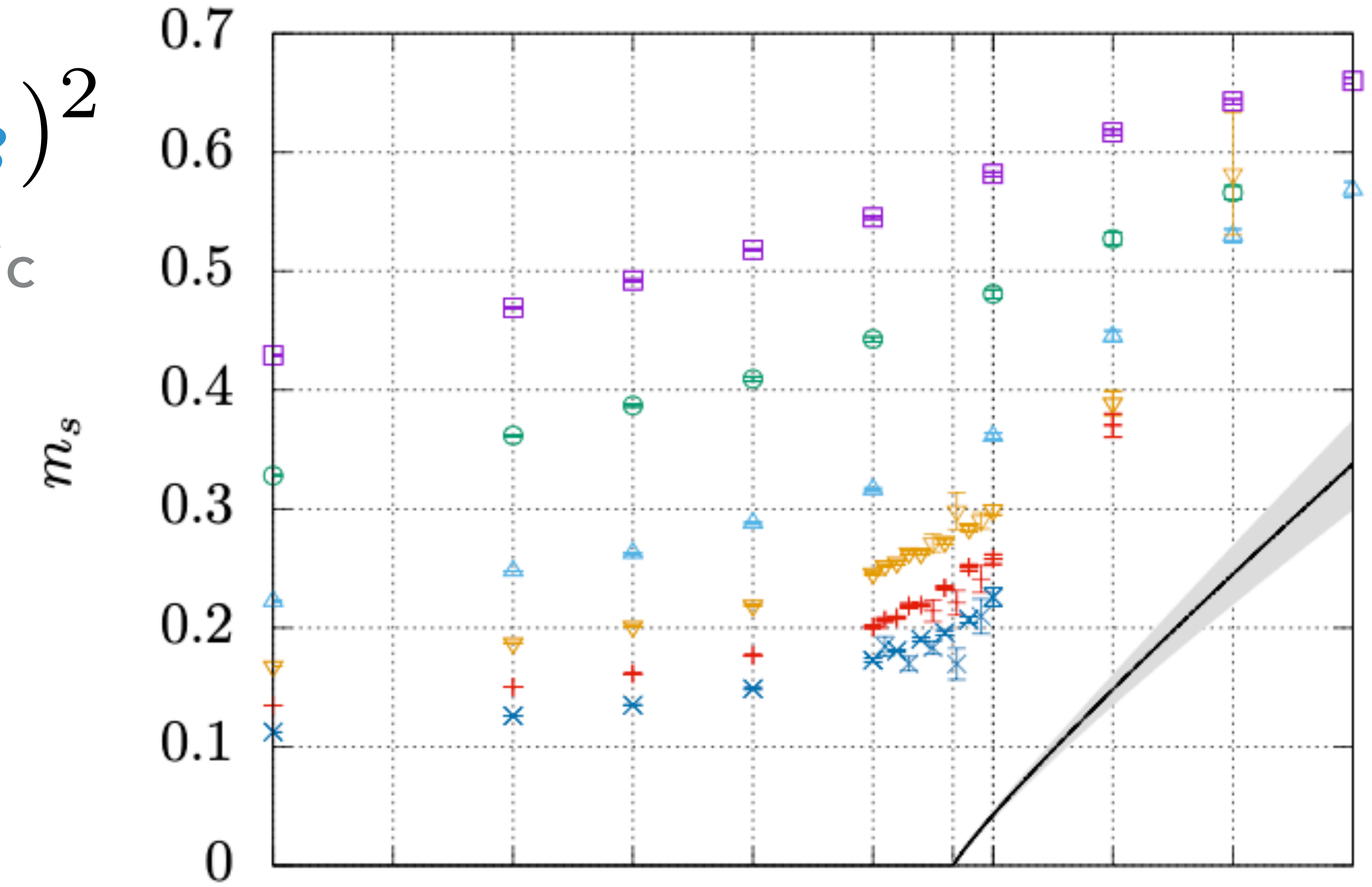


ZERO-TEMPERATURE LIMIT

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2105.06936

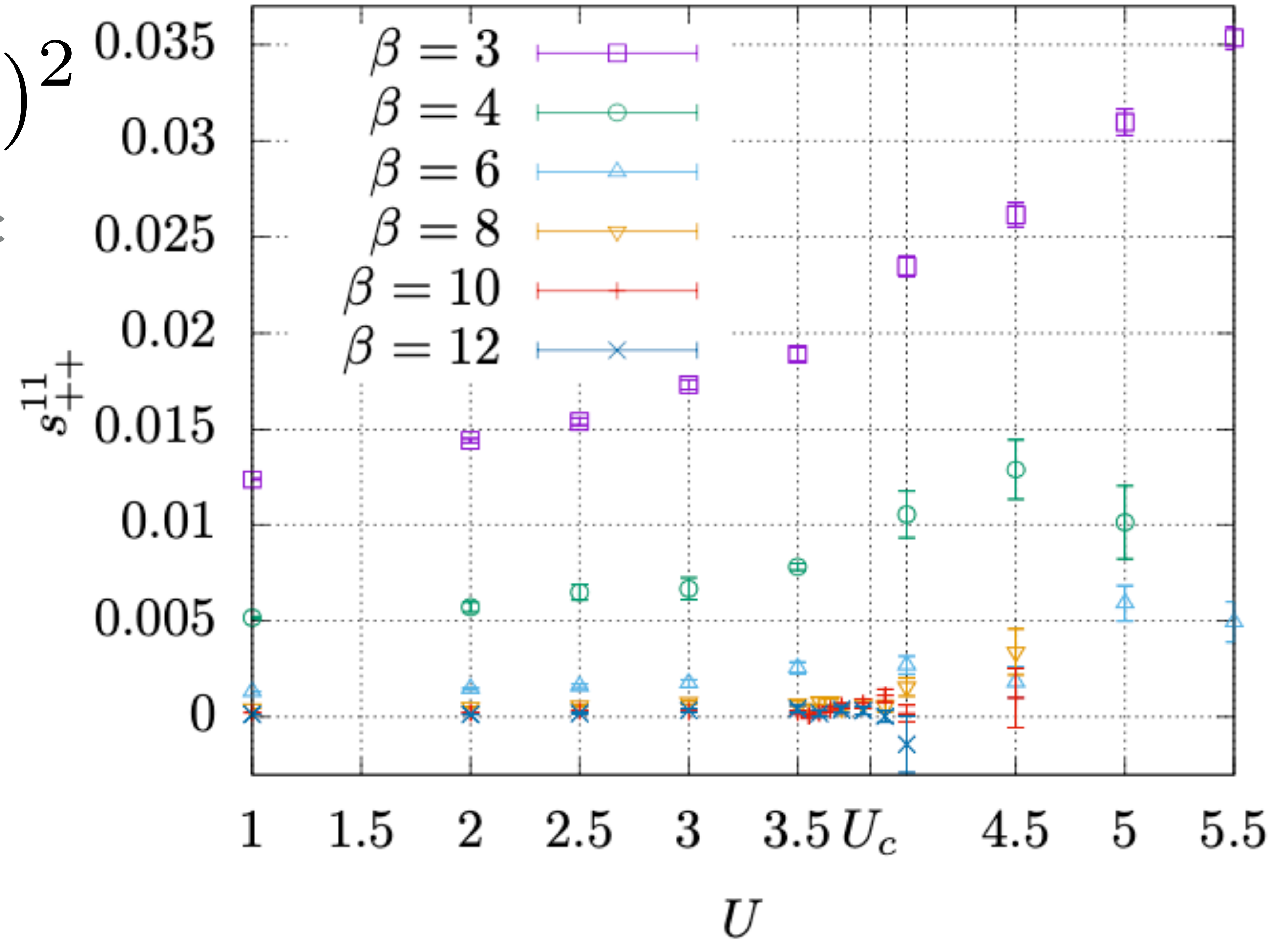
$\sim (\vec{S}_A - \vec{S}_B)^2$

antiferromagnetic



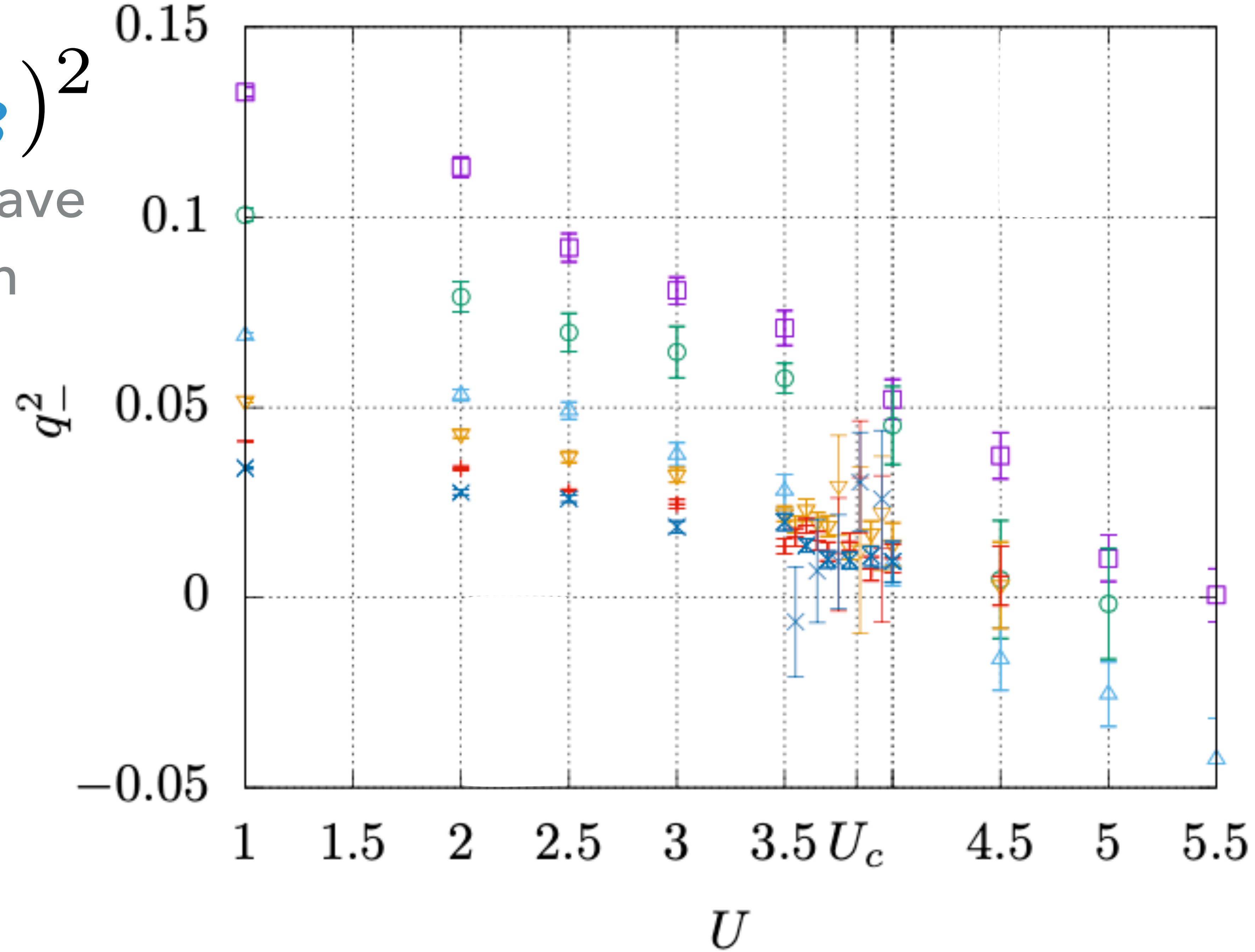
$\sim (\vec{S}_A + \vec{S}_B)^2$

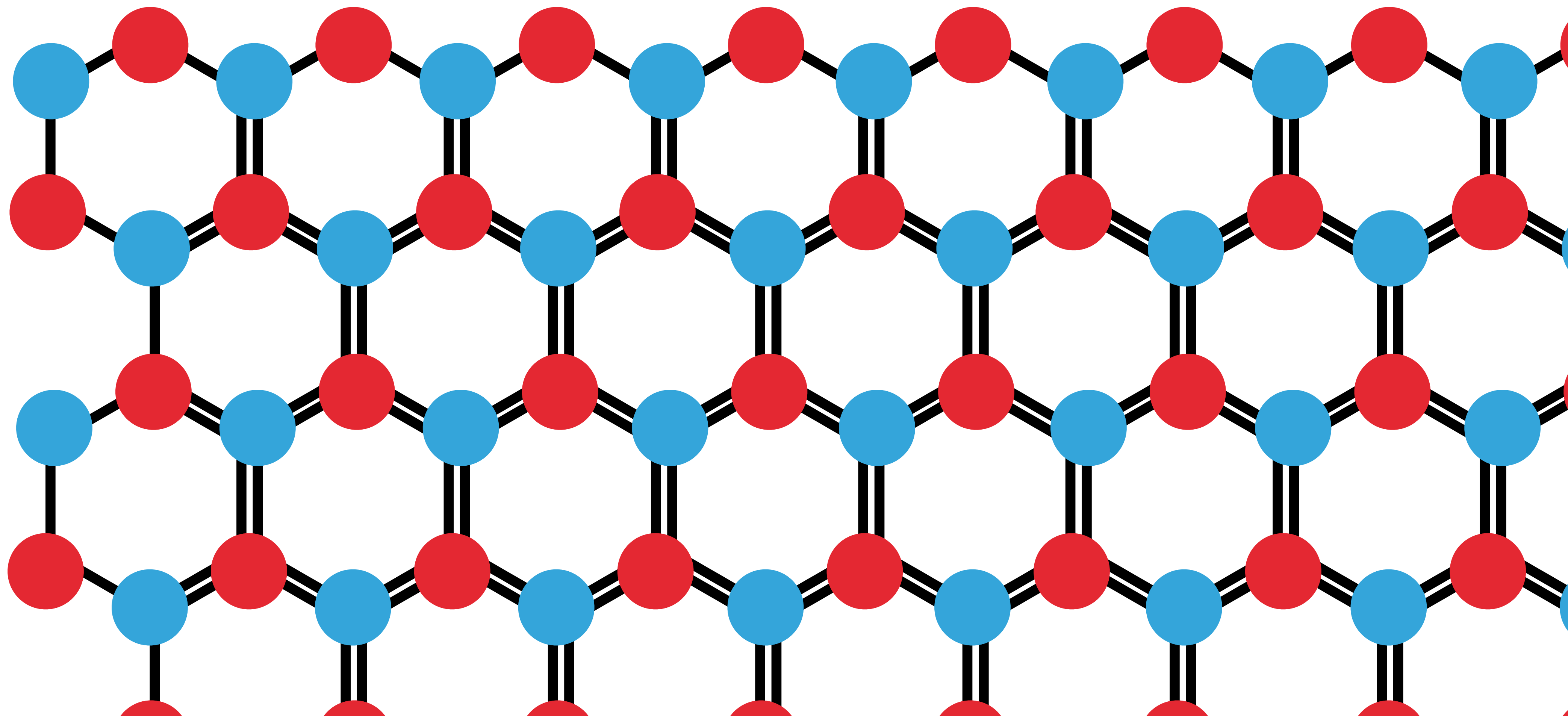
ferromagnetic



$\sim (\vec{Q}_A - \vec{Q}_B)^2$

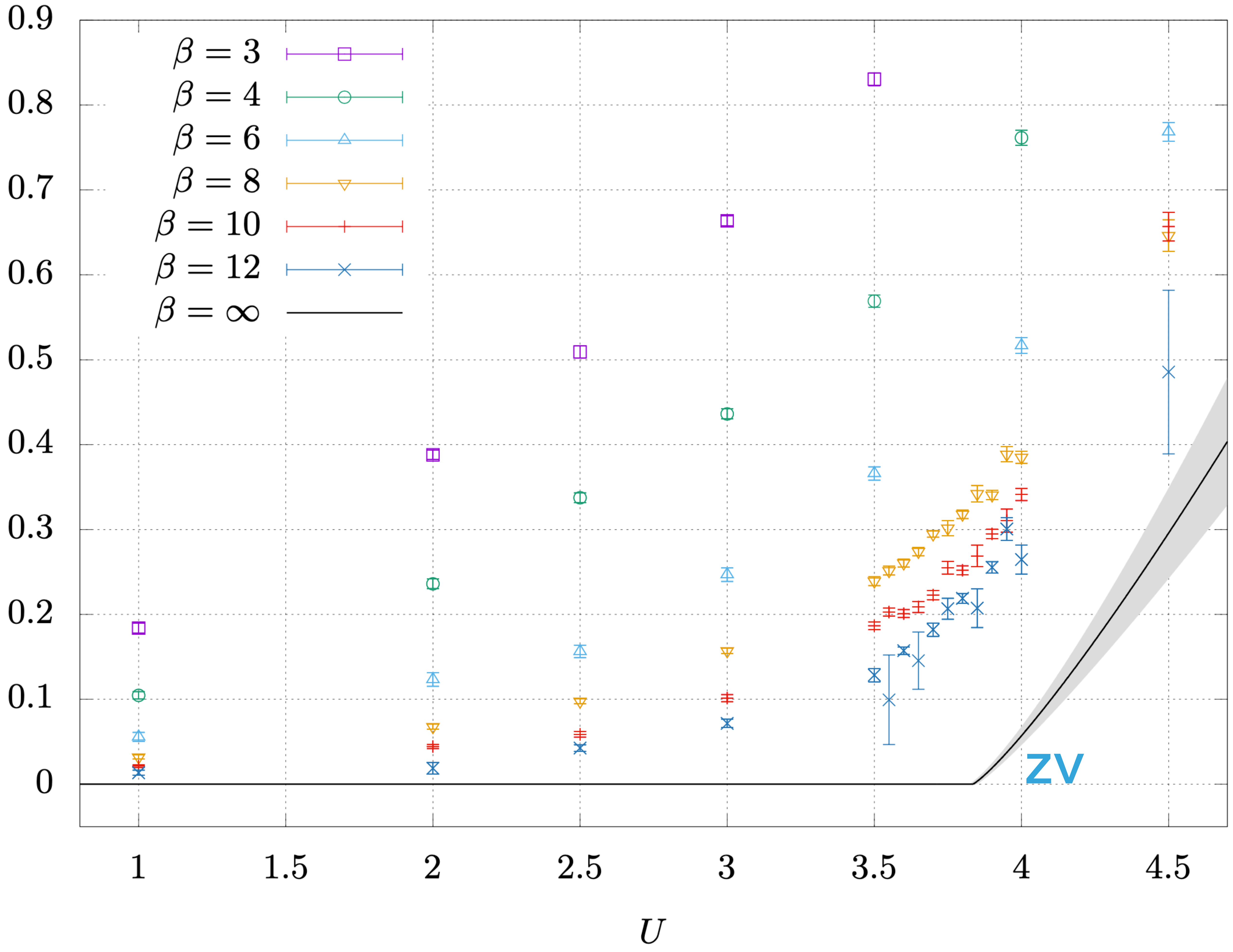
charge-density wave
charge separation



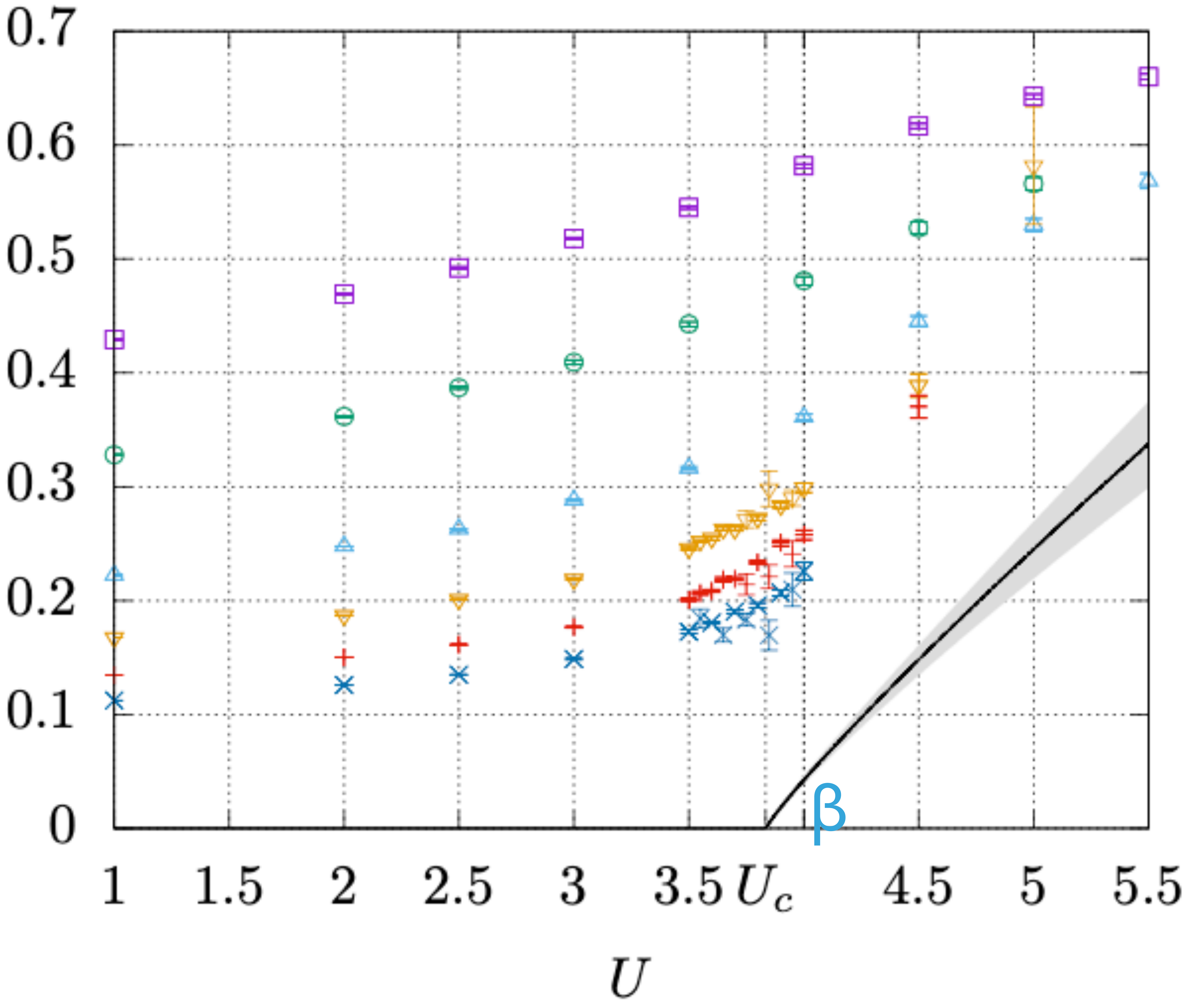


THE PHASE TRANSITION

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112
2105.06936



Δ_0



$\sim (\vec{S}_A - \vec{S}_B)^2$

antiferromagnetic

PHASE DIAGRAM

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112
2105.06936

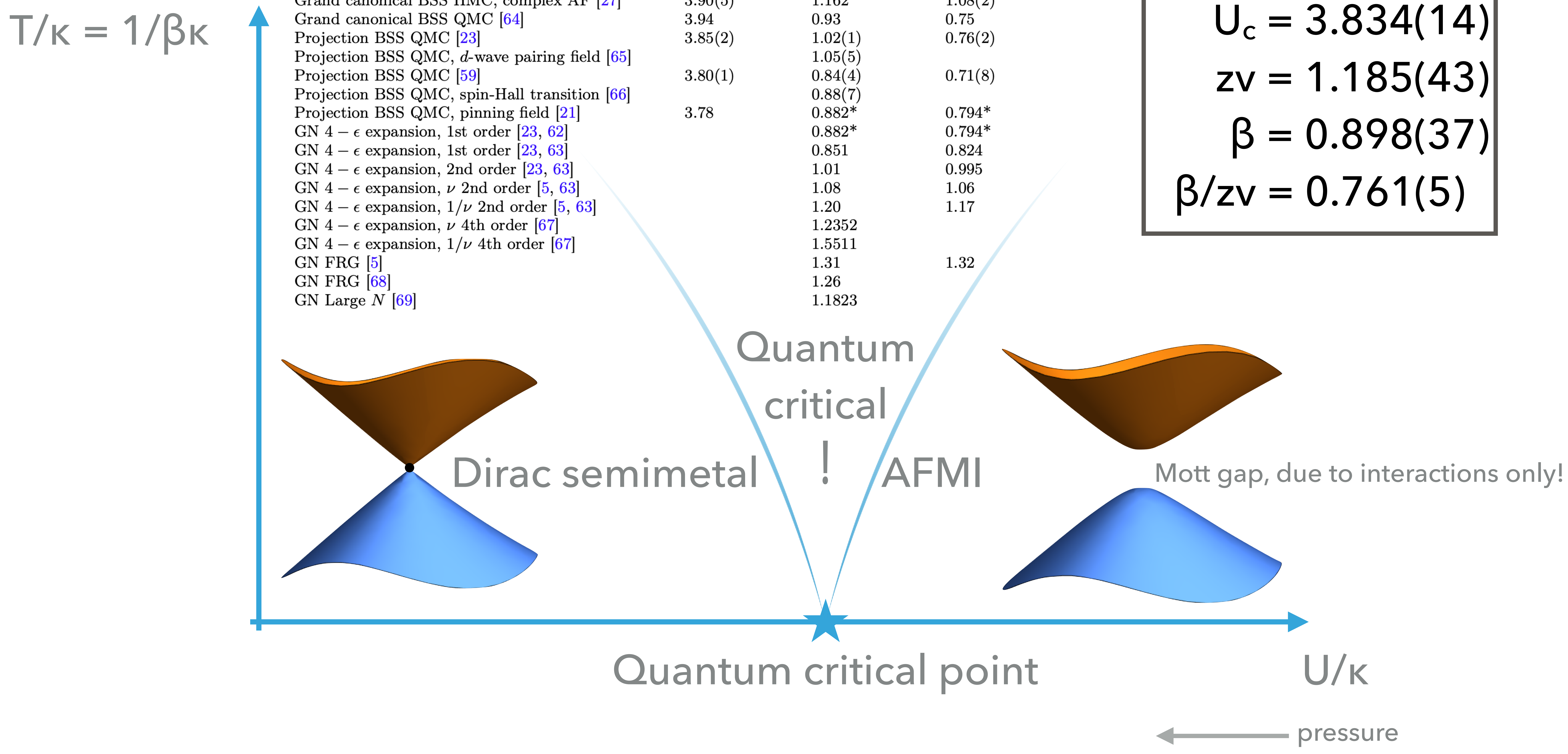
Method	U_c/κ	ν	β
Grand canonical BRS HMC (present work)	3.834(14)	1.185(43)†	1.095(37)‡
Grand canonical BSS HMC, complex AF [27]	3.90(5)	1.162	1.08(2)
Grand canonical BSS QMC [64]	3.94	0.93	0.75
Projection BSS QMC [23]	3.85(2)	1.02(1)	0.76(2)
Projection BSS QMC, *d*-wave pairing field [65]		1.05(5)	
Projection BSS QMC [59]	3.80(1)	0.84(4)	0.71(8)
Projection BSS QMC, spin-Hall transition [66]		0.88(7)	
Projection BSS QMC, pinning field [21]	3.78	0.882*	0.794*
GN $4-\epsilon$ expansion, 1st order [23, 62]		0.882*	0.794*
GN $4-\epsilon$ expansion, 1st order [23, 63]		0.851	0.824
GN $4-\epsilon$ expansion, 2nd order [23, 63]		1.01	0.995
GN $4-\epsilon$ expansion, ν 2nd order [5, 63]		1.08	1.06
GN $4-\epsilon$ expansion, $1/\nu$ 2nd order [5, 63]		1.20	1.17
GN $4-\epsilon$ expansion, ν 4th order [67]		1.2352	
GN $4-\epsilon$ expansion, $1/\nu$ 4th order [67]		1.5511	
GN FRG [5]		1.31	1.32
GN FRG [68]		1.26	
GN Large N [69]		1.1823	

$U_c = 3.834(14)$

$z\nu = 1.185(43)$

$\beta = 0.898(37)$

$\beta/z\nu = 0.761(5)$

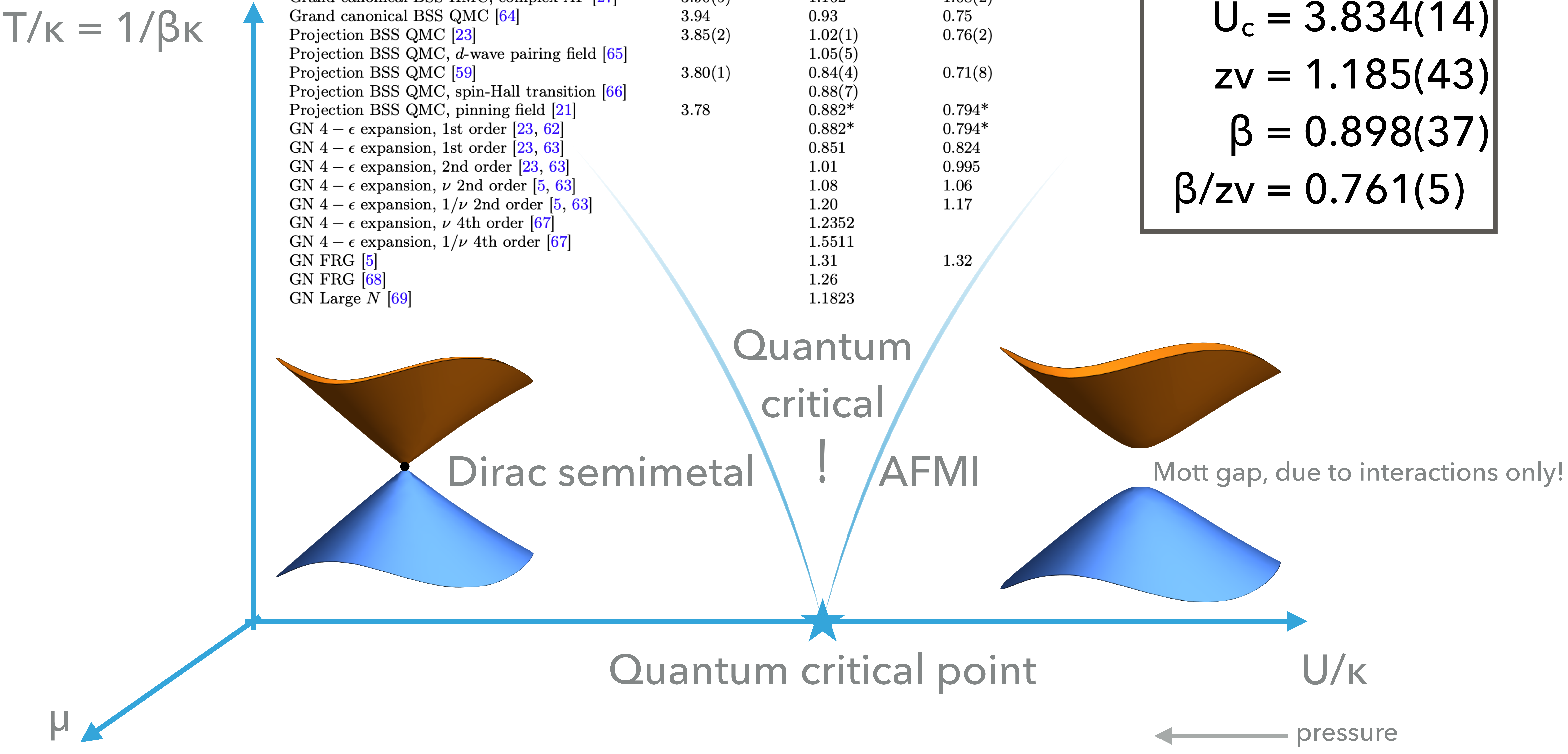


BEYOND HALF FILLING?

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112
2105.06936

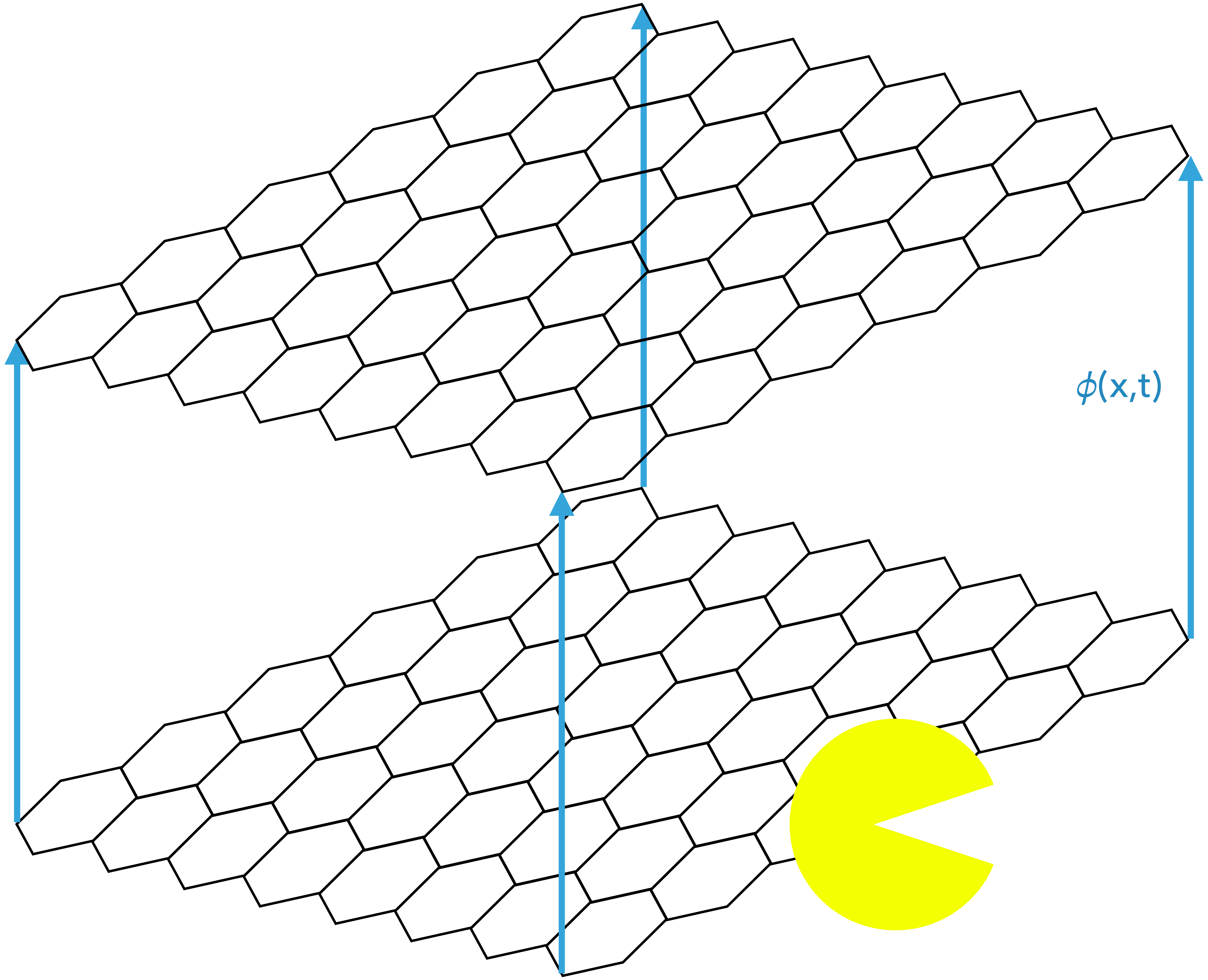
Method	U_c/κ	ν	β
Grand canonical BRS HMC (present work)	3.834(14)	1.185(43)†	1.095(37)‡
Grand canonical BSS HMC, complex AF [27]	3.90(5)	1.162	1.08(2)
Grand canonical BSS QMC [64]	3.94	0.93	0.75
Projection BSS QMC [23]	3.85(2)	1.02(1)	0.76(2)
Projection BSS QMC, *d*-wave pairing field [65]		1.05(5)	
Projection BSS QMC [59]	3.80(1)	0.84(4)	0.71(8)
Projection BSS QMC, spin-Hall transition [66]		0.88(7)	
Projection BSS QMC, pinning field [21]	3.78	0.882*	0.794*
GN $4-\epsilon$ expansion, 1st order [23, 62]		0.882*	0.794*
GN $4-\epsilon$ expansion, 1st order [23, 63]		0.851	0.824
GN $4-\epsilon$ expansion, 2nd order [23, 63]		1.01	0.995
GN $4-\epsilon$ expansion, ν 2nd order [5, 63]		1.08	1.06
GN $4-\epsilon$ expansion, $1/\nu$ 2nd order [5, 63]		1.20	1.17
GN $4-\epsilon$ expansion, ν 4th order [67]		1.2352	
GN $4-\epsilon$ expansion, $1/\nu$ 4th order [67]		1.5511	
GN FRG [5]		1.31	1.32
GN FRG [68]		1.26	
GN Large N [69]		1.1823	

$U_c = 3.834(14)$
$z\nu = 1.185(43)$
$\beta = 0.898(37)$
$\beta/z\nu = 0.761(5)$



SIGN PROBLEMS

IMPORTANCE SAMPLING THE PATH INTEGRAL



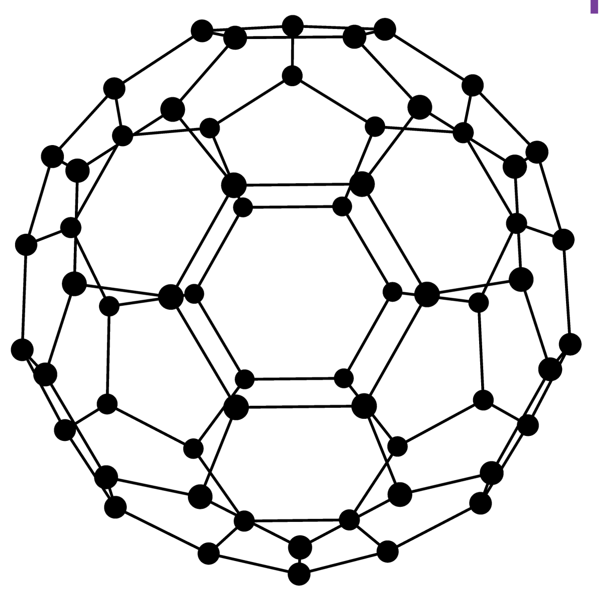
$$\mathcal{Z} \propto \int \mathcal{D}\phi \det\left(M[\phi, h, \mu]\; M^\dagger[\phi, h, -\mu]\right) e^{-\frac{1}{2}\sum_{xyt}\phi_{xt}V^{-1}_{xy}\phi_{yt}}$$

Probability?

$$\mathcal{Z} \propto \int \mathcal{D}\phi \det\left(M[+\phi, +h, +\mu]M[-\phi, -h, -\mu]\right) e^{-\frac{1}{2}\phi V^{-1}\phi}$$

Trade for M†[+φ, ...]

Flip on a bipartite lattice



No problem in the bipartite μ=0 case.

$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} e^{-iS^I}\rangle_R}{\langle e^{-iS^I}\rangle_R}$$

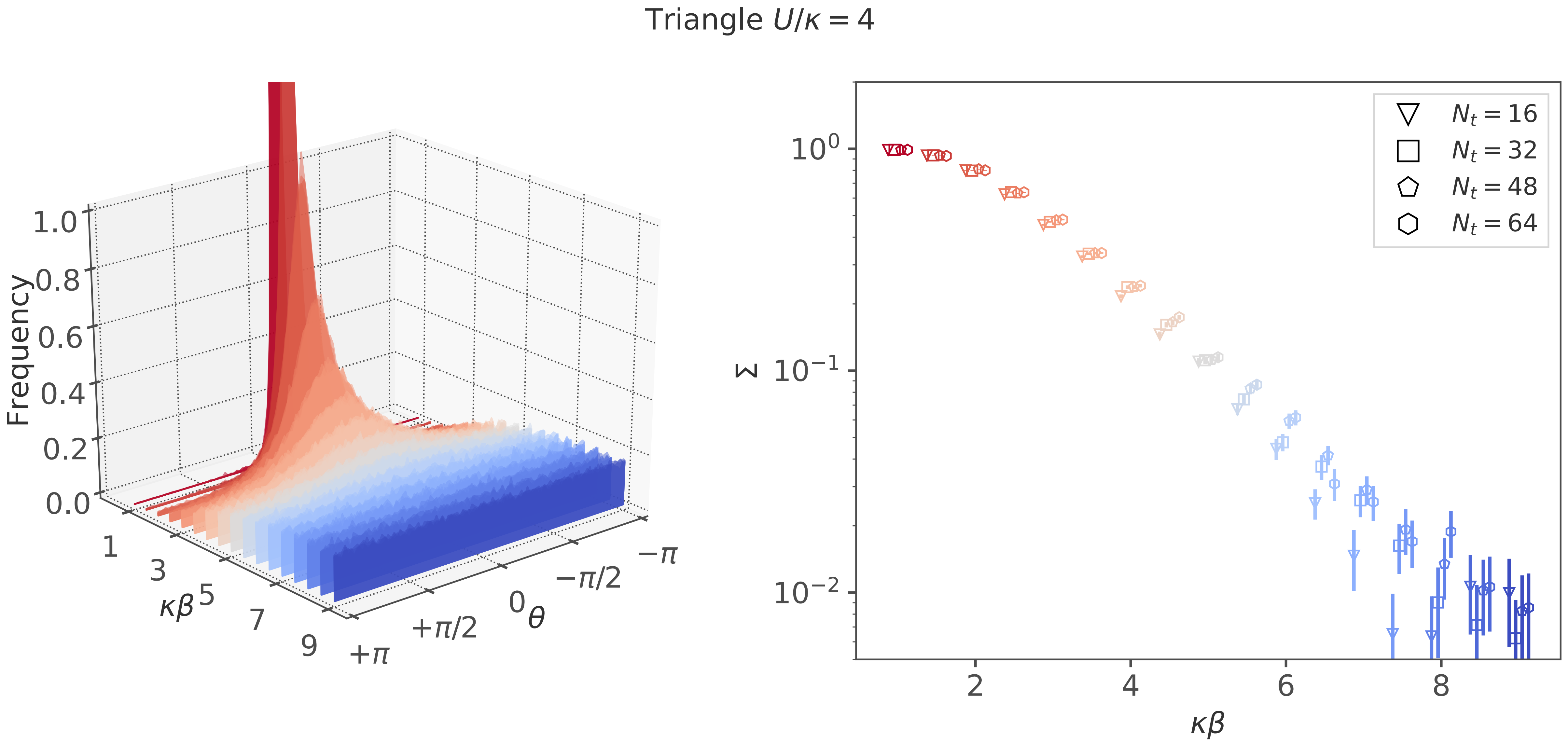
The average sign, or *statistical power* $\Sigma = \left|\langle e^{-iS^I}\rangle_R\right|$

COMPLEX WEIGHTS LEAD TO SIGN PROBLEMS

The average sign, or *statistical power* Σ

$$\Sigma = \left| \langle e^{-iS^I} \rangle_R \right|$$

is the ratio of two partition functions ~ differences of free energies
so is extensive in spacetime volume → exponentially decays



$$\mathcal{Z} \propto \int \mathcal{D}\phi \det\left(M[\phi, h, \mu]\, M^\dagger[\phi, h, -\mu]\right) e^{-\frac{1}{2}\sum_{xyt} \phi_{xt} V^{-1}_{xy} \phi_{yt}}$$

Probability?

Generate an *ensemble* for fixed U, β, N_t, ...

$$\{\phi_1,\ \phi_2,\ \cdots,\ \phi_N\}$$

Hybrid Monte Carlo

Estimate any observable

$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} e^{-iS^I} \rangle_R}{\langle e^{-iS^I} \rangle_R}$$

Importance sample according to the real part of the weight

Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221

SIGN OPTIMIZATION

Pick a simple contour deformation with few parameters λ.

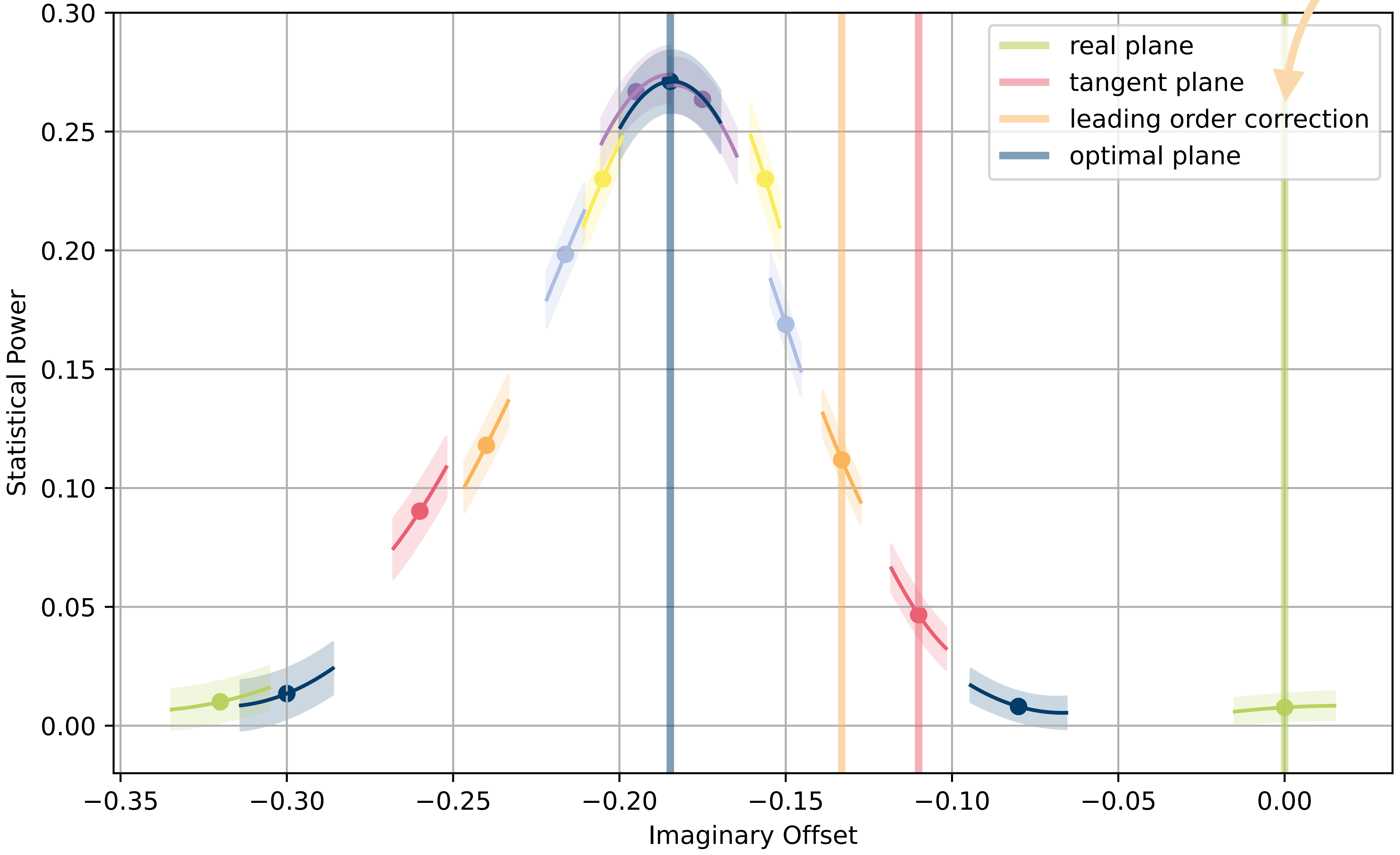
Example: the simplest imaginable deformation; integrate on a plane parallel to $\mathbb{R}^N$ offset by a constant imaginary piece

Gradient of Σ is sign-problem free!

$$\nabla_\lambda \log \Sigma(\lambda) = \left\langle \nabla_\lambda S_R - \mathrm{ReTr}\left[J^{-1}\nabla_\lambda J\right] \right\rangle_R$$

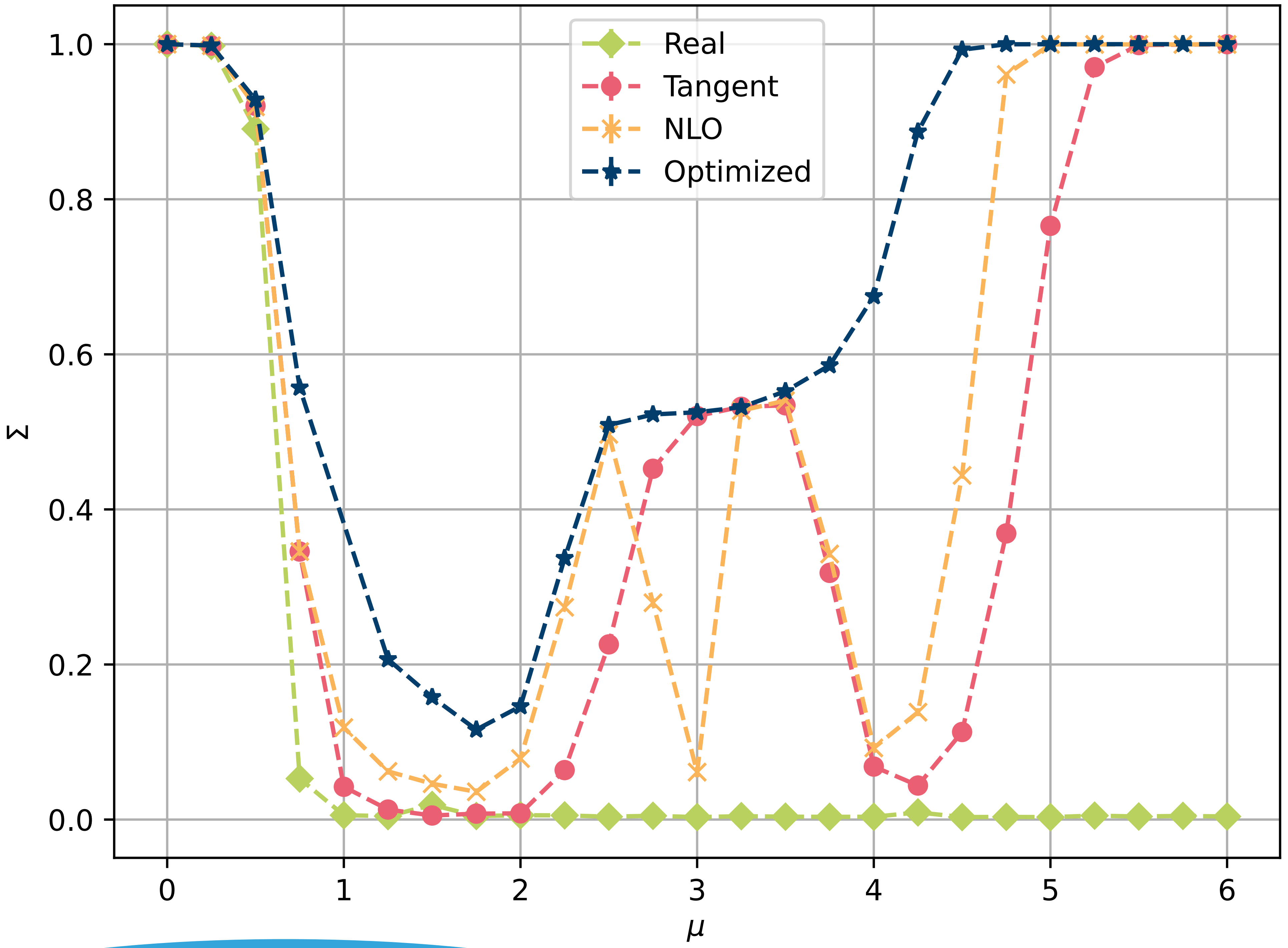
Alexandru, Bedaque, Lamm + Lawrence, PRD 97 094510 (2018)
1804.00697 10.1103/PhysRevD.97.094510

8-site honeycomb N_t=16 β=8 U=2 μ=1



Gäntgen et al. 2208.XXXX

Sort of like the one-loop effective potential



Unsupervised learning?

RESULTS

Gäntgen et al. 2208.XXXX

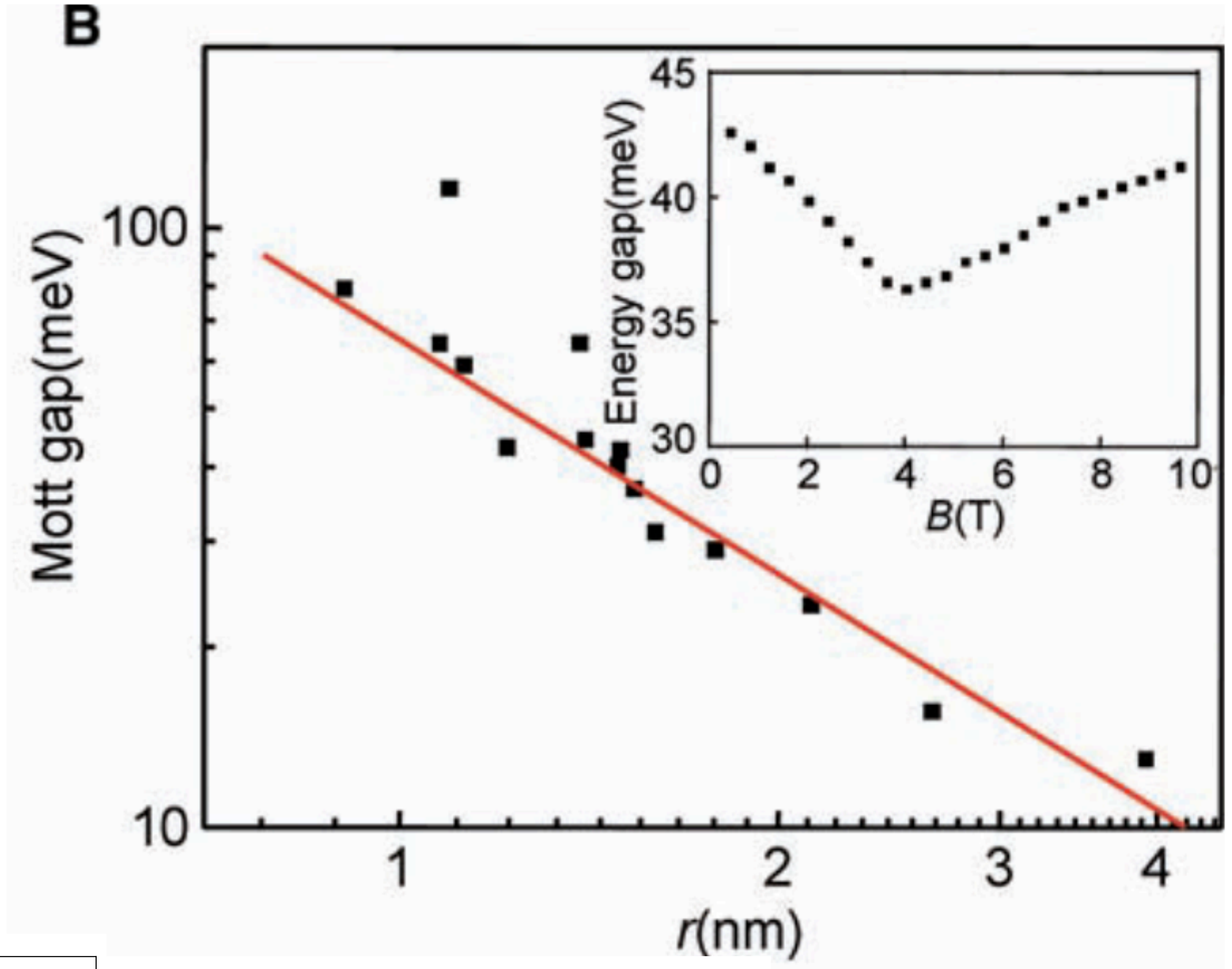
8-site honeycomb N_t=16 β=8 U=2 | C_{20} N_t=32 β=6 U=2 μ=1 | C_{60} N_t=32 β=6 U=2 μ=1

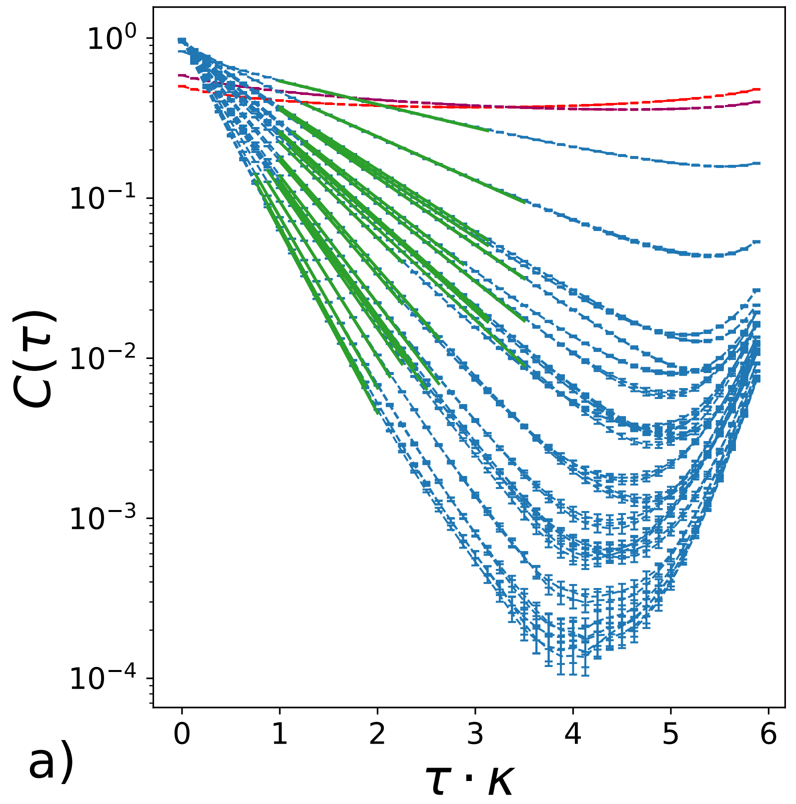
OUTLOOK

Deshpande et al., Science 323 5910 (2009) 10.1126/science.1165799
EB, Körber, Krieg, Labus, Lähde, Luu Lattice 2017 10.1051/epjconf/201817503009 1710.06213
+ work under way

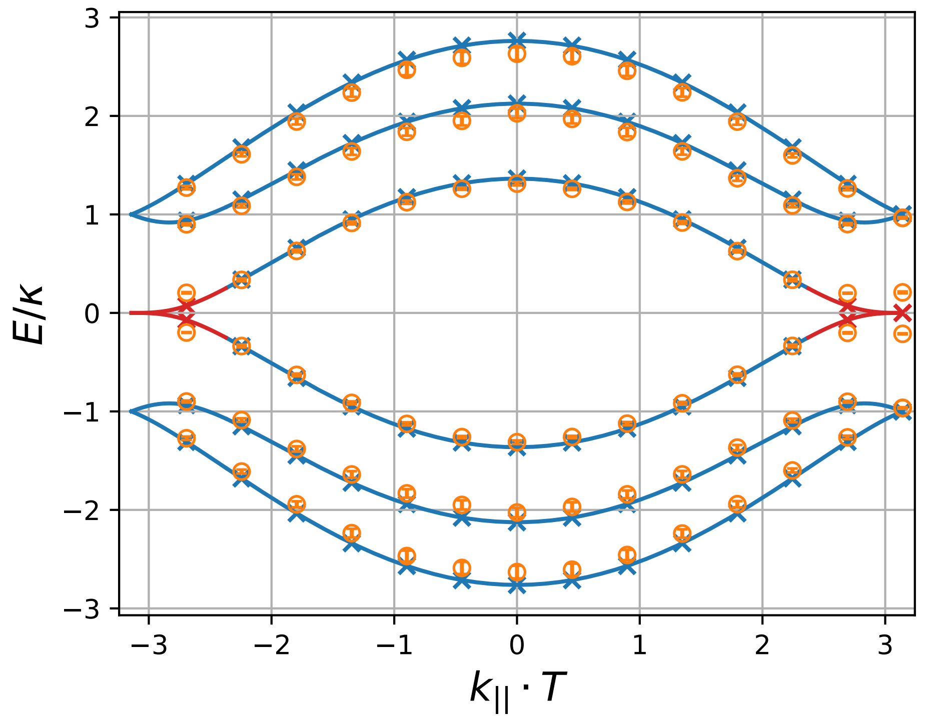
WHAT HUBBARD MODEL BEST DESCRIBES CARBON NANOSTRUCTURES?

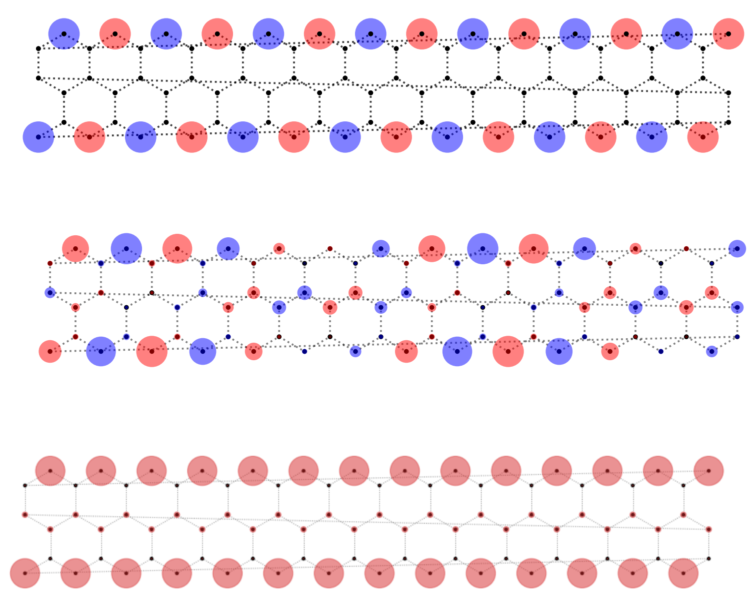
- Directly simulate nanotubes and reproduce the experimentally-observed gap's dependence on radius
- Extrapolate to r = ∞
- Are nonlocal interactions *really* needed? Can we exclude a Hubbard description of graphene from first principles?
- Study 'the' Hubbard graphene, carbon nanostructures, ribbons, topological structures
- DOPE!





a)

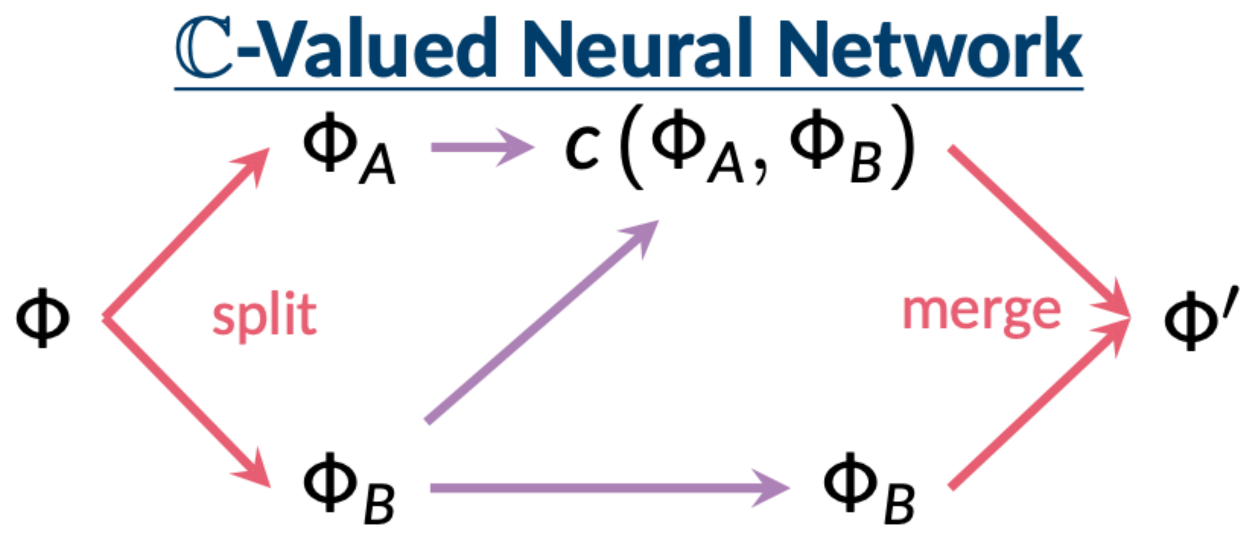




PERYLENE: MOLECULES IN SOLAR CELLS

effort led by Marcel Rodekamp

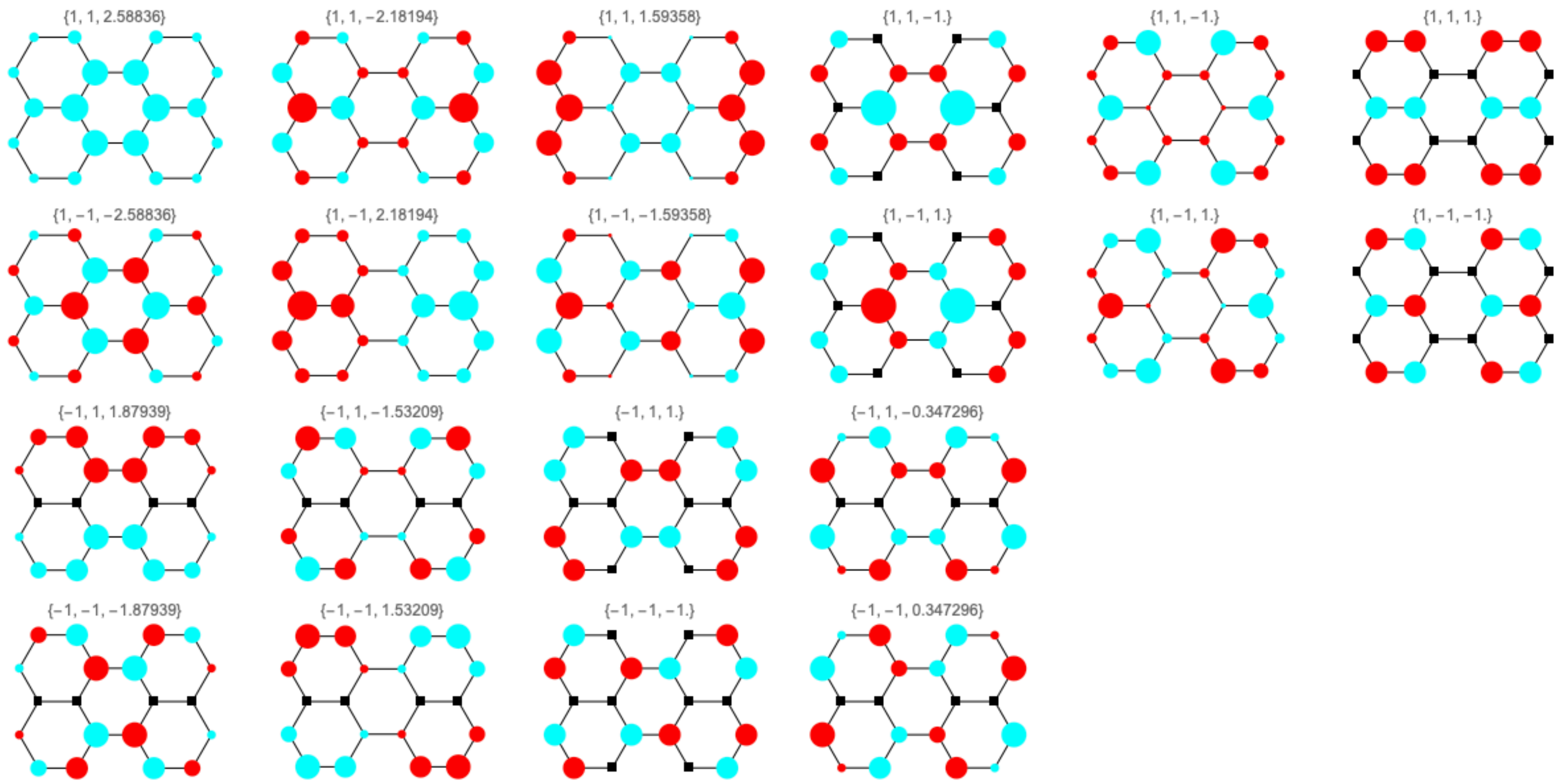
- Current state of the art from chemistry is ~DFT.
- Complex-valued, holomorphic, equivariant networks approximate the holomorphic flow

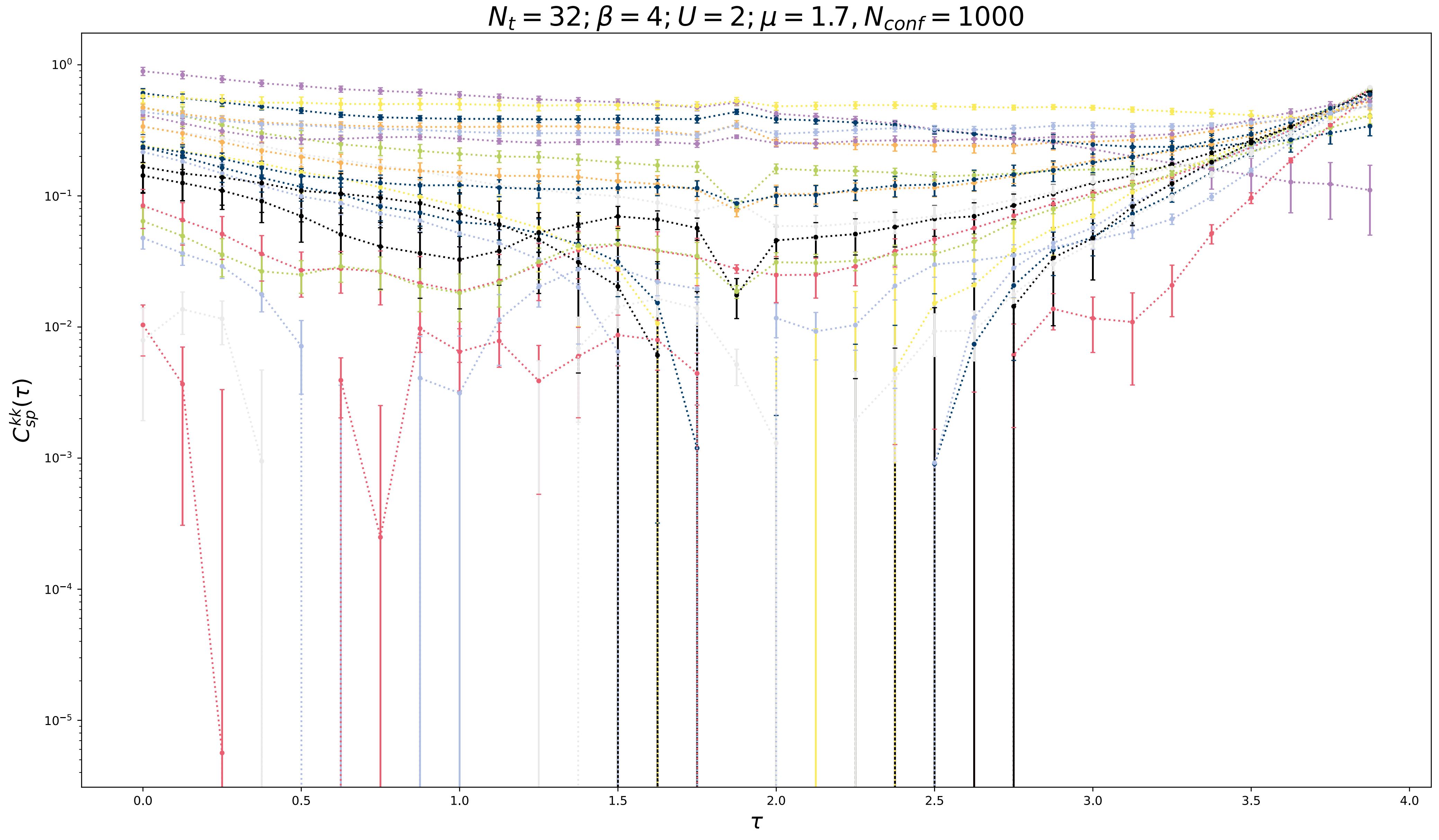


cf. normalizing flows

Alexandru, Bedaque, Lamm, Lawrence, Physical Review D 96, 094505 (2017) 1709.01971
Albergo, Kanwar, Shanahan, PRD 100, 034515 1904.12072
Rodekamp, EB, Gäntgen et al., PRB 106(12):125139 2203.00390

- Can we get the electromagnetic responses with doped molecules?





EQUIVARIANCE WITHOUT THINKING HARD ABOUT GROUP THEORY

$NN : \phi \longrightarrow \phi$ Equivariance: $NN(T\phi) = T\, NN(\phi)$

Time translation, spatial symmetries, ...

Only put 'conventional' φ through the ML

- Enforce a convention - Find t such that $\Sigma_x |\varphi_{xt}|^2$ is maximal; shift by –t.
- Apply network - Weights, biases, nonlinearities
- Undo convention - Shift back by +t.

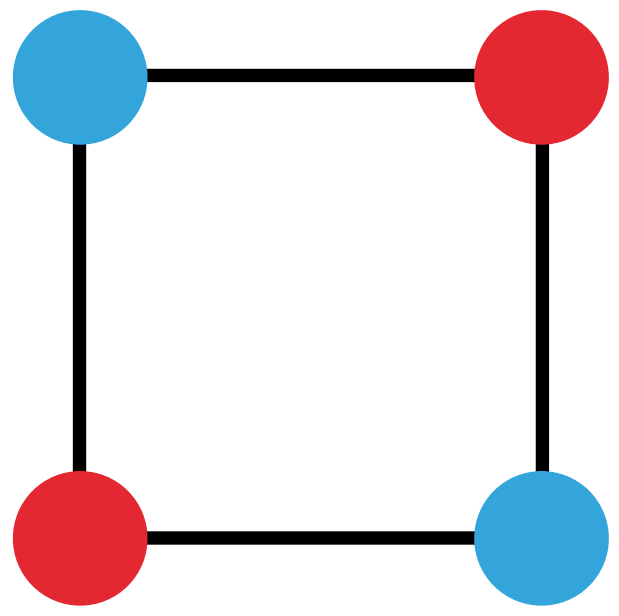
The more prescriptive your convention the more equivariance you enjoy.

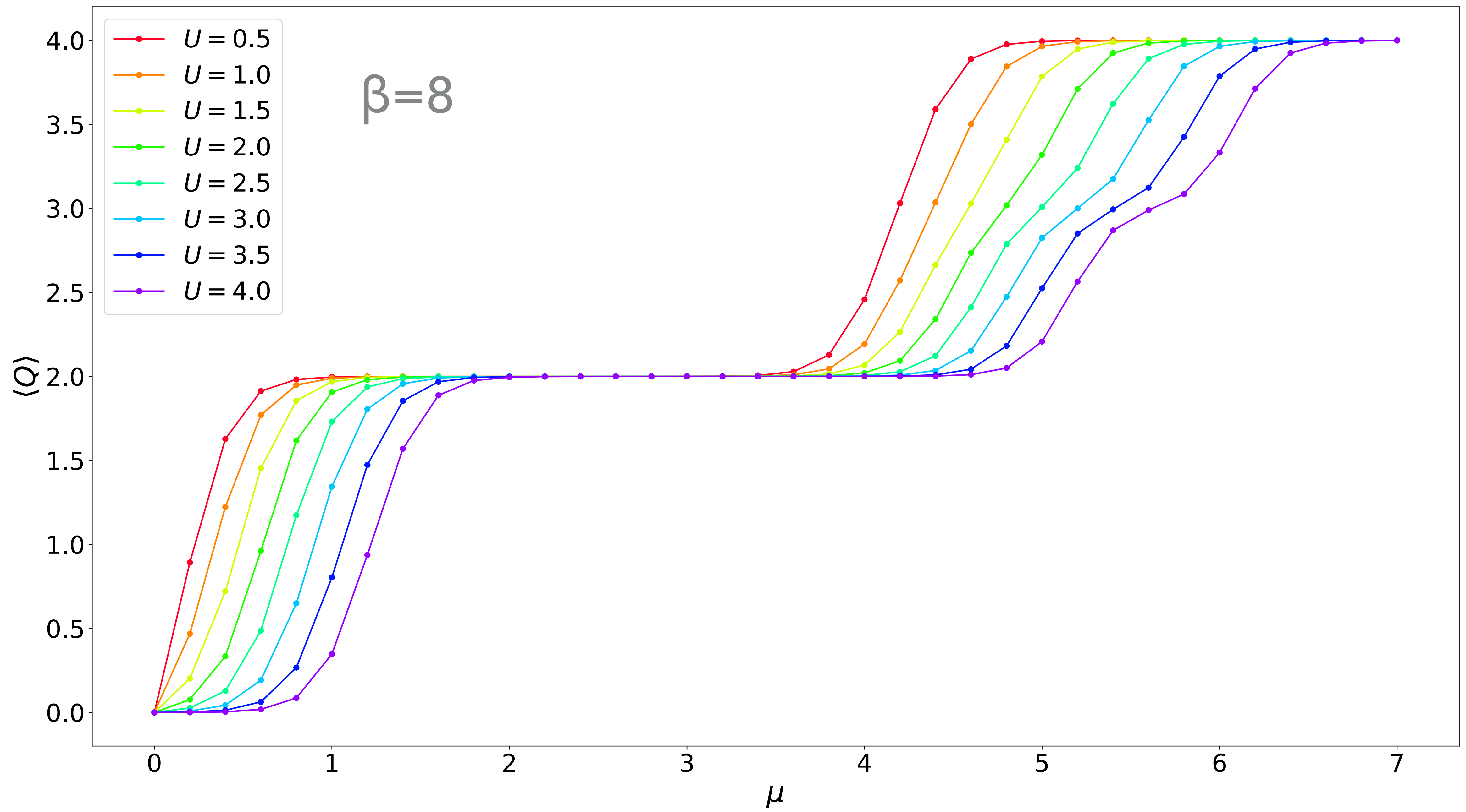
- Better for discrete / global symmetries!
- Annoying for gauge symmetries

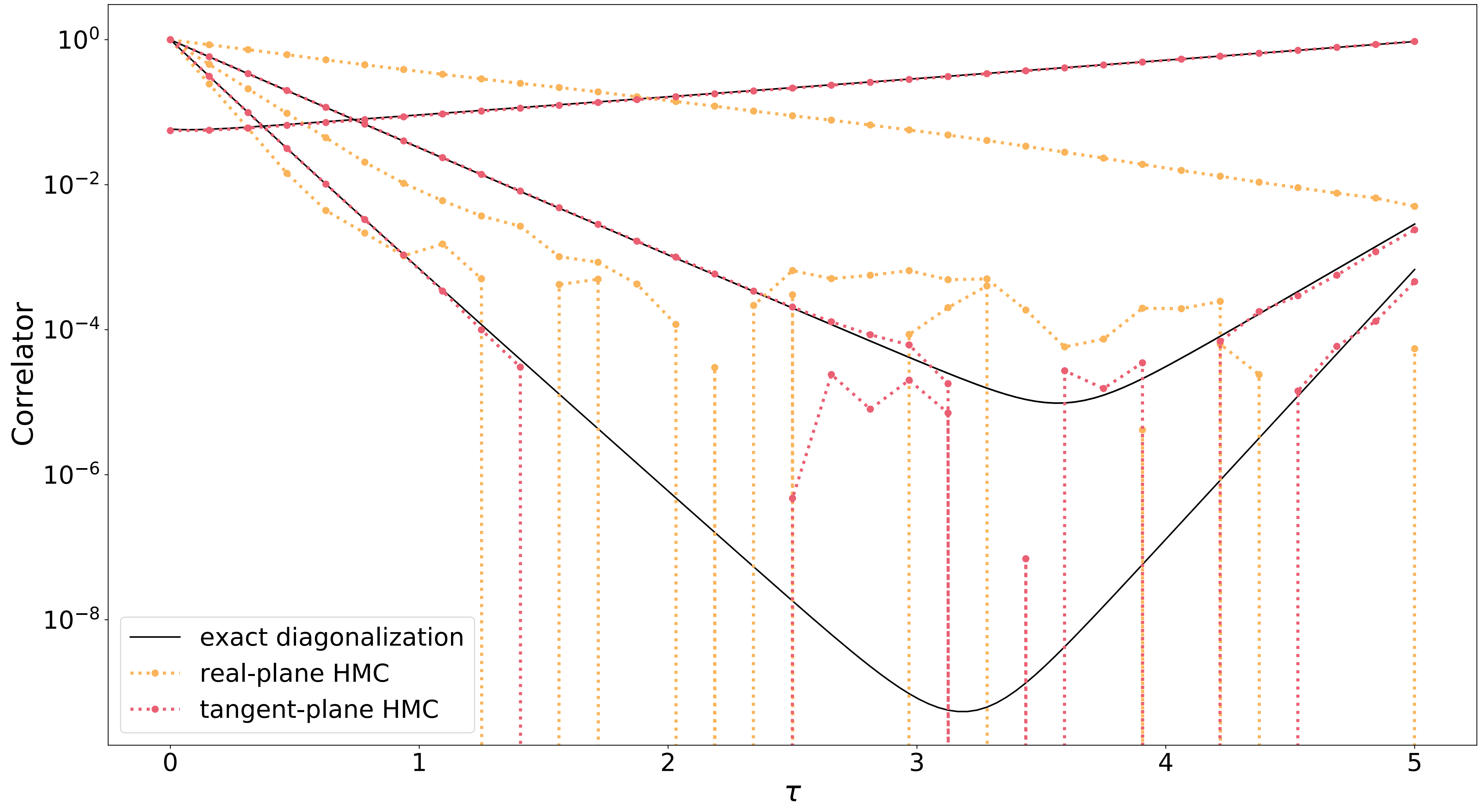
Kanwar et al. PRL 125 121601 (2020)

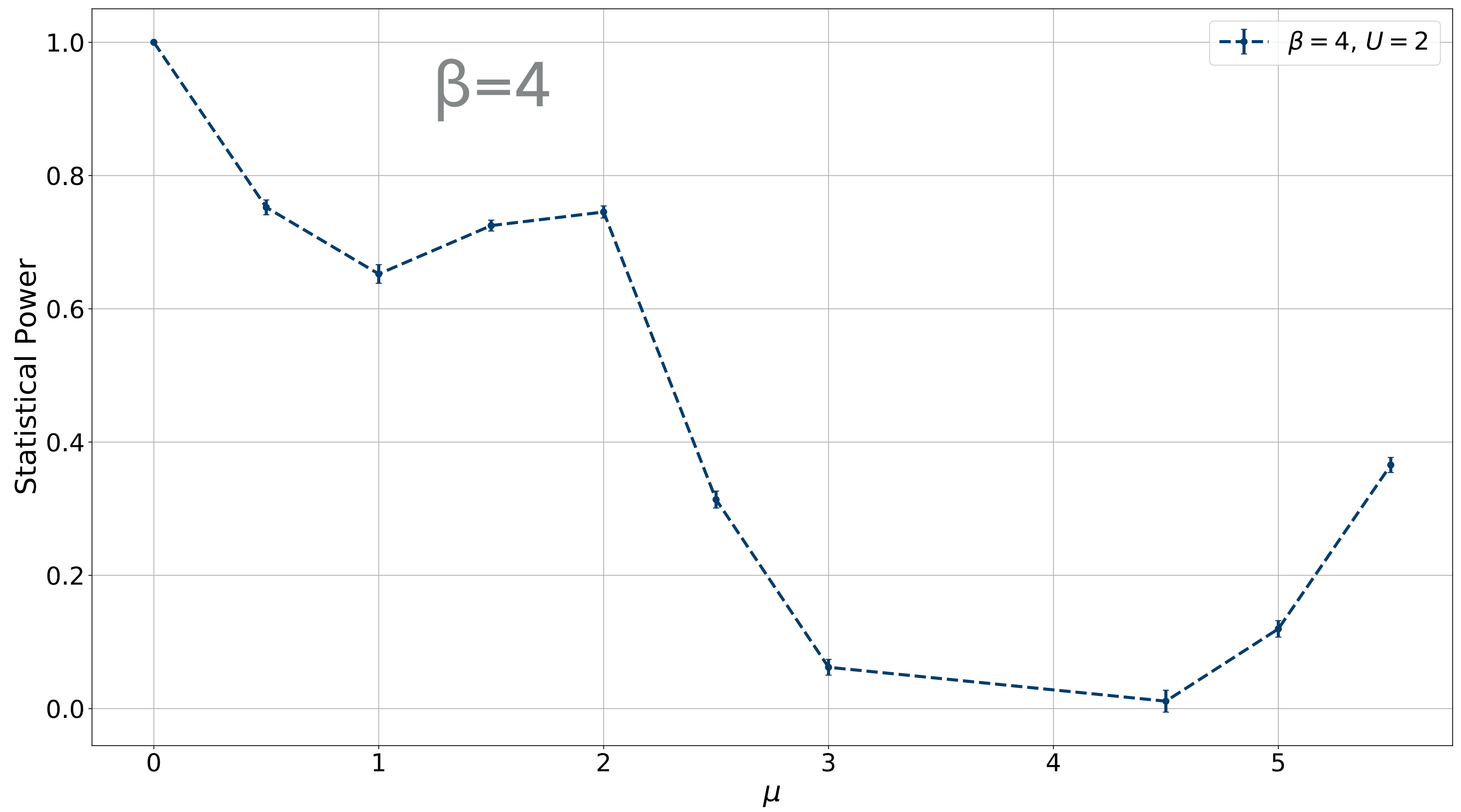
SQUARE LATTICE: HIGH T_C SUPERCONDUCTORS?

Figures taken from C. Gäntgen's master's thesis







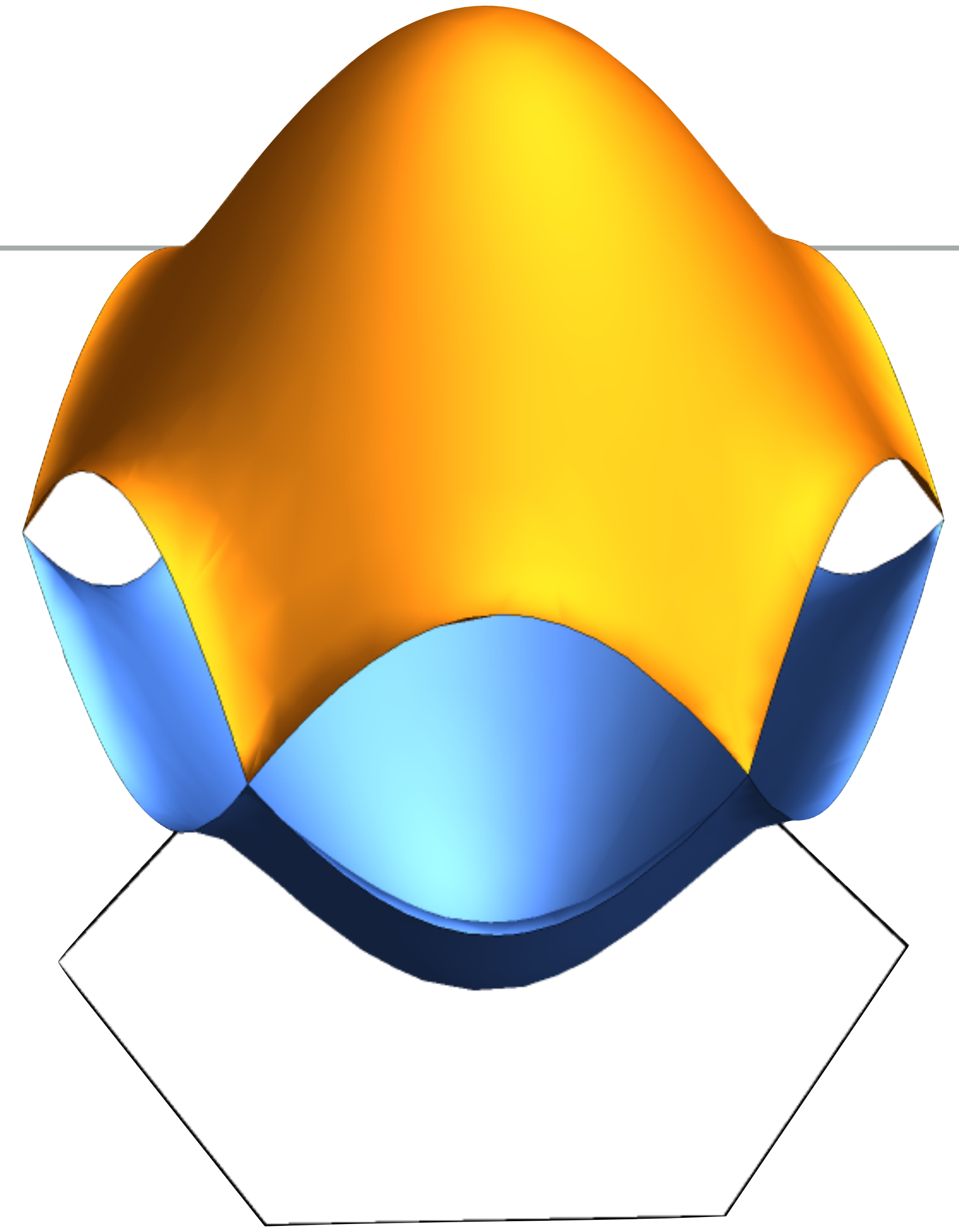


THE HUBBARD MODEL

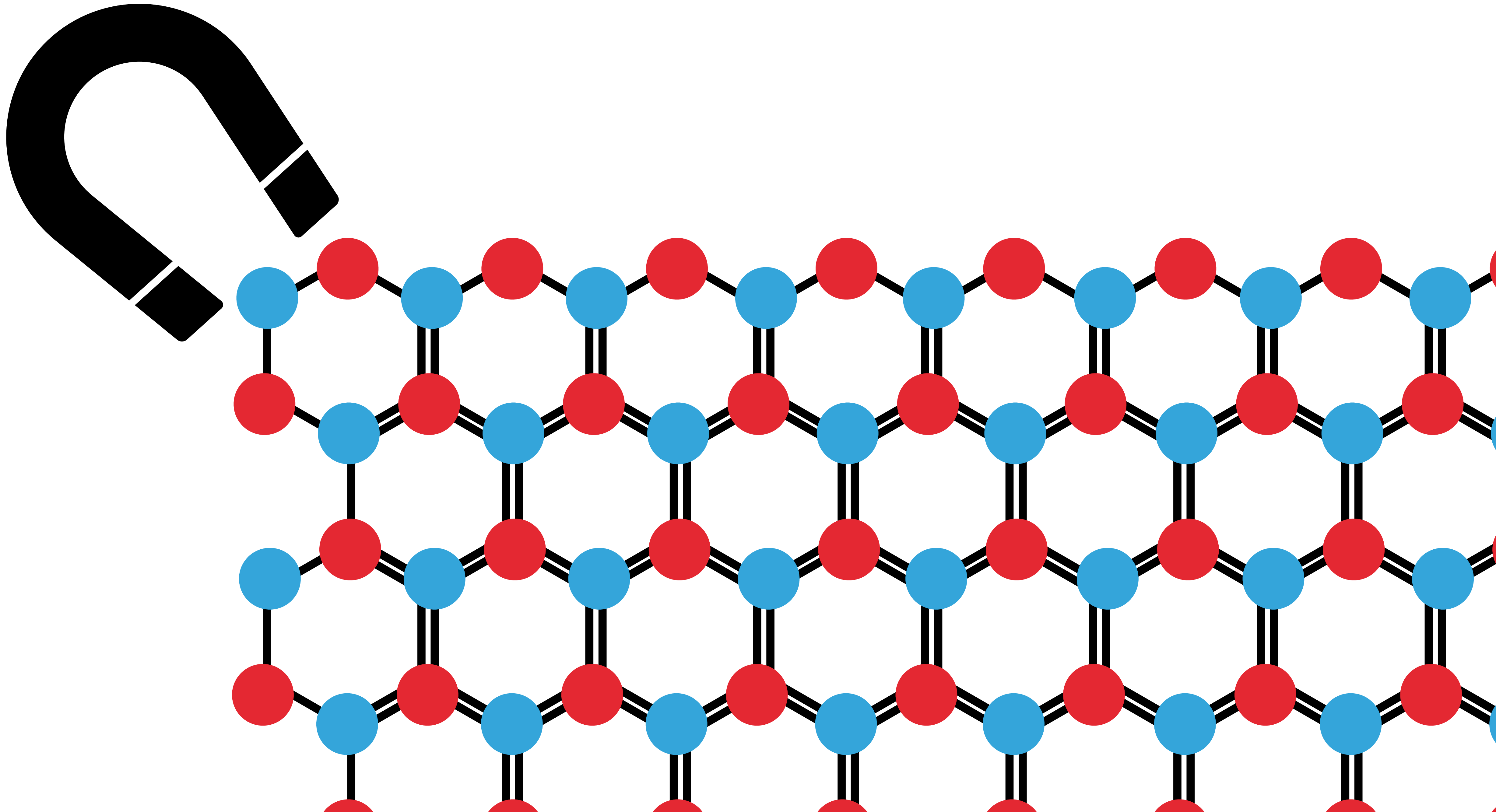
BACKUP SLIDES

OTHER DIRECTIONS

STRUCTURE FACTORS, MATRIX ELEMENTS



- Anomalous dimension
- Measure one-body spectrum, especially near K, K'
- Quasiparticle weight
- Measure momentum-dependence spin-spin structure factors
- Matrix elements!
  Response to magnetic fields, ...



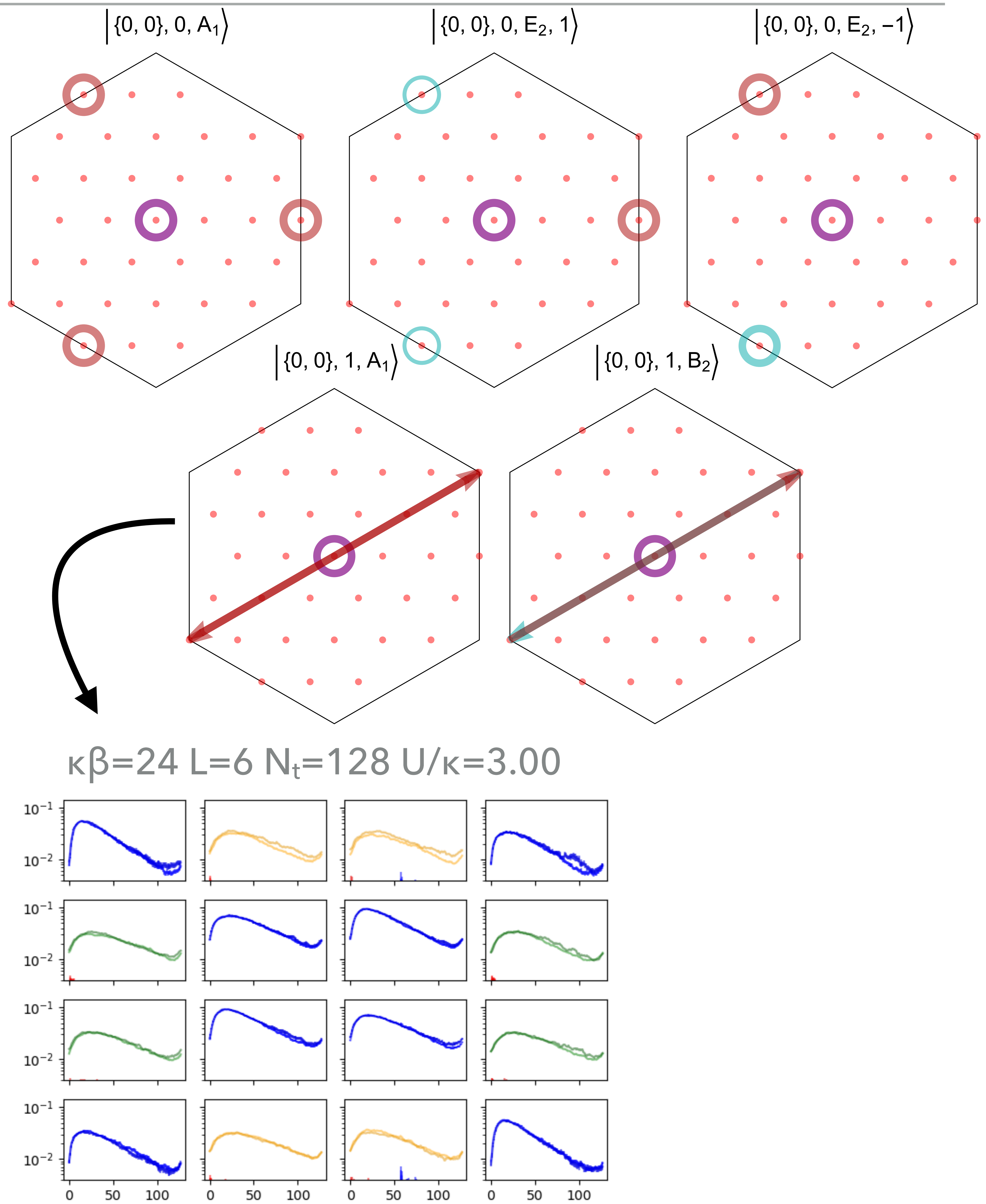
TWO-BODY PHYSICS

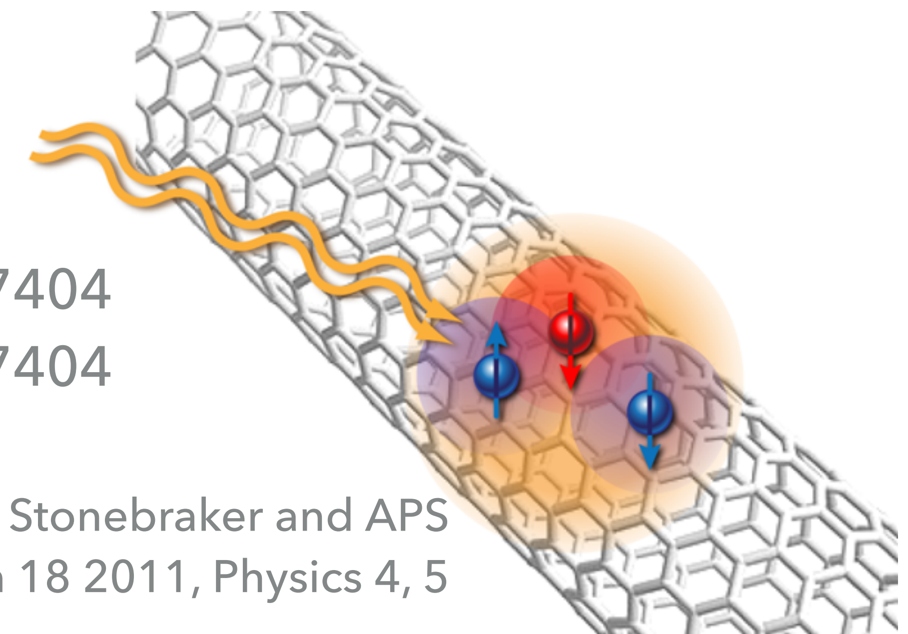
Varsano et al., Nature Communications 8:1461 Science 323 5910 (2009) 10.1038/s41467-017-01660-8
Petar Sinilkov, EB, et al. (2022?)

EXCITONS

- Measure two-body energy levels
- Many states in each sector of total crystal momenta, little group
- Leverage the analog of the finite-volume LQCD formalism (Lüscher's method) for two-body phase shifts.
- Resonances? Bound states?
- … trions?

Matsunaga, Matsuda, and Kanemitsu PRL 106, 037404
10.1103/PhysRevLett.106.037404





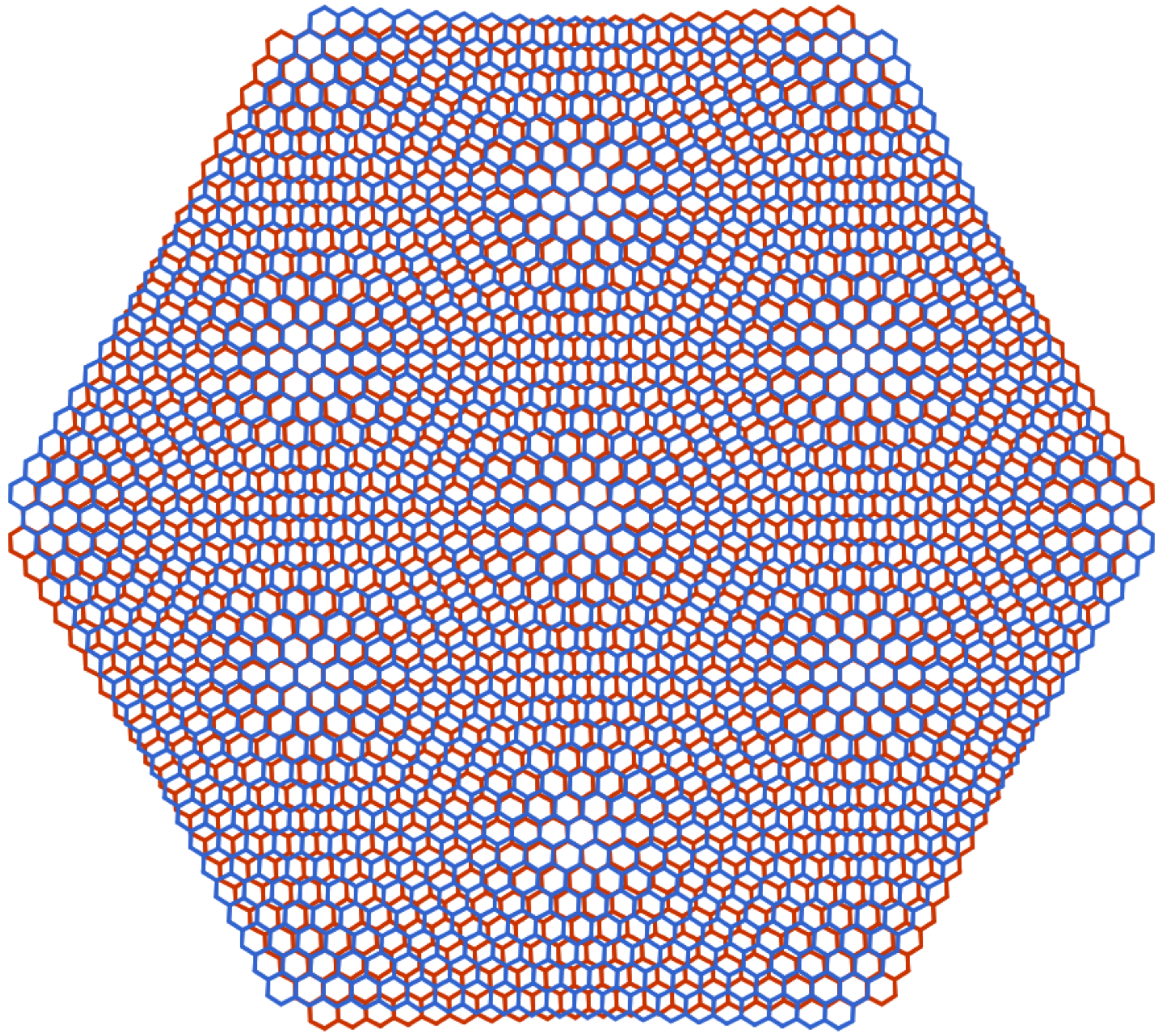
Alan Stonebraker and APS
Jan 18 2011, Physics 4, 5

OTHER MATERIALS / LATTICES

DIRECT EXPLORATION OF HUBBARD SYSTEMS

We can take the temporal continuum limit with $2{\times}102^2$ ~ 20000 ions !

- Add screened Coulomb
- Transition metal oxides (heavy fermions)
- Lanthanide materials (Kondo insulators)
- Perovskites (high-T_c superconductors) on a square / checkerboard lattice
- Magic-angle Moiré superlattices



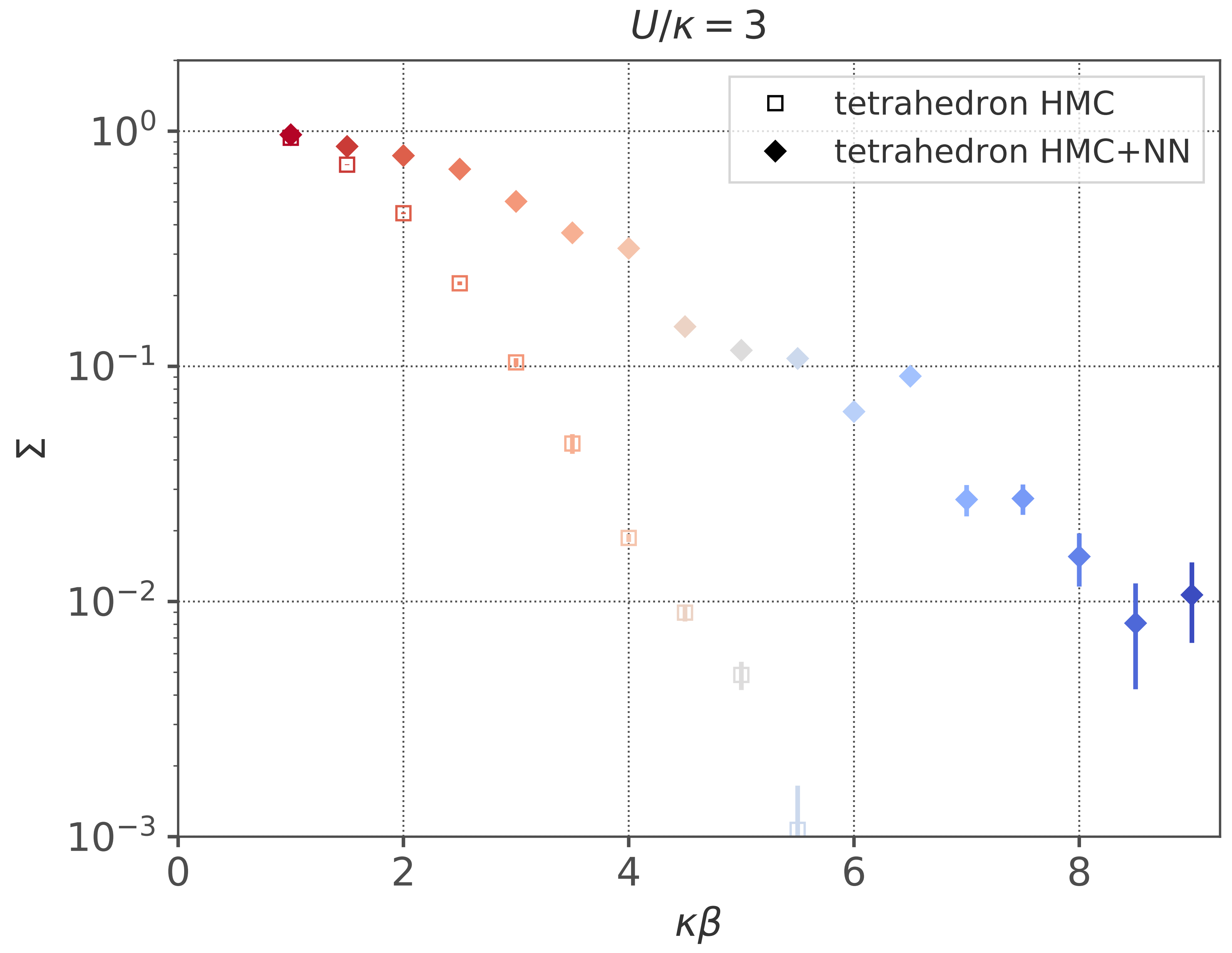
everettyou.github.io

NEW ALGORITHMS UNLOCK NEW PHYSICS

$$\mathcal{Z} \propto \int \mathcal{D}\phi \det\left(M[\phi, h, \mu]\; M^{\dagger}[\phi, -h, -\mu]\right) e^{-\frac{1}{2}\sum_{xyt} \phi_{xt} V^{-1}_{xy} \phi_{yt}}$$

average phase = Σ

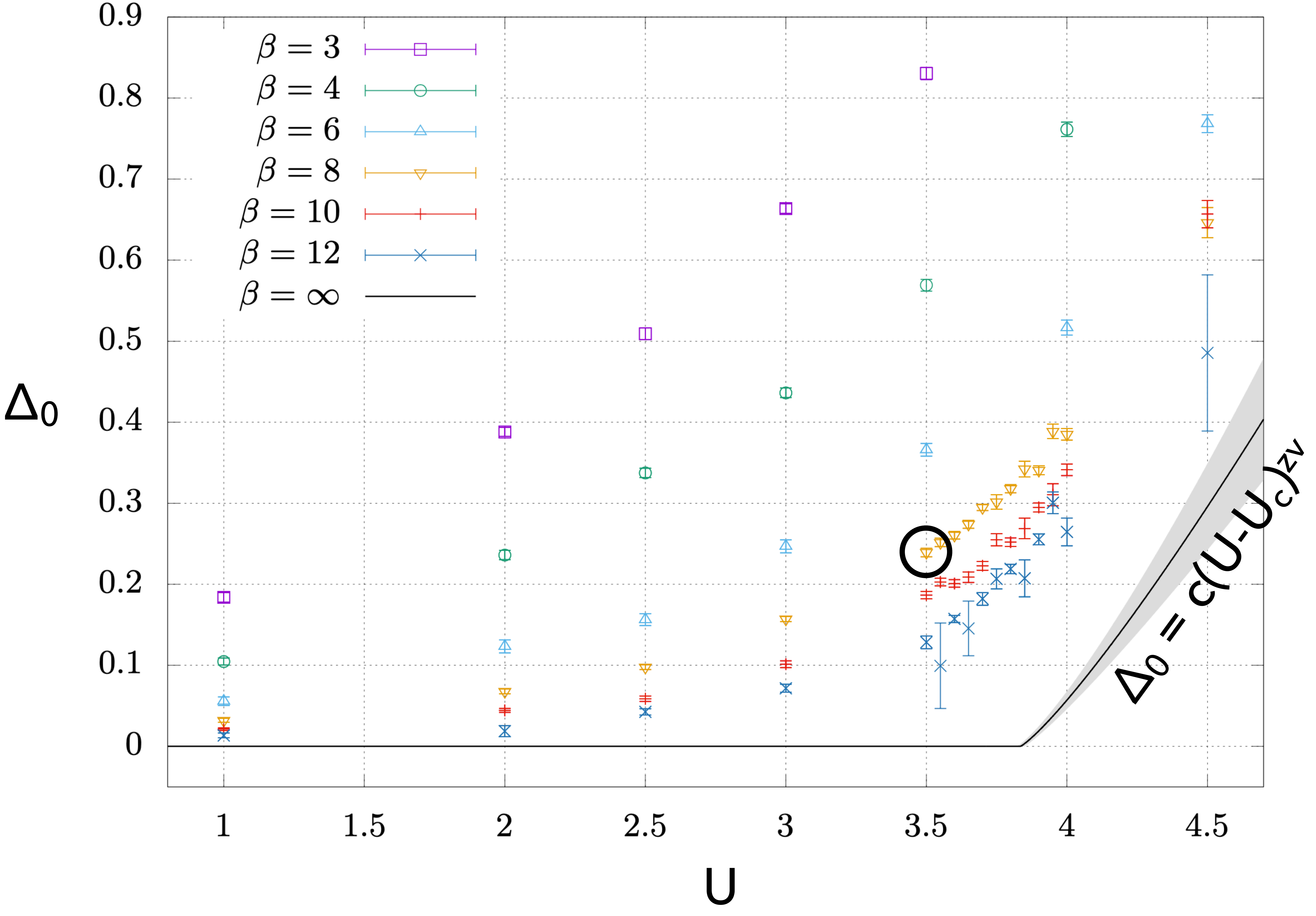
- Non-bipartite, frustrated systems (fullerenes, triangular, kagome lattices)
- Break half-filling requirement (doping, semiconductors)
- Opportunities for machine learning, Lefschetz thimbles, … (interdisciplinary applicability to QCD)
- Real-time physics via Schwinger-Keldysh?



FINITE SIZE SCALING

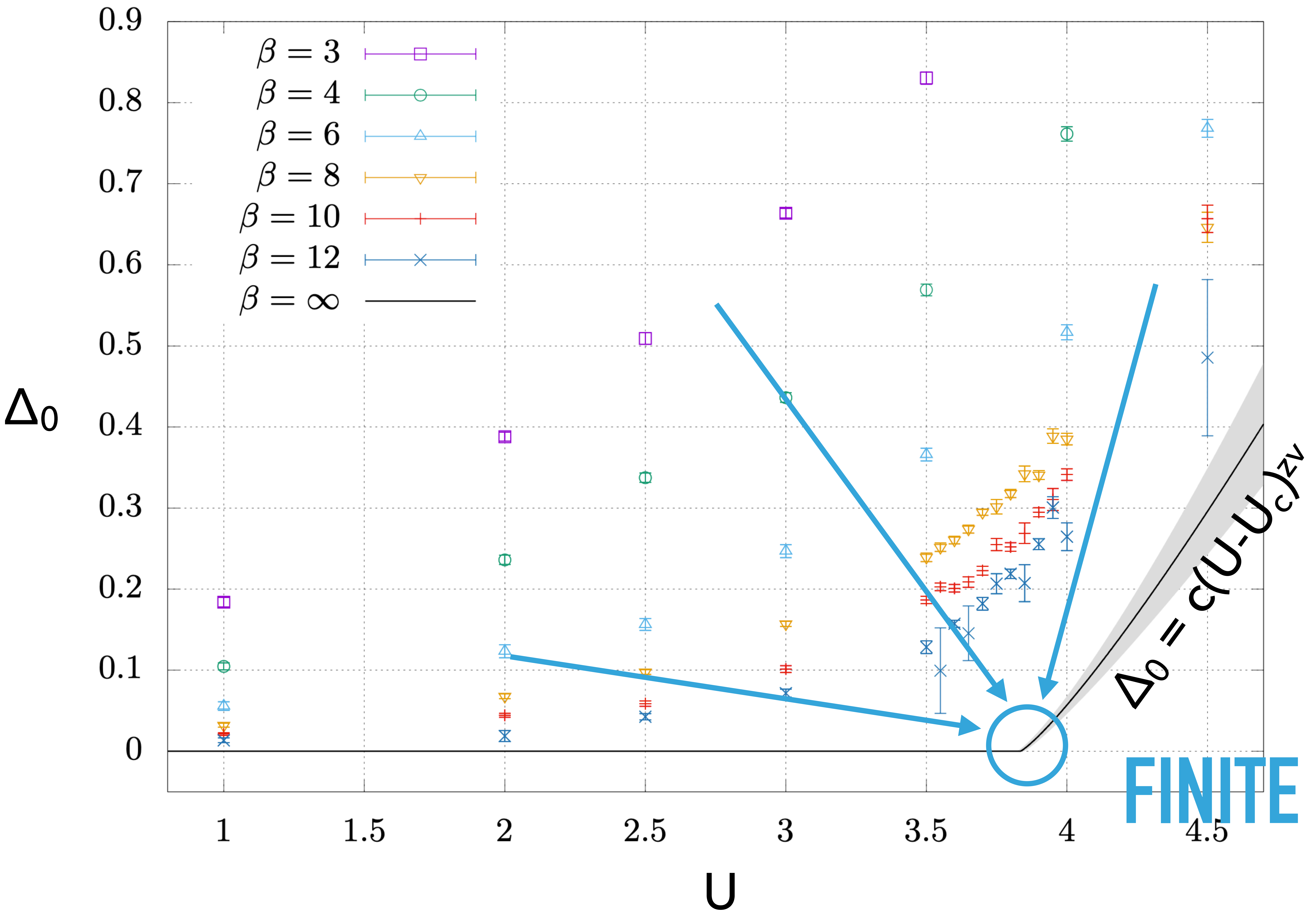
THERMODYNAMIC LIMIT

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112



THERMODYNAMIC LIMIT

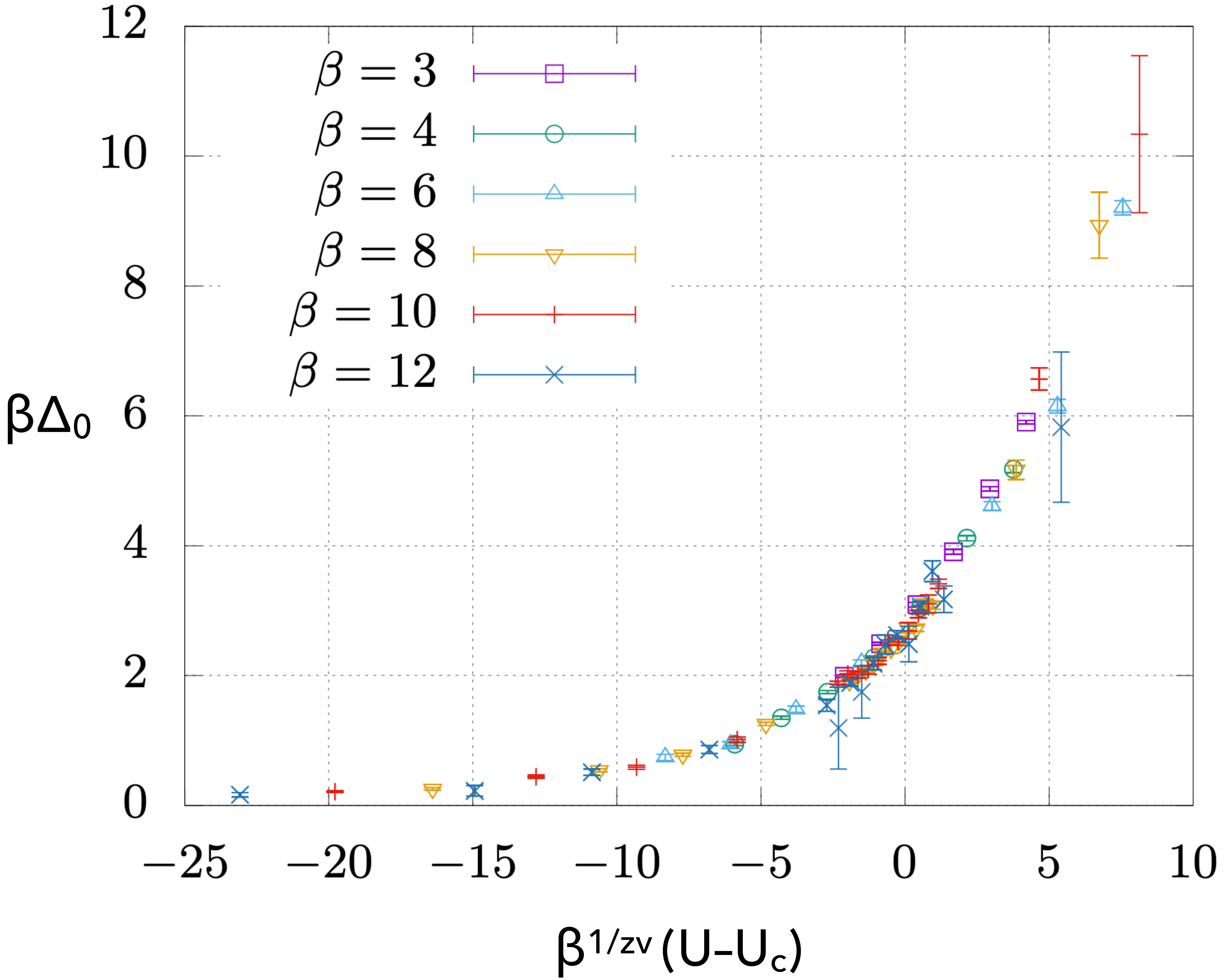
Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112



FINITE SIZE SCALING

FINITE-SIZE SCALING

Assaad and Herbut, PRX 3, 031010 (2013) 1304.6340
Wang, Corboz, and Troyer, New J. Phys 16, 103008 (2014) 1407.0029
Otsuka, Yunoki, Sorella, PRX 6, 011029 (2016) 1510.08593



$U_c = 3.834(14)$
$z\nu = 1.185(43)$

FINITE-SIZE SCALING MEAN-FIELD Δ/U

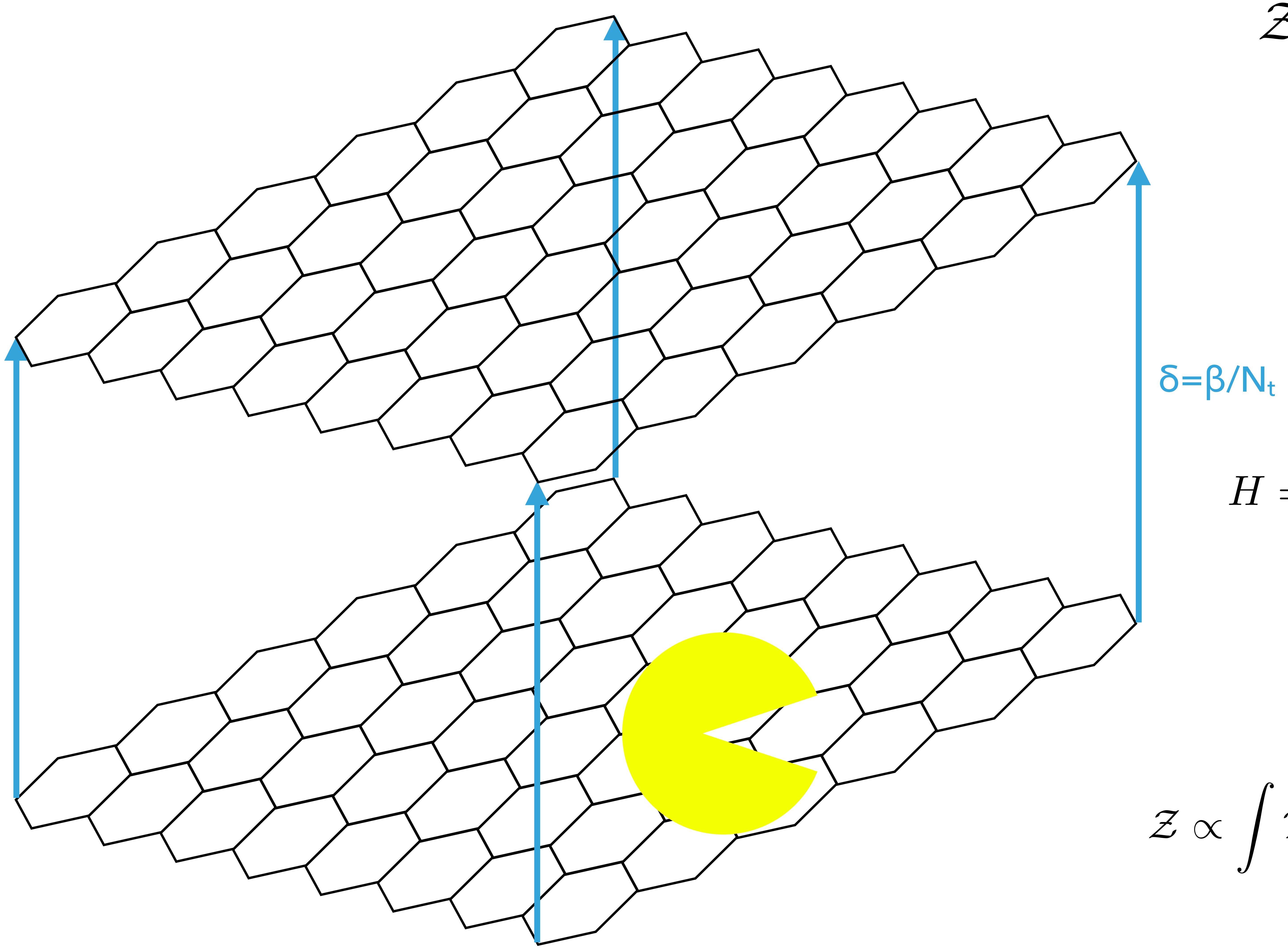
Assaad and Herbut, PRX 3, 031010 (2013) 1304.6340

$U_c = 3.834(14)$
$z\nu = 1.185(43)$
$\tilde{\beta} = 1.095(37)$

$\tilde{\beta}$ is the critical exponent for $\langle m_s \rangle$

HMC + DISCRETIZATION

FORMULATING THE PATH INTEGRAL



$$\mathcal{Z} = \mathrm{tr}\left[e^{-\beta H}\right]$$

Grassmannian coherent state identity

$$\mathbb{1} = \int \left[\prod_x d\psi_x^*\, d\psi_x\, d\eta_x^*\, d\eta_x\right] e^{-\sum_x \psi_x^* \psi_x + \eta_x^* \eta_x} |\psi, \eta\rangle\langle\psi, \eta|$$

$$H = \sum_{xy} \left(a_x^\dagger h_{xy} a_y + b_x^\dagger h_{xy} b_y\right) + \frac{1}{2} \sum_{xy} \rho_x V_{xy} \rho_y - \mu Q$$

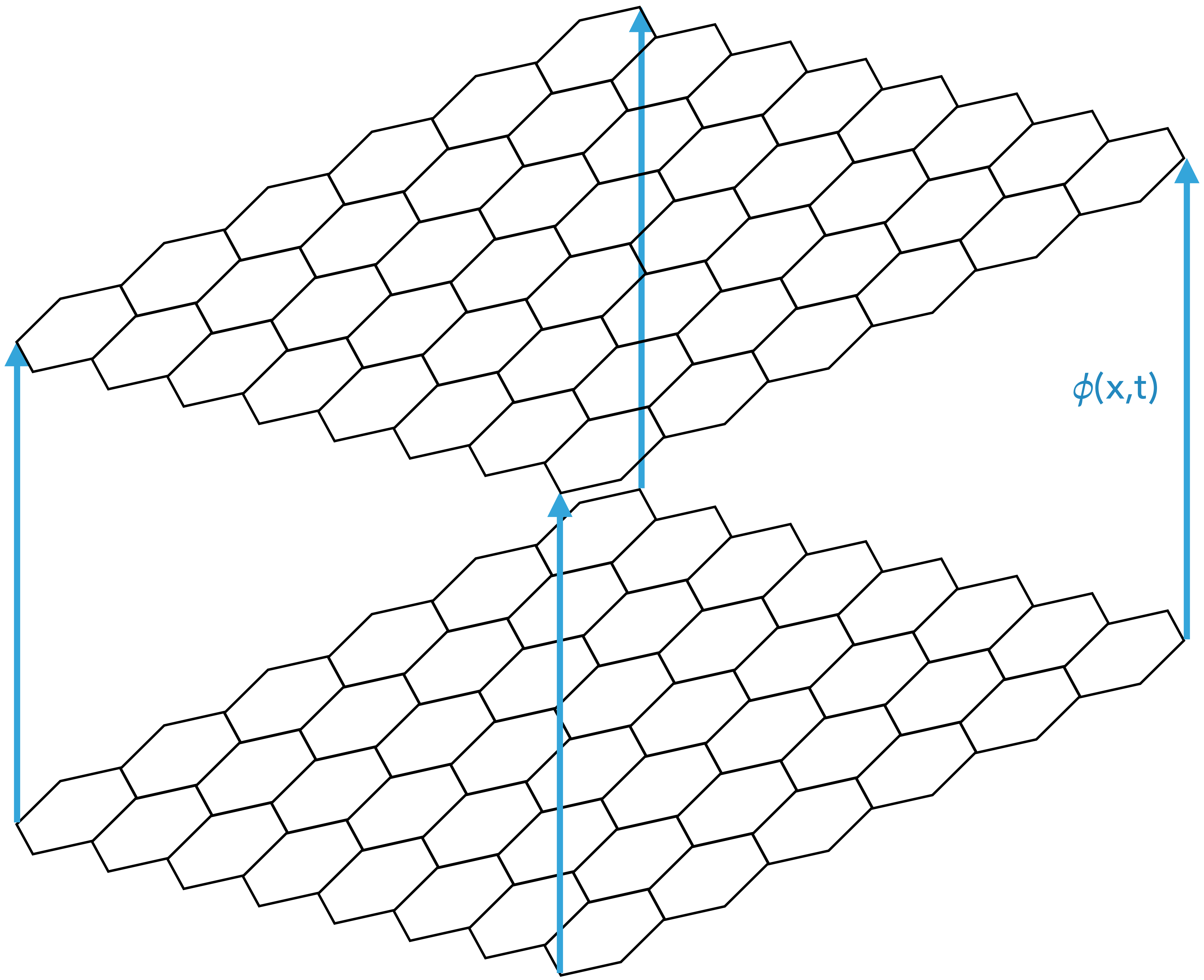
Linearize with Hubbard-Stratonovich transformation

$$\mathcal{Z} \propto \int \mathcal{D}\phi \,\det\left(M[\phi, h, \mu]\; M^\dagger[\phi, h, -\mu]\right) e^{-\frac{1}{2}\sum_{xyt} \phi_{xt} V_{xy}^{-1} \phi_{yt}}$$

Easy to change the interaction

IMPORTANCE SAMPLING THE PATH INTEGRAL

Duane, Kennedy, Pendleton, and Roweth, PLB 195 216-222 (1987)
10.1016/0370-2693(87)91197-X



$$\mathcal{Z} \propto \int \mathcal{D}\phi \det\left(M[\phi, h, \mu]\, M^\dagger[\phi, h, -\mu]\right) e^{-\frac{1}{2}\sum_{xyt} \phi_{xt} V^{-1}_{xy} \phi_{yt}}$$

Probability

Generate an *ensemble* for fixed U, β, N_t, ...

$$\{\phi_1,\ \phi_2,\ \cdots,\ \phi_N\}$$

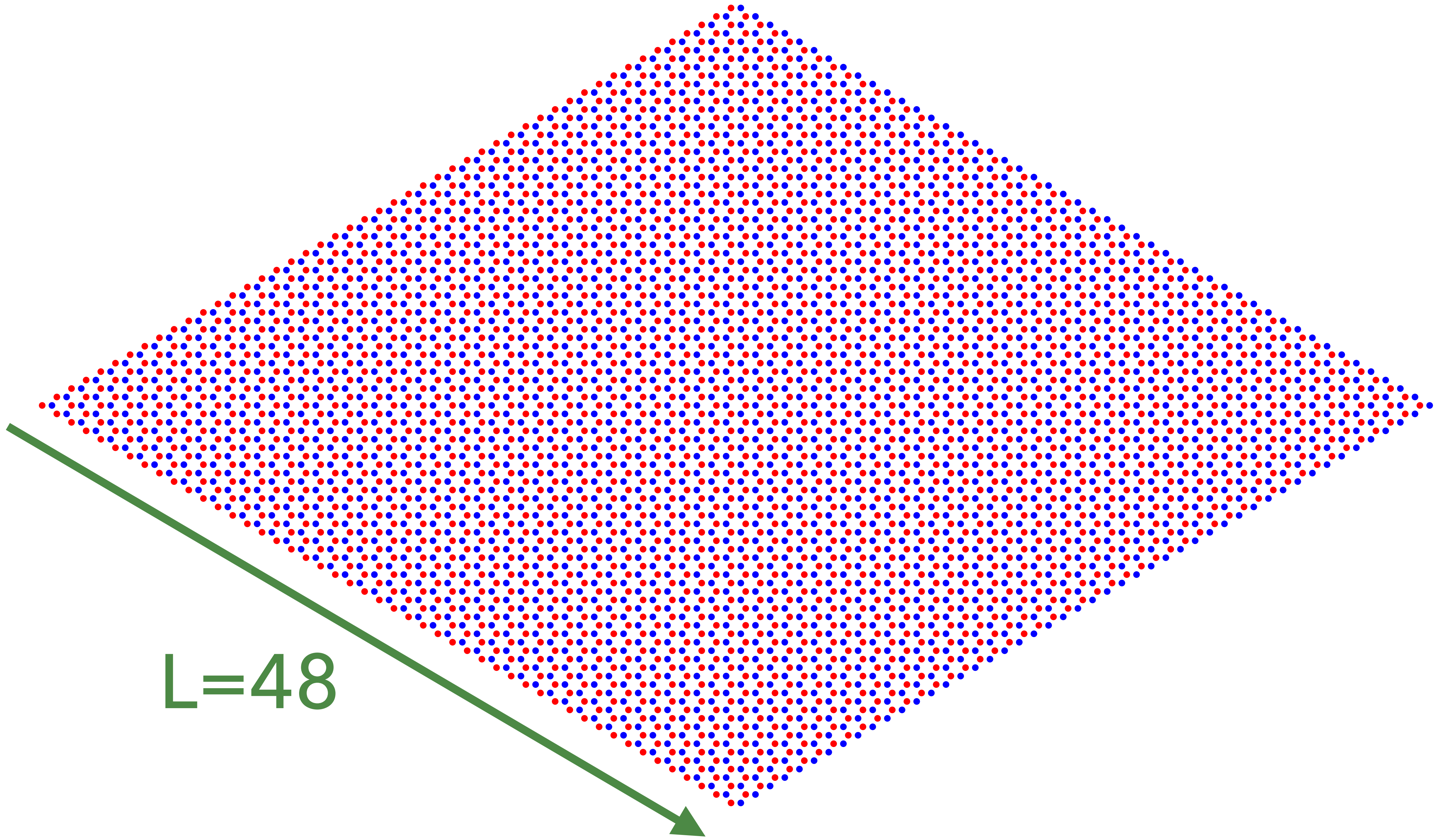
Hybrid Monte Carlo ~ $V^{5/4}$

Estimate any observable

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int d\mathcal{Z}\ \mathcal{O}[\phi]$$

$$= \frac{1}{N} \sum_i^N \mathcal{O}[\phi_i]$$

HMC SCALES VERY MILDLY!

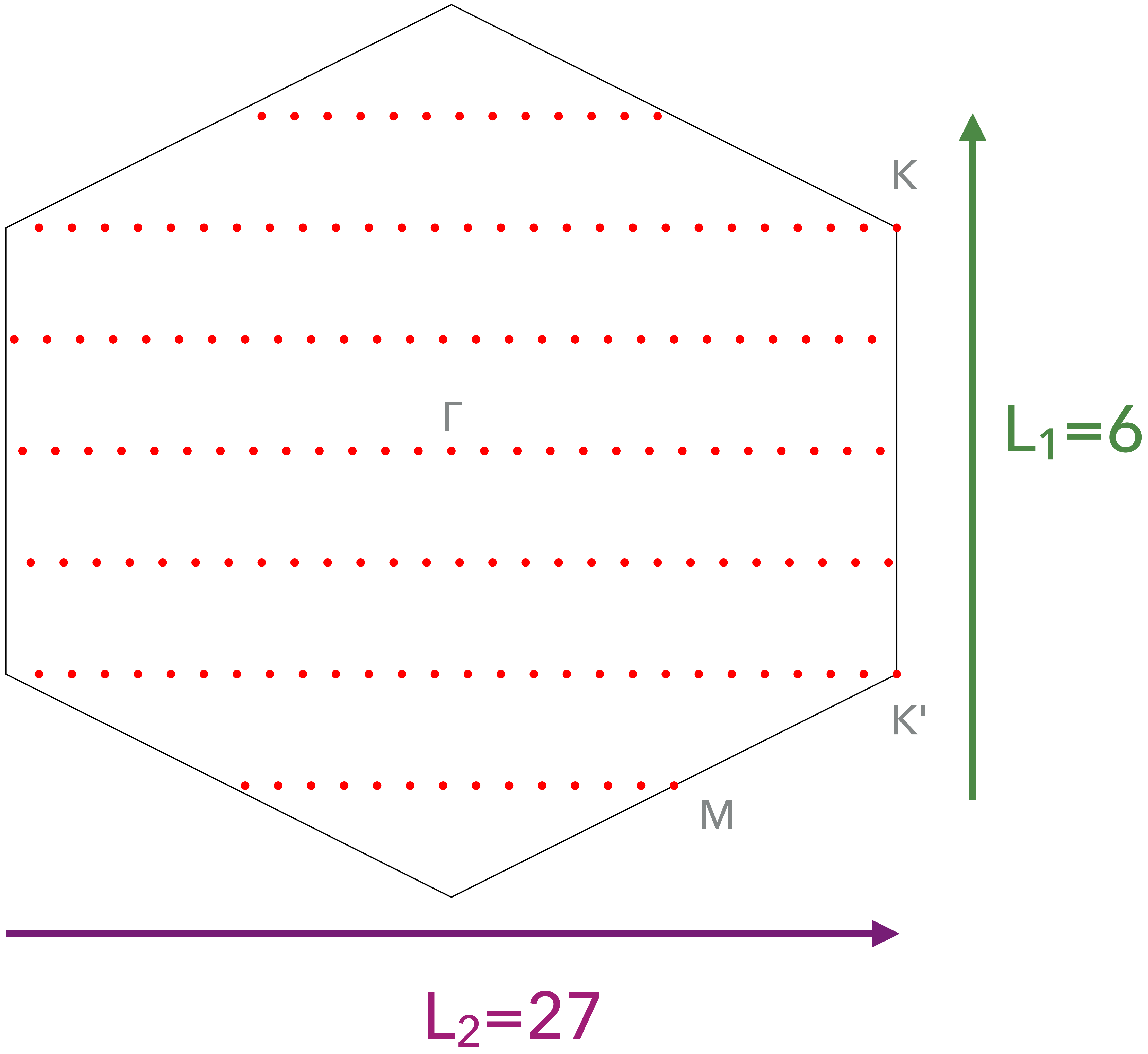


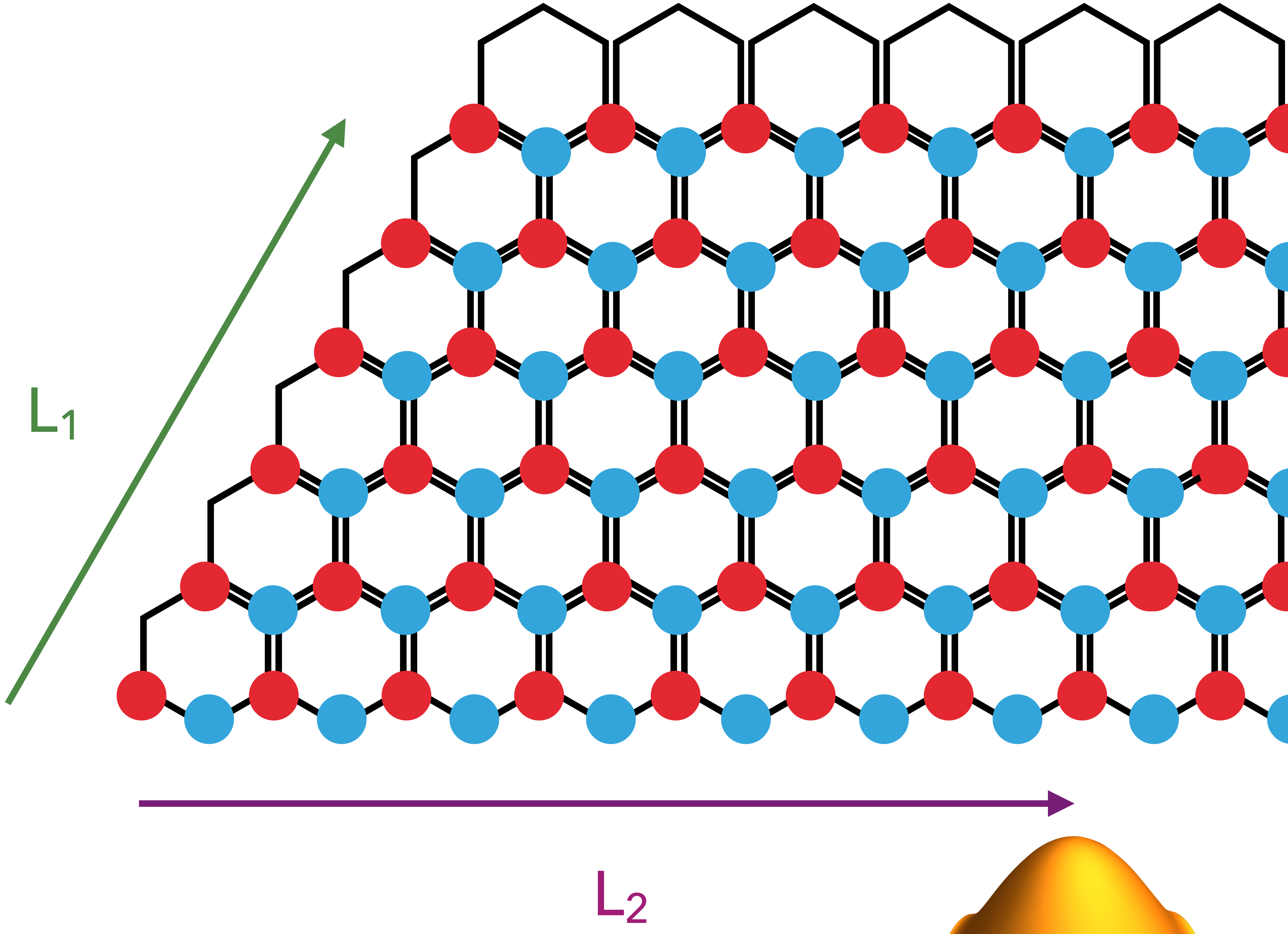
- sparse M
- simulate directly at $m_s = 0$
- Cost ~ $V^{5/4}$

HMC SCALES VERY MILDLY!

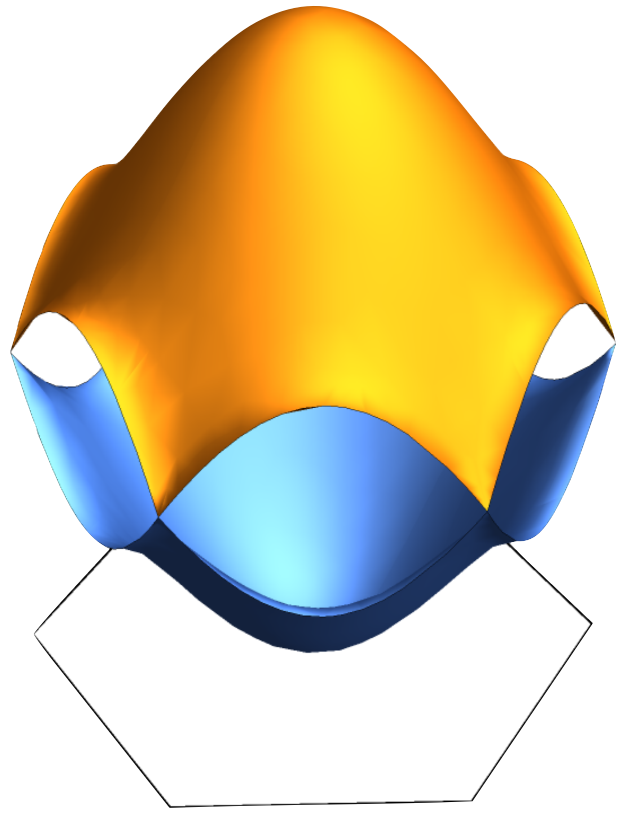
- sparse M
- simulate directly at $m_s = 0$
- Cost ~ $V^{5/4}$

BRILLOUIN ZONE





- $L_1 = L_2$ for graphene sheets. Can also make nanotubes
- Would-be Dirac points are directly accessible when $L_1, L_2 \equiv 0 \pmod 3$



HMC + ERGODICITY

HYBRID MONTE CARLO

Multiply by $\mathbb{1} = \frac{1}{(2\pi)^{N/2}} \int \mathcal{D}p \, e^{-\frac{p^2}{2}}$

$$\mathcal{Z} \propto \int \mathcal{D}\phi \, \det\left(M[\phi, h, \mu] \, M^\dagger[\phi, h, -\mu]\right) e^{-\frac{1}{2}\sum_{xyt} \phi_{xt} V^{-1}_{xy} \phi_{yt}}$$

Probability

Sample p according to the gaussian

Evolve all the ϕ according to

$$\mathcal{H} = \frac{p^2}{2} + \frac{1}{2}\phi V^{-1}\phi - \log\det M[\phi, h, \mu] M^\dagger[\phi, h, -\mu]$$

Accept / reject as in Metropolis-Hastings, with $\mathcal{H}$ as the energy

Refresh p according to the gaussian...

Generate an *ensemble* for fixed U, β, N_t, ...

$$\{\phi_1, \ \phi_2, \ \cdots, \ \phi_N\}$$

Hybrid Monte Carlo

Estimate any observable

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int d\mathcal{Z} \, \mathcal{O}[\phi]$$

$$= \frac{1}{N} \sum_i^N \mathcal{O}[\phi_i] + O\left(\frac{1}{\sqrt{N}}\right)$$

HYBRID MONTE CARLO

Duane, Kennedy, Pendleton, and Roweth, PLB 195 216-222 (1987)
10.1016/0370-2693(87)91197-X

Multiply by $\mathbb{1} = \frac{1}{(2\pi)^{N/2}} \int \mathcal{D}p \, e^{-\frac{p^2}{2}}$

$$\mathcal{Z} \propto \int \mathcal{D}\phi \, \det \left(M[\phi, h, \mu] \, M^\dagger[\phi, h, -\mu] \right) e^{-\frac{1}{2} \sum_{xyt} \phi_{xt} V^{-1}_{xy} \phi_{yt}}$$

Probability

Sample p according to the gaussian

Evolve all the ϕ according to

$$\mathcal{H} = \frac{p^2}{2} + \frac{1}{2} \phi V^{-1} \phi - \log \det M[\phi, h, \mu] M^\dagger[\phi, h, -\mu]$$

Accept / reject as in Metropolis-Hastings, with $\mathcal{H}$ as the energy

Refresh p according to the gaussian...

Generate an *ensemble* for fixed U, β, N_t, ...

$$\{\phi_1, \ \phi_2, \ \cdots, \ \phi_N\}$$

Hybrid Monte Carlo

Estimate any observable

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int d\mathcal{Z} \; \mathcal{O}[\phi]$$

$$= \frac{1}{N} \sum_i^N \mathcal{O}[\phi_i] + O\left(\frac{1}{\sqrt{N}} \right)$$

ERGODICITY OF HYBRID MONTE CARLO

Multiply by $\mathbb{1} = \frac{1}{(2\pi)^{N/2}} \int \mathcal{D}p \; e^{-\frac{p^2}{2}}$

$$\mathcal{Z} \propto \int \mathcal{D}\phi \; \det \left(M[\phi, h, \mu] \; M^\dagger[\phi, h, -\mu] \right) e^{-\frac{1}{2} \sum_{xyt} \phi_{xt} V^{-1}_{xy} \phi_{yt}}$$

Sample *p* according to the gaussian

Evolve all the ϕ according to

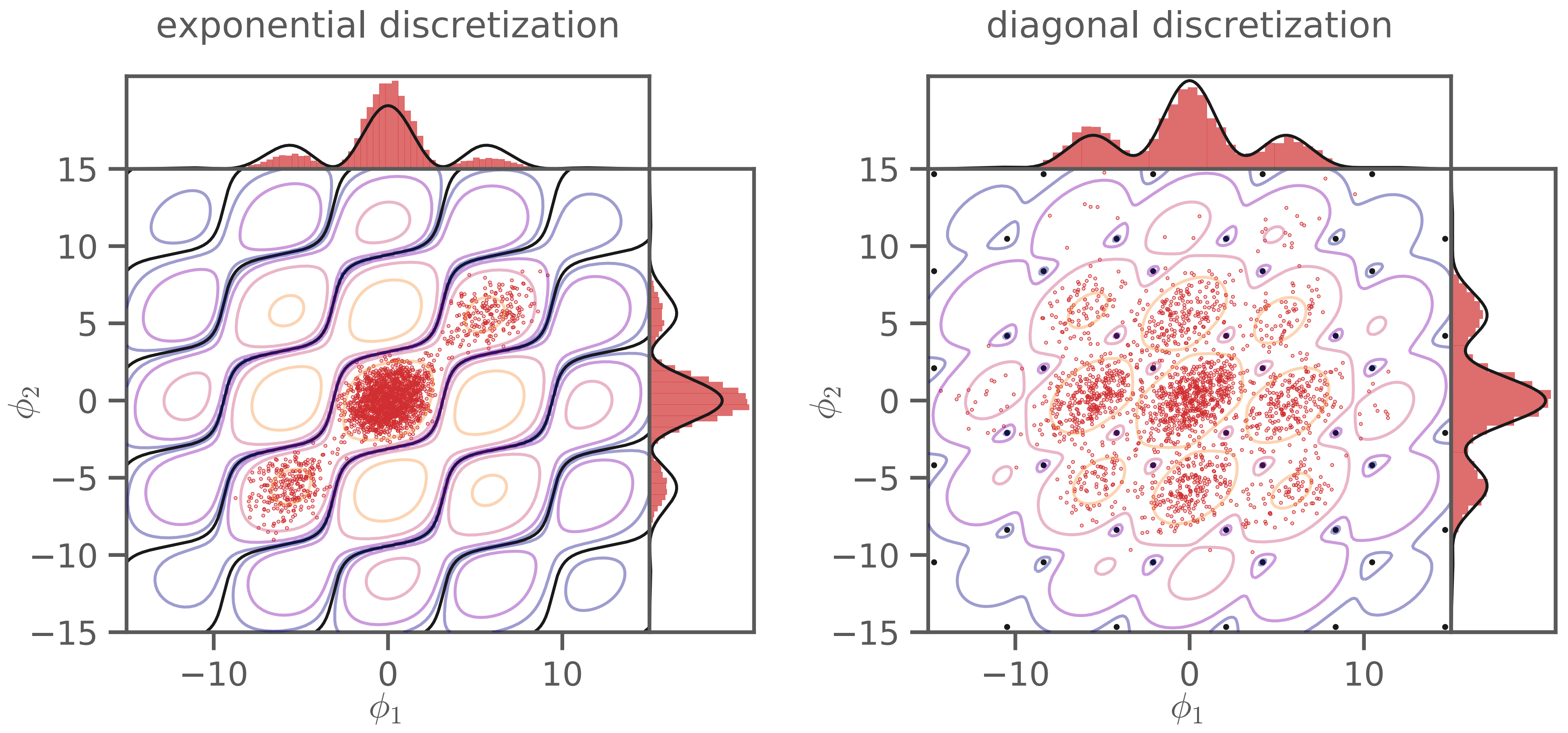
$$\mathcal{H} = \frac{p^2}{2} + \frac{1}{2} \phi V^{-1} \phi - \log \det M[\phi, h, \mu] M^\dagger[\phi, h, -\mu]$$

Potential

If the potential has infinite codimension-1 surfaces (the determinant vanishes), the evolution might not be able reach all ϕ, and the method has a bias.

- Depends on the discretization of the fermion operator M
- When μ≠0 action is complex

Nx=2 Nt=1 U/κ = 18, κβ=1



By universality, barriers appear in the continuum limit

CHOICE OF DISCRETIZATION IS A BALANCING ACT

Exponential $$M[\phi]_{x't',xt} = \delta_{x'x}\delta_{t't} - \left[e^{h}\right]_{x'x} e^{i\phi_{xt}} B_{t'}\delta_{t',t+1}$$

Meng, Lang, Wessel, Assaad, Muramatsu, Nature 464 847-851 (2010) 10.1038/nature08942

(complex ϕ) Beyl, Goth, Assaad, PRB 97 085144 (2018) 10.1103/PhysRevB.97.085144

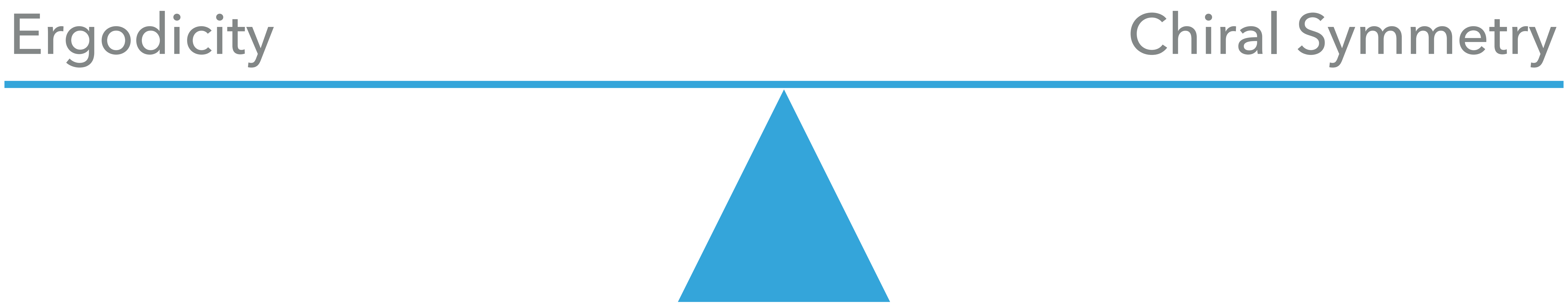
Ulybyshev and Valgushev, 1712.02188

Diagonal $$M[\phi]_{x't',xt} = (\delta_{x'x} - h_{x'x})\delta_{t't} - e^{i\phi_{xt}} B_{t'}\delta_{t',t+1}$$

Brower, Rebbi, Schaich PoS LATTICE2011 056 (2011) 1204.5424

Luu and Lähde, PRB 93, 155106 (2016) 10.1103/PhysRevB.93.155106

EB, Körber, Krieg, Labus, Lähde, Luu, Lattice 2017 10.1051/epjconf/201817503009



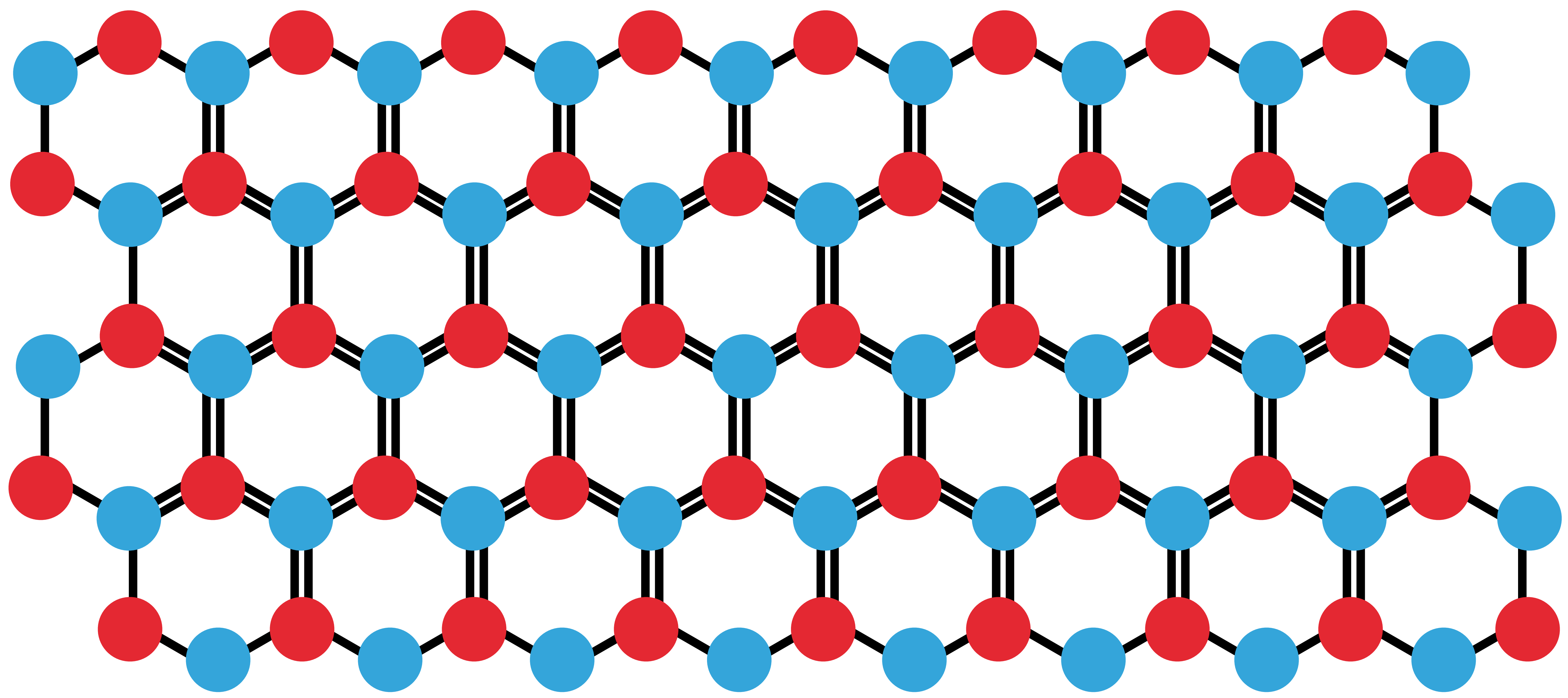
Beyl, Goth, Assaad (above)

Wynen, EB, Körber, Lähde, Luu PRB 100 075141 10.1103/PhysRevB.100.075141

MIXED DIFFERENCING

Brower, Rebbi, Schaich PoS LATTICE2011 056 (2011) 1204.5424
Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112

$$M_{x't',xt} = \delta_{x'x}\left(\delta_{t',t-1} - e^{i\phi_{x't'}}\delta_{t',t}\right)$$
$$M_{x't',xt} = \delta_{x'x}\left(\delta_{t',t} - e^{i\phi_{x't'}}\delta_{t',t+1}\right)$$
$$M_{x't',xt} = -h_{x',x}\delta_{t't}$$
$$M_{x't',xt} = -h_{x',x}\delta_{t't}$$



- time continuum limit δ → 0 is faster than forward (or backward) differencing.

- produces a dynamically-generated normal-ordering term

- simulate directly at $m_s = 0$

- HMC scales very mildly

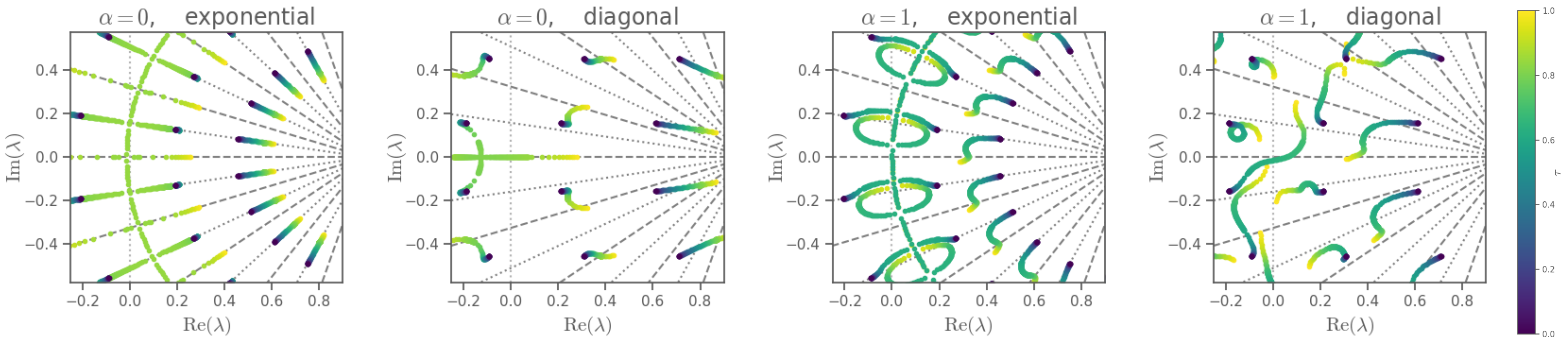
SYMMETRY CONSTRAINS M EIGENSPECTRUM

Exponential $$M[\phi]_{x't',xt} = \delta_{x'x}\delta_{t't} - \left[e^{h}\right]_{x'x} e^{i\phi_{xt}} B_{t'}\delta_{t',t+1}$$

Eigenvalue identity of the characteristic polynomial P[ϕ] $P[\phi](s) \sim P[\phi](1/s^*)^*$

Diagonal $$M[\phi]_{x't',xt} = (\delta_{x'x} - h_{x'x})\delta_{t't} - e^{i\phi_{xt}} B_{t'}\delta_{t',t+1}$$

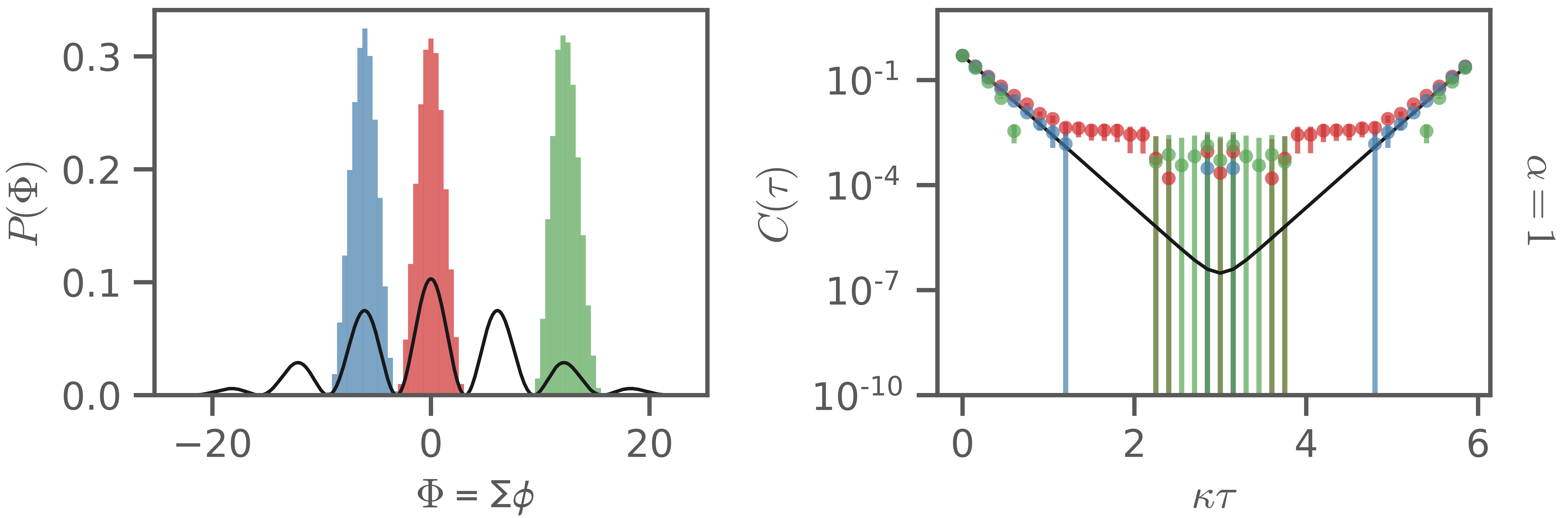
No such identity



$N_x = 4$, $N_t=20$, $\kappa\beta = 4$ Wynen, EB, Körber, Lähde, Luu PRB 100 075141 10.1103/PhysRevB.100.075141

ERGODICITY PROBLEMS LEAD TO BIASES

$$N_x = 1,\ N_t = 40, \quad U/\kappa = 10,\ \kappa\beta = 6$$

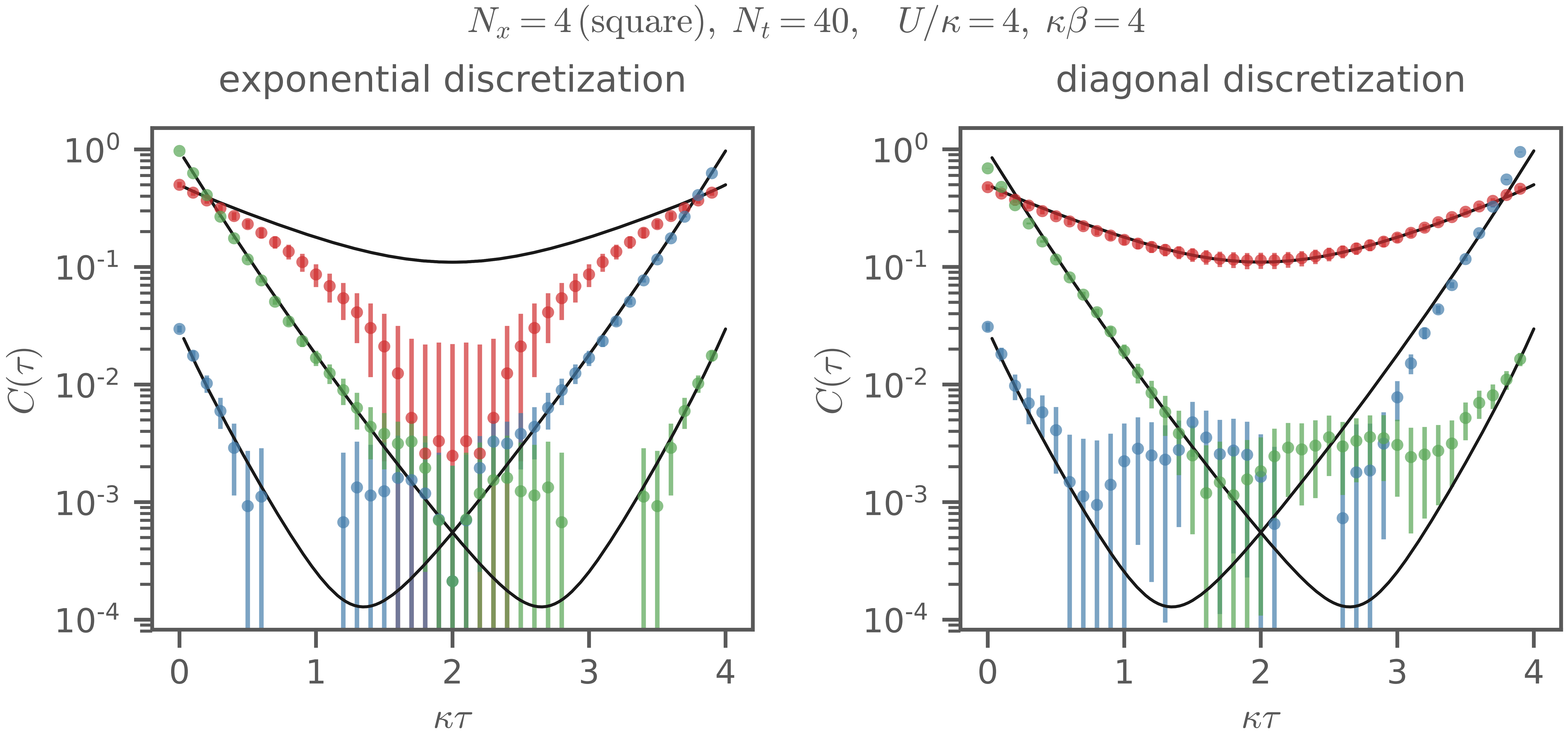


Wynen, EB, Körber, Lähde, Luu PRB 100 075141 10.1103/PhysRevB.100.075141

ERGODICITY PROBLEMS LEAD TO BIASES

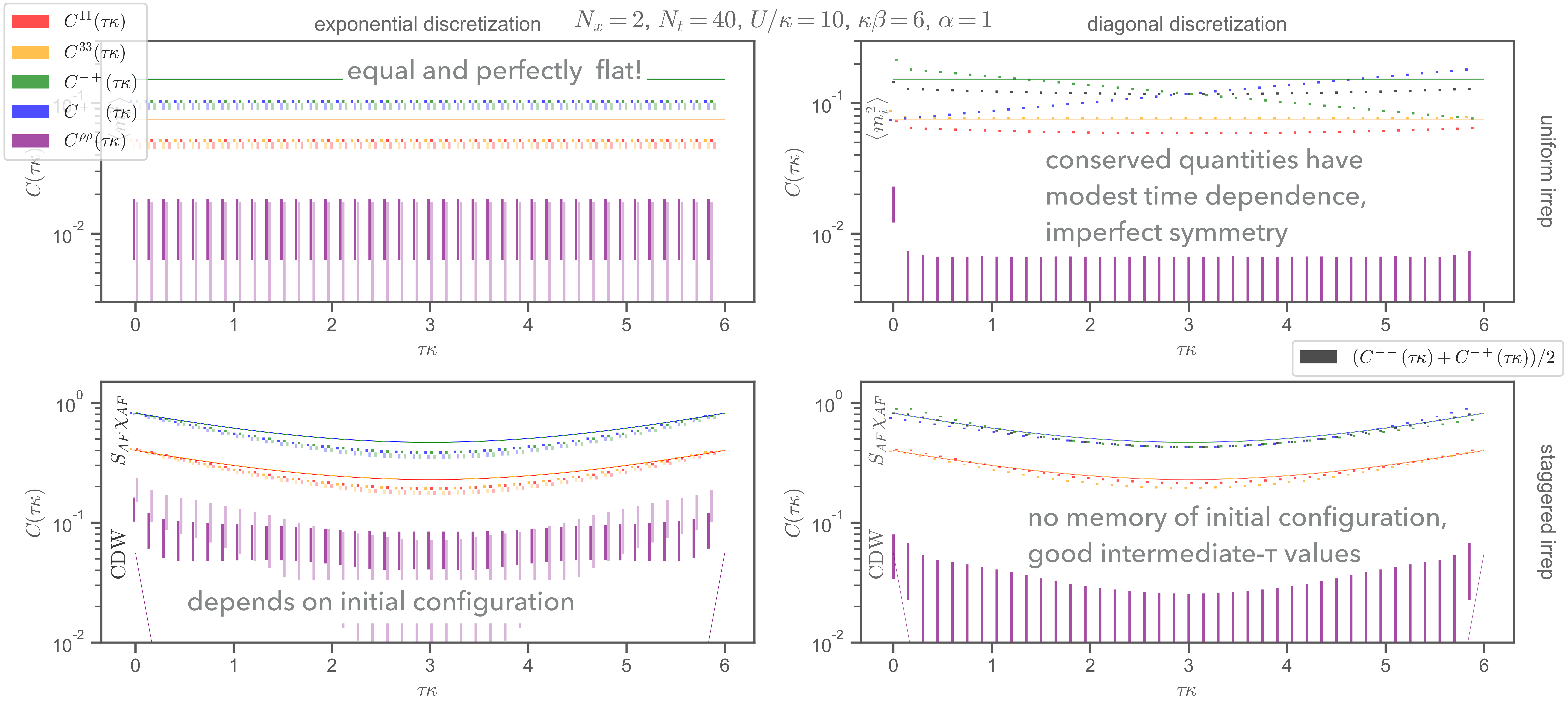
Exponential $M[\phi]_{x't',xt} = \delta_{x'x}\delta_{t't} - \left[e^{h}\right]_{x'x} e^{i\phi_{xt}} B_{t'}\delta_{t',t+1}$

Diagonal $M[\phi]_{x't',xt} = (\delta_{x'x} - h_{x'x})\delta_{t't} - e^{i\phi_{xt}} B_{t'}\delta_{t',t+1}$



Wynen, EB, Körber, Lähde, Luu PRB 100 075141 10.1103/PhysRevB.100.075141

CHOICE OF DISCRETIZATION IS A BALANCING ACT



Wynen, EB, Körber, Lähde, Luu PRB 100 075141 10.1103/PhysRevB.100.075141

HMC + SOLVERS

ACCELERATING HYBRID MONTE CARLO

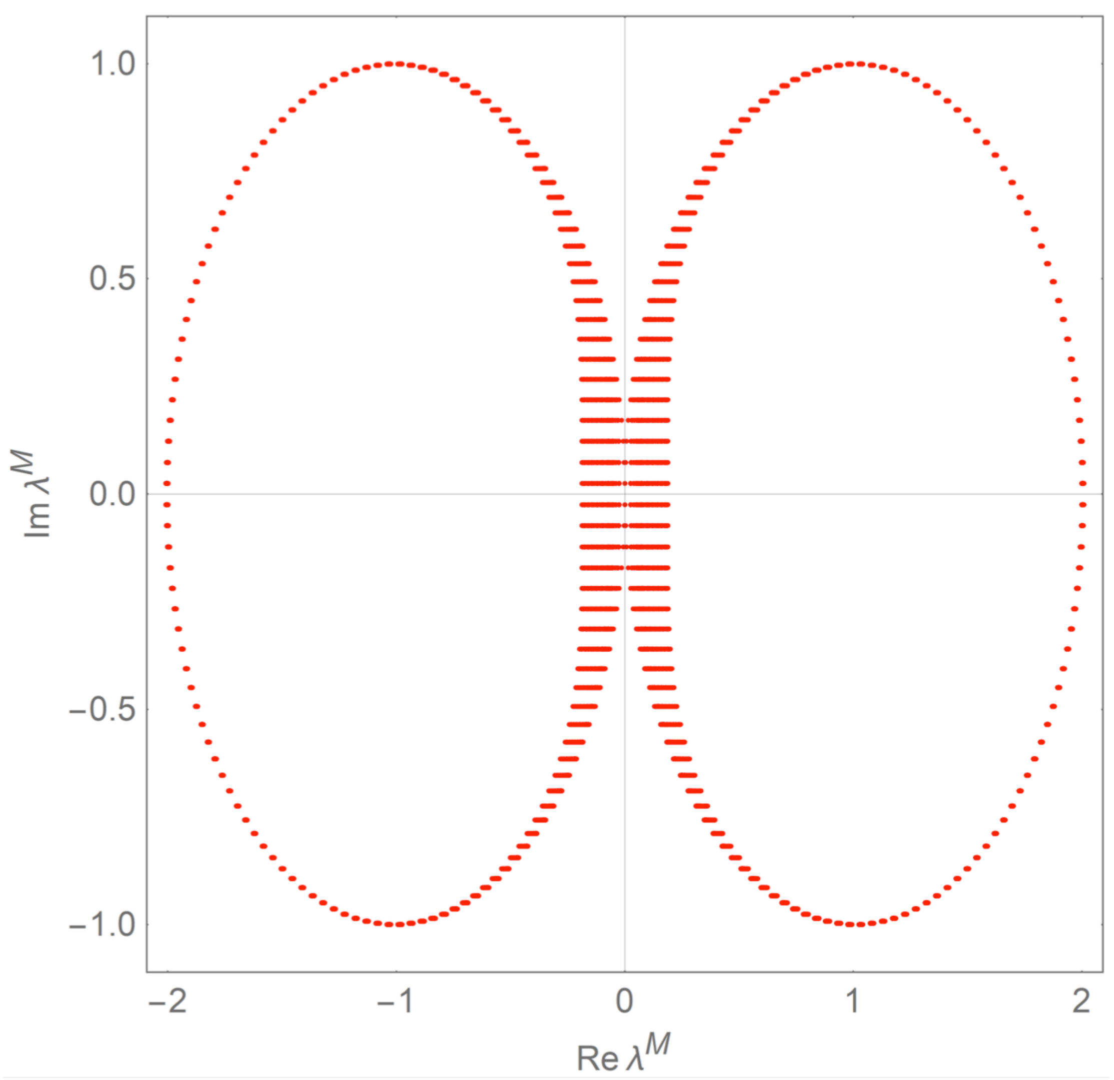
Multiply by $\mathbb{1} = \frac{\det\left(M[m_s]M^\dagger[m_s]\right)}{\det\left(M[m_s]M^\dagger[m_s]\right)}$

$m_s=0$

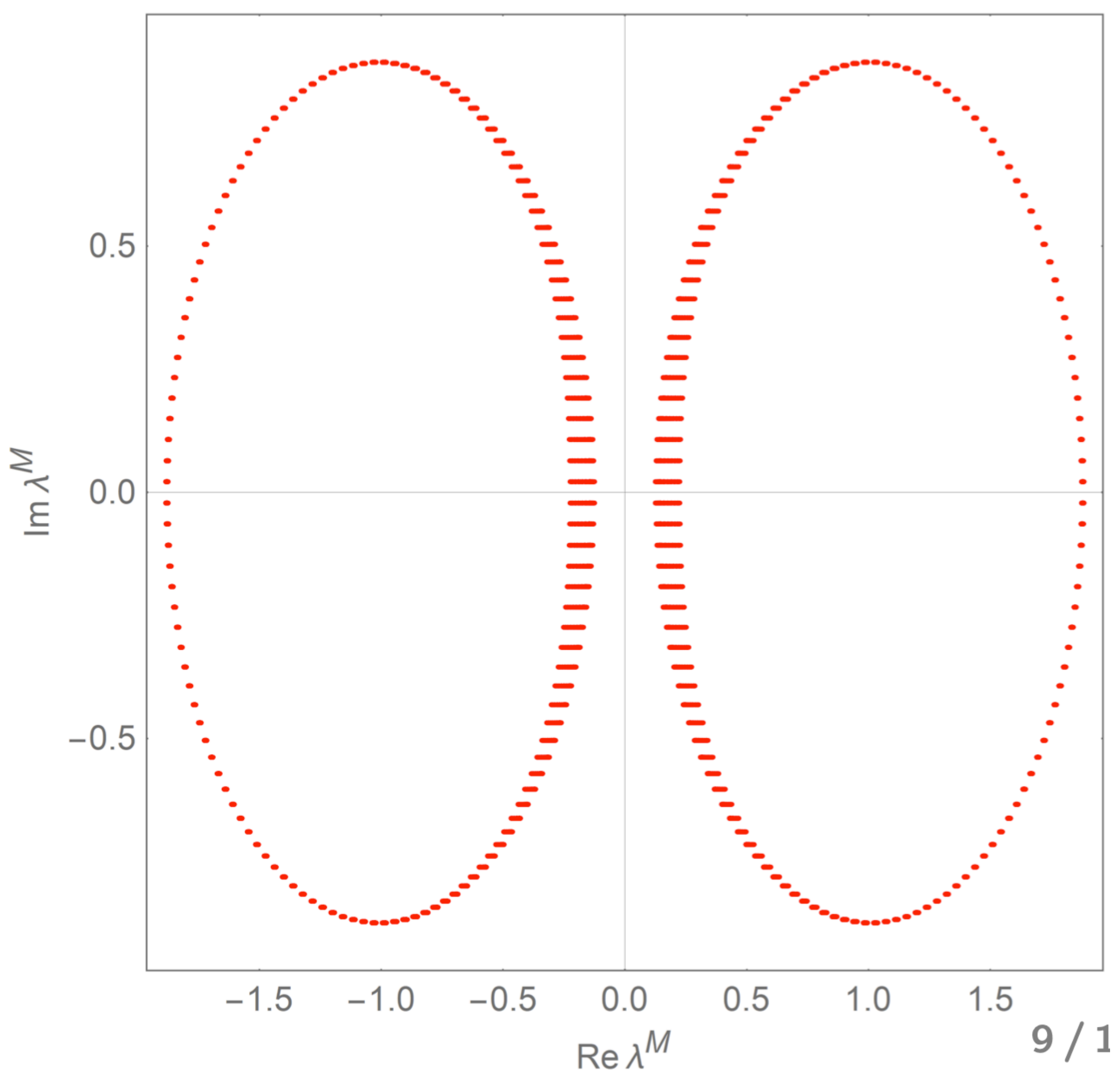
$$\mathcal{Z} \propto \int \mathcal{D}\phi \det\left(M[\phi,h,\mu]\ M^\dagger[\phi,h,-\mu]\right) e^{-\frac{1}{2}\sum_{xyt}\phi_{xt}V^{-1}_{xy}\phi_{yt}}$$

Probability

$m_s=0$



$m_s\neq0$



Generate an *ensemble* for fixed U, β, N_t, ...

$$\{\phi_1,\ \phi_2,\ \cdots,\ \phi_N\}$$

Hybrid Monte Carlo

Estimate any observable

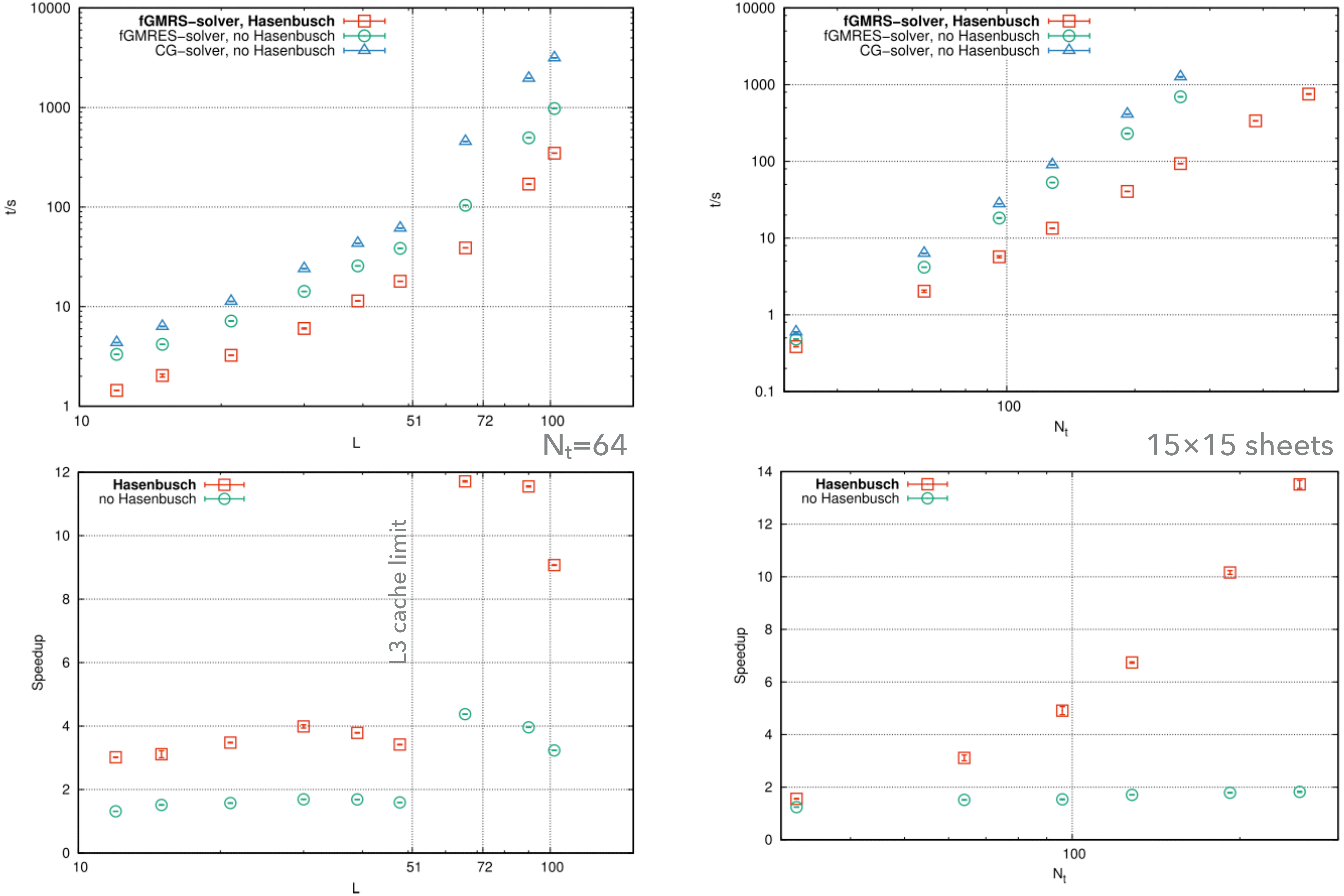
$$\langle\mathcal{O}\rangle = \frac{1}{\mathcal{Z}}\int d\mathcal{Z}\ \mathcal{O}[\phi]$$

$$= \frac{1}{N}\sum_i^N \mathcal{O}[\phi_i] + O\left(\frac{1}{\sqrt{N}}\right)$$

- Condition number is much better
- det(m_s = 0) / det($m_s \neq 0$) is close to 1

Hasenbusch, PLB 519 (1) (2001) 10. 1016/S0370-2693(01)01102-9 hep-lat/0107019
Krieg, Luu, Ostmeyer, Papaphilippou, Urbach Comp. Phys. Comm 236 (2019) 1804.07195

SCALING OF HASENBUSCH SOLVER

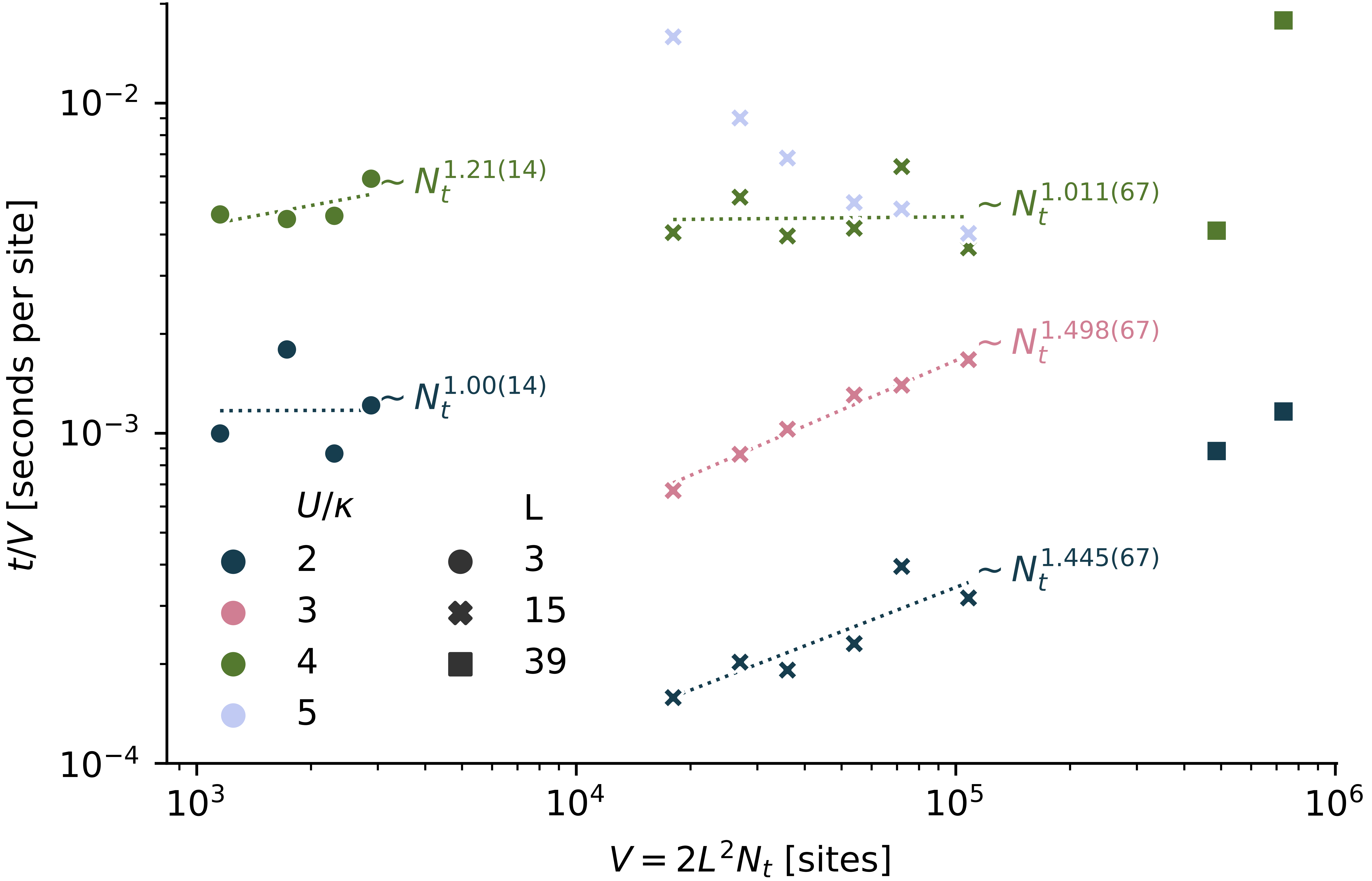


Krieg, Luu, Ostmeyer, Papaphilippou, Urbach Comp. Phys. Comm 236 (2019) 1804.07195

SCALING OF HMC

Beyl, Goth, Assaad, PRB 97 085144 (2018) 10.1103/PhysRevB.97.085144
found unfavorable scaling ~ $V^{2.5\text{-}3.0}$ for HMC with complexified ϕ

HMC IS EXPECTED TO SCALE LIKE $V^{5/4}$



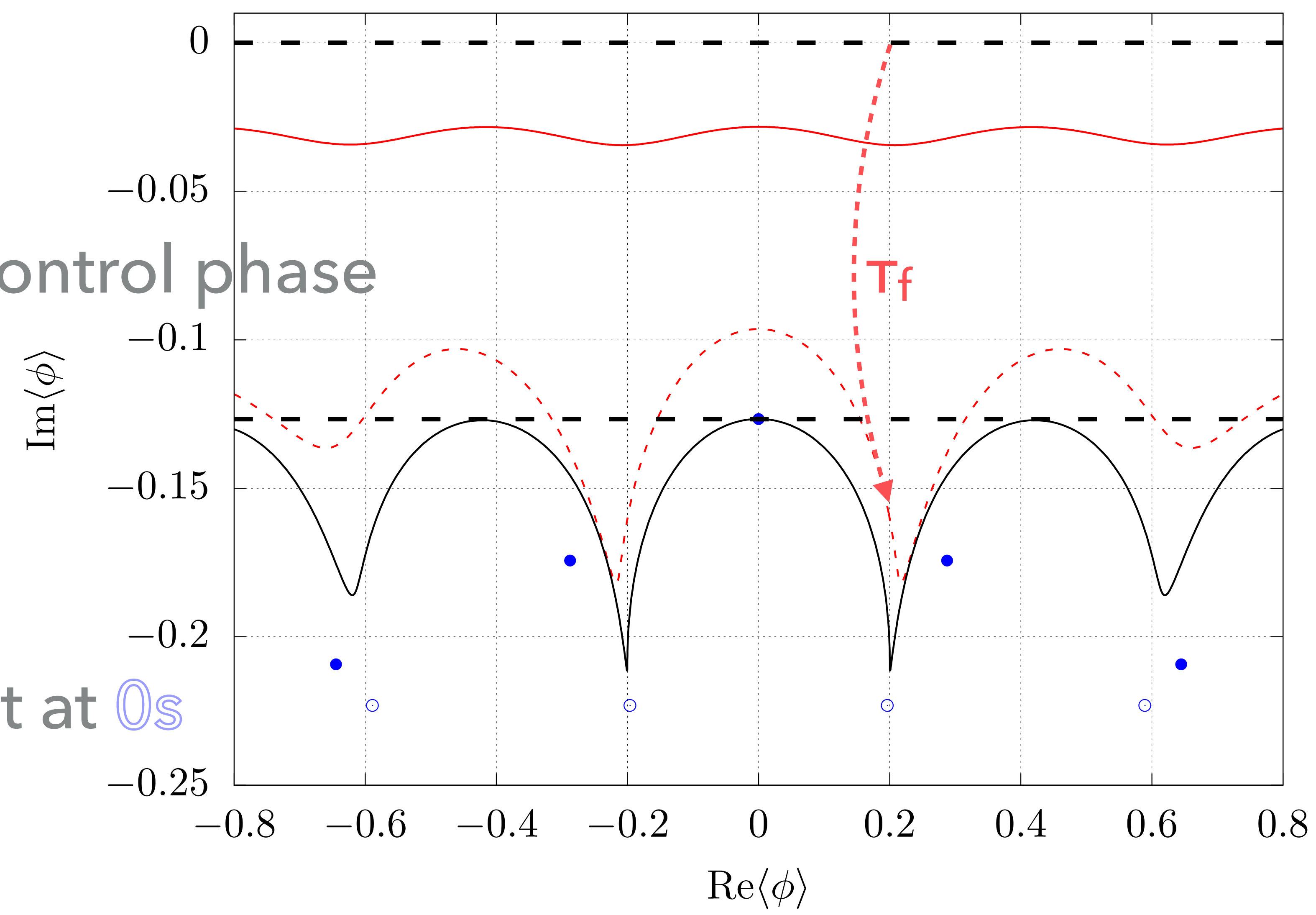
Creutz, PRD 38 1228 (1988) 10.1103/PhysRevD.38.1228

FLOW + ERGODICITY

LEFSCHETZ THIMBLES HAVE CONSTANT SIGN

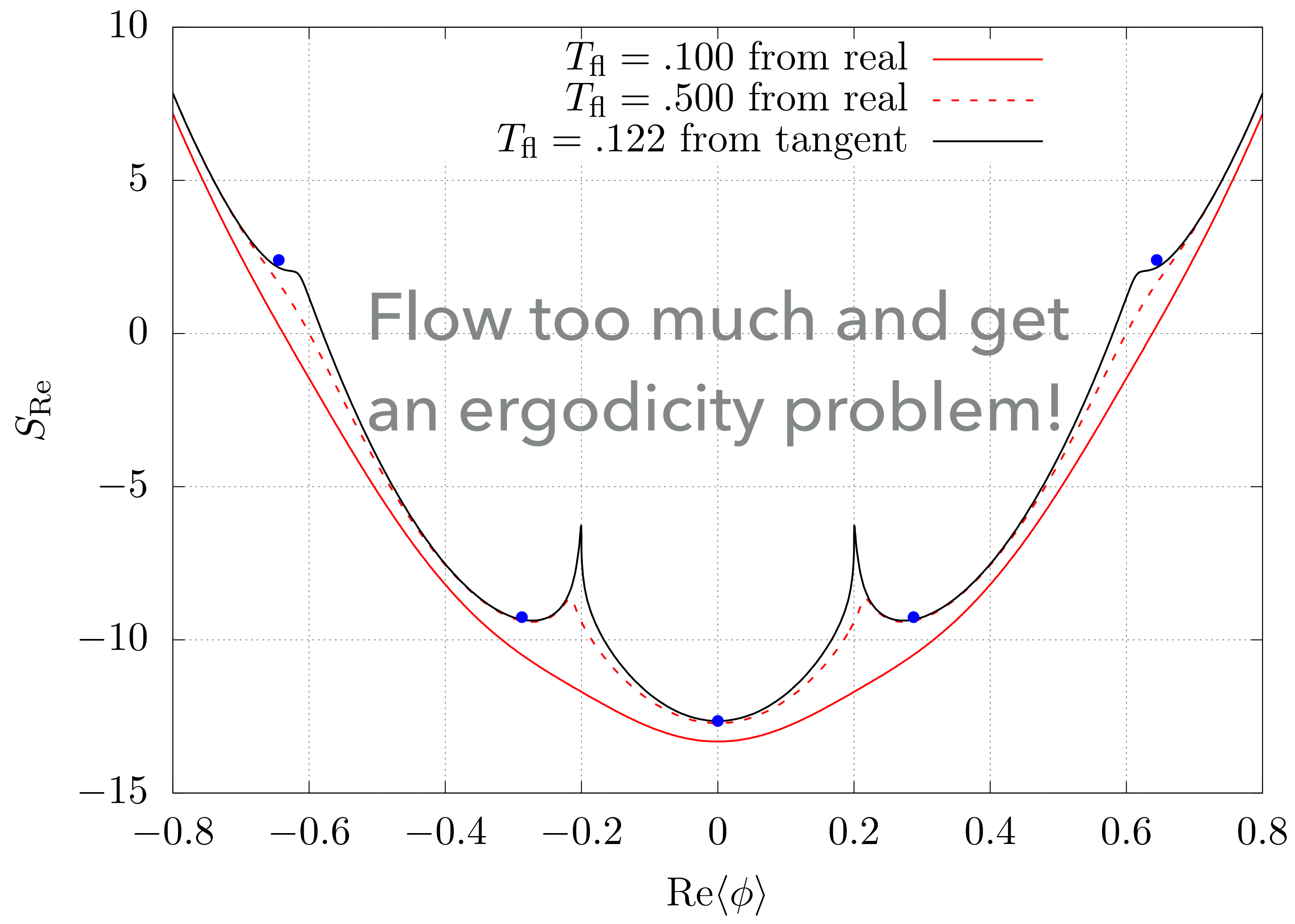
Critical points control phase

Thimbles meet at 0s

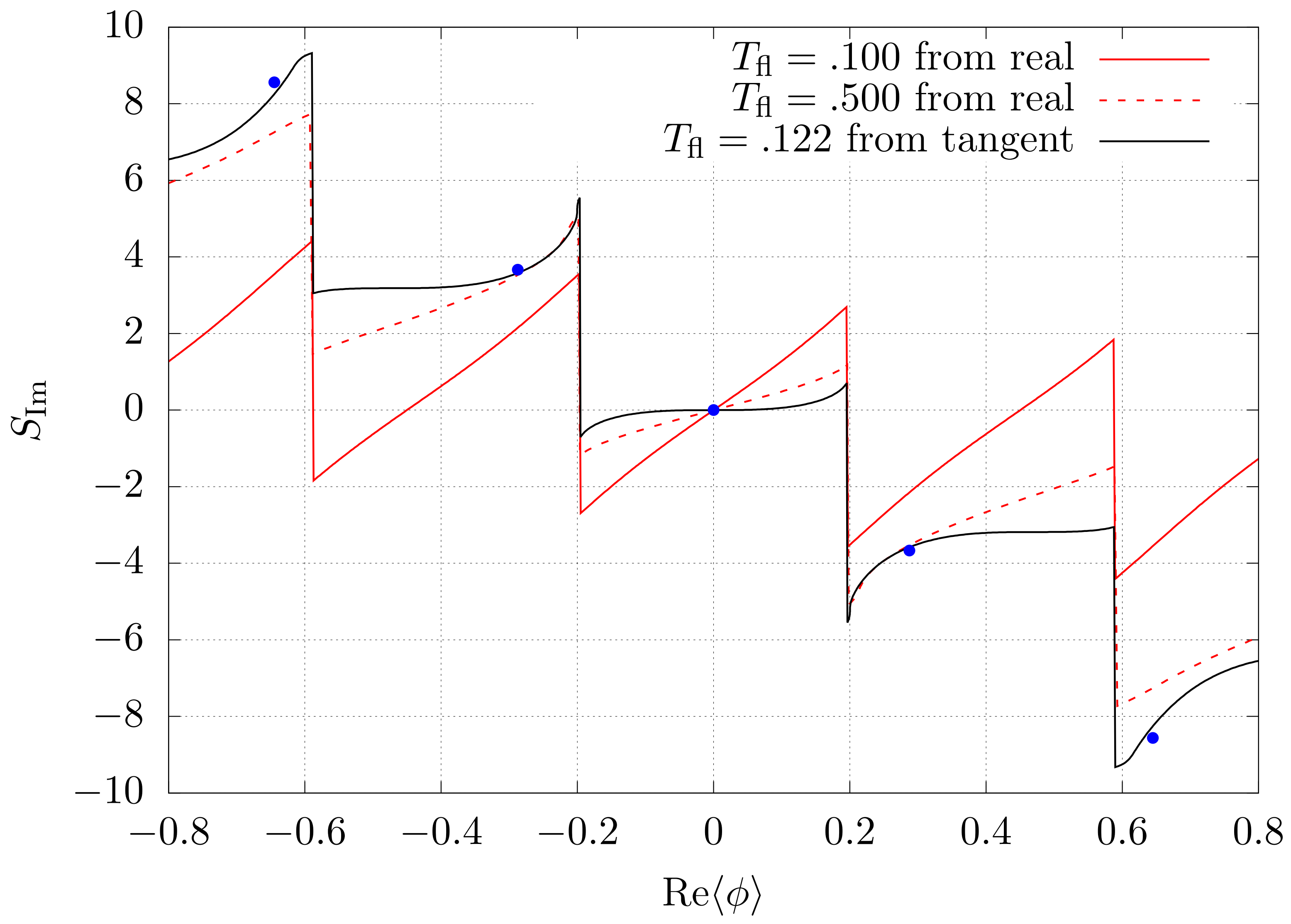


Complexify ϕ, try to integrate on steepest-descent analogues called *Lefschetz thimbles*, fixed points of holomorphic flow

$$\frac{\mathrm{d}\phi^R}{\mathrm{d}\tau_f} = \pm\frac{\partial S^R}{\partial \phi^R_i} = \pm\frac{\partial S^I}{\partial \phi^I_i} \qquad \frac{\mathrm{d}\phi^I}{\mathrm{d}\tau_f} = \pm\frac{\partial S^R}{\partial \phi^I_i} = \mp\frac{\partial S^I}{\partial \phi^R_i}$$



Flow too much and get an ergodicity problem!



As you flow to the thimbles, phases become constant.

Cristoforetti, Di Renzo, Scorzato PRD 86, 074506 10.1103/PhysRevD.86.074506 1205.3996

Alexandru, Başar, Bedaque, Warrington 2007.05436

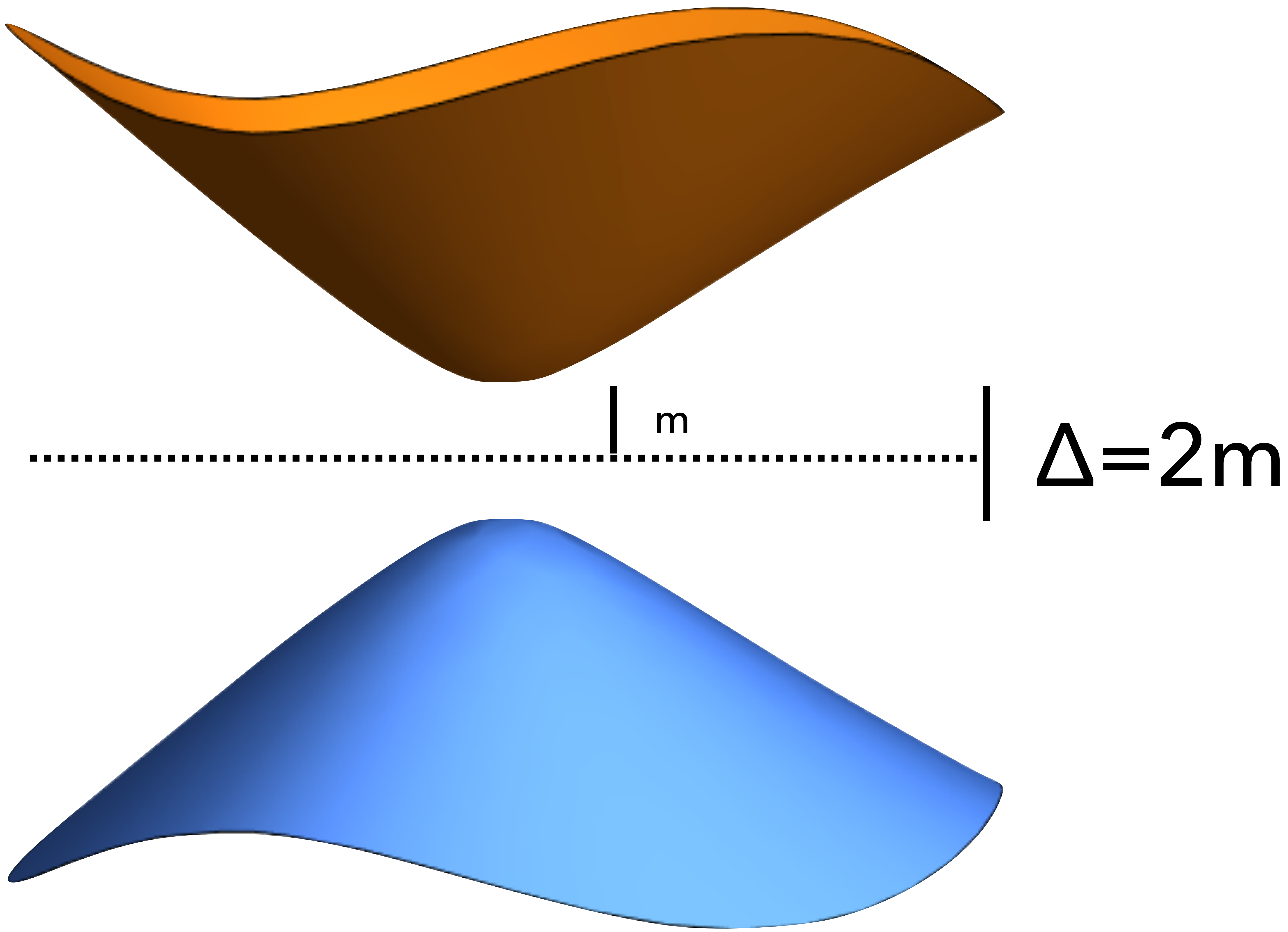
RESULTS

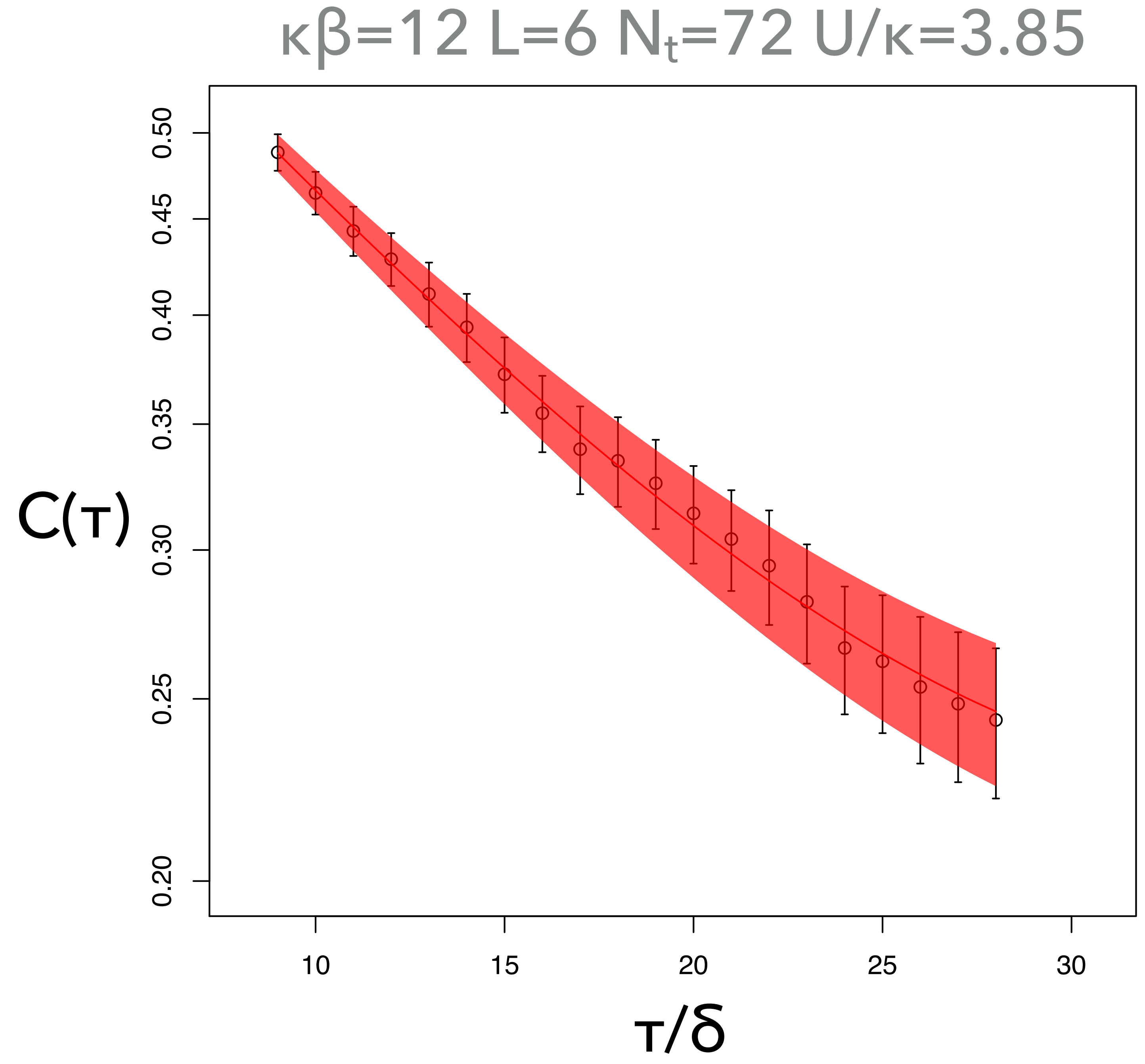
EFFECTIVE MASS

$$C_k^{AB}(\tau) = \left\langle \left(\sum_y e^{-iky} a_y^{A\dagger}(\tau) \right) \left(\sum_x e^{ikx} a_x^B(0) \right) \right\rangle = \frac{1}{\mathcal{Z}} \text{tr}\left[a_k^{A\dagger} e^{-H\tau} a_k^B e^{-H(\beta-\tau)} \right] = \frac{1}{\mathcal{Z}} \sum_{\alpha n} \left\langle \alpha \middle| a_k^{A\dagger} \middle| n \right\rangle \left\langle n \middle| a_k^B \middle| \alpha \right\rangle e^{-(E_n - E_\alpha)\tau} e^{-E_\alpha \beta}$$

$$\lim_{\tau\to\infty} -\partial_t \ln \lim_{\beta\to\infty} C_k^{AB}(\tau) = (E_1 - E_\Omega) = m$$

$$C_k^{AB}(\tau) = \left\langle \sum_t \left(M_{AB}^{-1} \right)_{k,t+\tau;k,t} \right\rangle$$





EFFECTIVE MASS

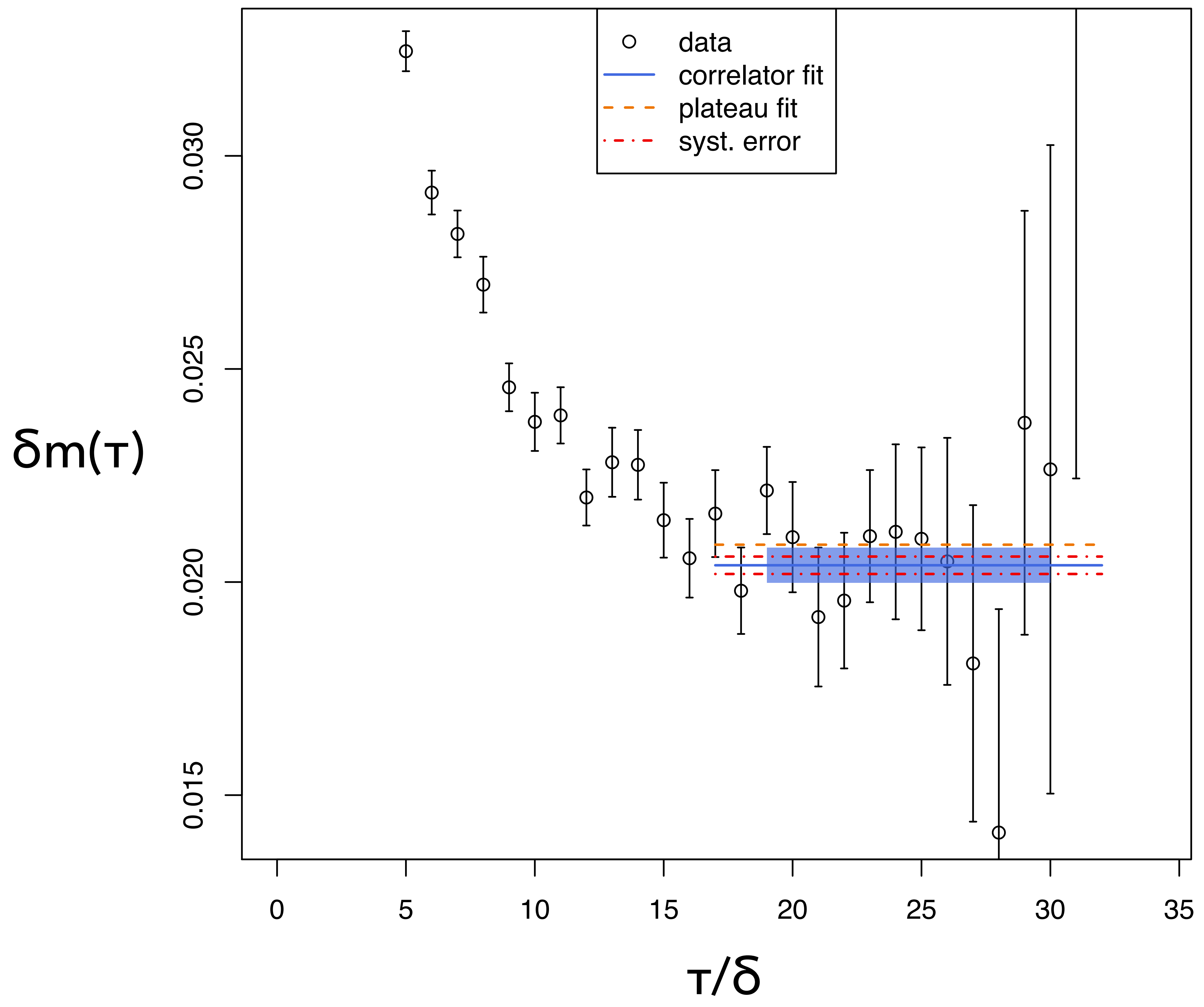
Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112

$$C_k^{AB}(\tau) = \left\langle \left(\sum_y e^{-iky} a_y^{A\dagger}(\tau) \right) \left(\sum_x e^{ikx} a_x^B(0) \right) \right\rangle = \frac{1}{\mathcal{Z}} \mathrm{tr} \left[a_k^{A\dagger} e^{-H\tau} a_k^B e^{-H(\beta-\tau)} \right] = \frac{1}{\mathcal{Z}} \sum_{\alpha n} \left\langle \alpha \middle| a_k^{A\dagger} \middle| n \right\rangle \left\langle n \middle| a_k^B \middle| \alpha \right\rangle e^{-(E_n-E_\alpha)\tau} e^{-E_\alpha \beta}$$

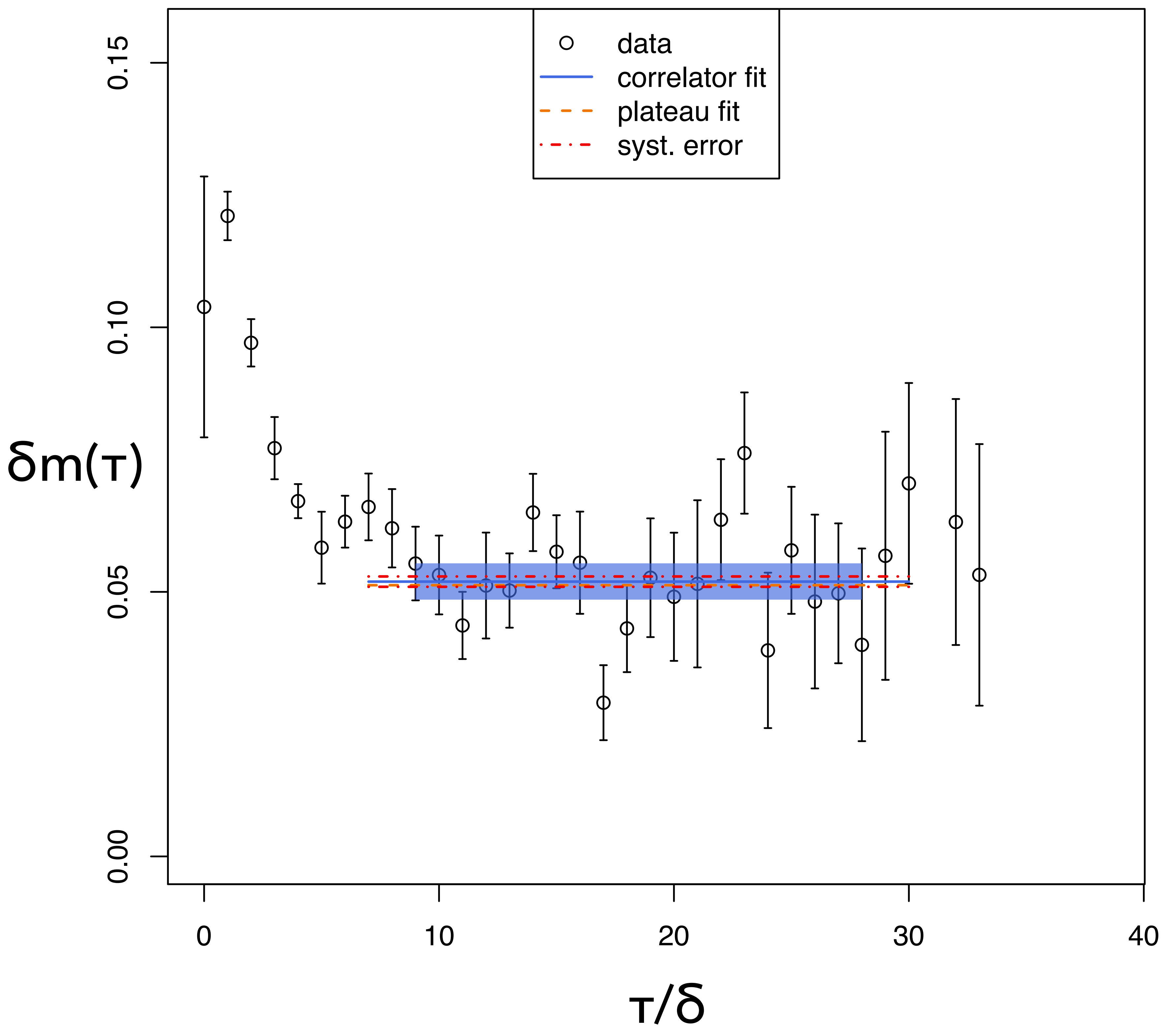
$$C_k^{AB}(\tau) = \left\langle \sum_t \left(M_{AB}^{-1}\right)_{k,t+\tau;k,t} \right\rangle$$

$$\lim_{\tau\to\infty} -\partial_t \ln \lim_{\beta\to\infty} C_k^{AB}(\tau) = (E_1 - E_\Omega) = m$$

κβ=8 L=15 N_t=64 U/κ=3.5

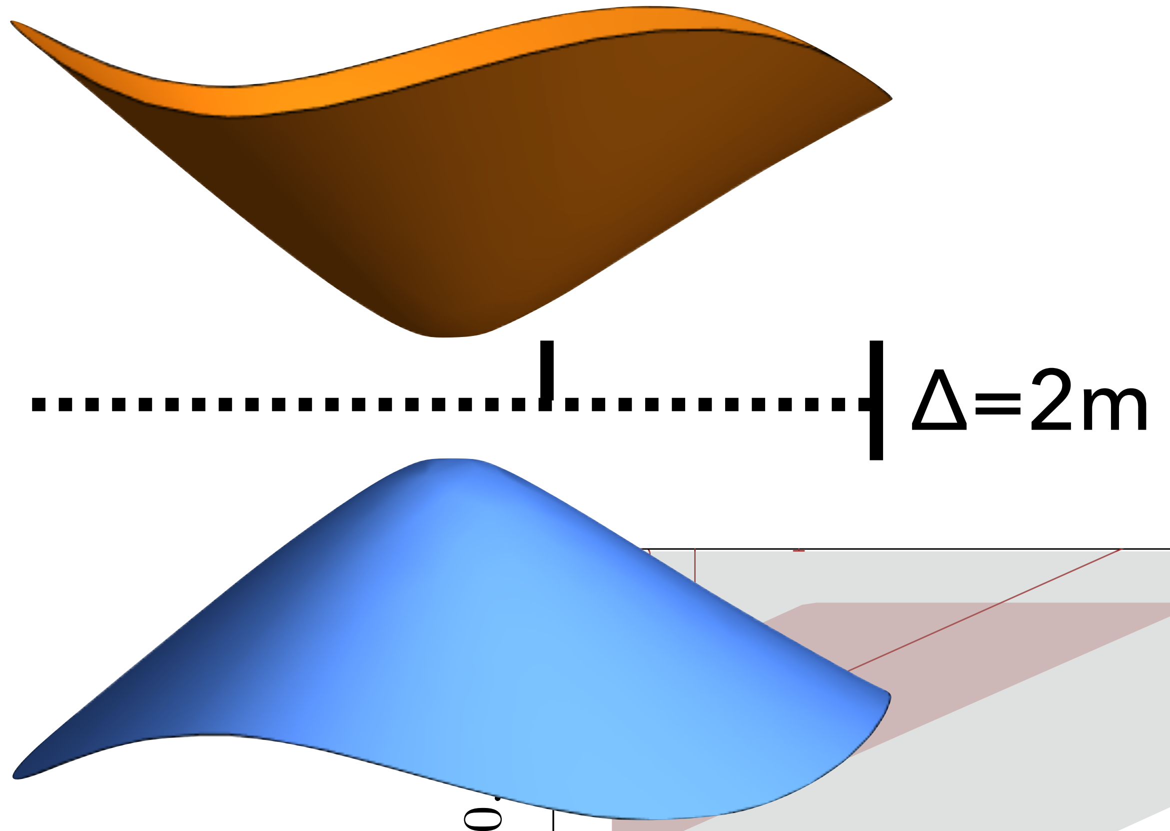


κβ=12 L=6 N_t=72 U/κ=3.85

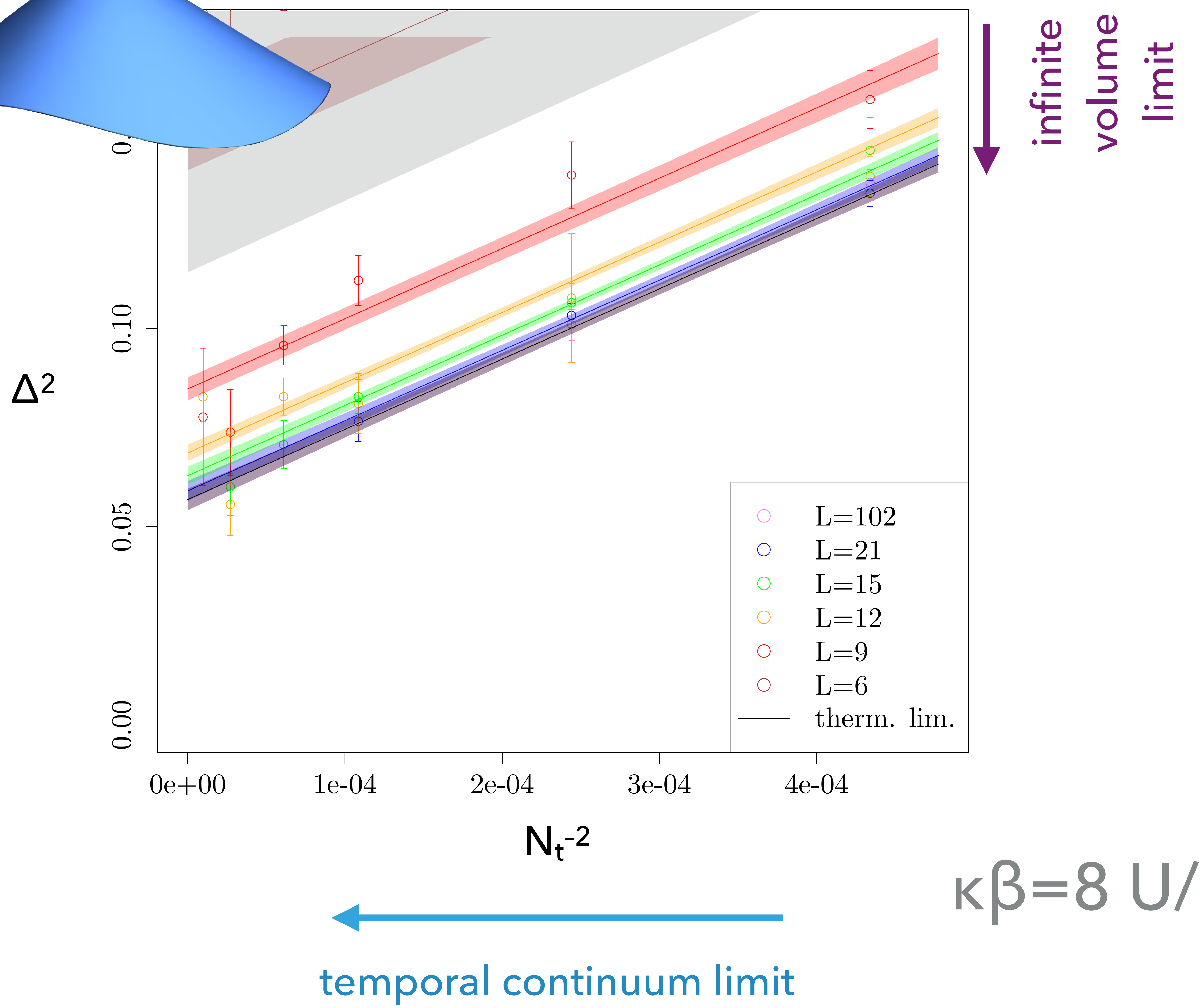


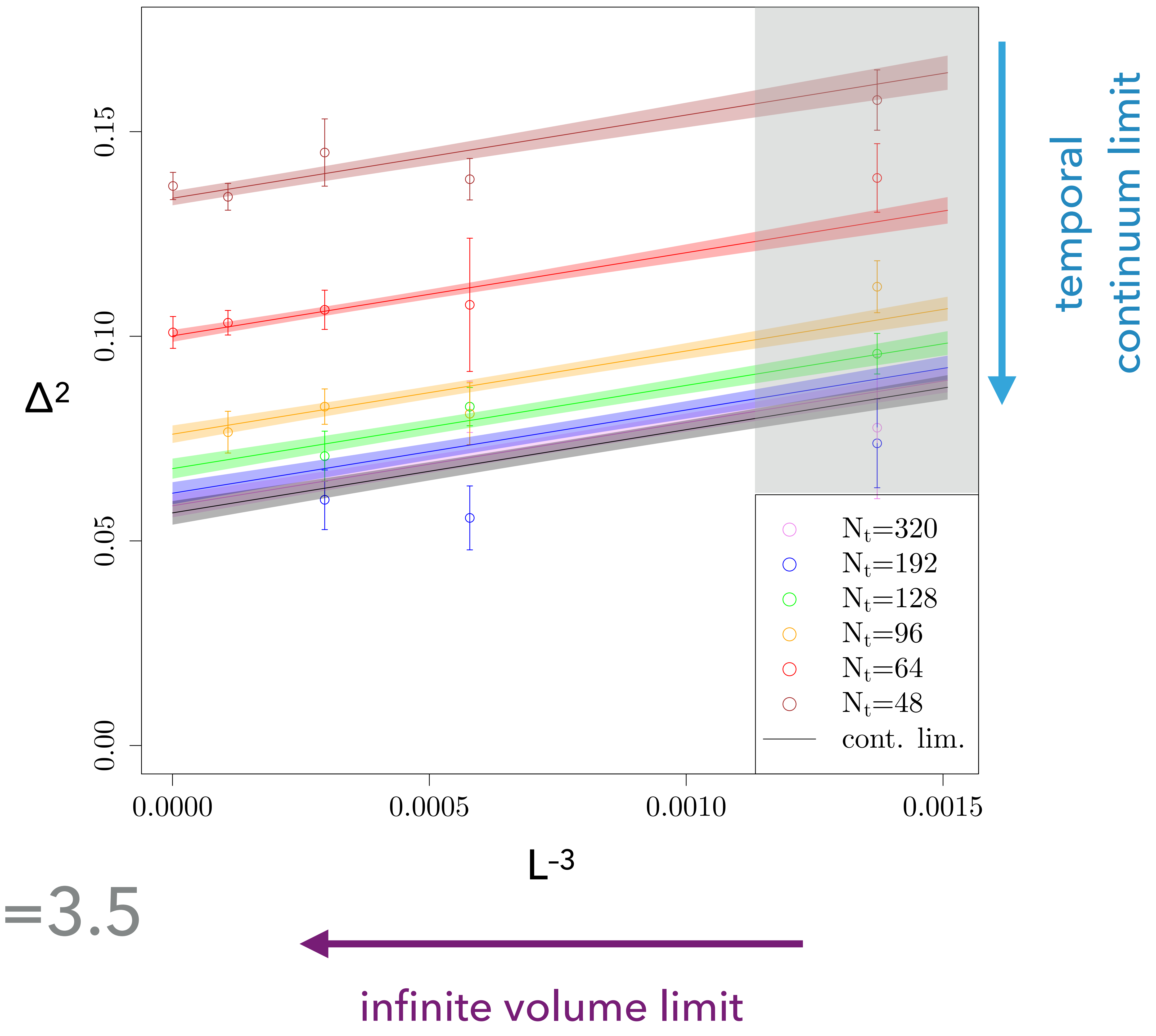
SYSTEMATIC EXTRAPOLATION

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112



$$\Delta^2(L, N_t) = \Delta_0^2 + \frac{c_0}{N_t^2} + \frac{c_1}{L^3} + \cdots$$

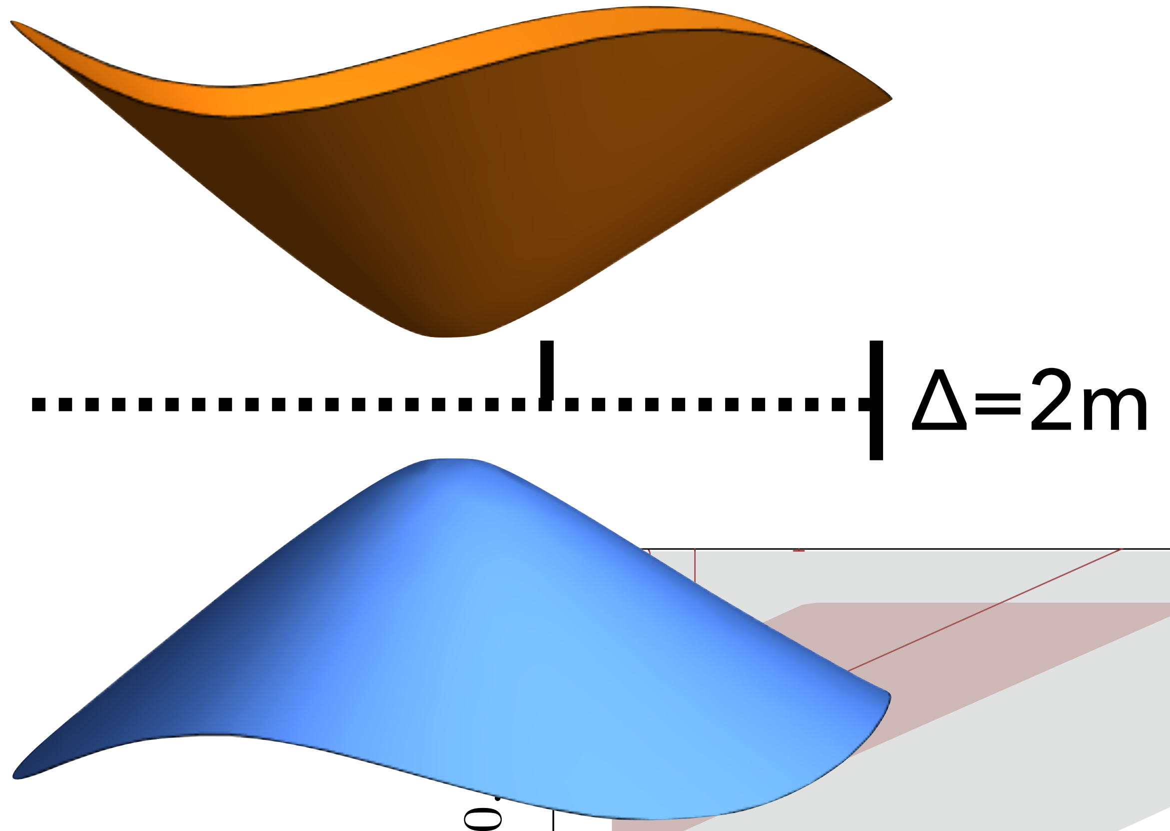




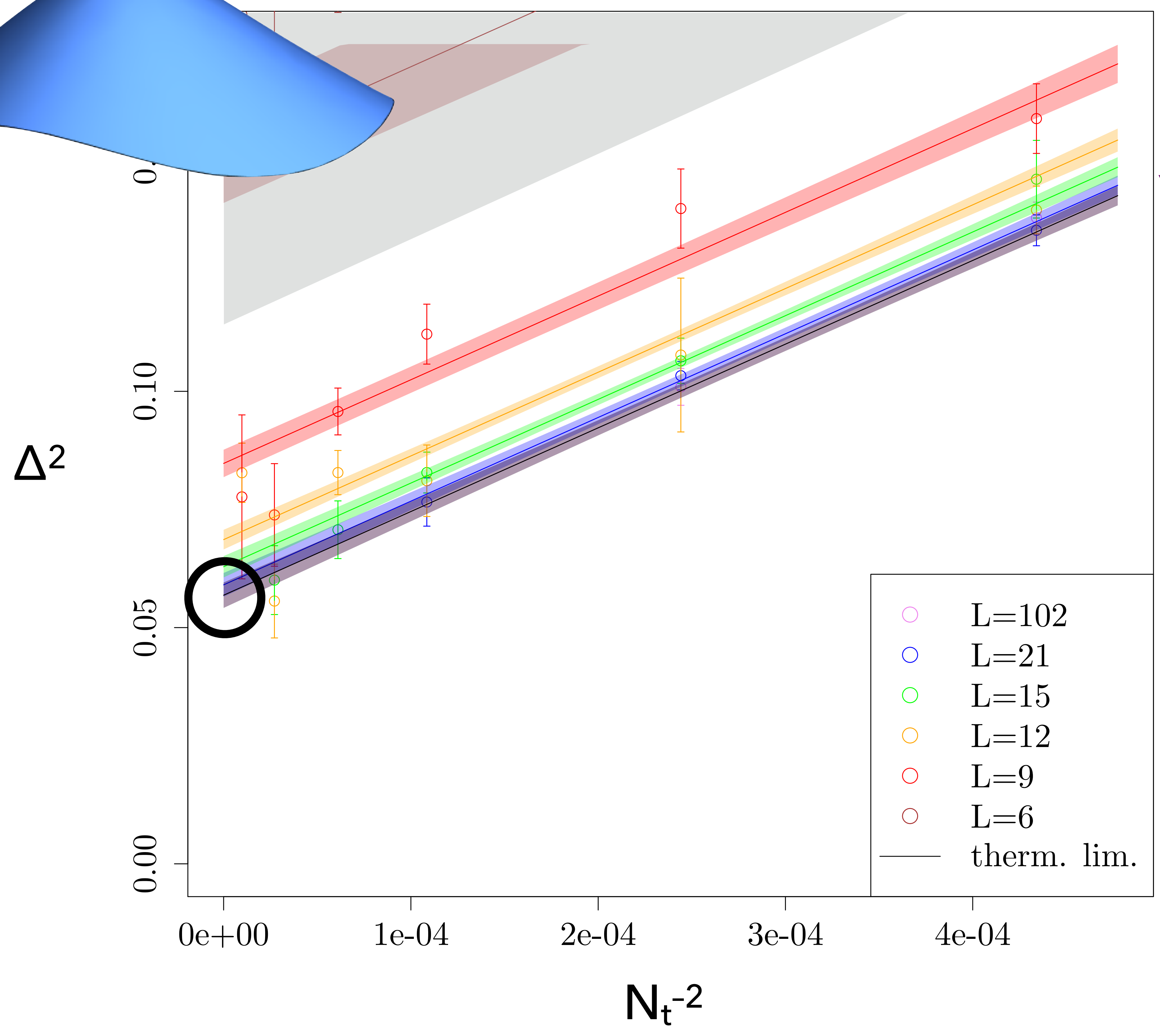
κβ=8 U/κ=3.5

SYSTEMATIC EXTRAPOLATION

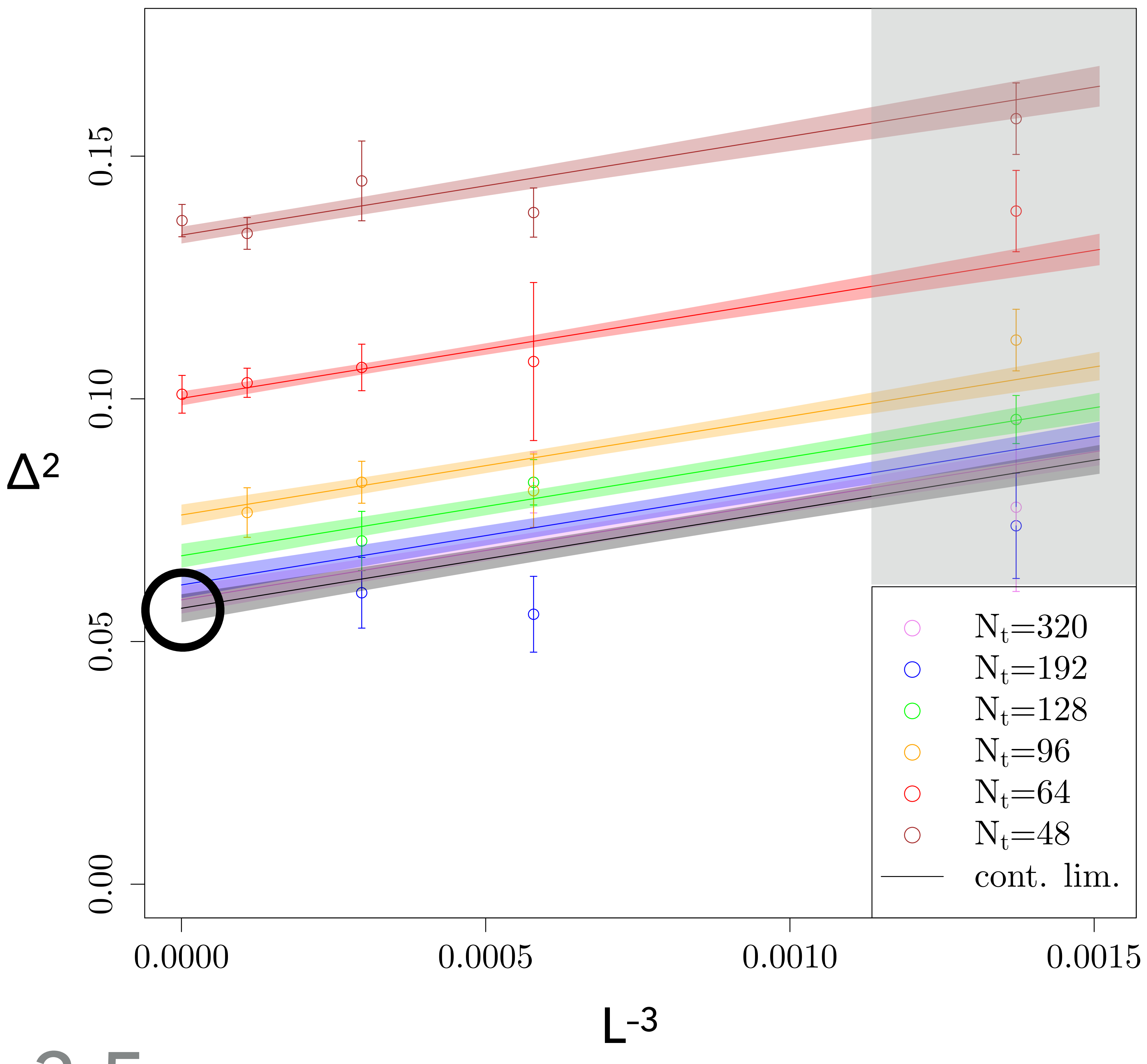
Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112



$$\Delta^2(L, N_t) = \Delta_0^2 + \frac{c_0}{N_t^2} + \frac{c_1}{L^3} + \cdots$$



infinite volume limit



temporal continuum limit

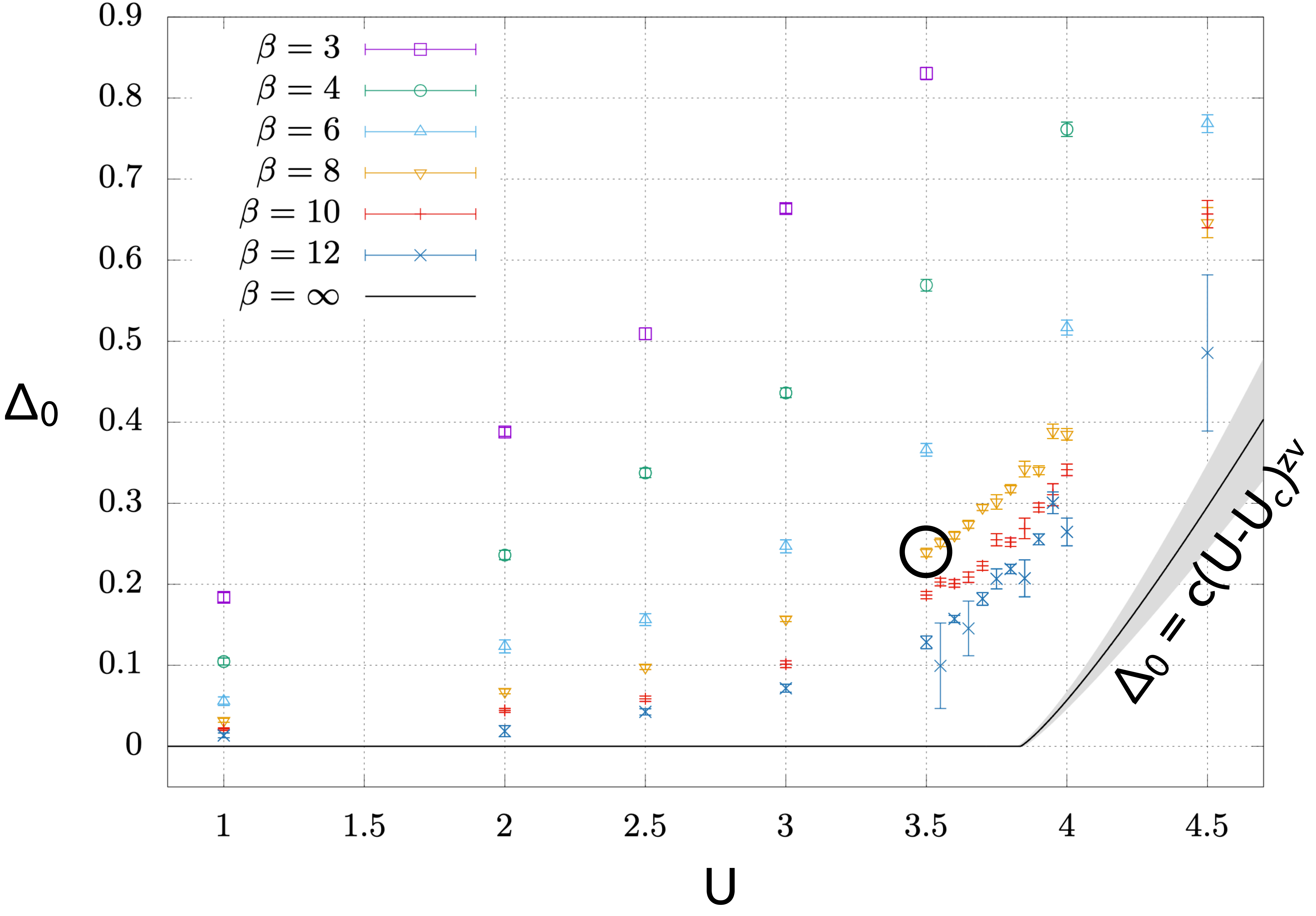
$\kappa\beta=8$ $U/\kappa=3.5$

temporal continuum limit

infinite volume limit

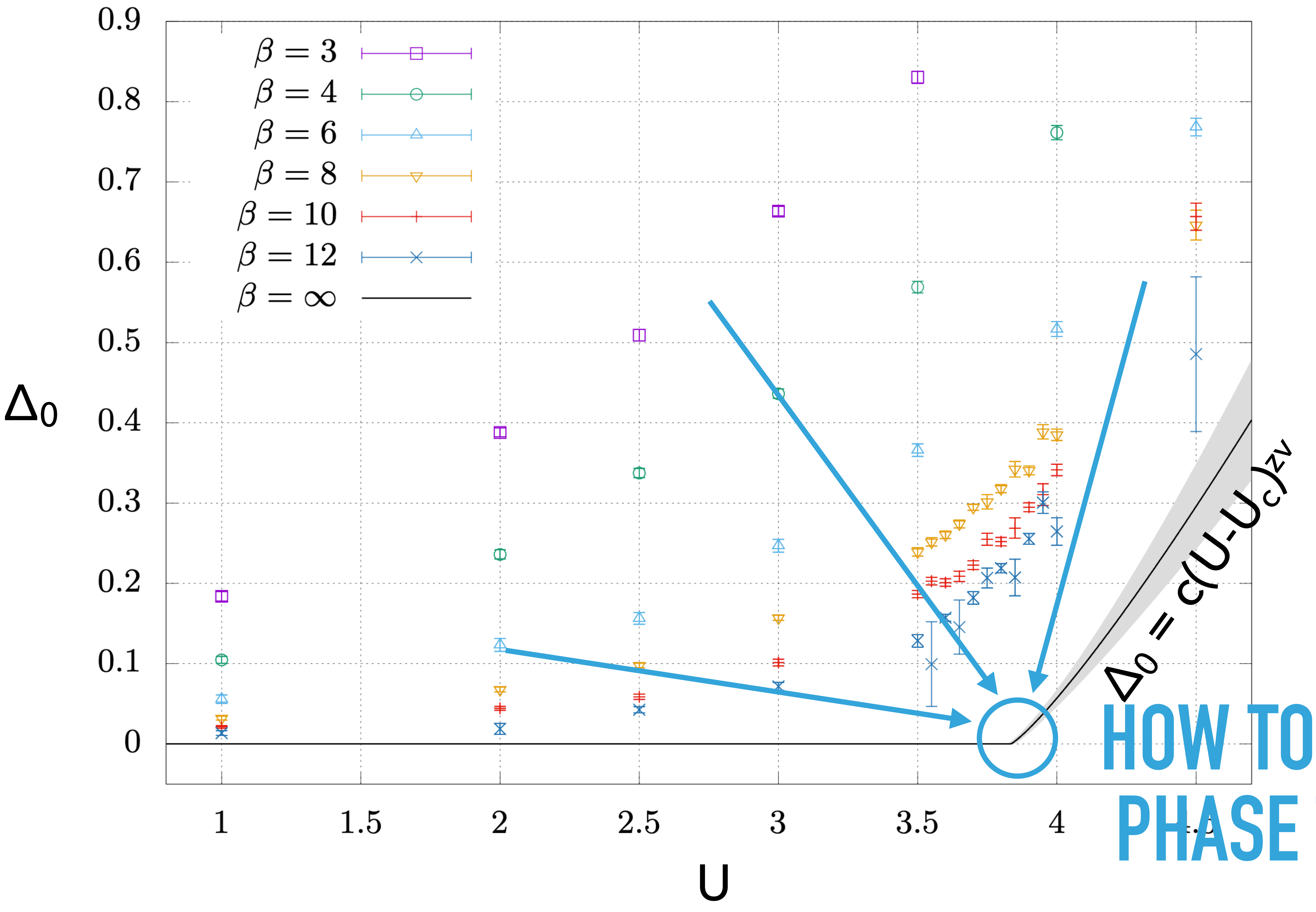
THERMODYNAMIC LIMIT

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112



THERMODYNAMIC LIMIT

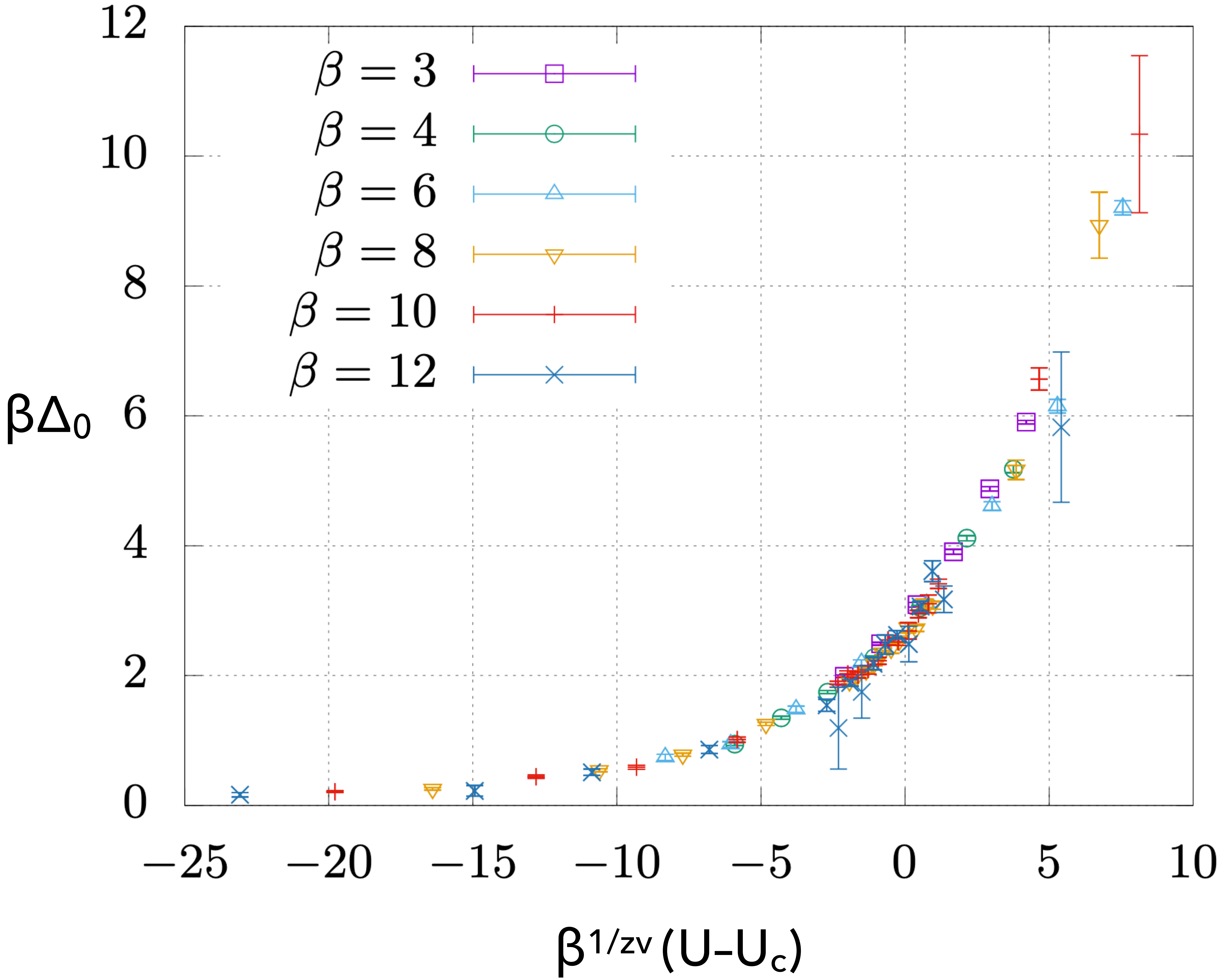
Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112



HOW TO EXTRACT THE PHASE TRANSITION?

FINITE-SIZE SCALING

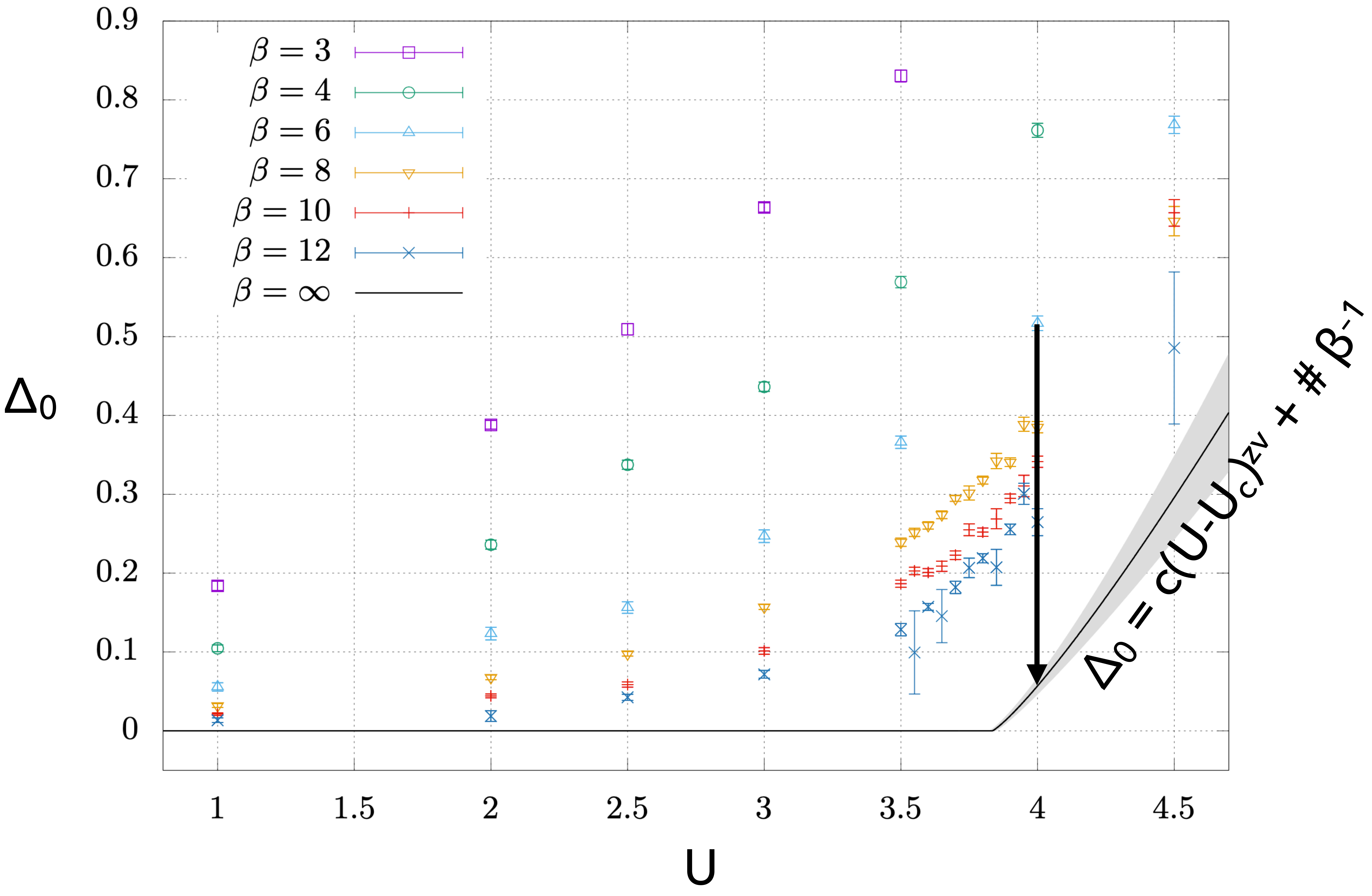
Assaad and Herbut, PRX 3, 031010 (2013) 1304.6340
Wang, Corboz, and Troyer, New J. Phys 16, 103008 (2014) 1407.0029
Otsuka, Yunoki, Sorella, PRX 6, 011029 (2016) 1510.08593



$U_c = 3.834(14)$
$z\nu = 1.185(43)$

ZERO-TEMPERATURE LIMIT

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112

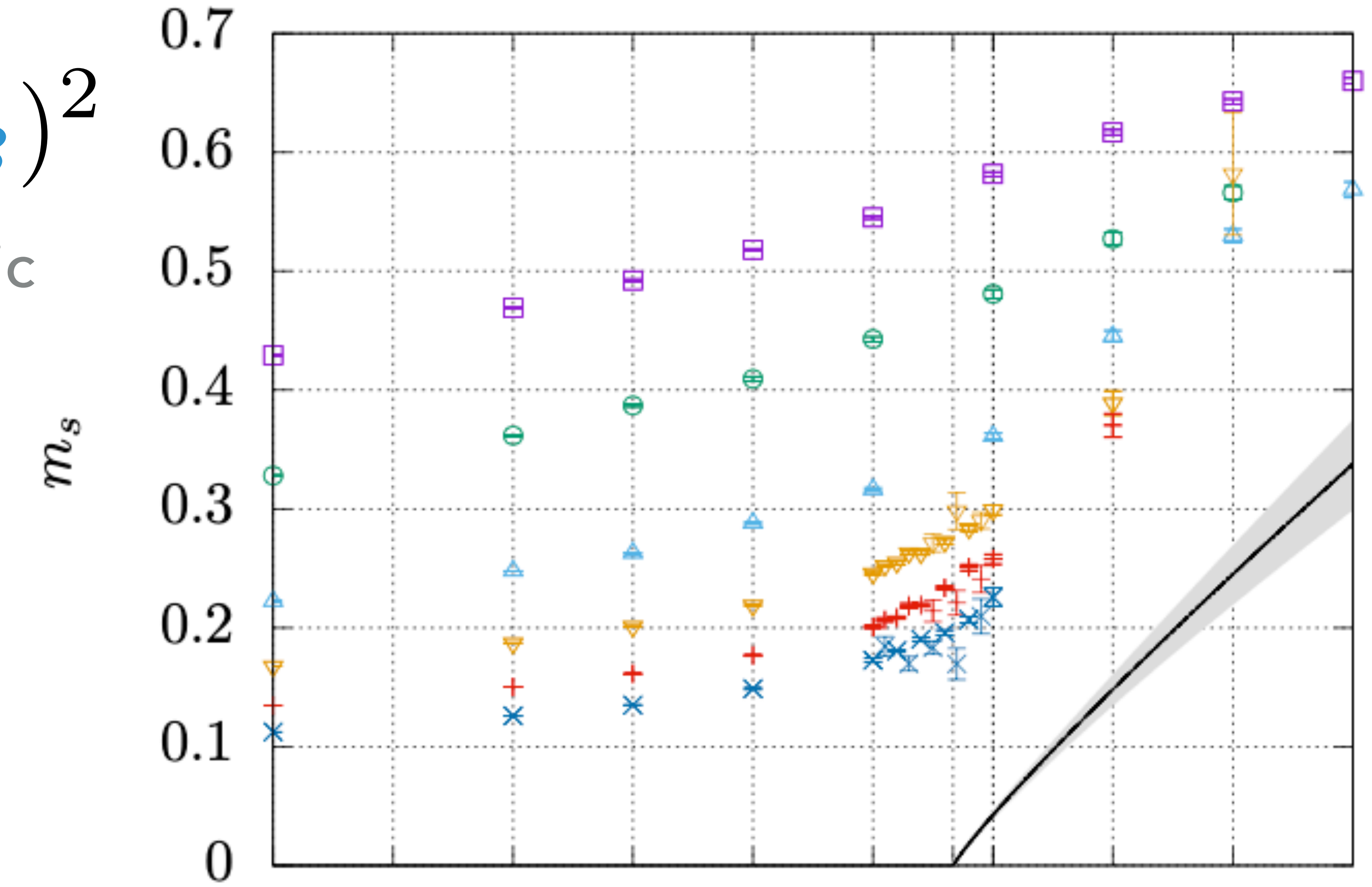


ZERO-TEMPERATURE LIMIT

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2105.06936

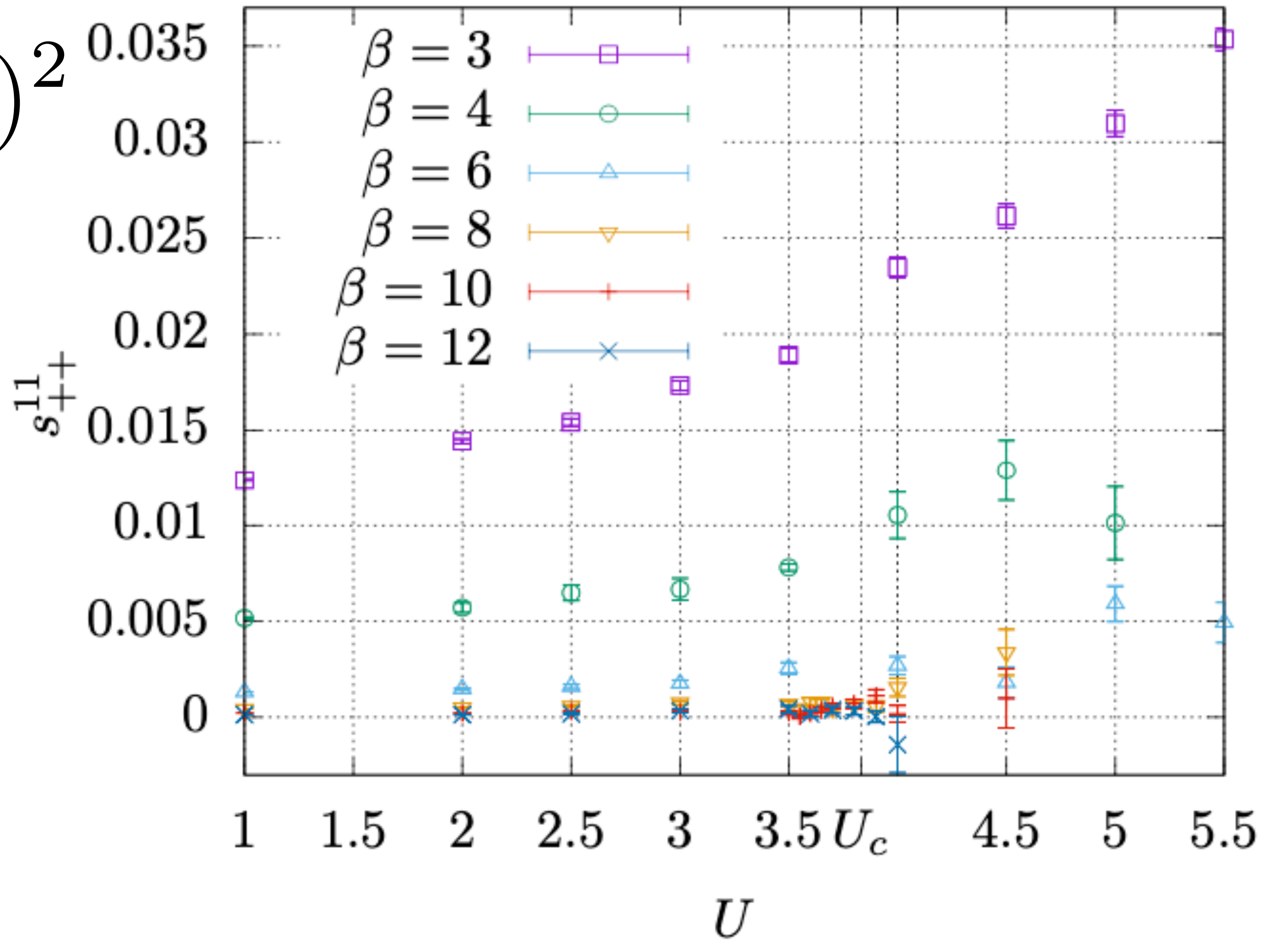
$\sim (\vec{S}_A - \vec{S}_B)^2$

antiferromagnetic



$\sim (\vec{S}_A + \vec{S}_B)^2$

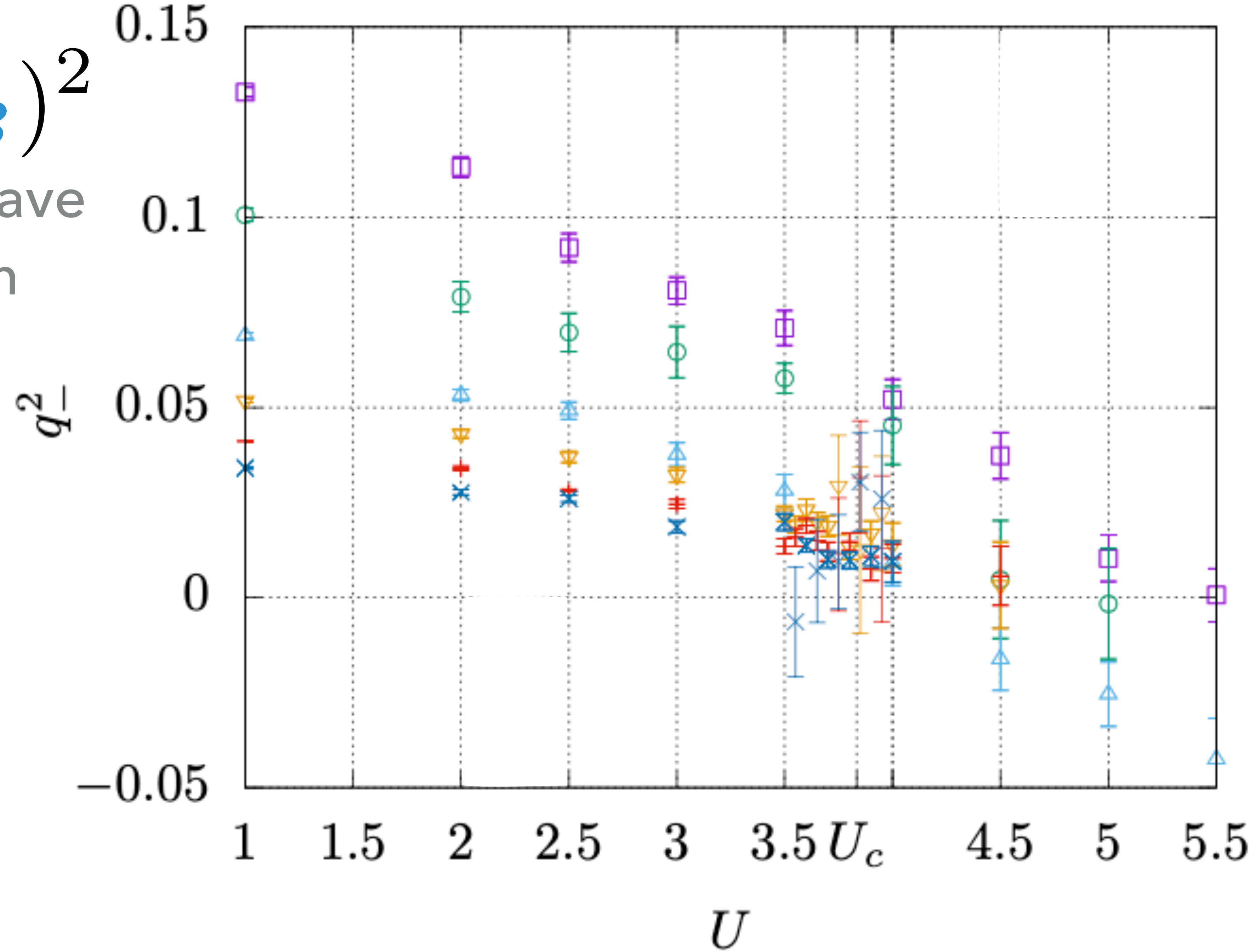
ferromagnetic

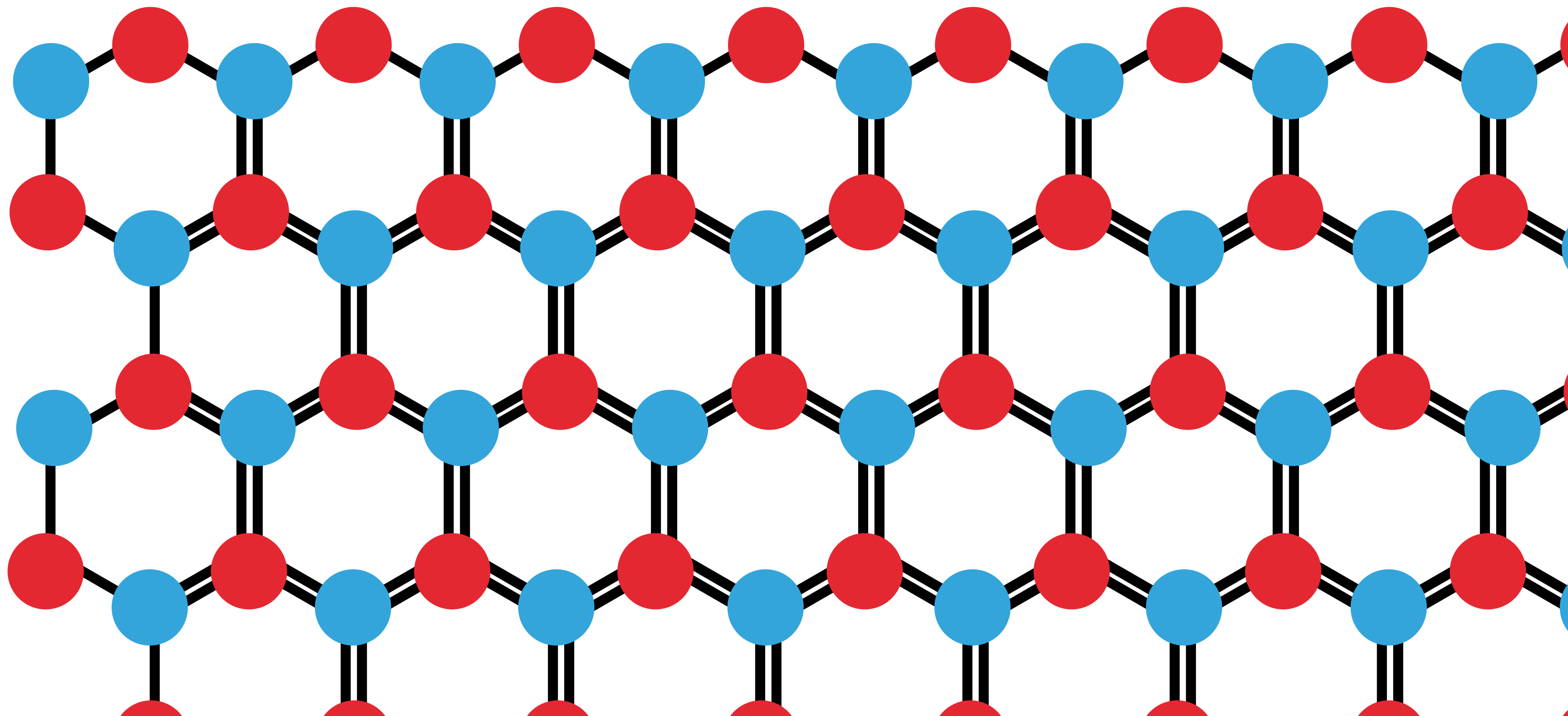


$\sim (\vec{Q}_A - \vec{Q}_B)^2$

charge-density wave

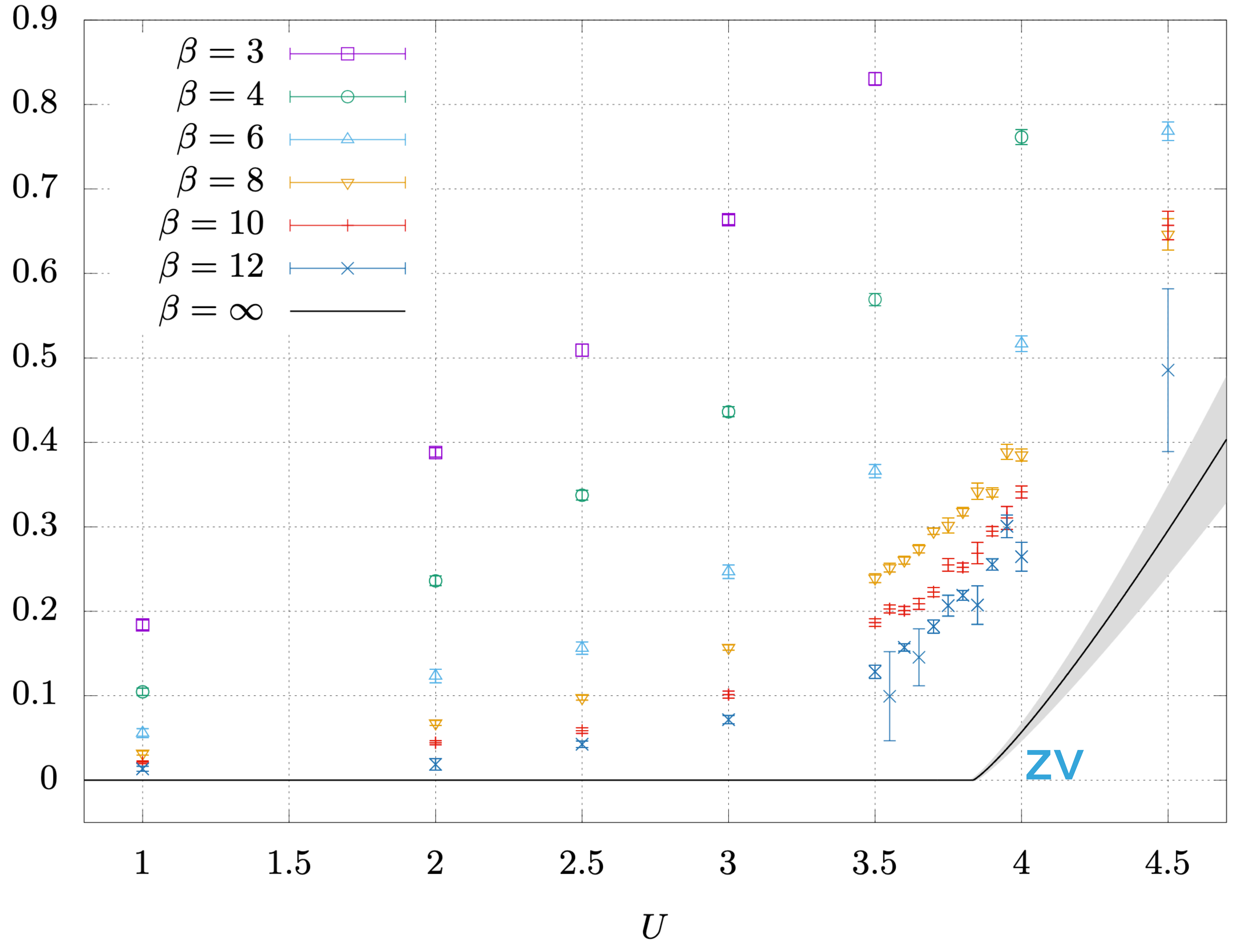
charge separation



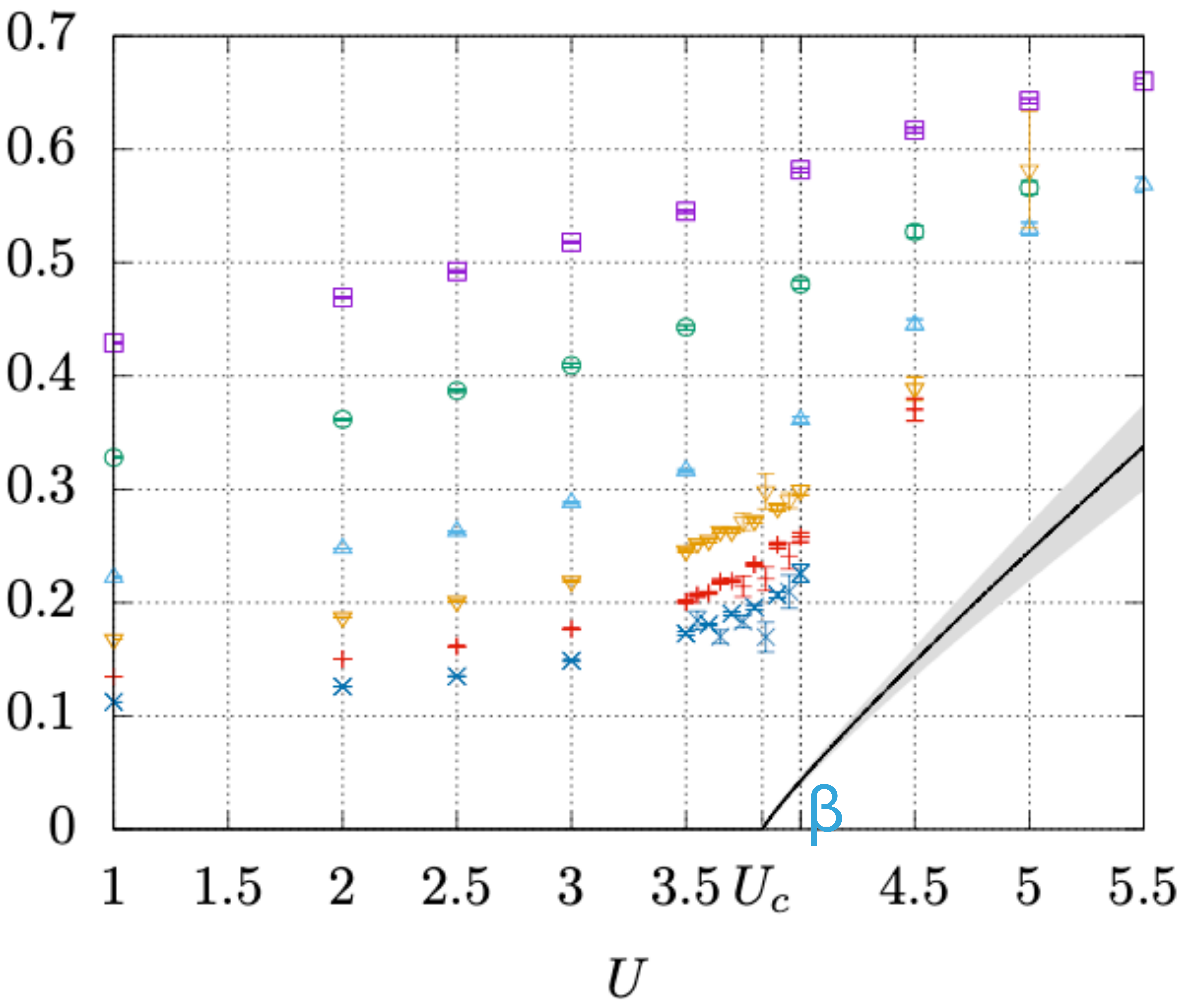


THE PHASE TRANSITION

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112
2105.06936



Δ_0



$\sim (\vec{S}_A - \vec{S}_B)^2$

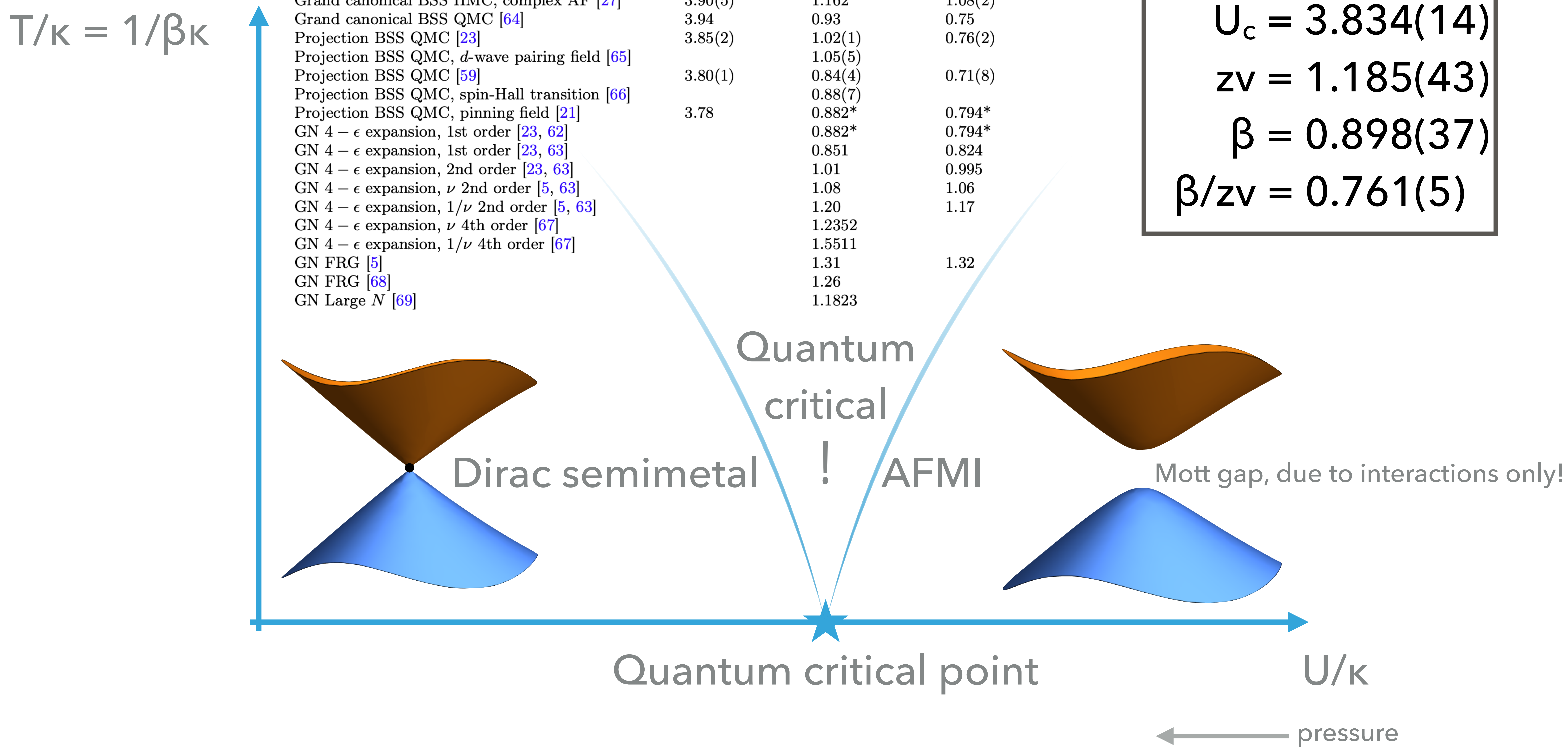
antiferromagnetic

PHASE DIAGRAM

Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112
2105.06936

Method	U_c/κ	ν	β
Grand canonical BSS HMC, complex AF [27]	3.90(5)	1.162	1.08(2)
Grand canonical BSS QMC [64]	3.94	0.93	0.75
Projection BSS QMC [23]	3.85(2)	1.02(1)	0.76(2)
Projection BSS QMC, d-wave pairing field [65]		1.05(5)	
Projection BSS QMC [59]	3.80(1)	0.84(4)	0.71(8)
Projection BSS QMC, spin-Hall transition [66]		0.88(7)	
Projection BSS QMC, pinning field [21]	3.78	0.882*	0.794*
GN $4-\epsilon$ expansion, 1st order [23, 62]		0.882*	0.794*
GN $4-\epsilon$ expansion, 1st order [23, 63]		0.851	0.824
GN $4-\epsilon$ expansion, 2nd order [23, 63]		1.01	0.995
GN $4-\epsilon$ expansion, ν 2nd order [5, 63]		1.08	1.06
GN $4-\epsilon$ expansion, $1/\nu$ 2nd order [5, 63]		1.20	1.17
GN $4-\epsilon$ expansion, ν 4th order [67]		1.2352	
GN $4-\epsilon$ expansion, $1/\nu$ 4th order [67]		1.5511	
GN FRG [5]		1.31	1.32
GN FRG [68]		1.26	
GN Large N [69]		1.1823	

$U_c = 3.834(14)$
$z\nu = 1.185(43)$
$\beta = 0.898(37)$
$\beta/z\nu = 0.761(5)$



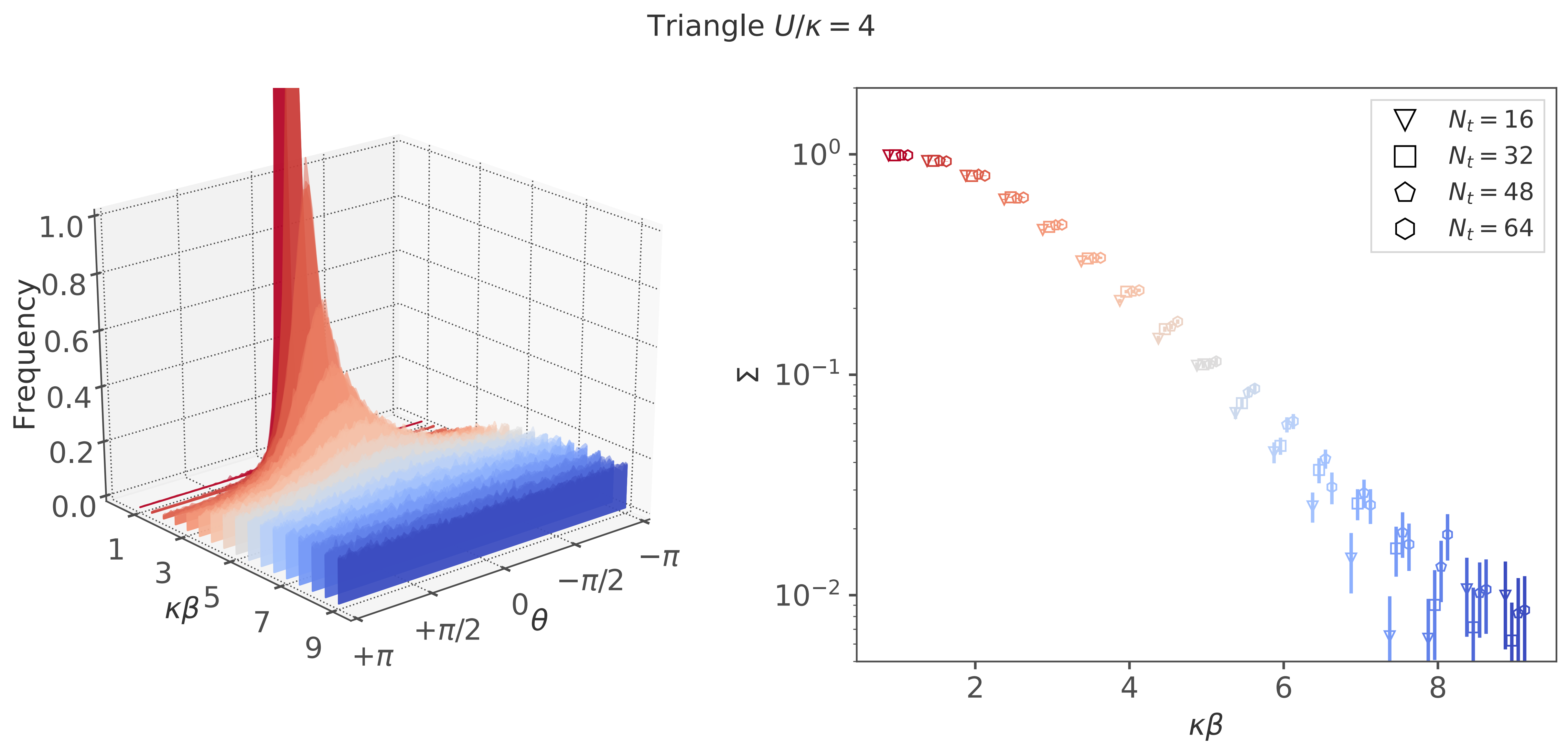
SIGN PROBLEMS

COMPLEX WEIGHTS LEAD TO SIGN PROBLEMS

The average sign, or *statistical power* Σ

$$\Sigma = \left|\langle e^{-iS^I}\rangle_R\right|$$

is the ratio of two partition functions ~ differences of free energies
so is extensive in spacetime volume → exponentially decays



$$\mathcal{Z} \propto \int \mathcal{D}\phi \; \det\left(M[\phi,h,\mu]\; M^\dagger[\phi,h,-\mu]\right) e^{-\frac{1}{2}\sum_{xyt}\phi_{xt}V^{-1}_{xy}\phi_{yt}}$$

Probability?

Generate an *ensemble* for fixed U, β, N_t, …

$$\{\phi_1,\ \phi_2,\ \cdots,\ \phi_N\}$$

Hybrid Monte Carlo

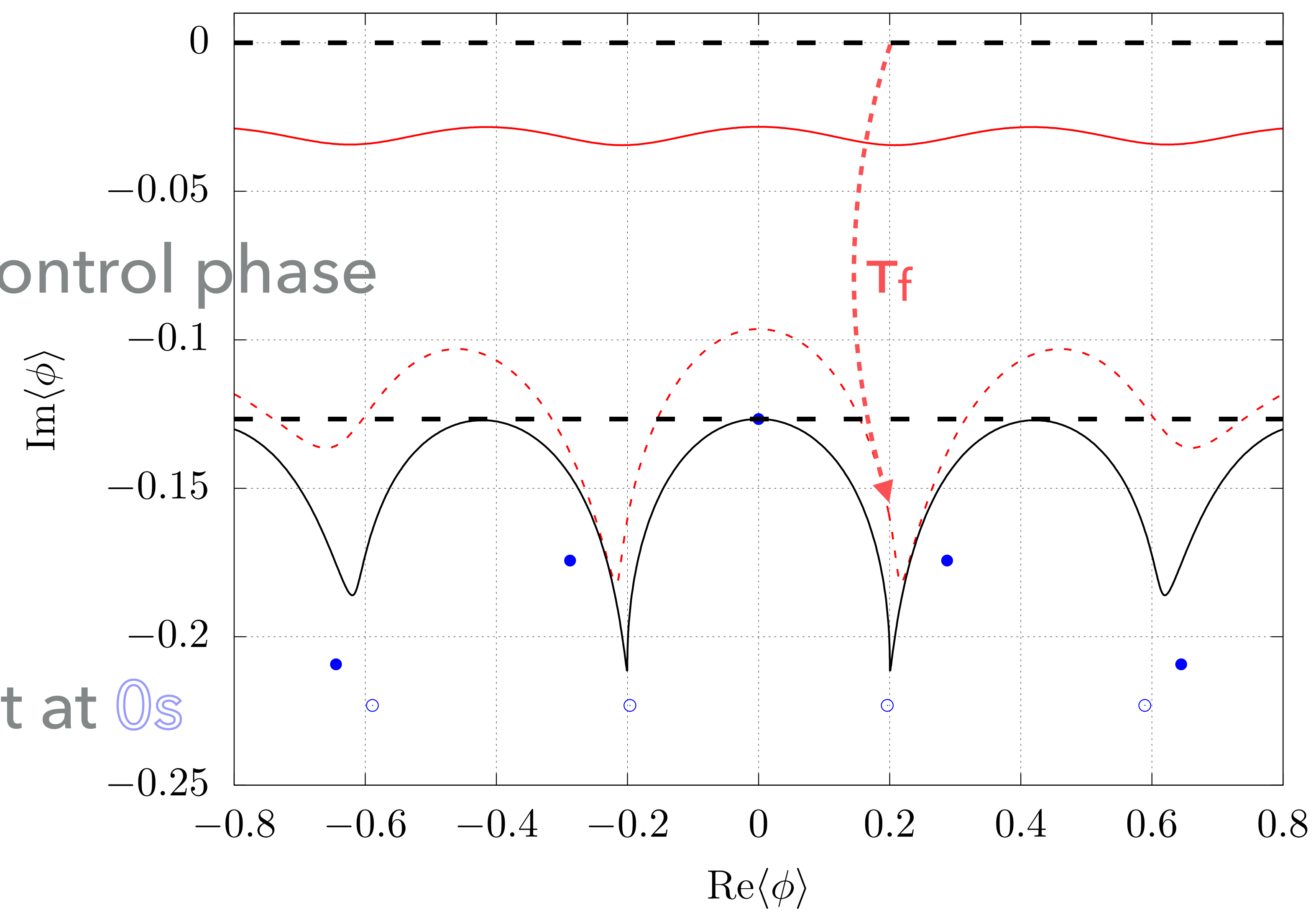
Estimate any observable

$$\langle\mathcal{O}\rangle = \frac{\left\langle \mathcal{O}e^{-iS^I}\right\rangle_R}{\left\langle e^{-iS^I}\right\rangle_R}$$

Importance sample according to the real part of the weight

Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221

LEFSCHETZ THIMBLES HAVE CONSTANT SIGN



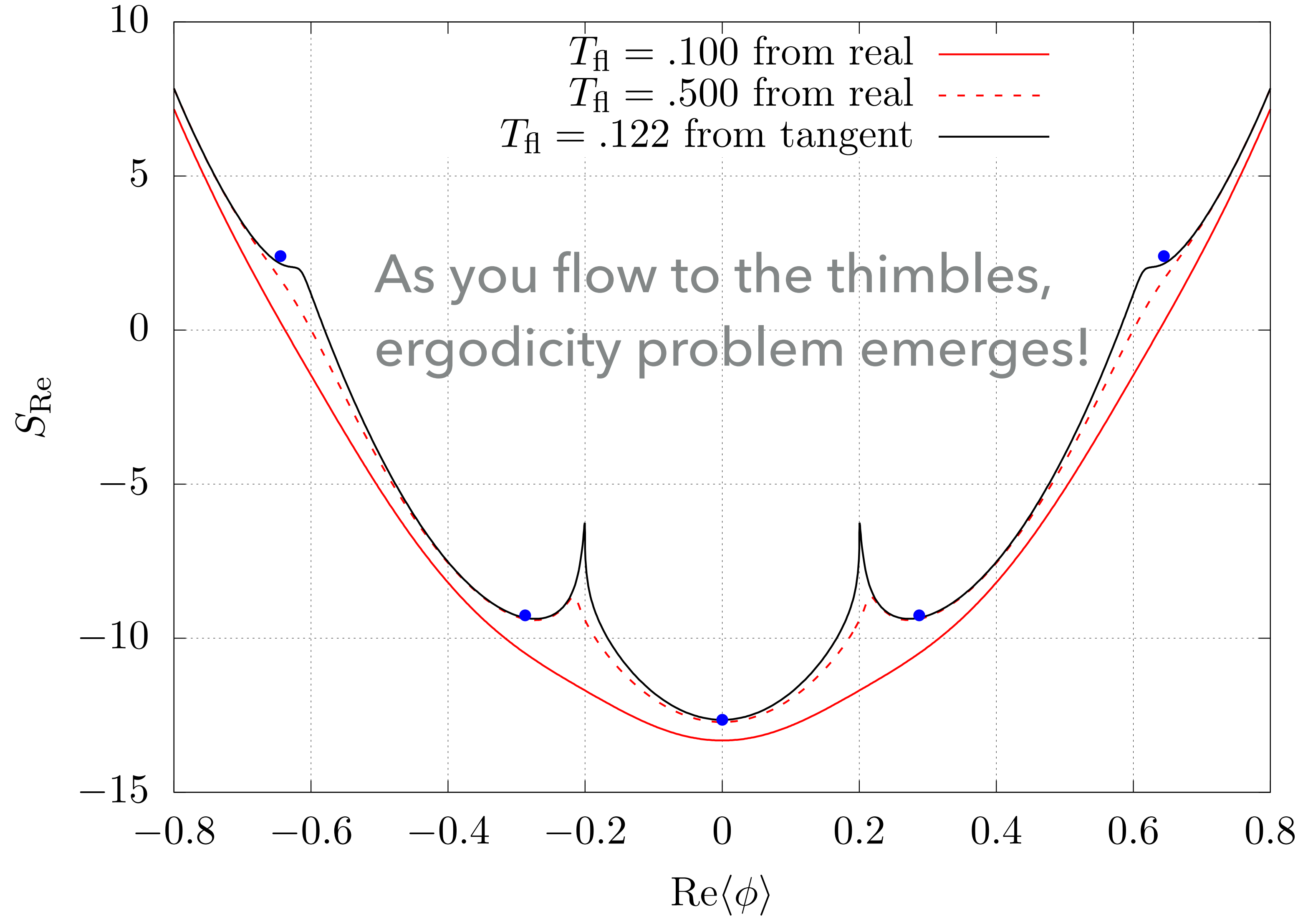
Critical points control phase

Thimbles meet at 0s

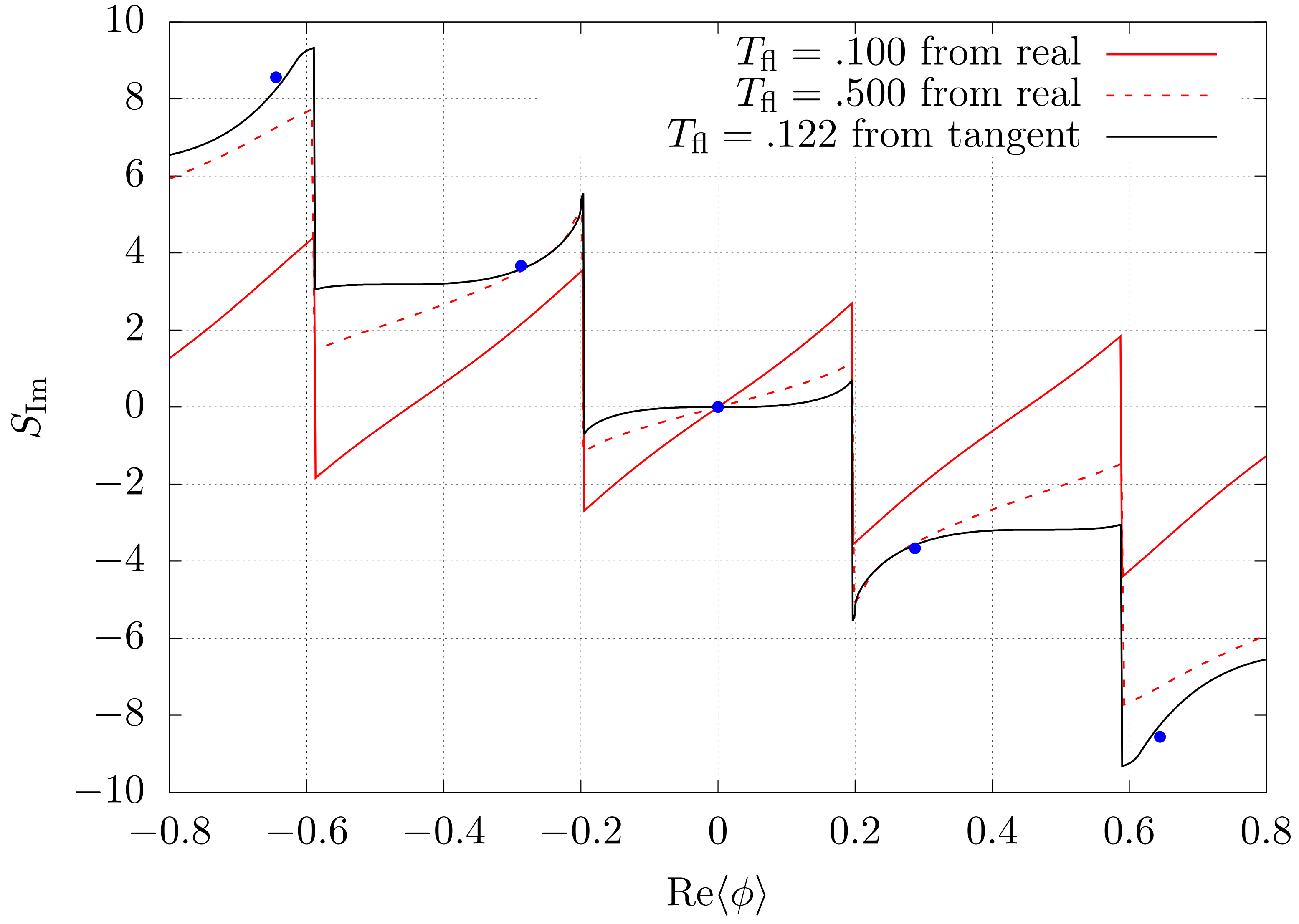
$$\mathcal{Z} \propto \int \mathcal{D}\phi \det\left(M[\phi,h,\mu]\, M^\dagger[\phi,h,-\mu]\right) e^{-\frac{1}{2}\sum_{xyt} \phi_{xt} V^{-1}_{xy} \phi_{yt}}$$

Complexify ϕ, integrate on steepest-descent analogues called *Lefschetz thimbles*, fixed points of holomorphic flow

$$\frac{d\phi^R}{d\tau_f} = \pm\frac{\partial S^R}{\partial \phi_i^R} = \pm\frac{\partial S^I}{\partial \phi_i^I} \qquad \frac{d\phi^I}{d\tau_f} = \pm\frac{\partial S^R}{\partial \phi_i^I} = \mp\frac{\partial S^I}{\partial \phi_i^R}$$



As you flow to the thimbles, ergodicity problem emerges!

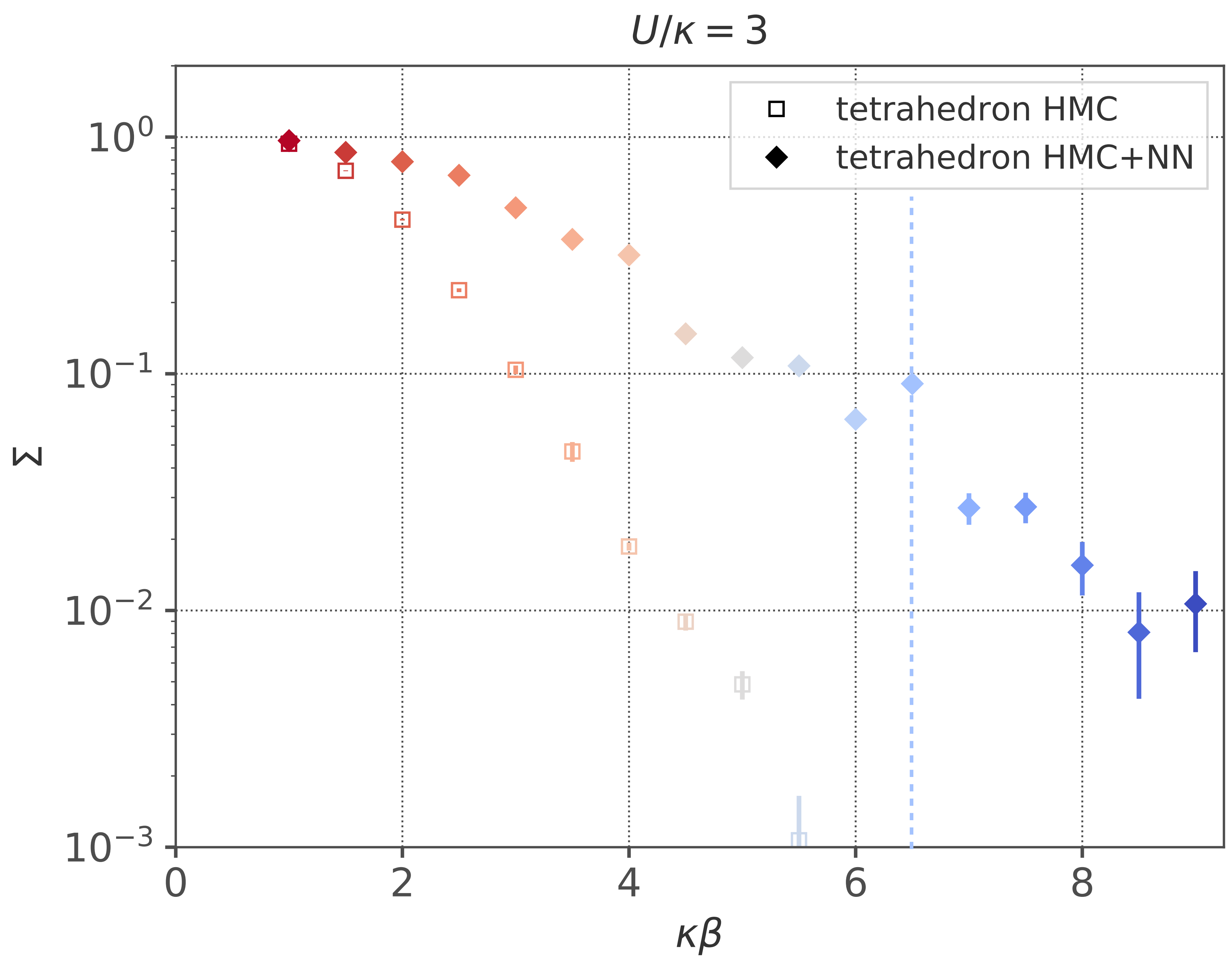


As you flow to the thimbles, phases become constant.

Cristoforetti, Di Renzo, Scorzato PRD 86, 074506 10.1103/PhysRevD.86.074506 1205.3996

Alexandru, Bedaque, Lamm, Lawrence PRD 96, 094505 (2017) 10.1103/PhysRevD.96.094505 1709.01971

MACHINE LEARNING FOR FAST FLOWS



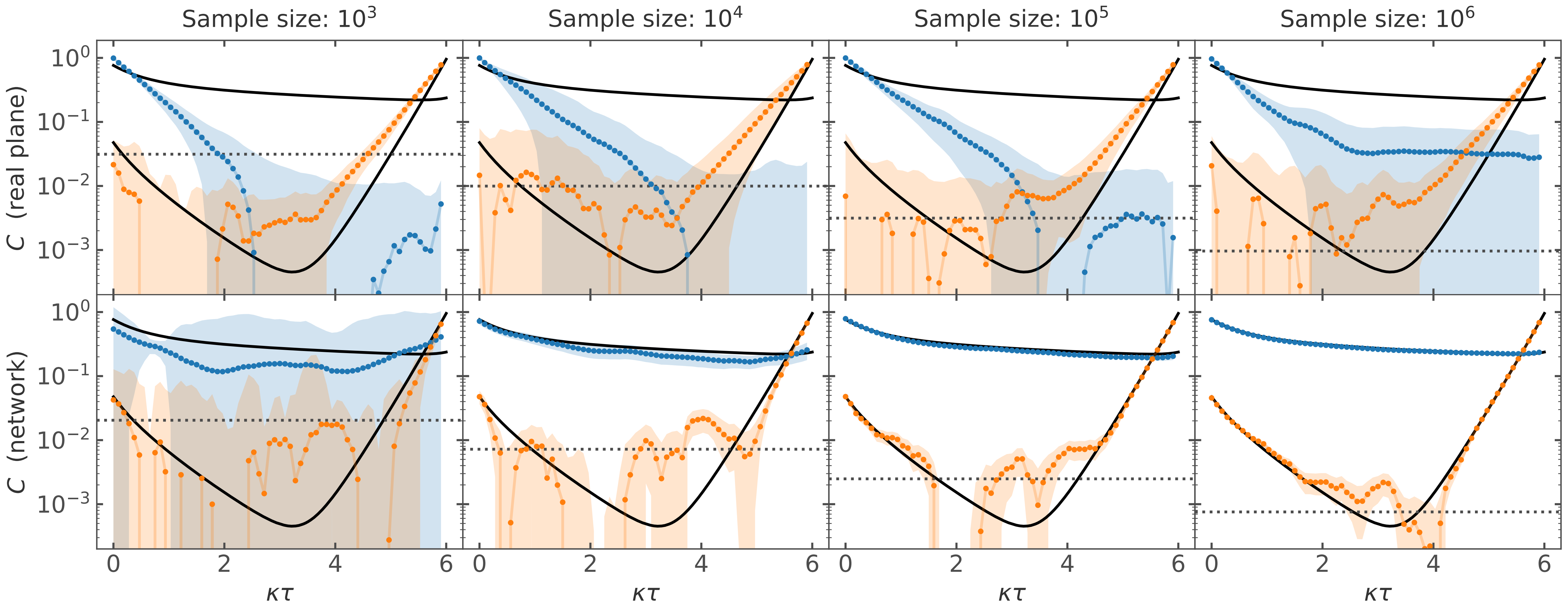
$$\mathcal{Z} \propto \int \mathcal{D}\phi \det\left(M[\phi,h,\mu]\, M^\dagger[\phi,h,-\mu]\right) e^{-\frac{1}{2}\sum_{xyt}\phi_{xt}V^{-1}_{xy}\phi_{yt}}$$

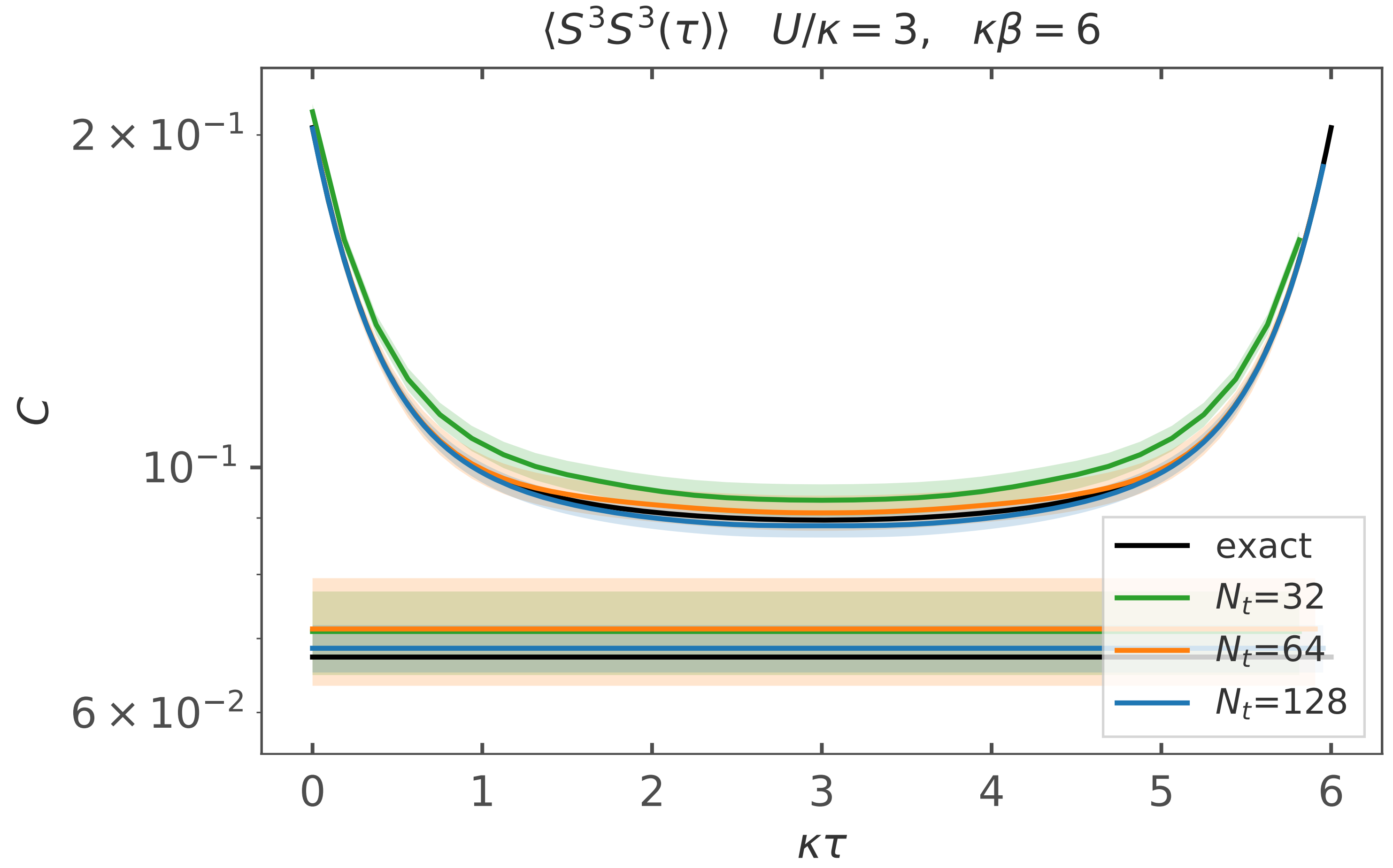
Complexify ϕ, integrate on steepest-descent analogues called *Lefschetz thimbles*, fixed points of holomorphic flow

$$\frac{\mathrm{d}\phi^R}{\mathrm{d}\tau_f} = \pm\frac{\partial S^R}{\partial \phi^R_i} = \pm\frac{\partial S^I}{\partial \phi^I_i} \qquad \frac{\mathrm{d}\phi^I}{\mathrm{d}\tau_f} = \pm\frac{\partial S^R}{\partial \phi^I_i} = \mp\frac{\partial S^I}{\partial \phi^R_i}$$

Flow is expensive and slow during HMC.
Use neural networks to approximate the thimble!

$\langle a_\tau a^\dagger \rangle$





Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221

SIGN PROBLEMS ABOUND

THE MOST INTERESTING PHYSICS REQUIRES NEW TOOLS

- Finite μ

Ulybyshev, Winterowd, Zafeiropolous PRD 101, 014508 (2020) 10.1103/PhysRevD.101.014508 1906.07678

- Non-bipartite lattices, fullerenes, …

Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221

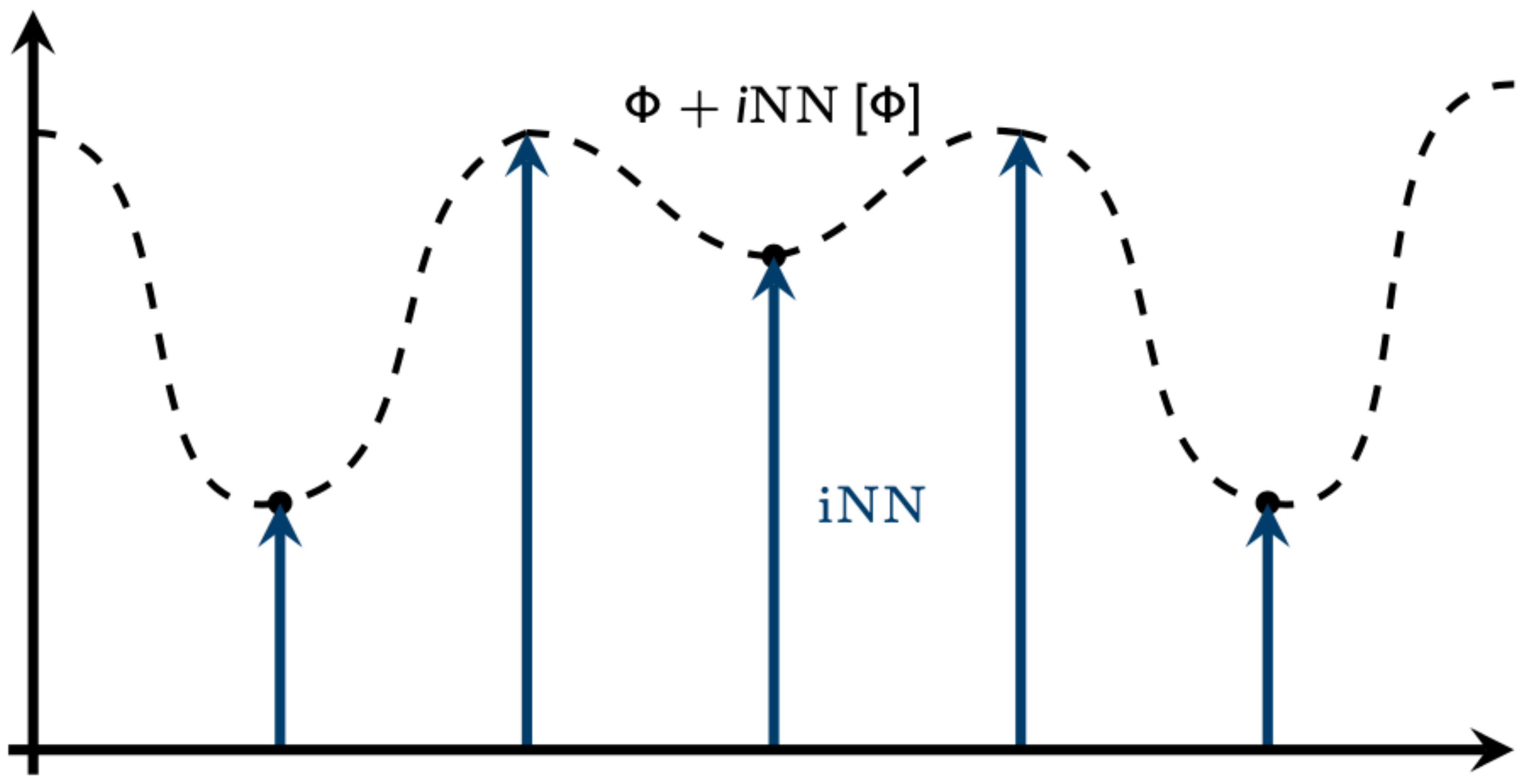
- Real-time

- Develop tools for QCD!

NETWORK ARCHITECTURES

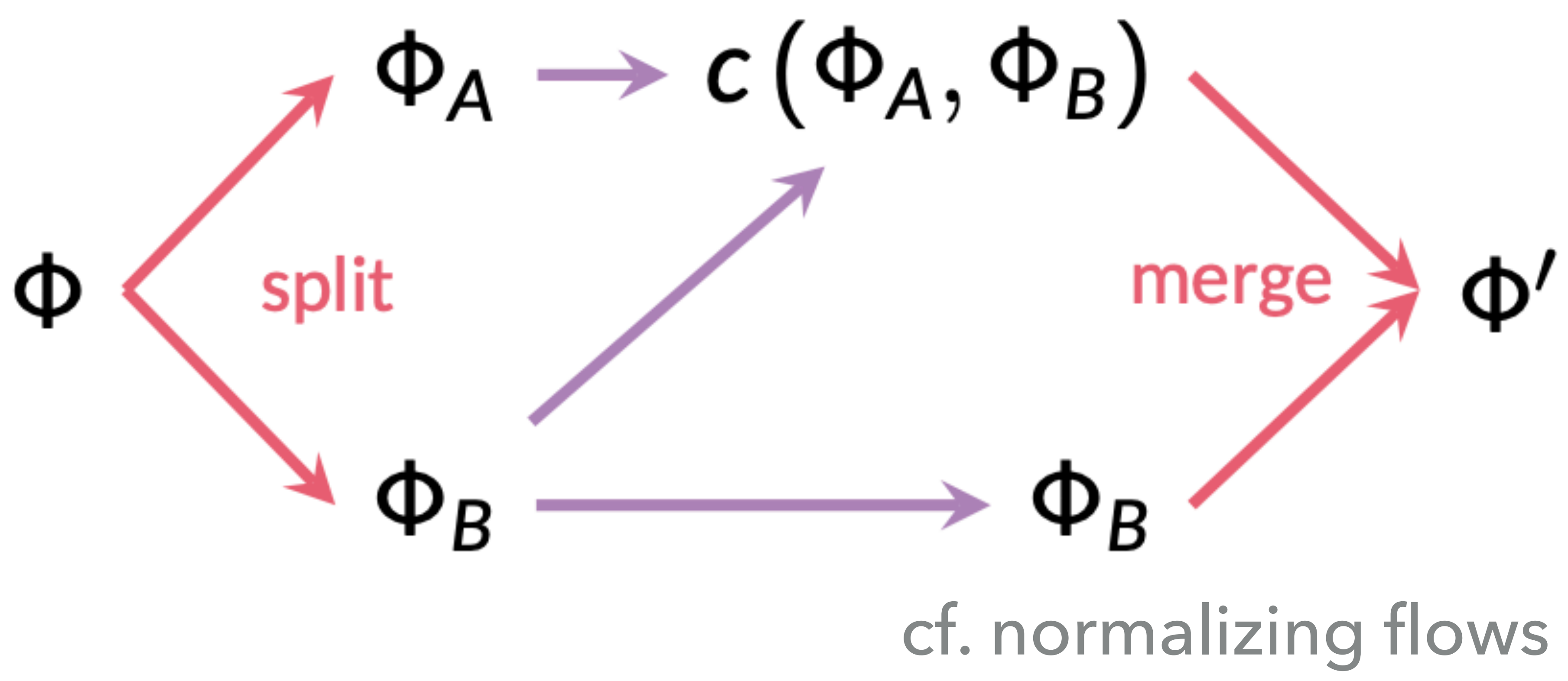
Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221
Rodekamp, EB, Gäntgen, Krieg, Luu, Ostmeyer 2203.00390

$\mathbb{R}$-Valued Neural Network



Train the network so that
- Input of the network is Re(Φ) at the end of the flow
- Output of the network is Im(Φ) at the end of the flow

$\mathbb{C}$-Valued Neural Network



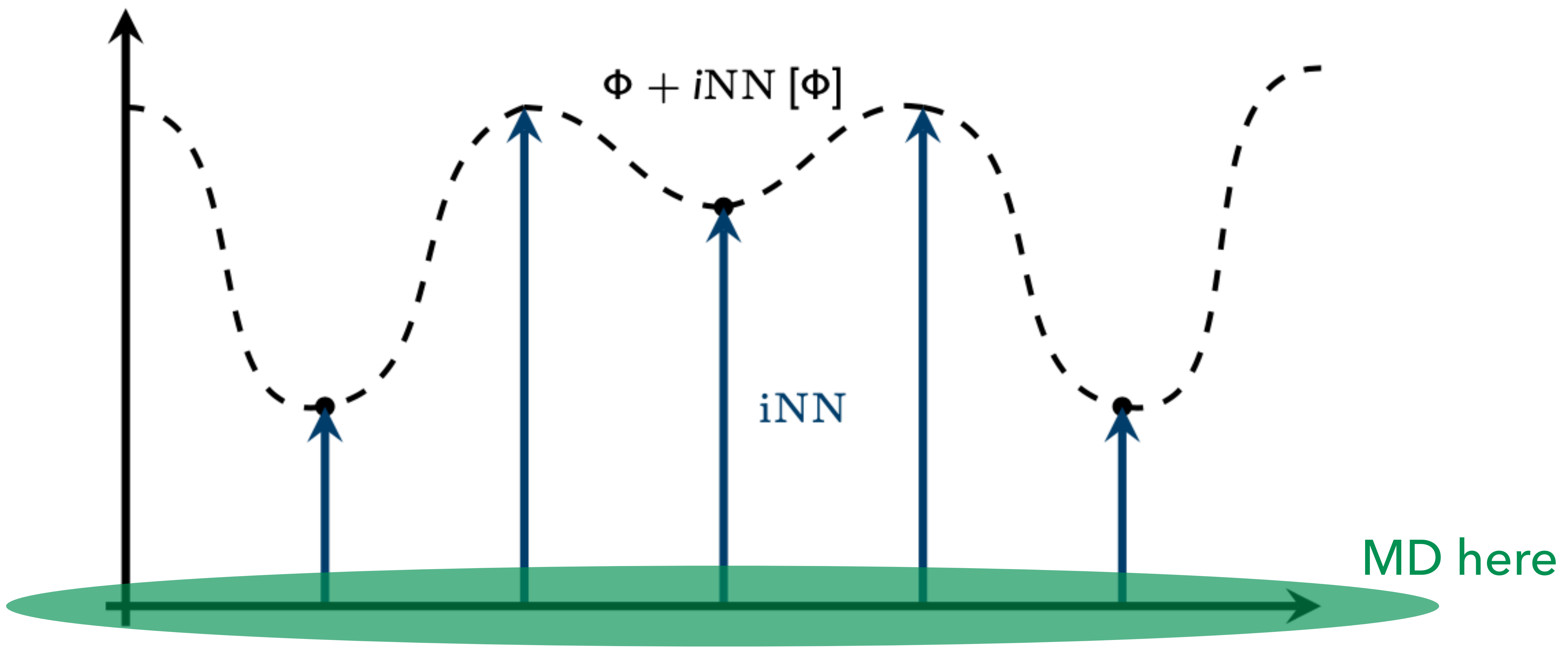
Train the network so that
- Input of the network is Φ at the start of the flow
- Output of the network is Φ at the end of the flow

Alexandru, Bedaque, Lamm, Lawrence, Physical Review D 96, 094505 (2017) 1709.01971
Albergo, Kanwar, Shanahan, PRD 100, 034515 1904.12072
Slide from M. Rodekamp, LATTICE 2022

NETWORK ARCHITECTURES

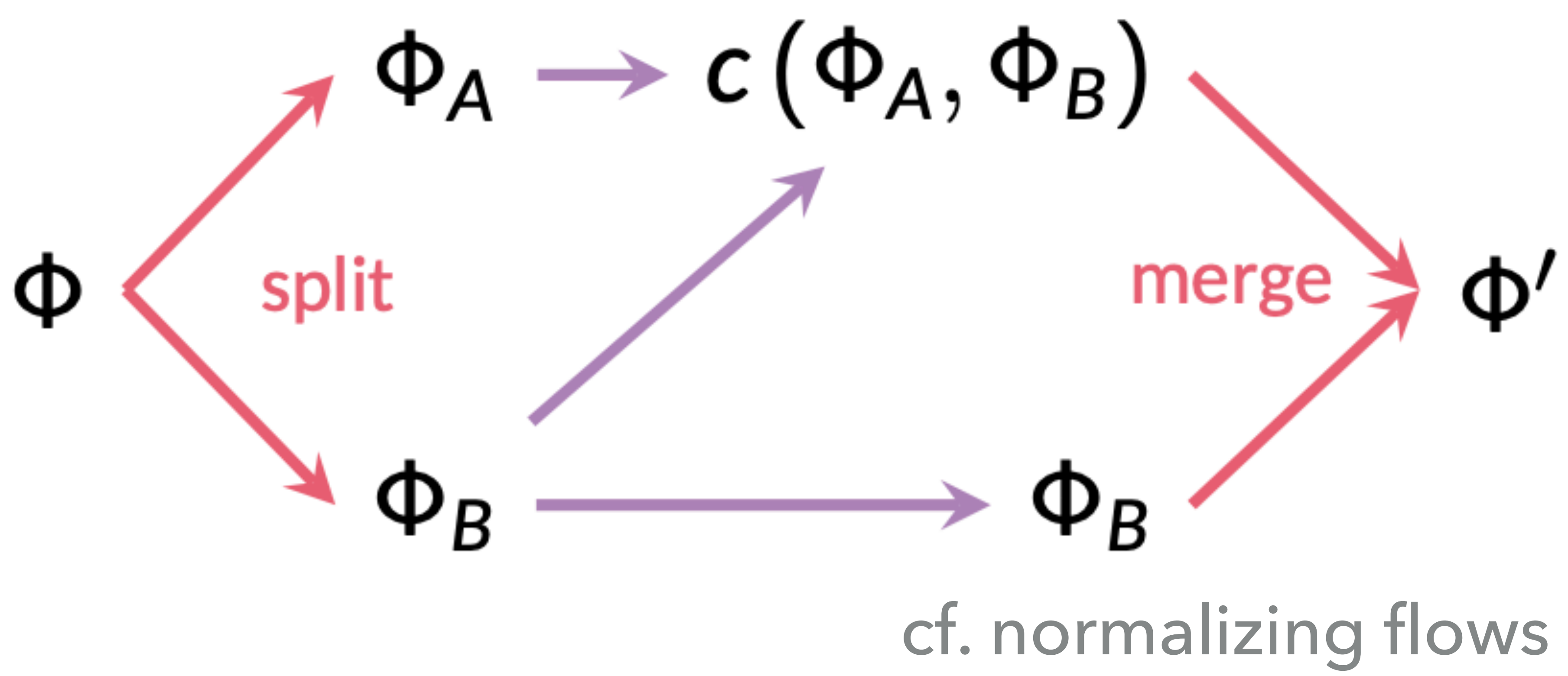
Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221
Rodekamp, EB, Gäntgen, Krieg, Luu, Ostmeyer 2203.00390

$\mathbb{R}$-Valued Neural Network



Train the network so that
- Input of the network is Re(Φ) at the end of the flow
- Output of the network is Im(Φ) at the end of the flow

$\mathbb{C}$-Valued Neural Network



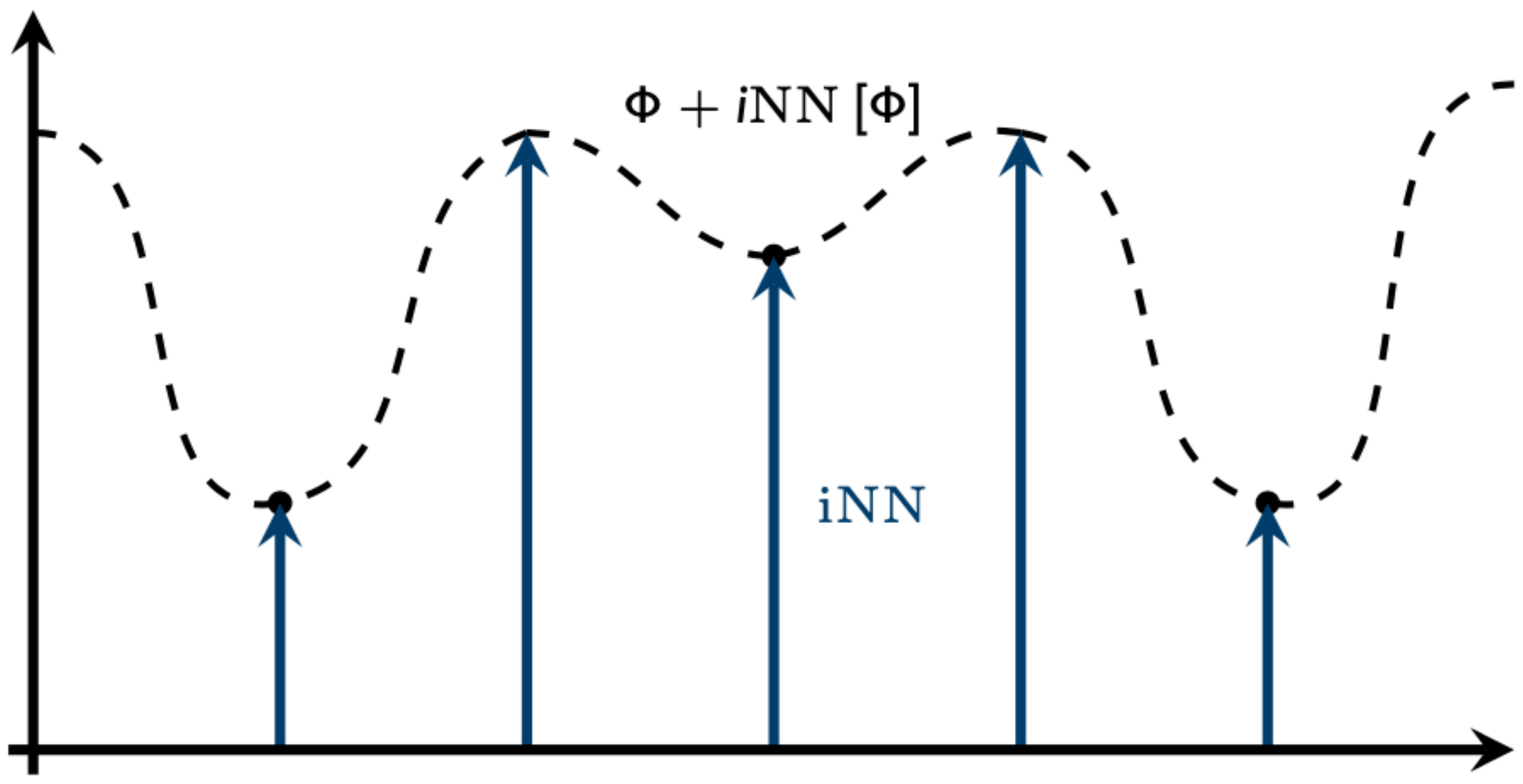
Train the network so that
- Input of the network is Φ at the start of the flow
- Output of the network is Φ at the end of the flow

Alexandru, Bedaque, Lamm, Lawrence, Physical Review D 96, 094505 (2017) 1709.01971
Albergo, Kanwar, Shanahan, PRD 100, 034515 1904.12072
Slide from M. Rodekamp, LATTICE 2022

NETWORK ARCHITECTURES

Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221
Rodekamp, EB, Gäntgen, Krieg, Luu, Ostmeyer 2203.00390

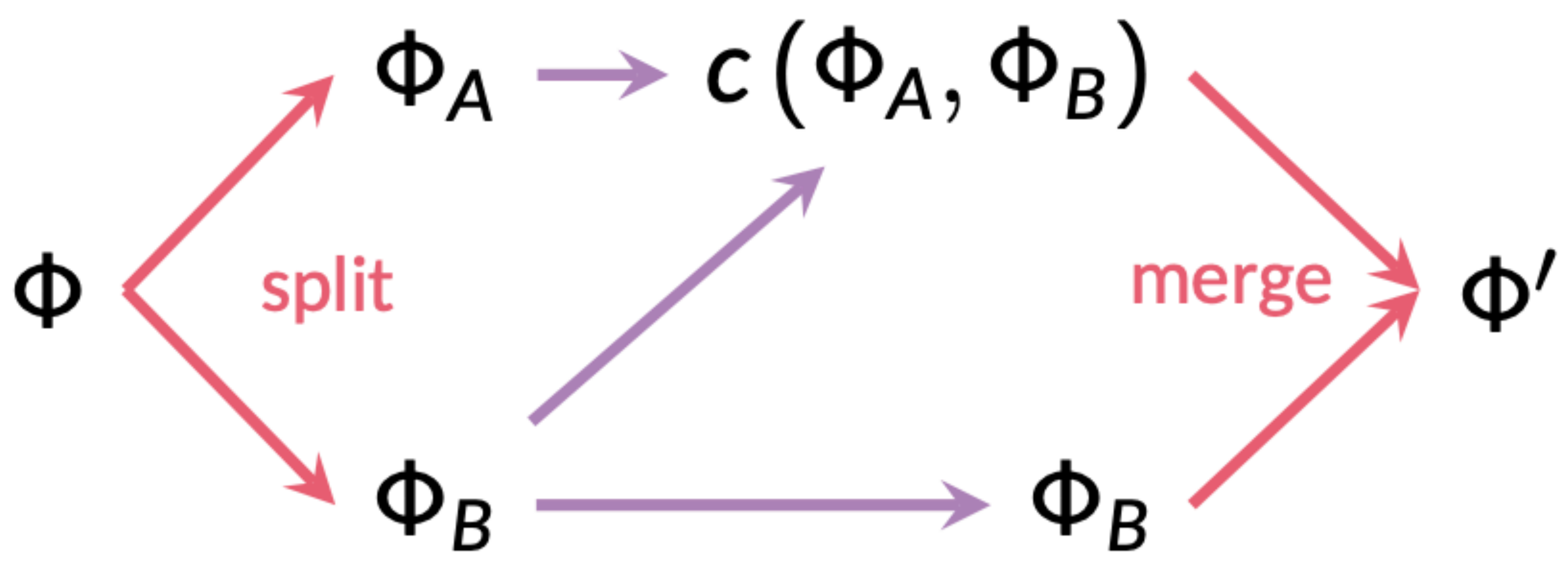
$\mathbb{R}$-Valued Neural Network



$$\mathbb{1} + i \begin{pmatrix} \frac{\partial \mathrm{NN}[\Phi]_0}{\partial \Phi_0} & \cdots & \frac{\partial \mathrm{NN}[\Phi]_{|\Lambda|}}{\partial \Phi_0} \\ \vdots & \ddots & \vdots \\ \frac{\partial \mathrm{NN}[\Phi]_0}{\partial \Phi_{|\Lambda|}} & \cdots & \frac{\partial \mathrm{NN}[\Phi]_{|\Lambda|}}{\partial \Phi_{|\Lambda|}} \end{pmatrix}$$

Jacobian is horrible: V^3

$\mathbb{C}$-Valued Neural Network



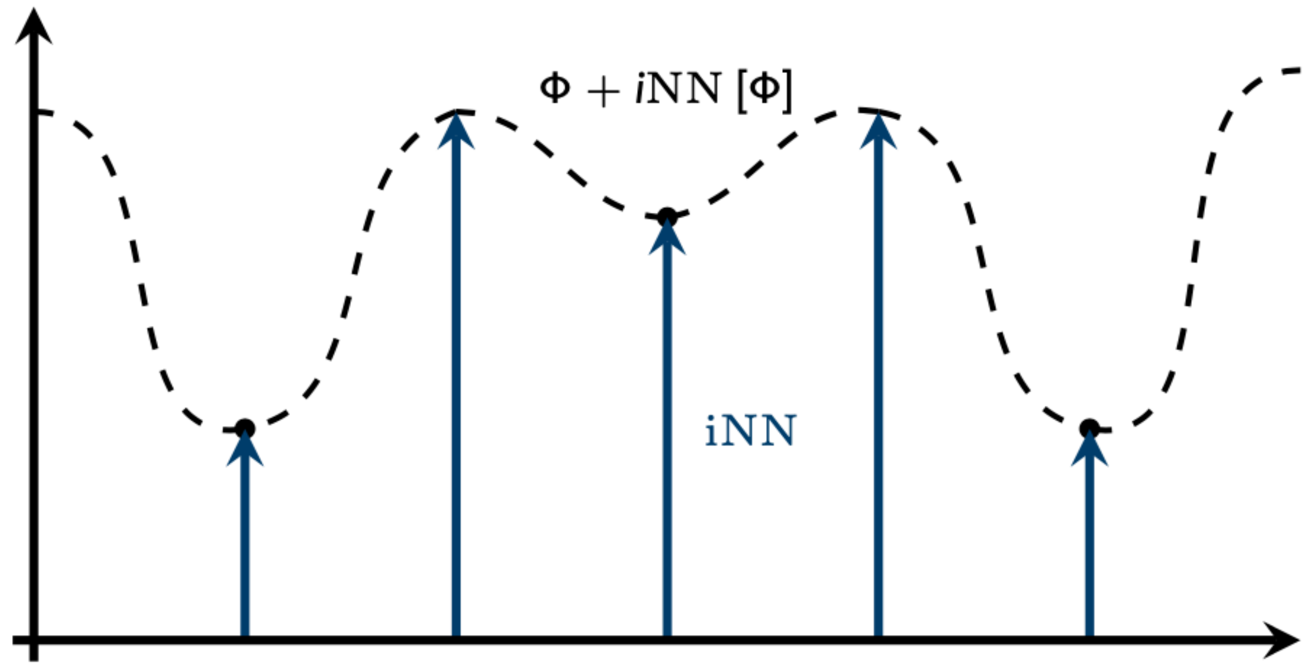
$$\begin{pmatrix} \frac{\partial c(\Phi_A, \Phi_B)}{\partial \Phi_A} & 0 \\ \star & \mathbb{1} \end{pmatrix}$$

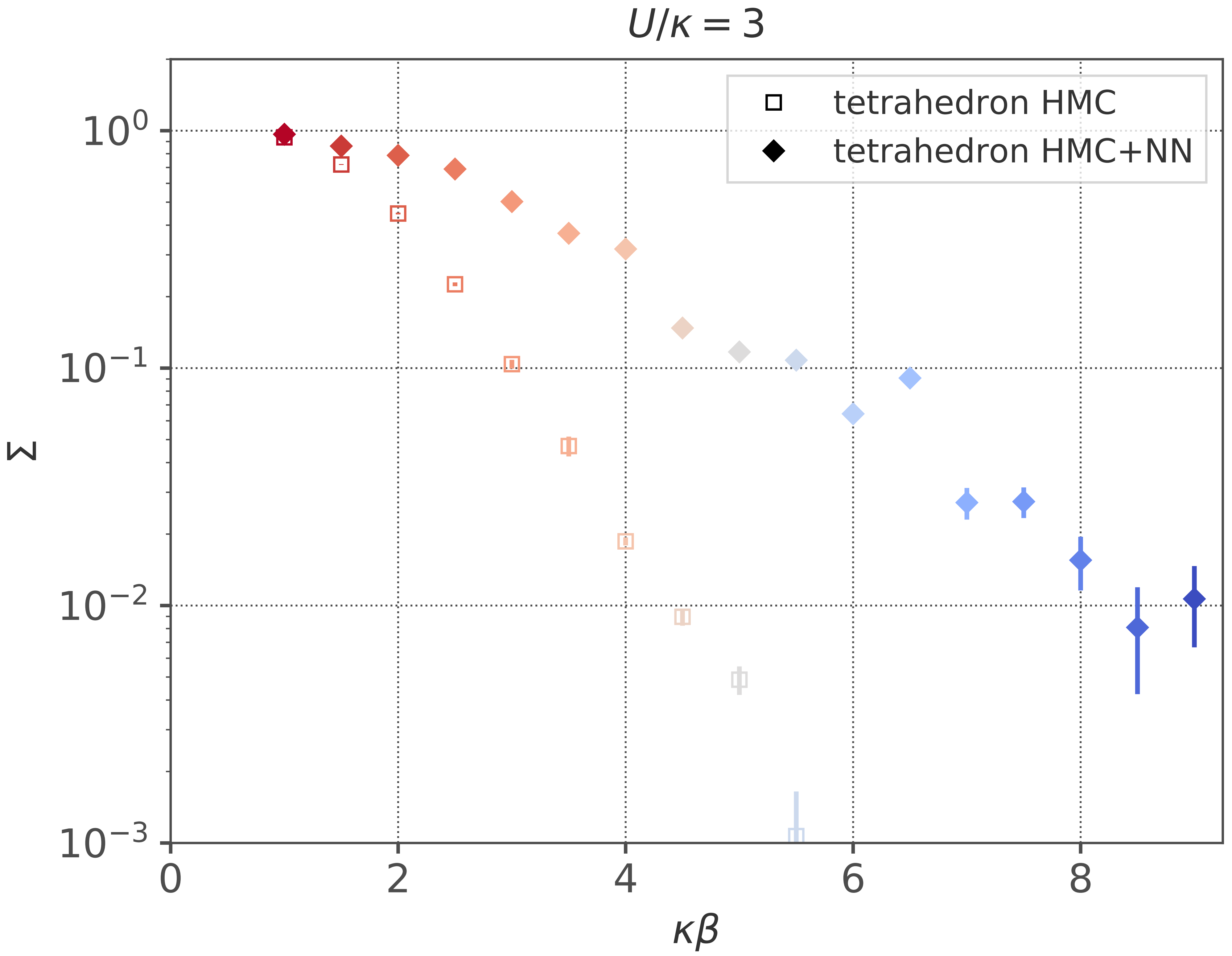
Jacobian is easy: V^1

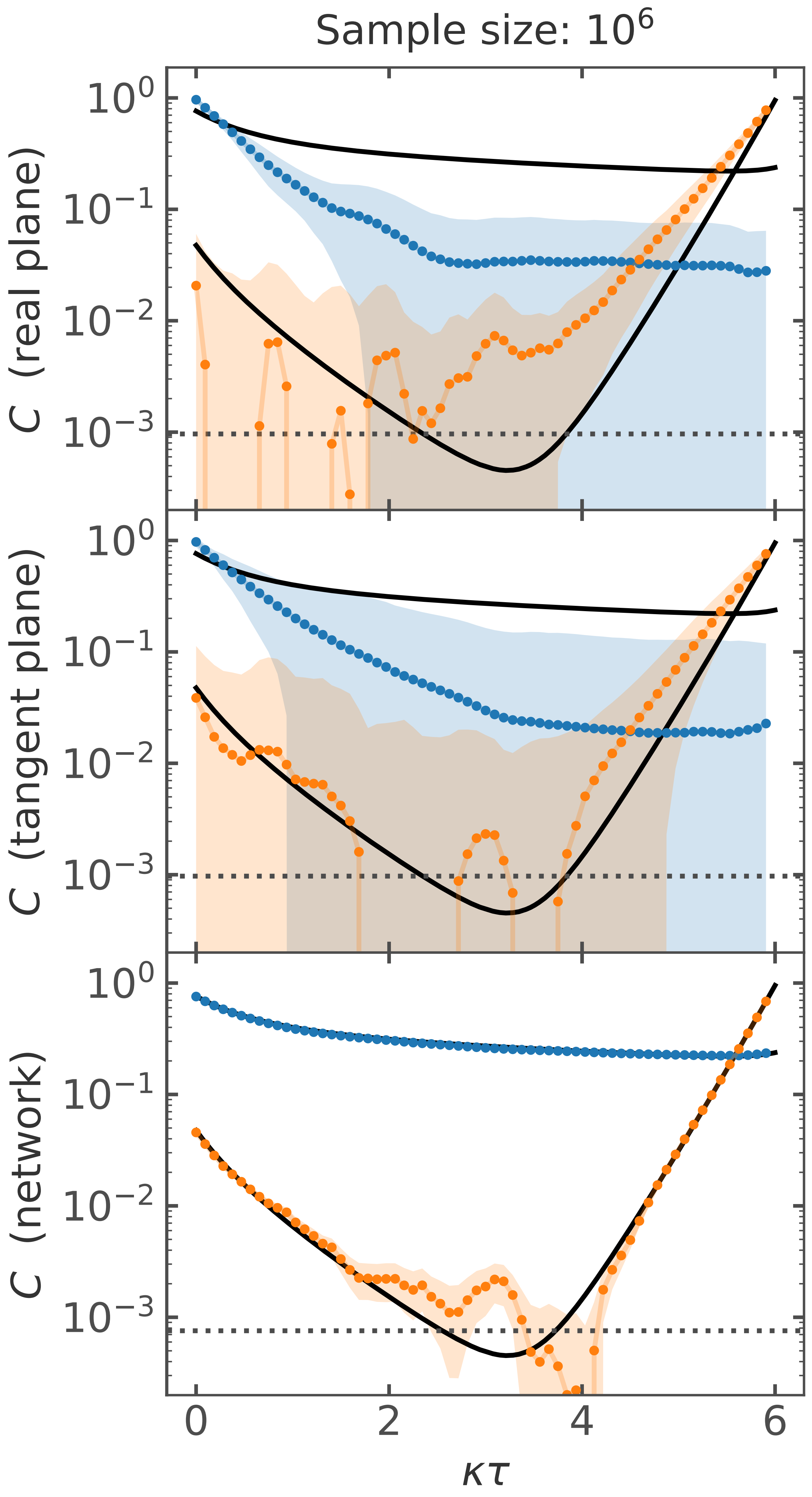
Slide from M. Rodekamp, LATTICE 2022

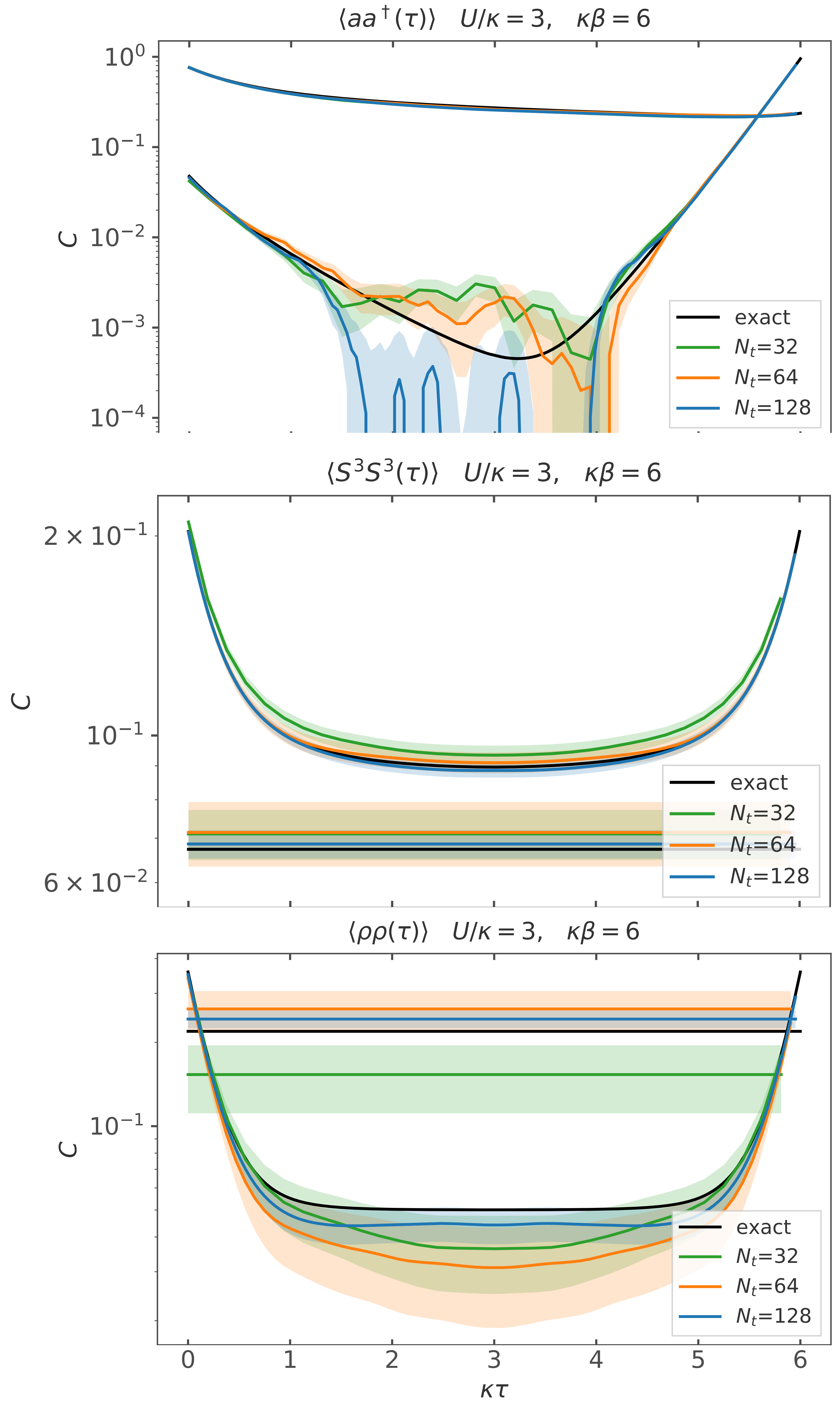
NONBIPARTITE EXAMPLES

Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221
Rodekamp, EB, Gäntgen, Krieg, Luu, Ostmeyer 2203.00390



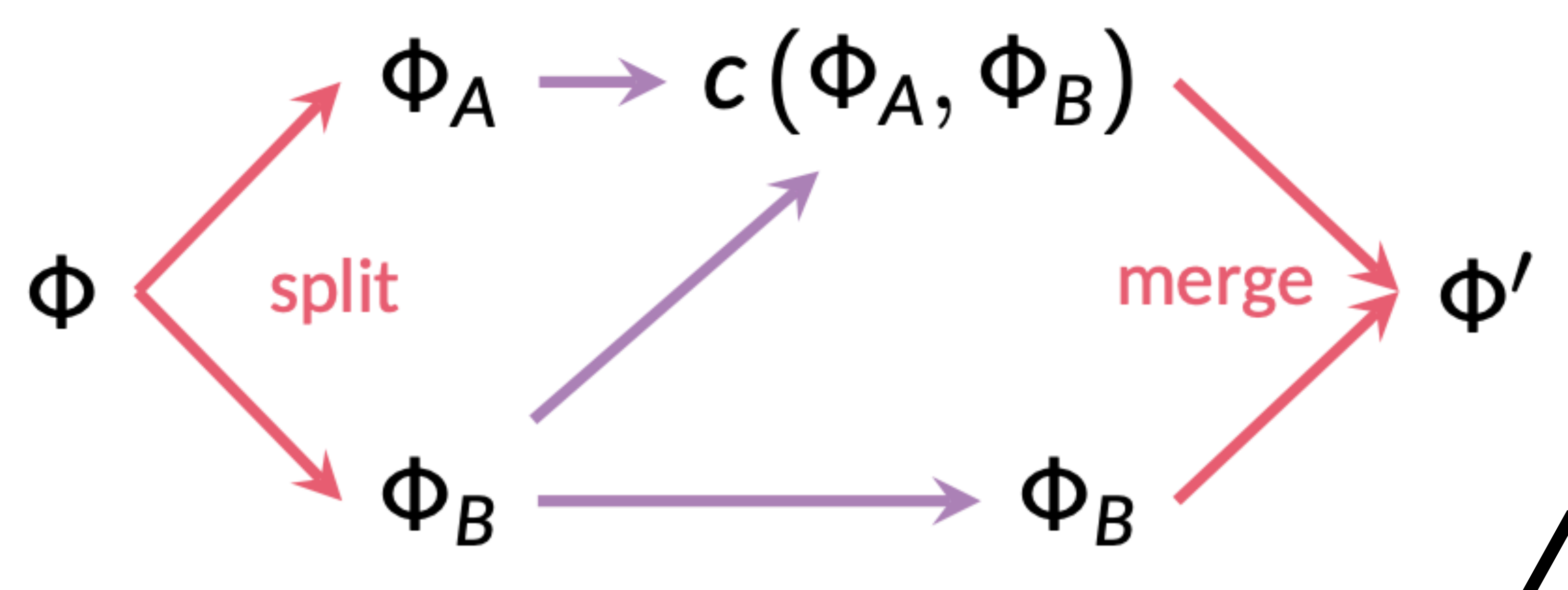


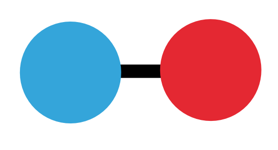


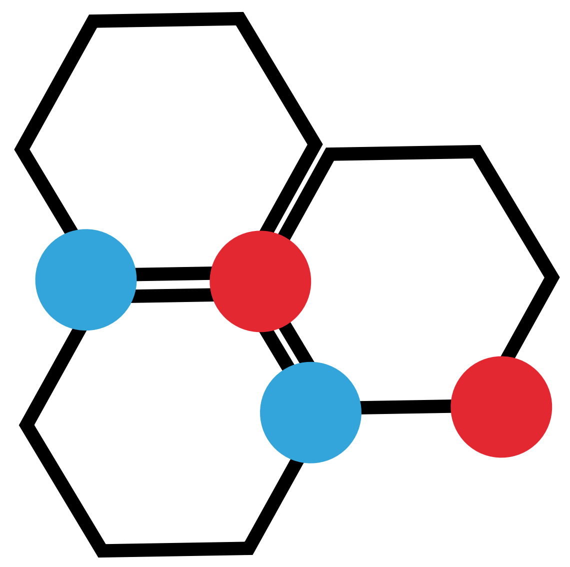


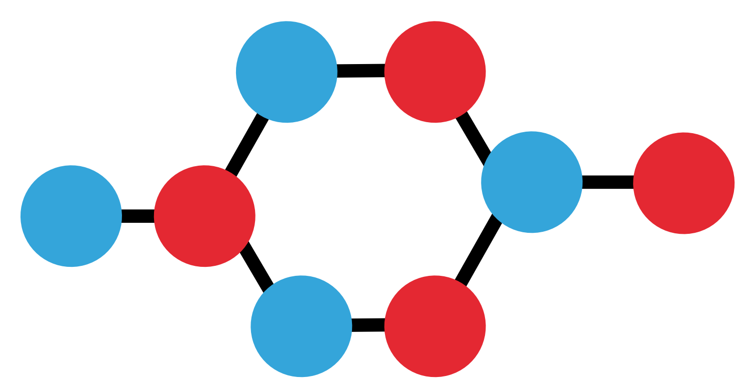
DOPED EXAMPLES

Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221
Rodekamp, EB, Gäntgen, Krieg, Luu, Ostmeyer 2203.00390

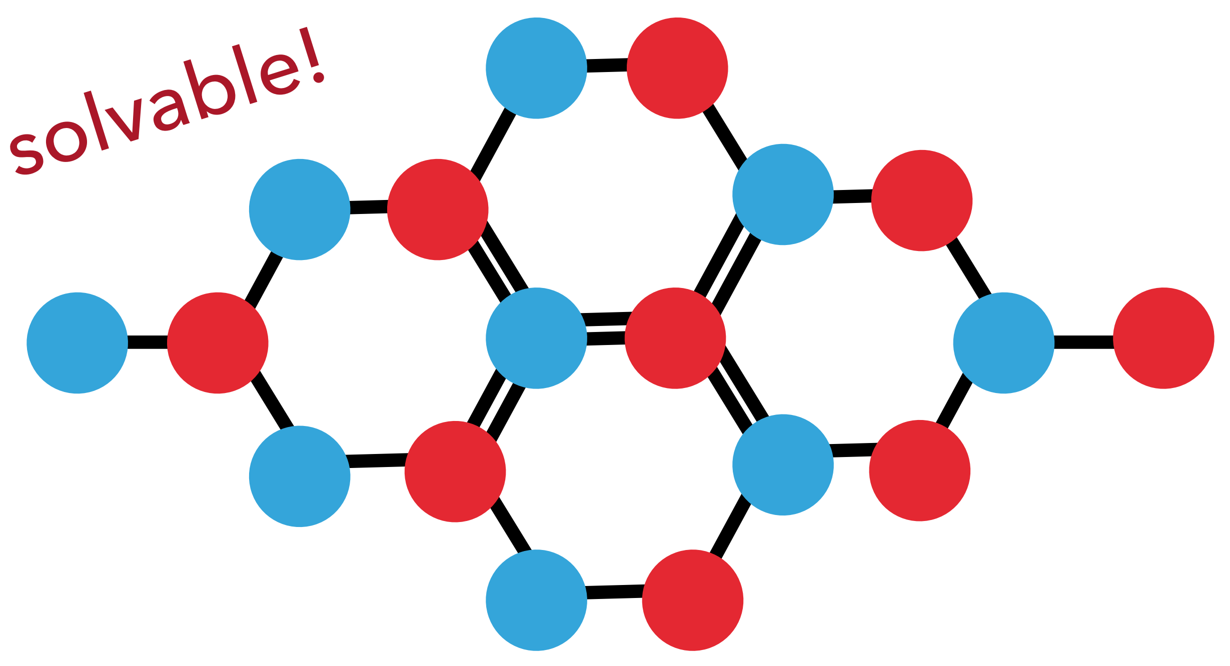






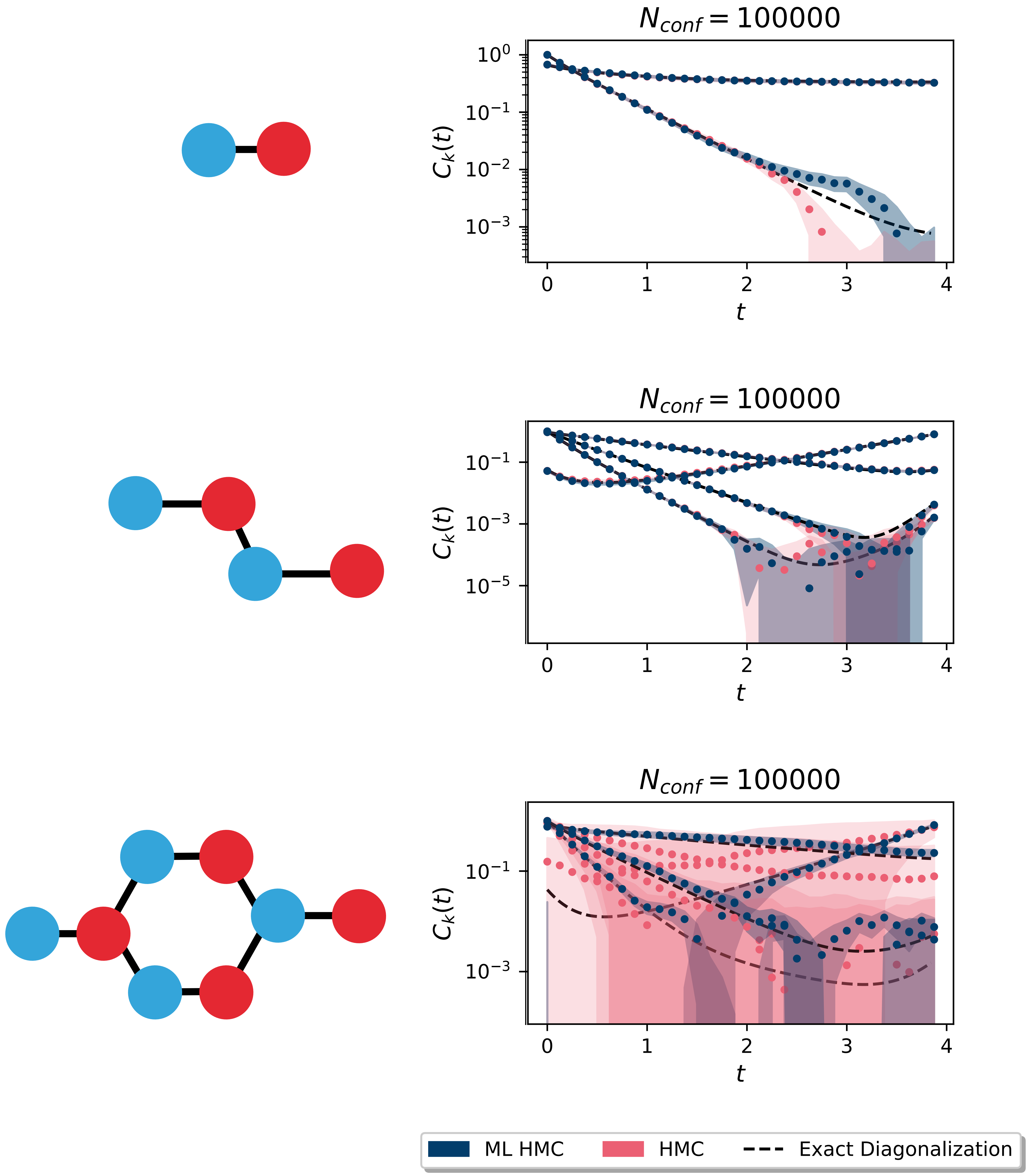


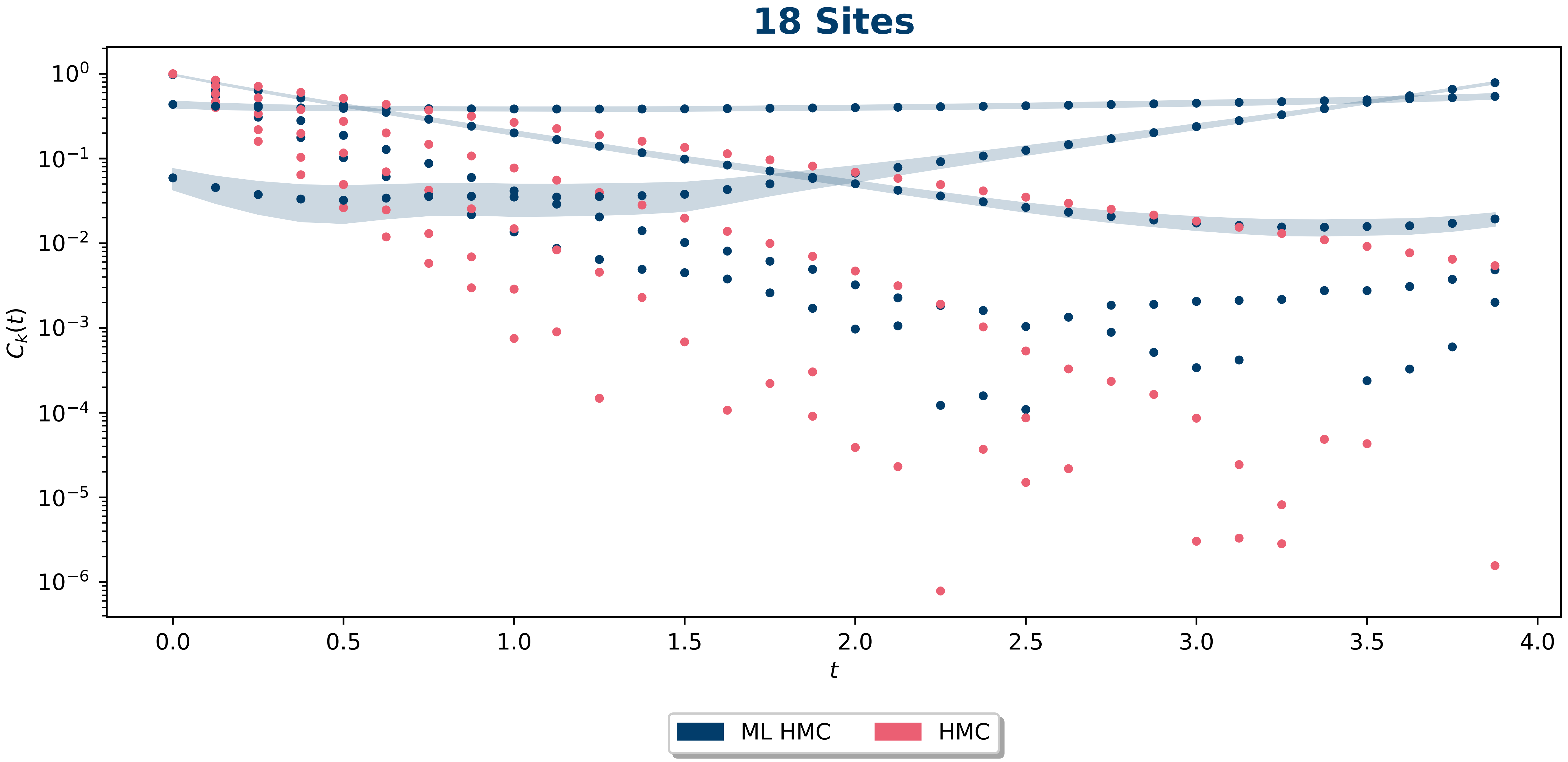
Not exactly solvable!



DOPED EXAMPLES

Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221
Rodekamp, EB, Gäntgen, Krieg, Luu, Ostmeyer 2203.00390





Not exactly solvable!