EVAN BERKOWITZ

INSTITUT FÜR KERNPHYSIK

INSTITUTE FOR ADVANCED SIMULATION, JÜLICH SUPERCOMPUTING CENTRE

FORSCHUNGSZENTRUM JÜLICH

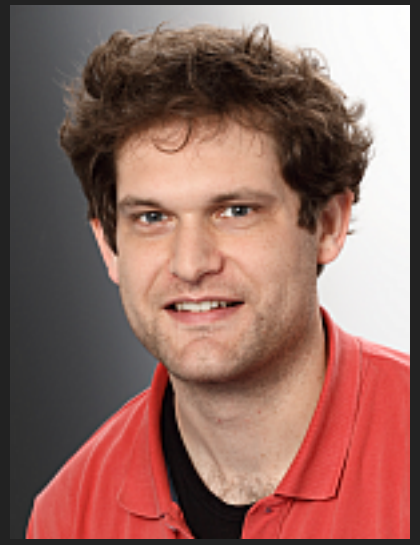
12 DECEMBER 2022

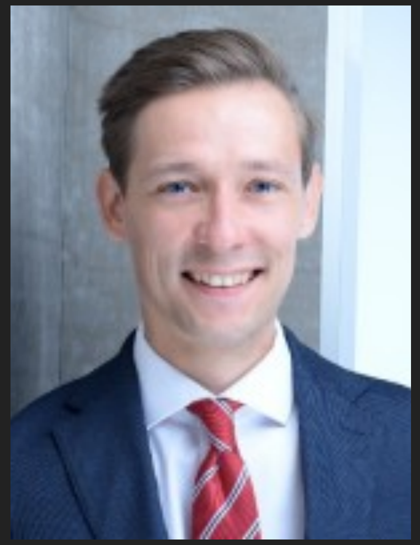
LEARNING ABOUT THE DOPED HUBBARD MODEL

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

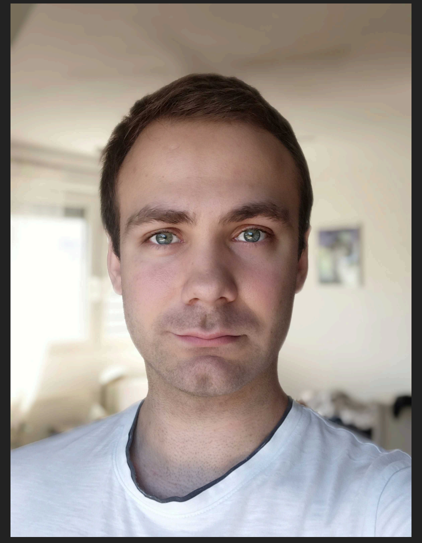
2005.11112 Ostmeyer, EB, Krieg, Lähde, Luu, Urbach, PRB 102:245105 10.1103/PhysRevB.102.245105

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; accepted in PRB


Marcel Rodekamp


Christoph Gäntgen

LEARNING ABOUT THE DOPED HUBBARD MODEL

L. Ron Hubbard House
Washington DC

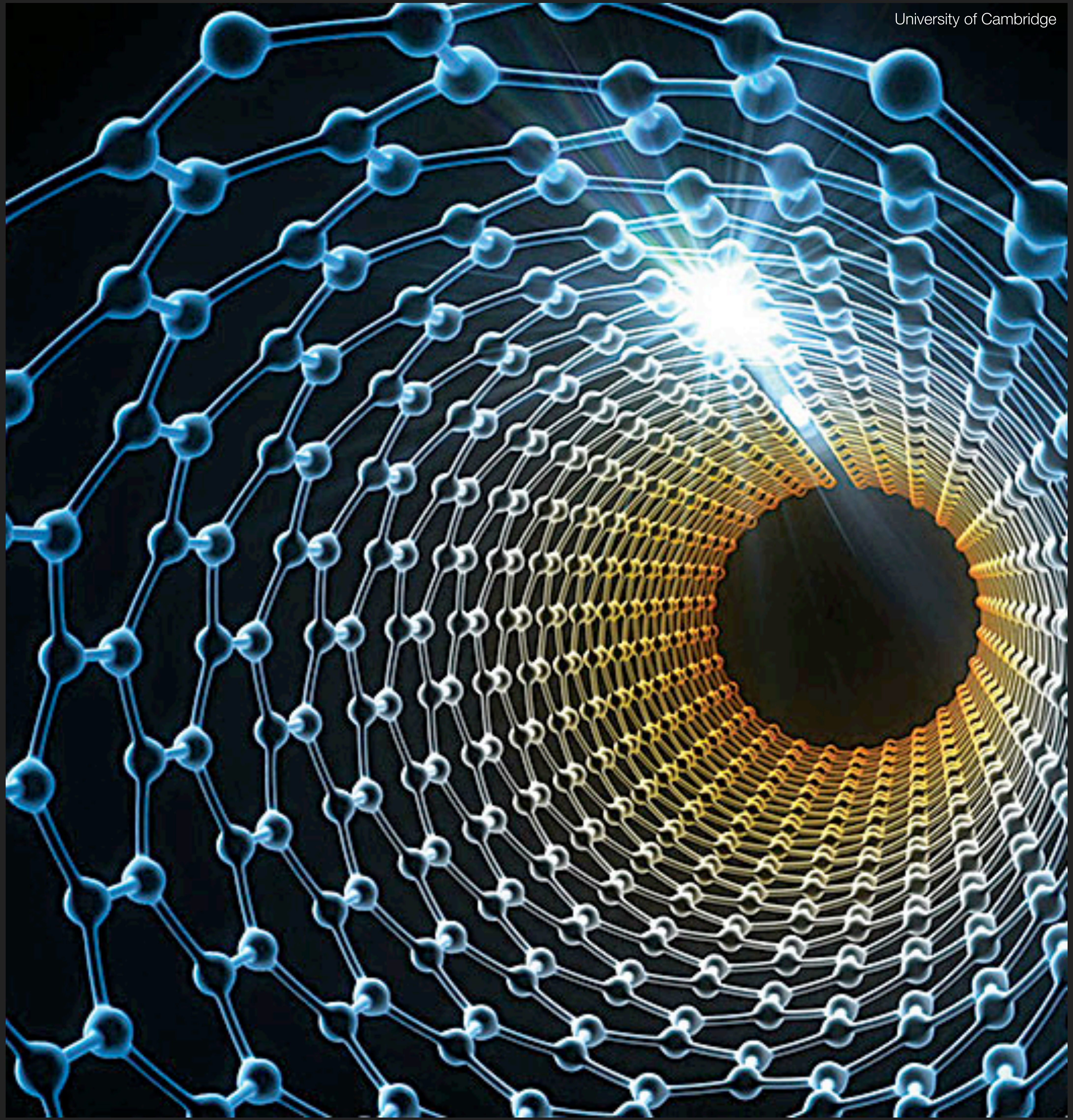
THE HUBBARD MODEL

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



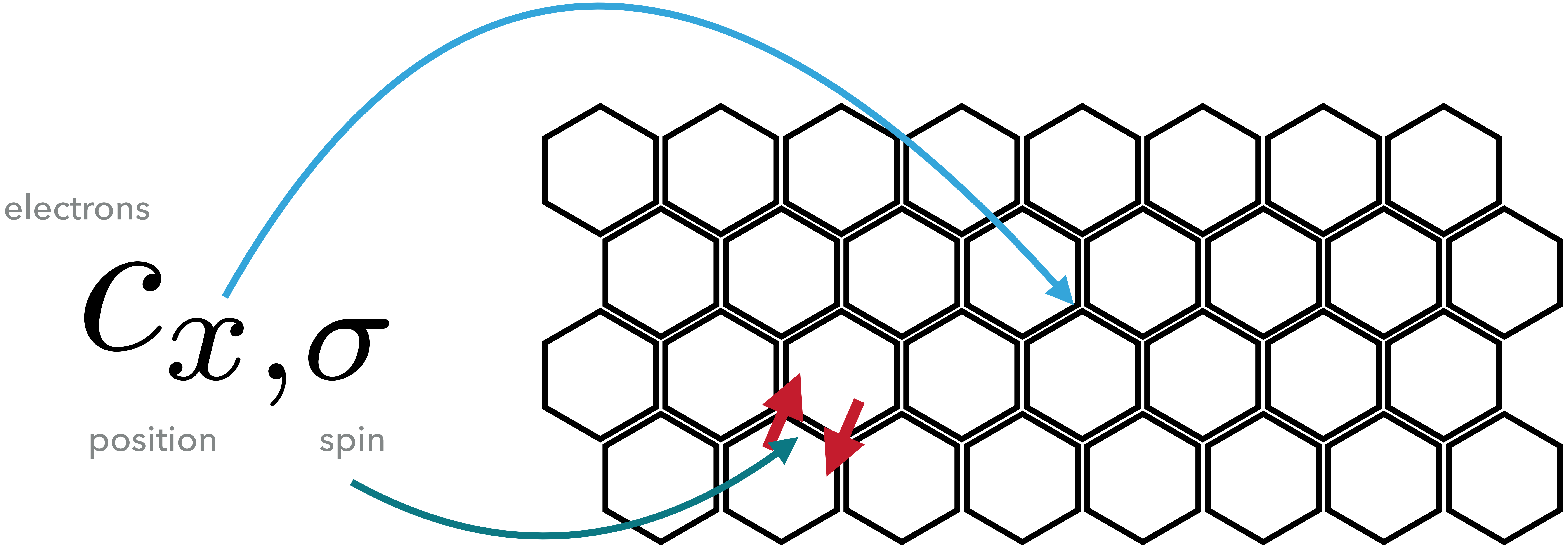
Hubbard Gold Medal of Anne Morrow Lindbergh

THE HUBBARD MODEL

BACKGROUND

THE TIGHT-BINDING MODEL

Bloch Zeit. für Physik 52 555-600 1929



Tight Binding

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

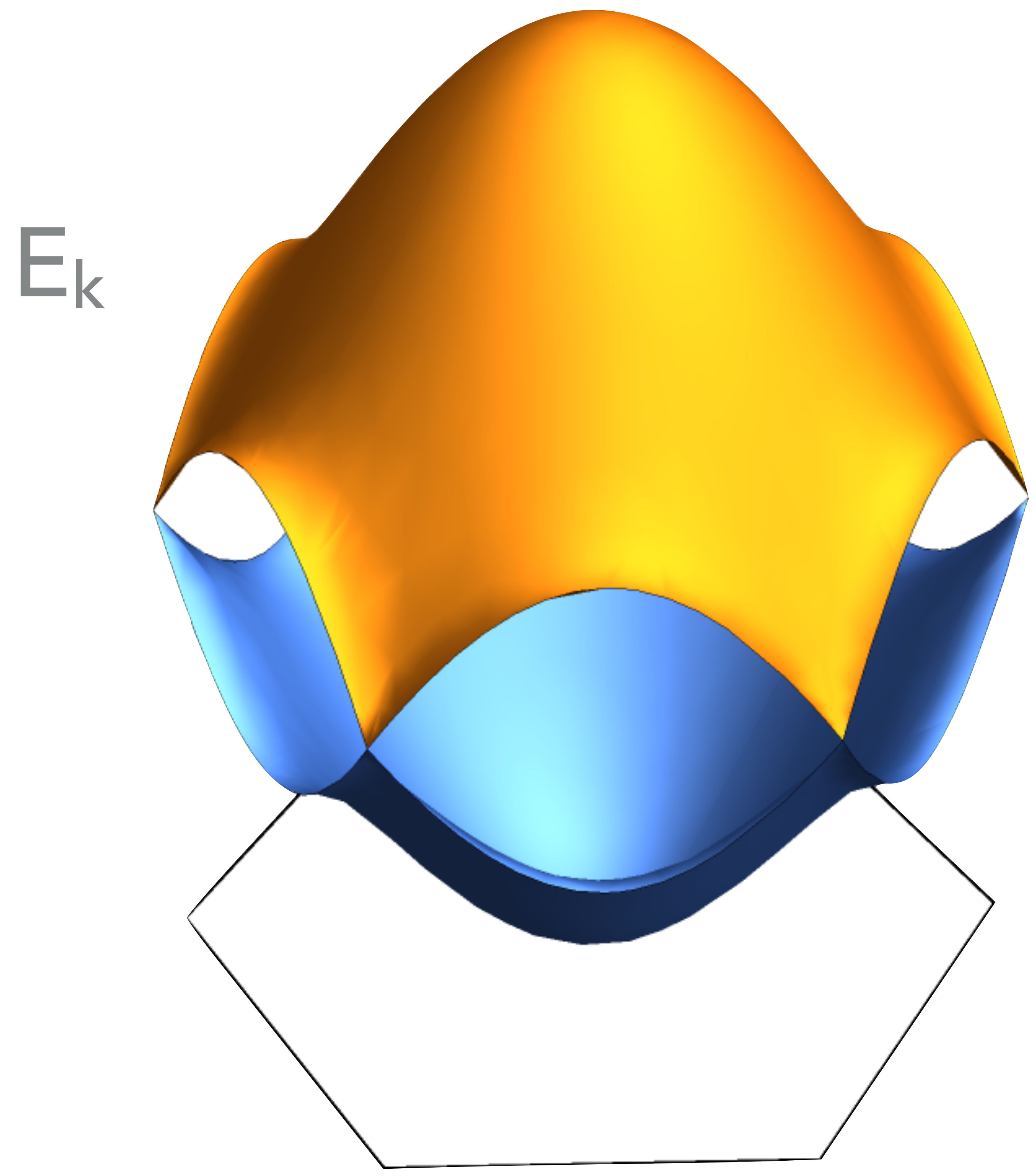
$$h_{xy} = \kappa \delta_{\langle xy \rangle}$$

Nearest-neighbor hopping

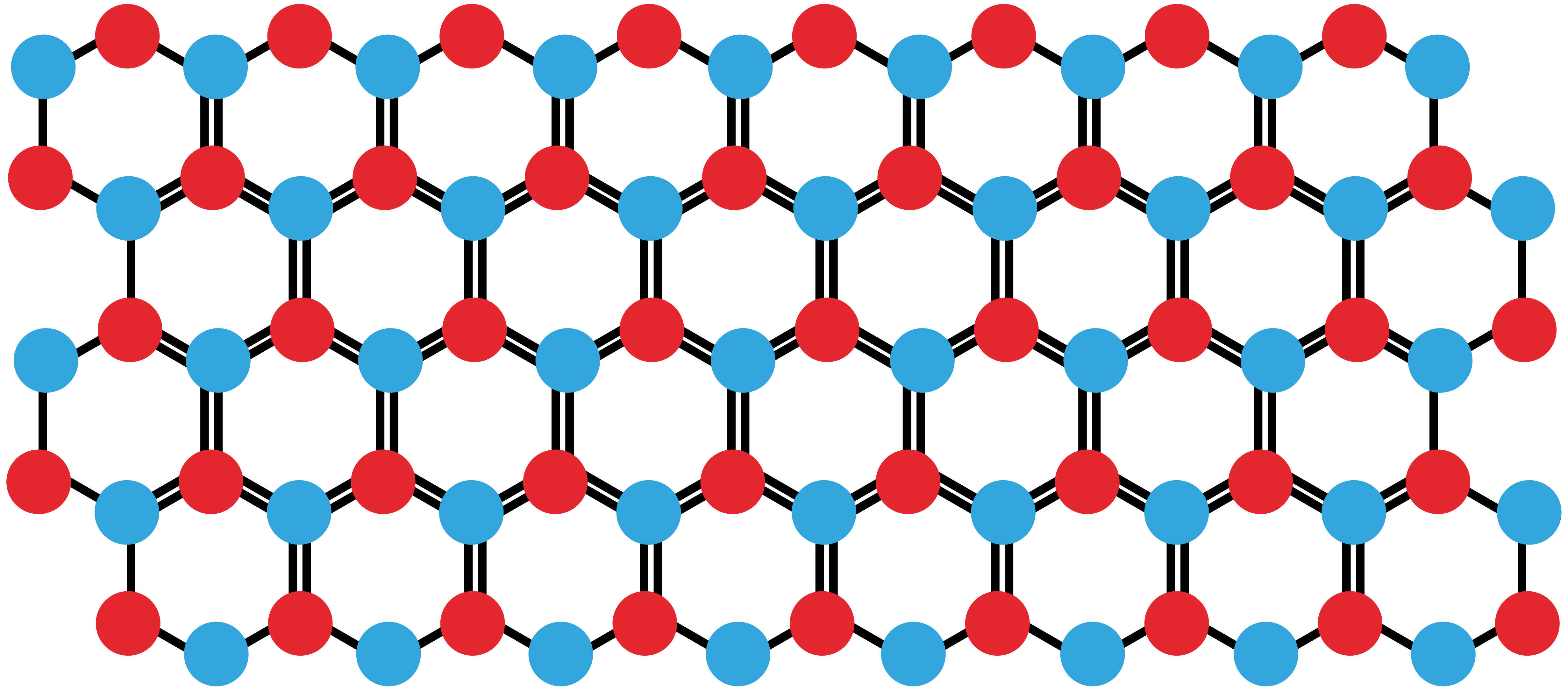
- Honeycomb:
  - triangular Bravais lattice
  - 2 sites per cell

THE TIGHT-BINDING MODEL

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



Brillouin Zone (BZ)

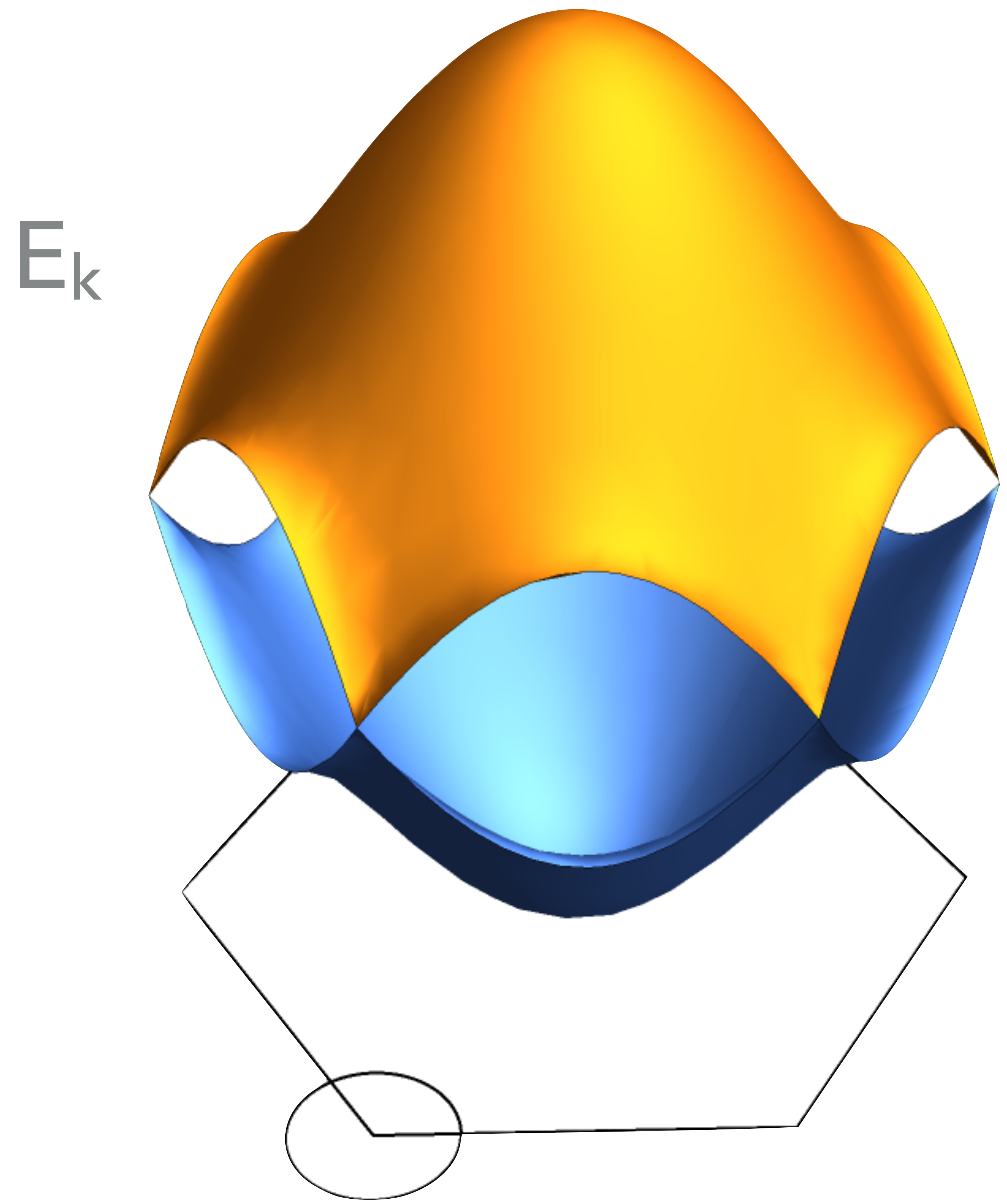


$$H_0 = -\sum_{x,y,\sigma} c^{\dagger}_{x,\sigma} h_{xy} c_{y,\sigma}$$

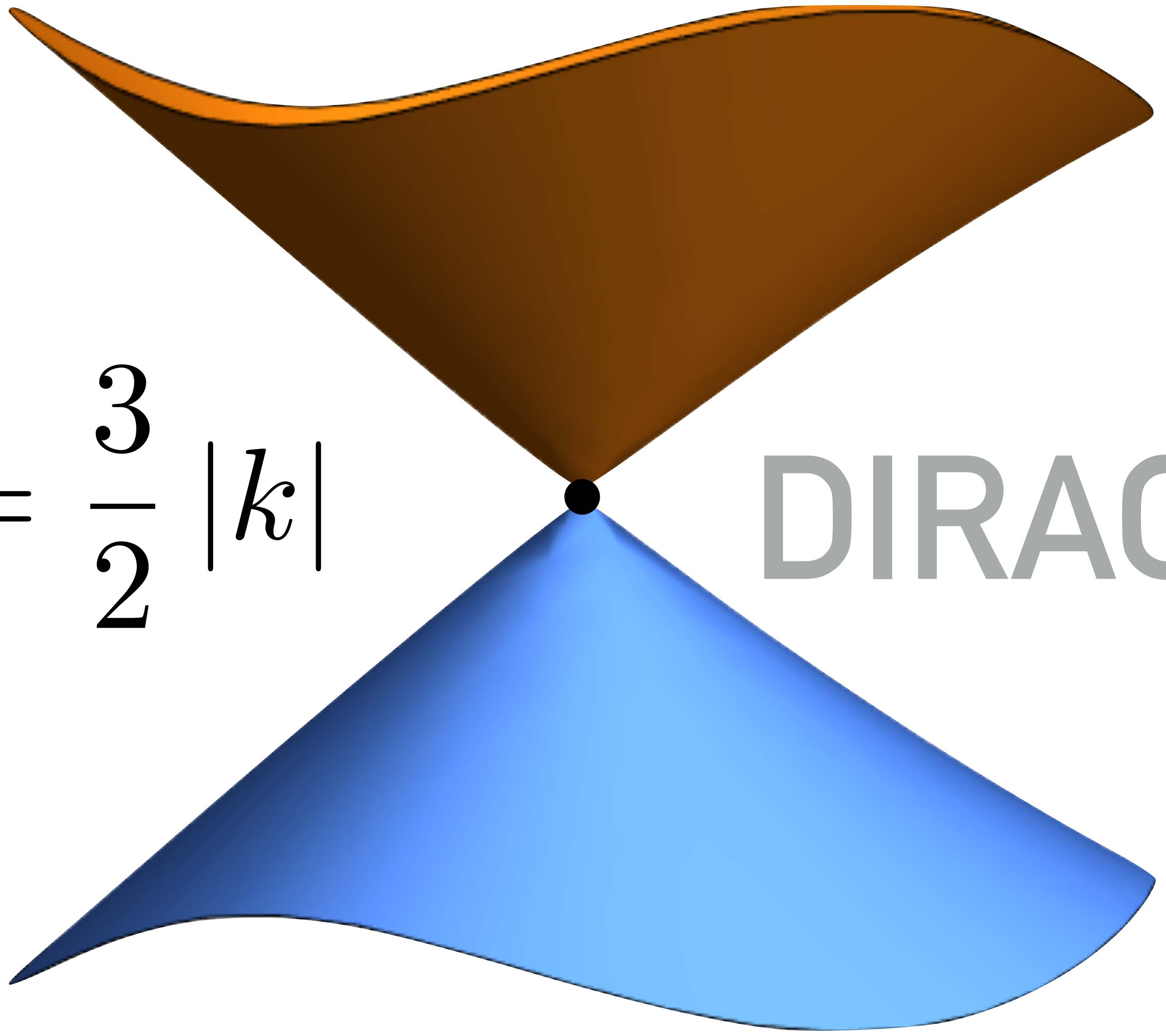
$$E_k/\kappa = \pm\sqrt{3 + 2\left(\cos\left(\frac{3}{2}k_x + \frac{\sqrt{3}}{2}k_y\right) + \cos\left(\frac{3}{2}k_x - \frac{\sqrt{3}}{2}k_y\right) + \cos\left(\sqrt{3}k_y\right)\right)}$$

THE TIGHT-BINDING MODEL

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



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



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

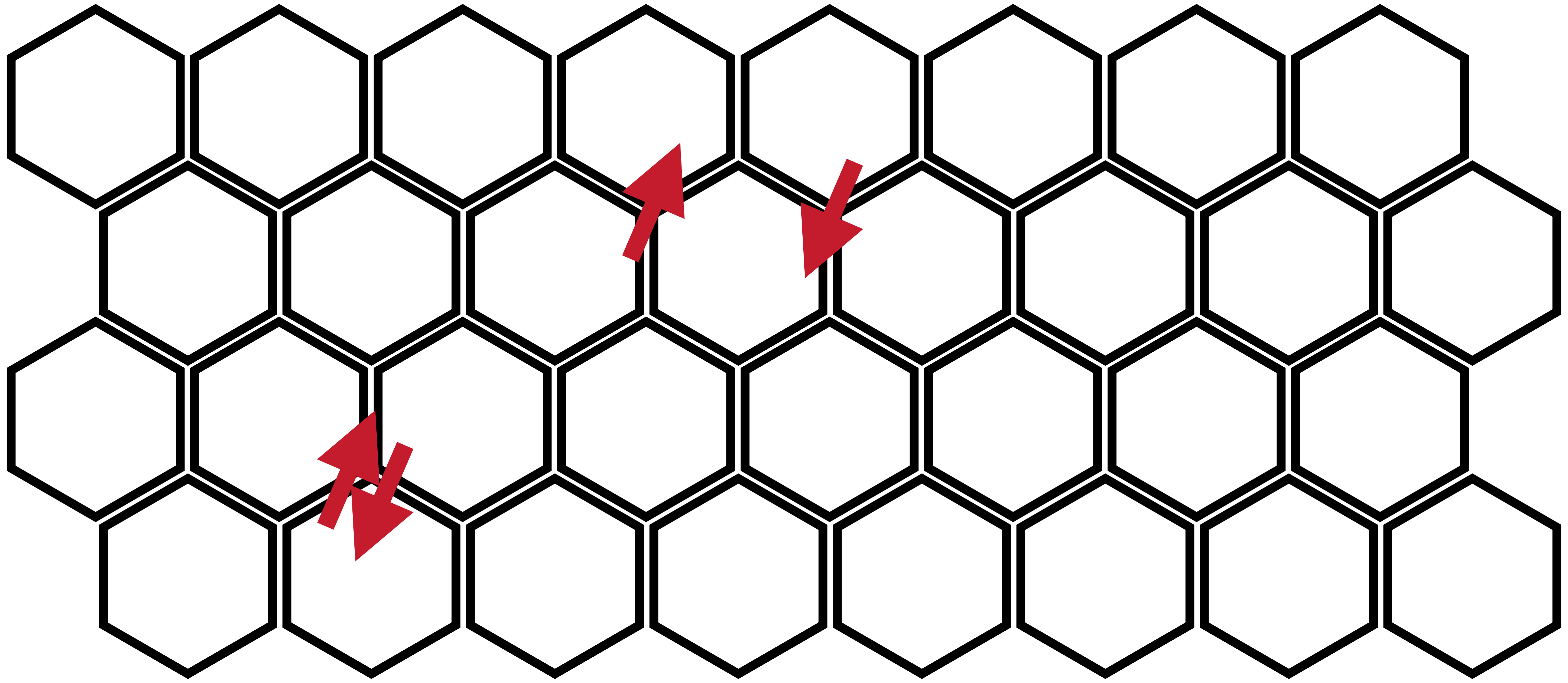
THE HUBBARD MODEL

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

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

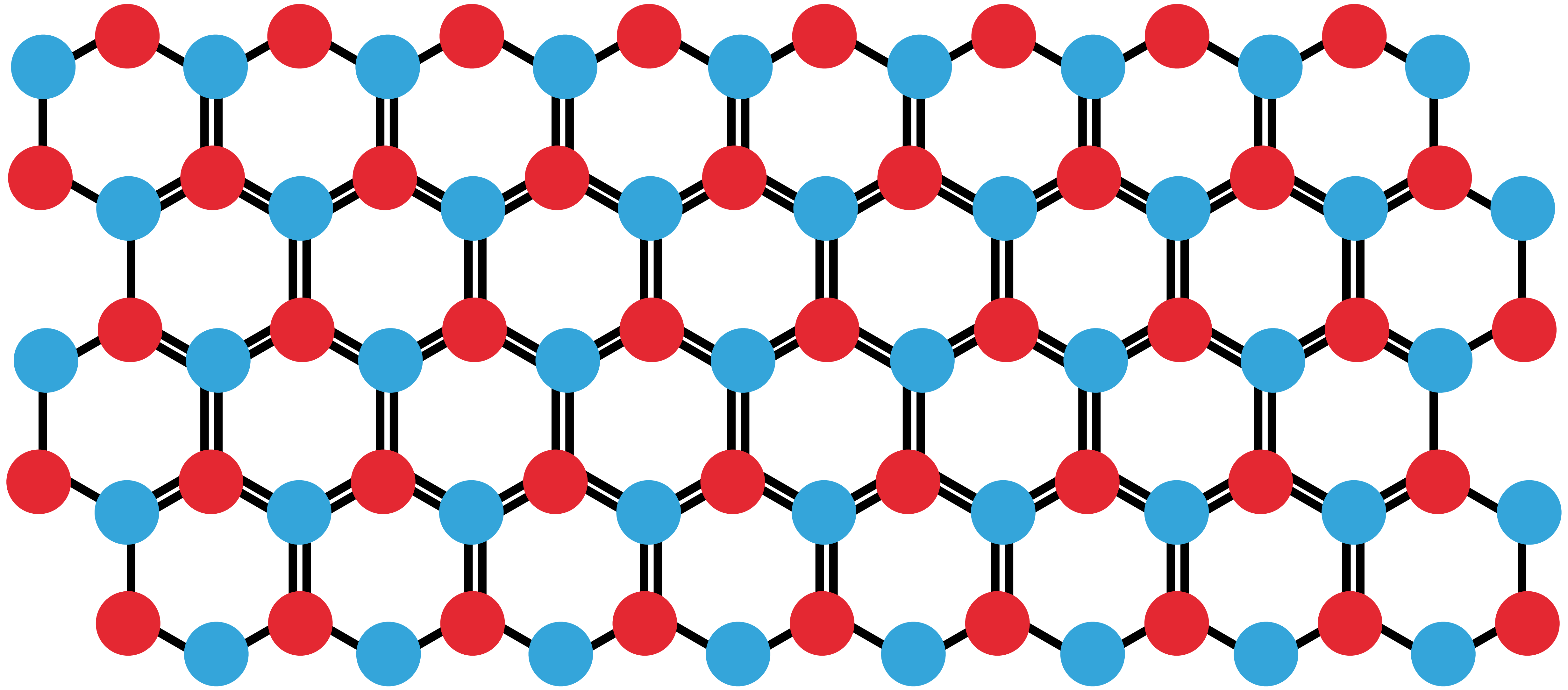
Half-filling: $\mu_\rho = 0$

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

−1

antiferromagnetic (Mott) insulator! (AFMI)

THE HUBBARD MODEL

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

Bipartite lattice!

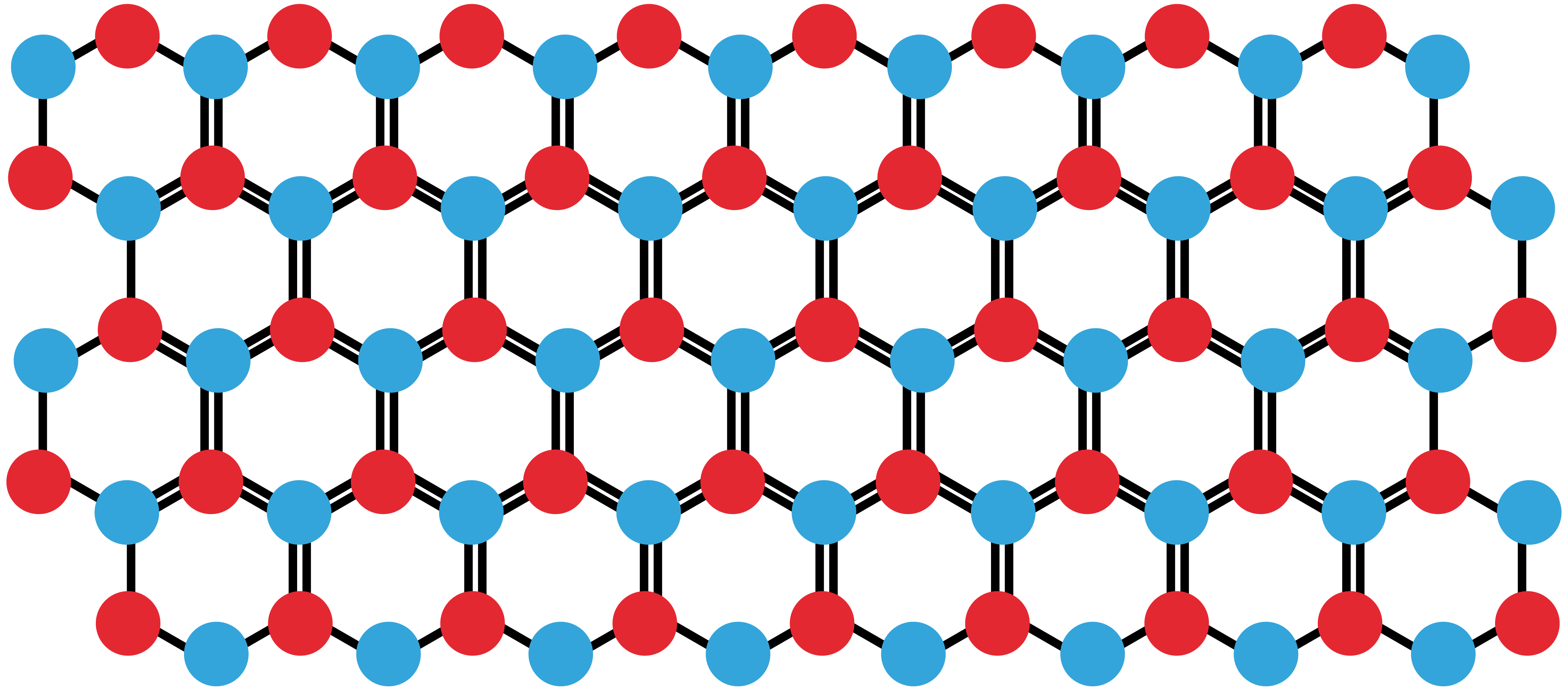
$$a_x = c_{x\uparrow} \qquad a_x^\dagger = c_{x\uparrow}^\dagger$$

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

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

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

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



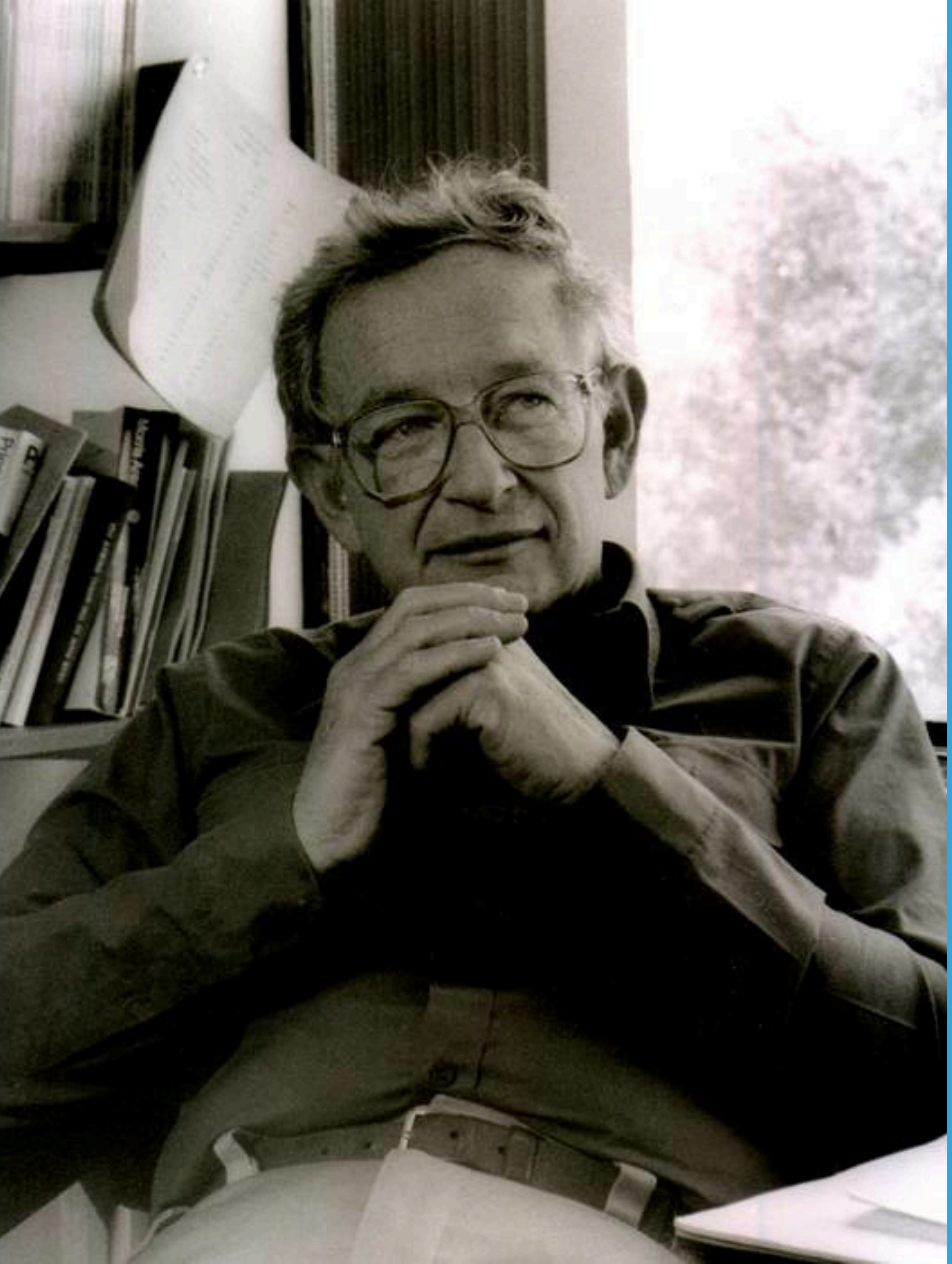
Half filling: ⟨ρ⟩= 0 $\qquad \rho_x = n_x^a - n_x^b$

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



[THE HUBBARD MODEL] 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.

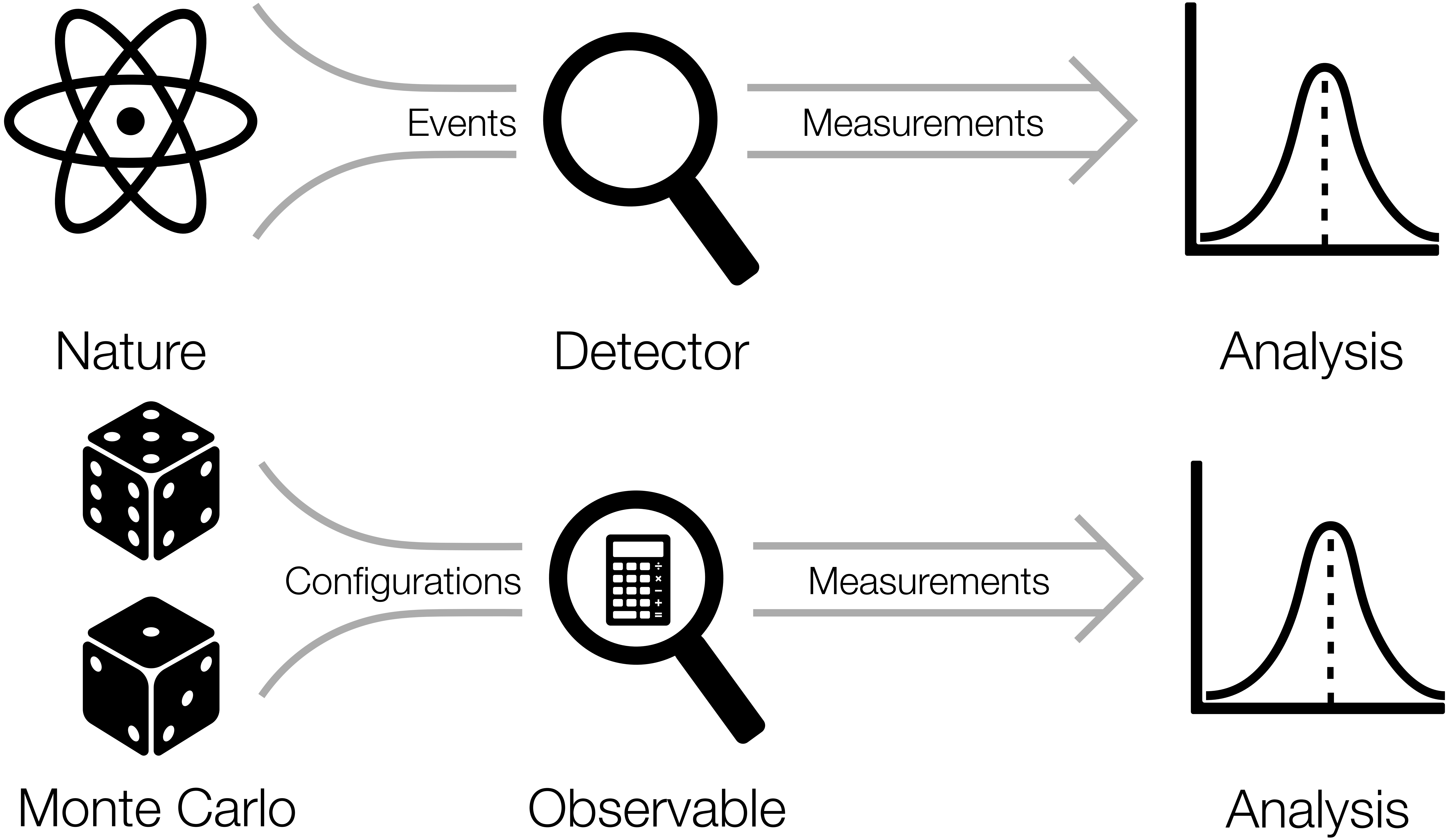
Philip W. Anderson

Nobel Lecture

8 December 1977

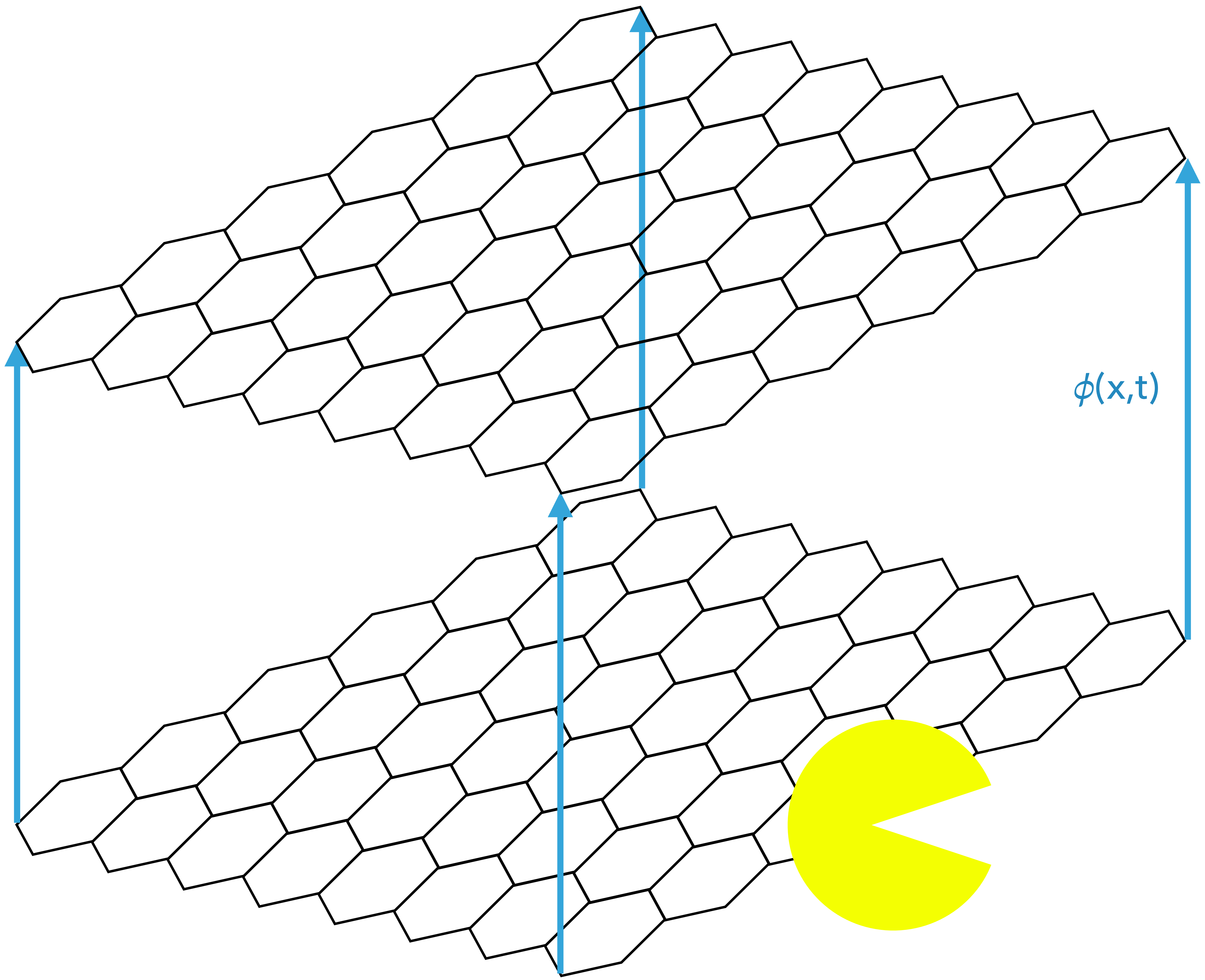
MARKOV CHAIN MONTE CARLO

✓ Statistical errors are improved with run time (budget)
✓ Systematic errors are understood + controlled



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

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

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

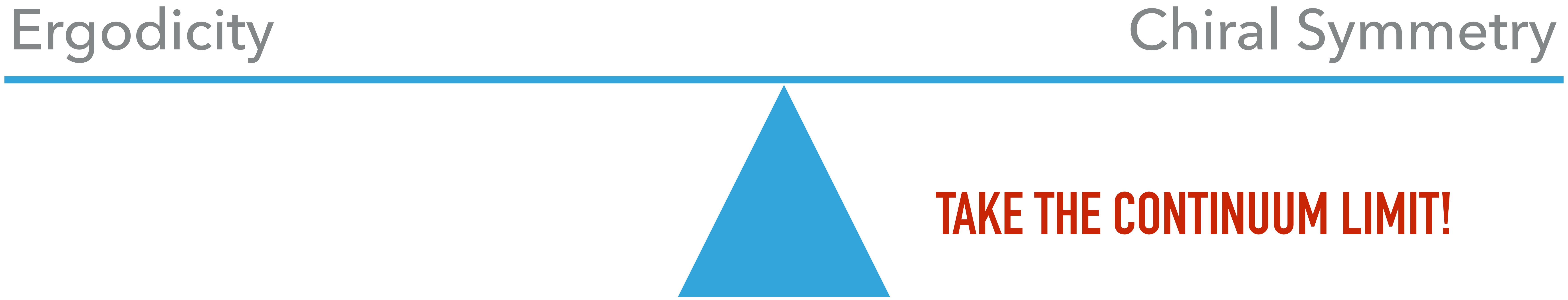
DISCRETIZATION

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

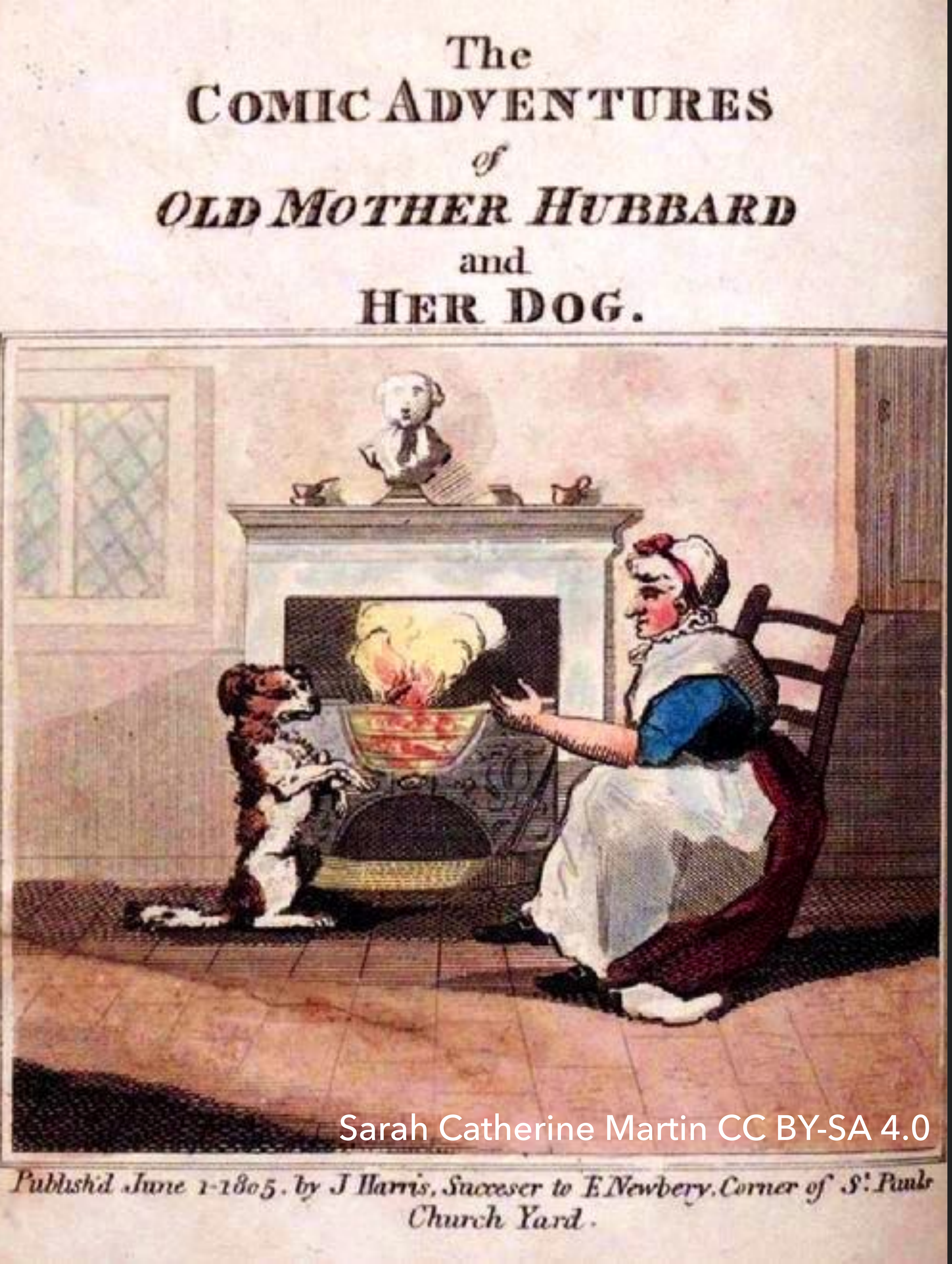
Meng, Lang, Wessel, Assaad, Muramatsu, Nature 464 847-851 (2010) 10.1038/nature08942
complex ϕ Beyl, Goth, Assaad, PRB 97 085144 (2018) 10.1103/PhysRevB.97.085144
Ulybyshev and Valgushev, 1712.02188

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



THE HUBBARD MODEL

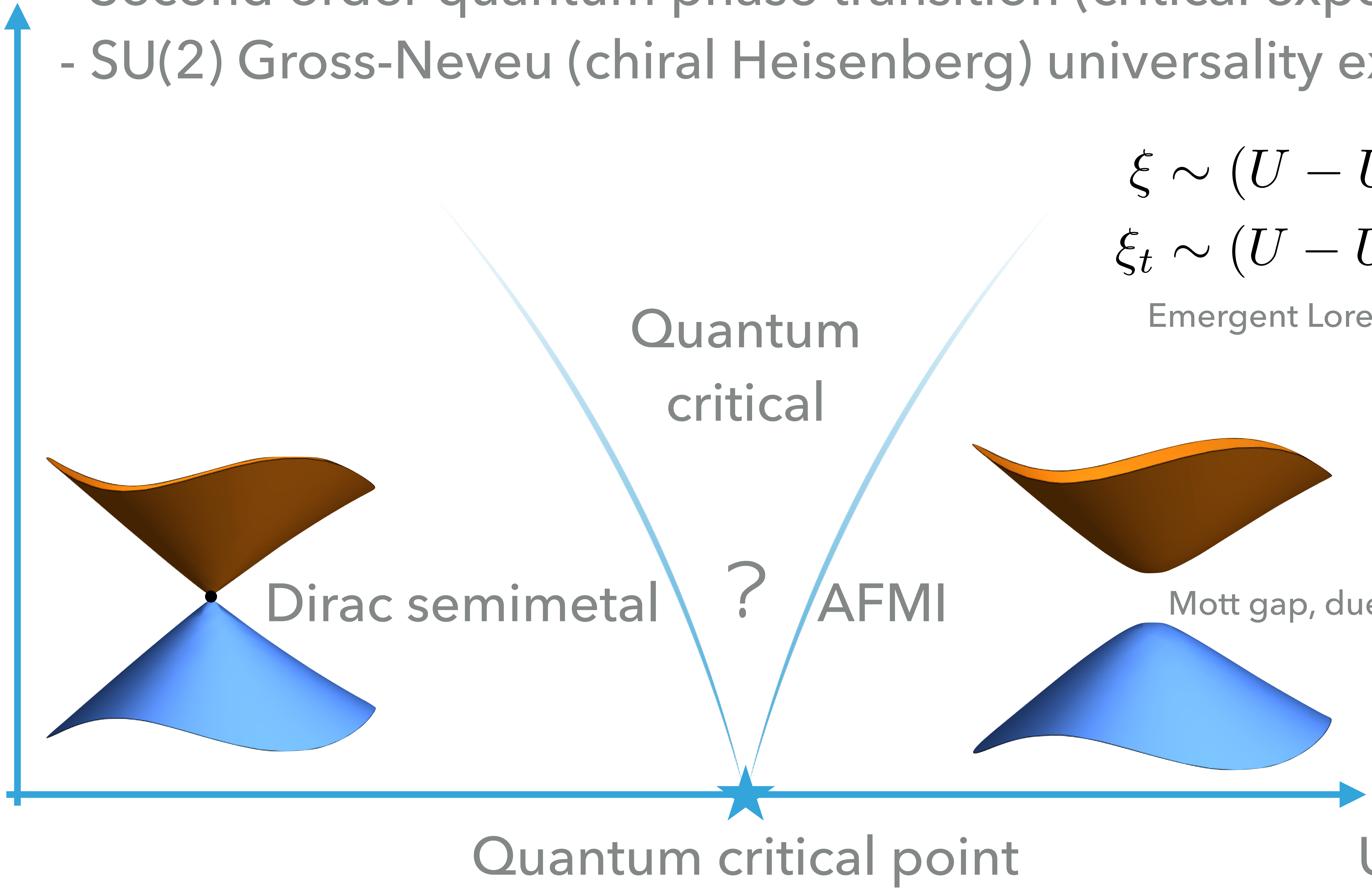
SIGN-PROBLEM-FREE RESULTS

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

T/κ = 1/βκ



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

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

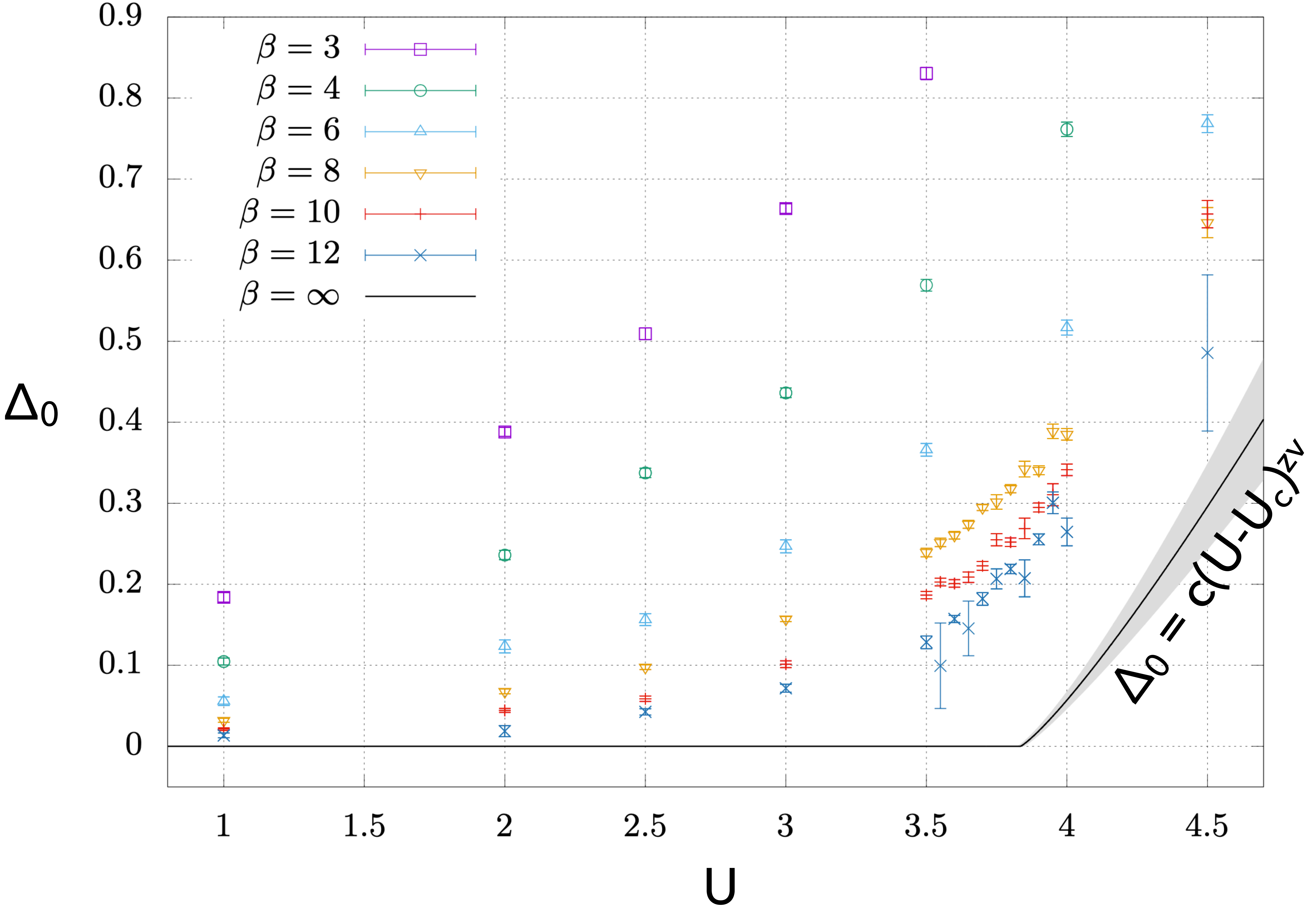
Emergent Lorentz symmetry: z=1

Mott gap, due to interactions only!

pressure

THERMODYNAMIC LIMIT

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



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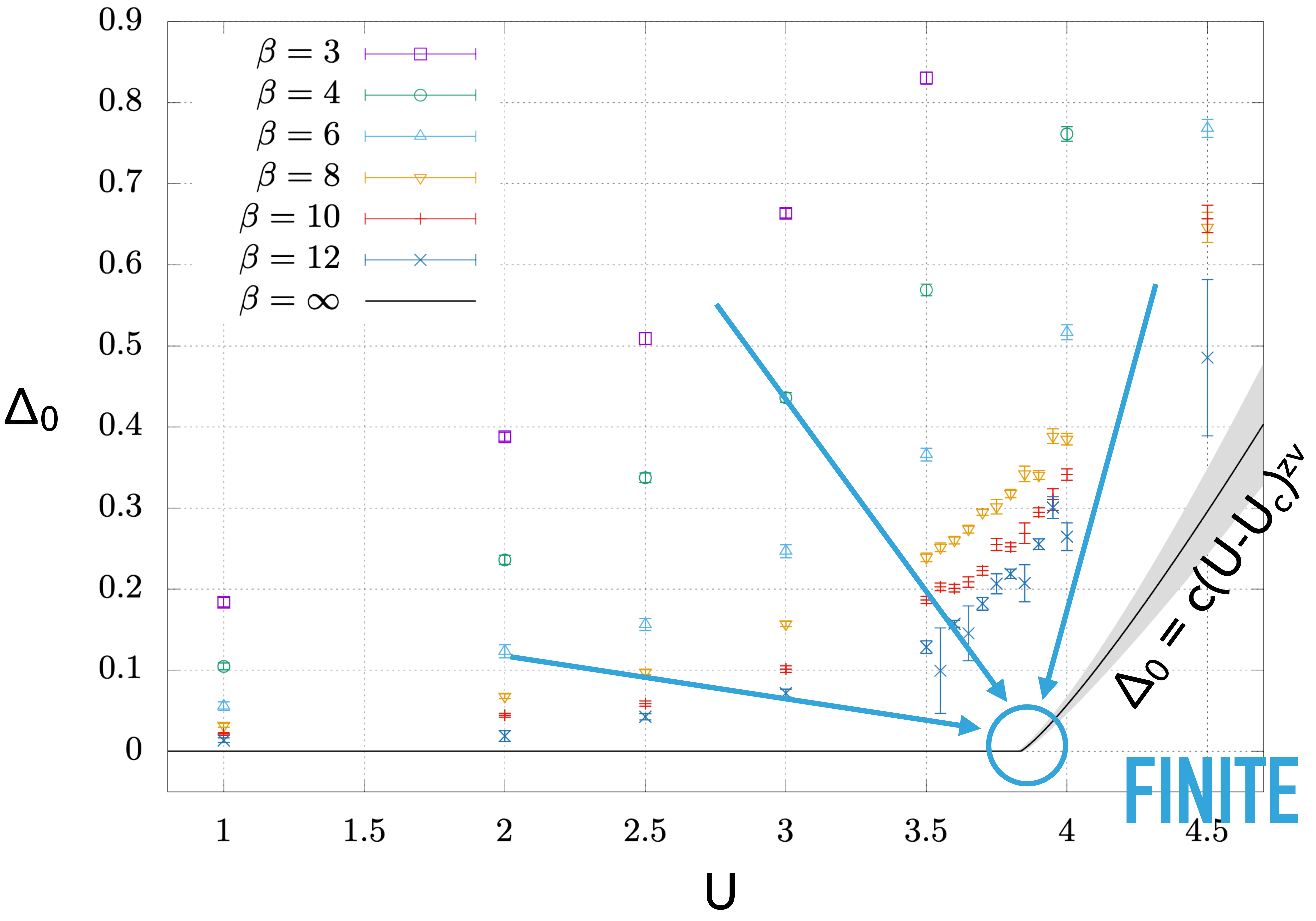
Ostmeyer, EB, Krieg, Lähde, Luu, Urbach 2005.11112



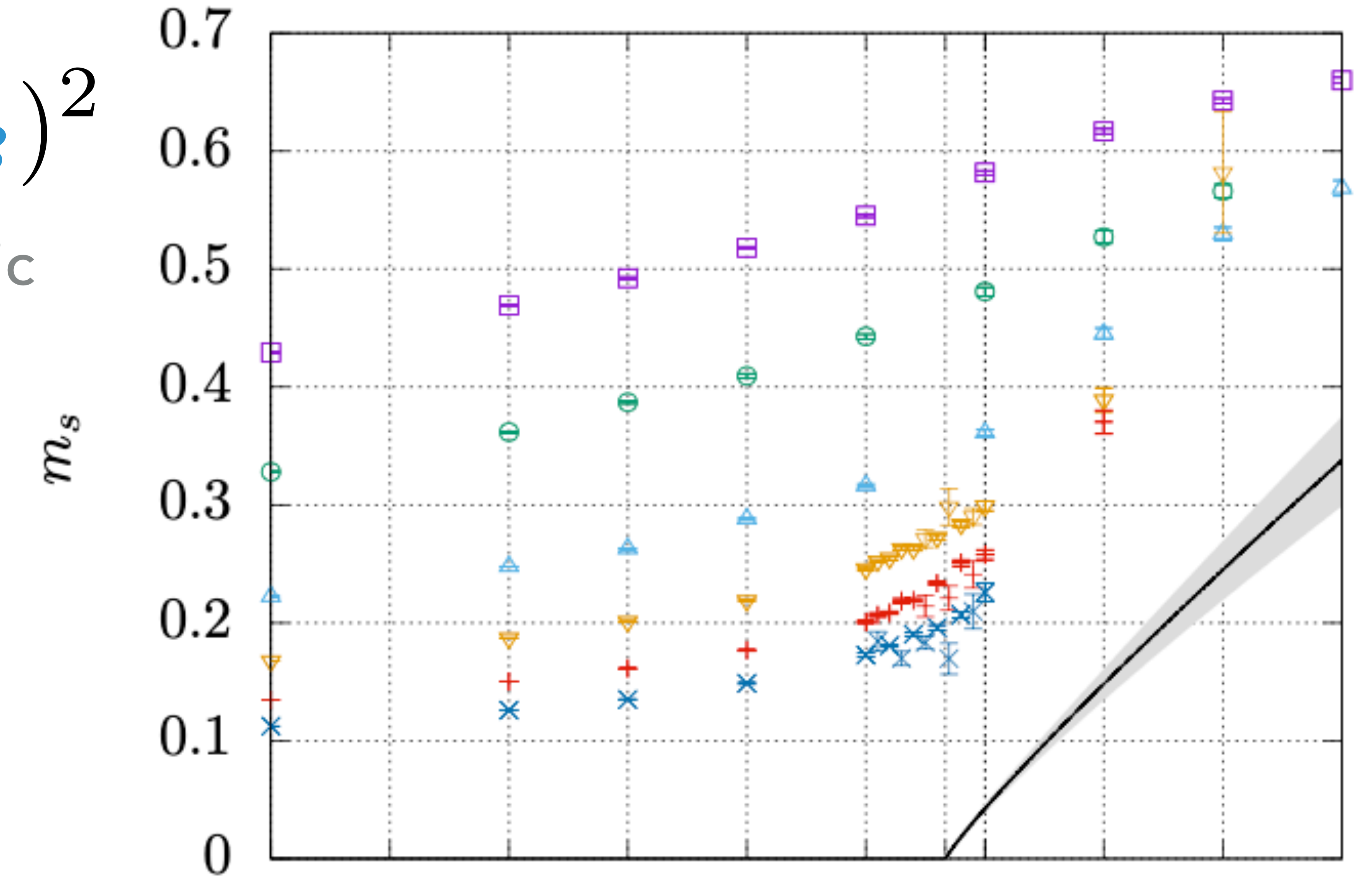
FINITE SIZE SCALING

ZERO-TEMPERATURE LIMIT

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

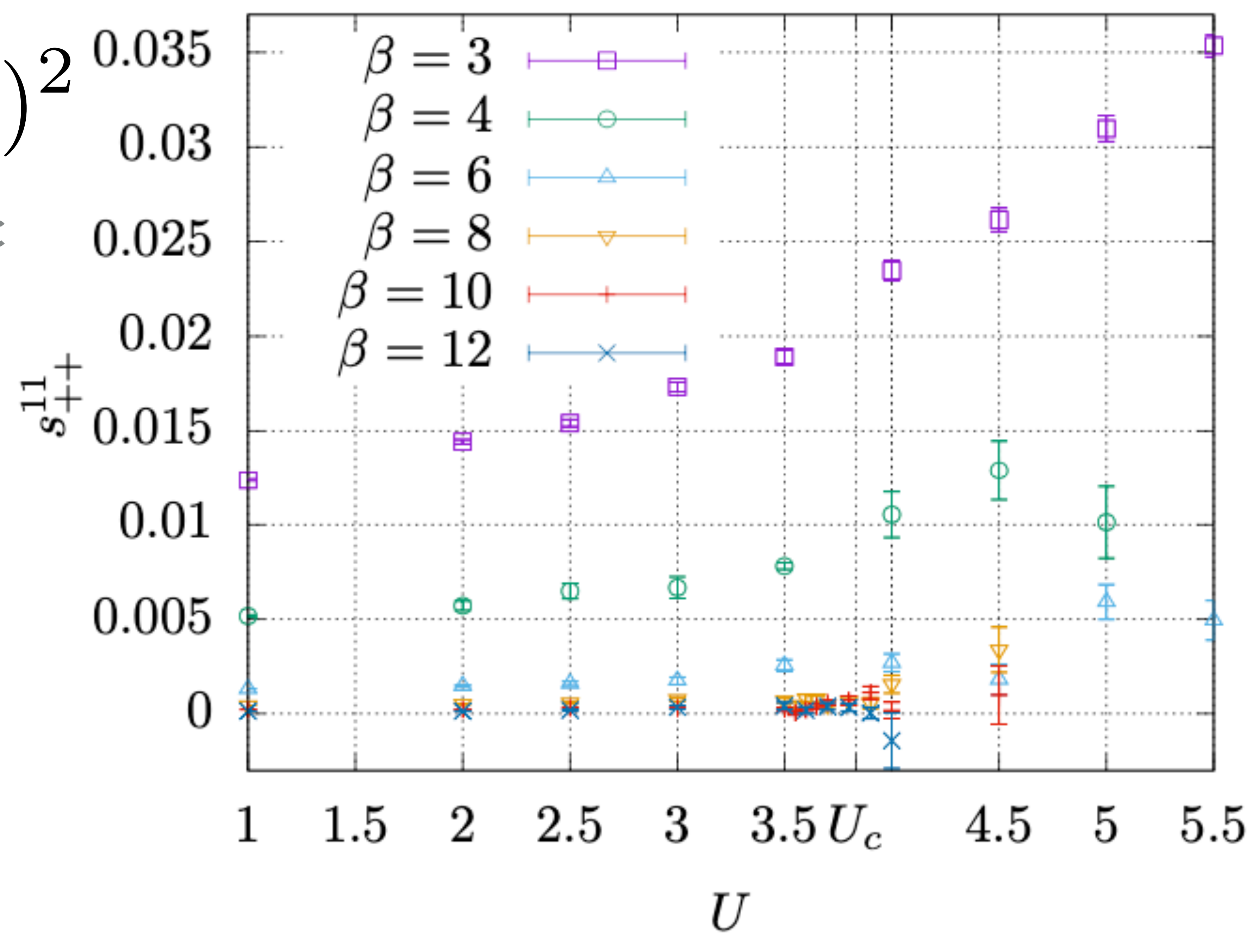
$\sim (\vec{S}_A - \vec{S}_B)^2$

antiferromagnetic



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

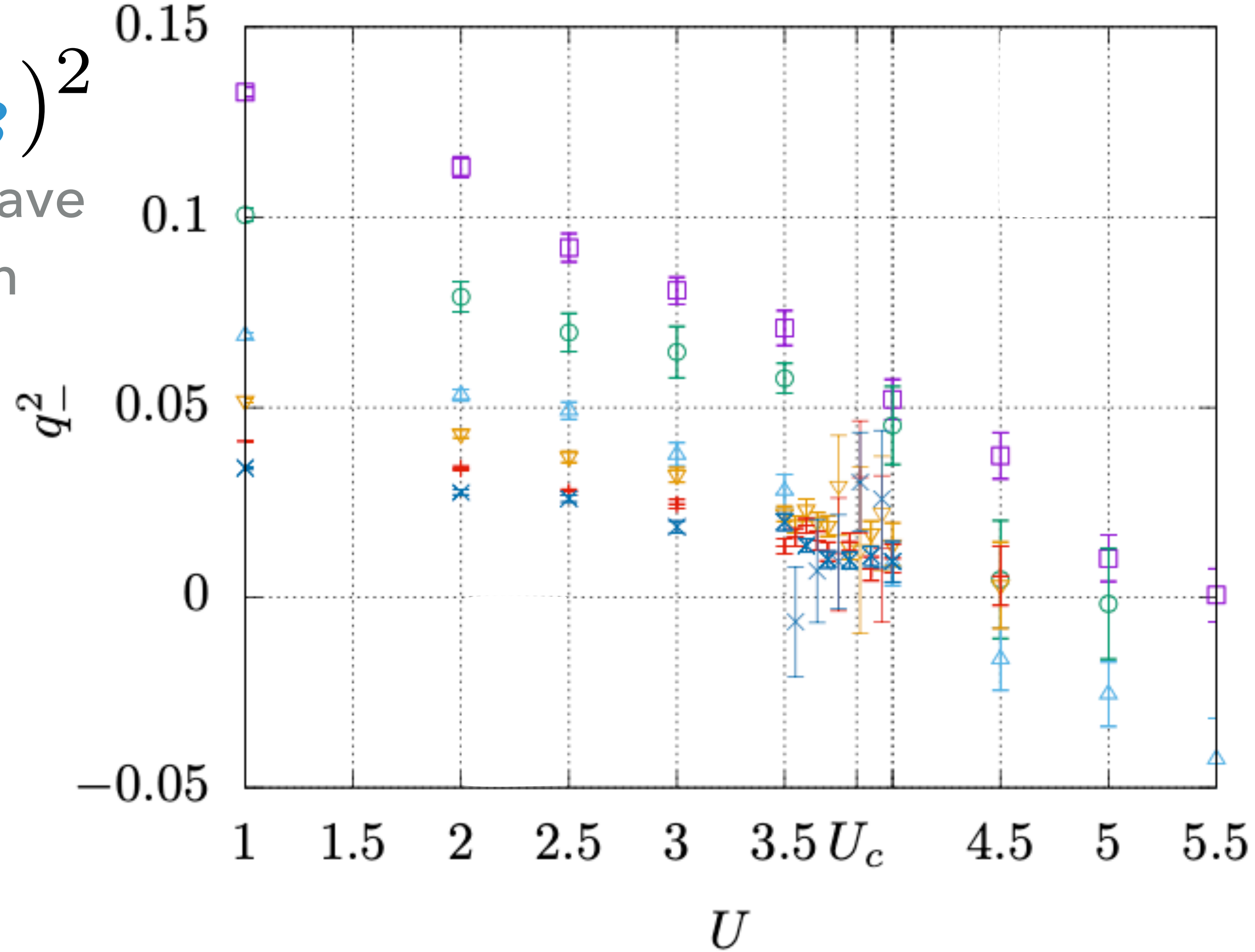
ferromagnetic

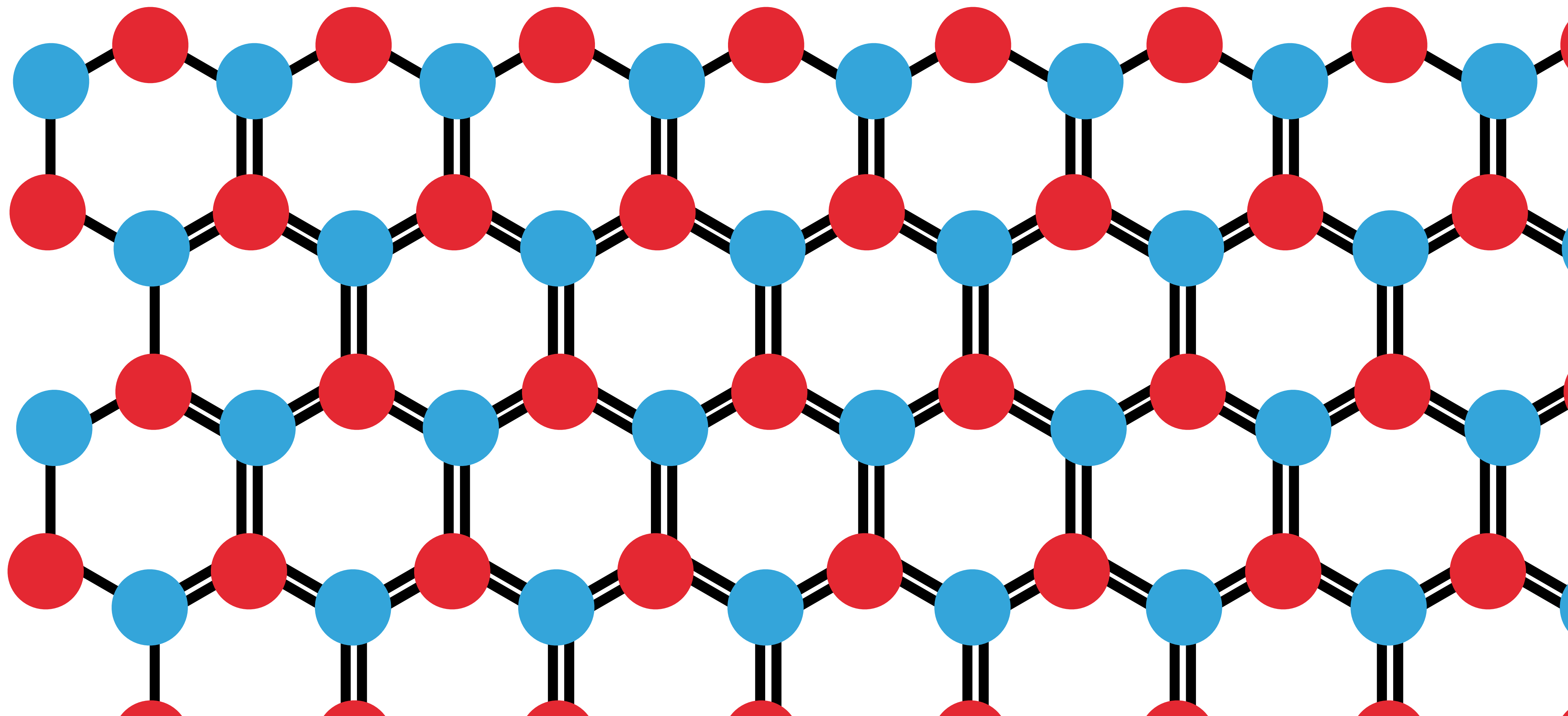


$\sim (\vec{Q}_A - \vec{Q}_B)^2$

charge-density wave

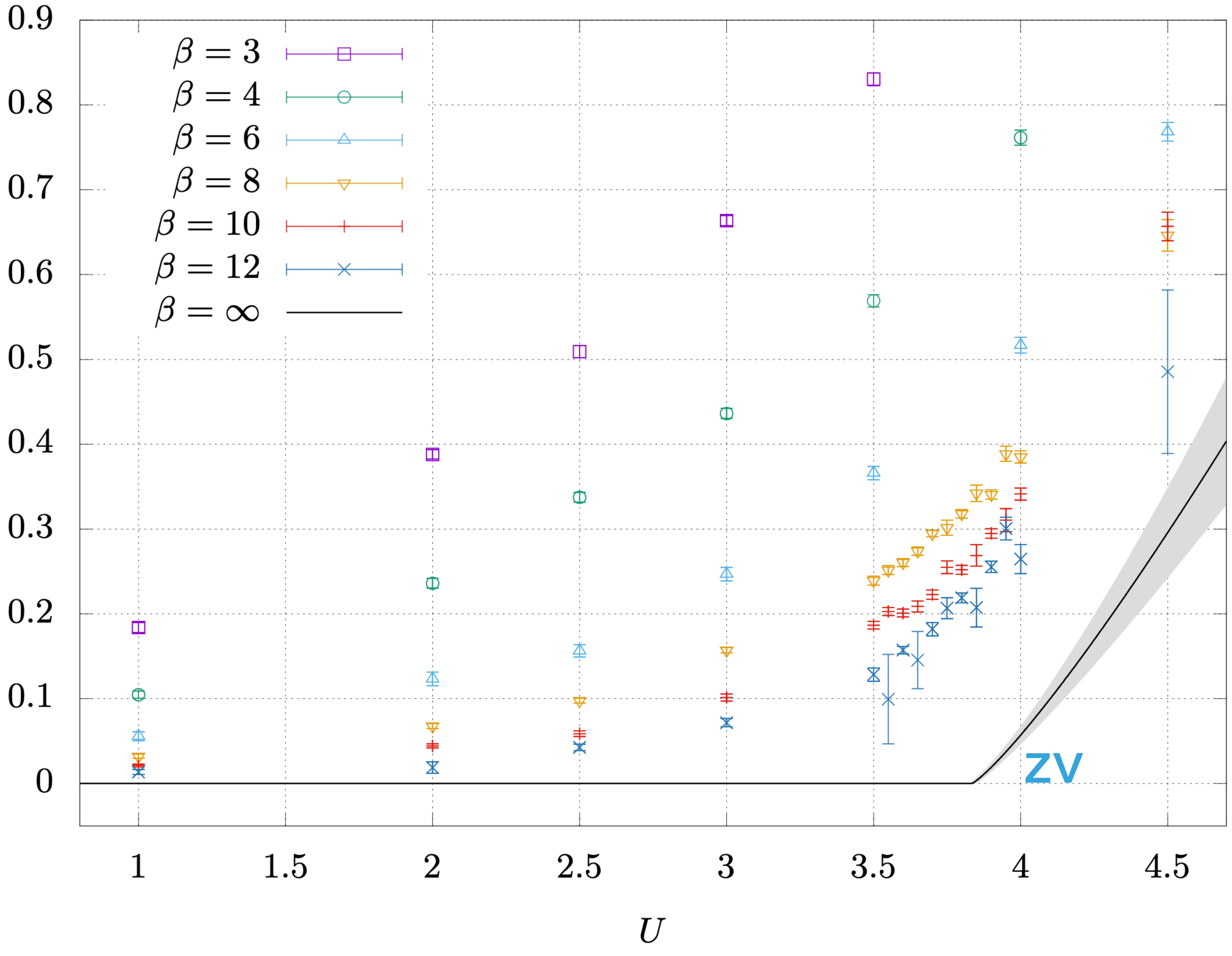
charge separation



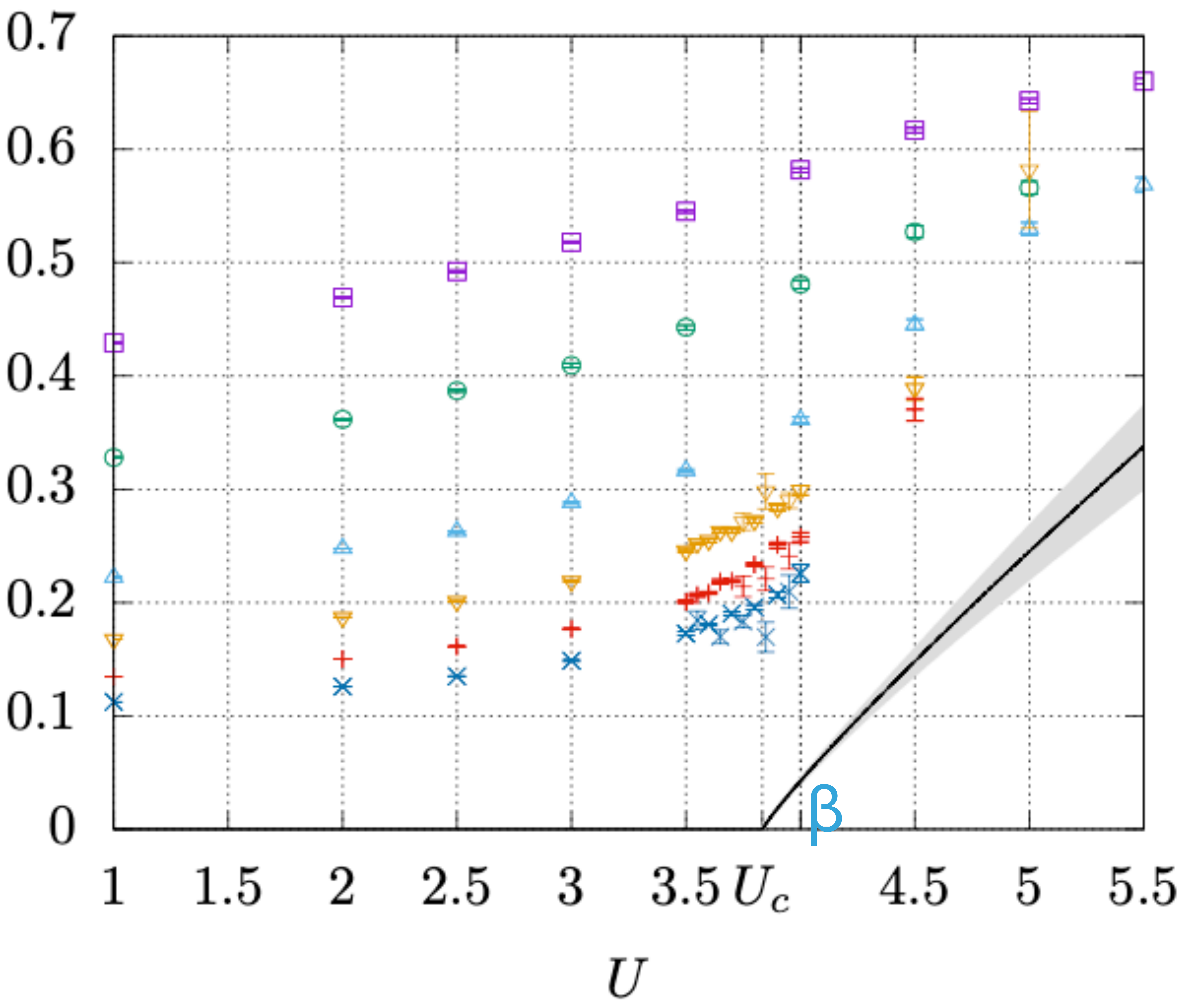


THE PHASE TRANSITION

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



Δ_0



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

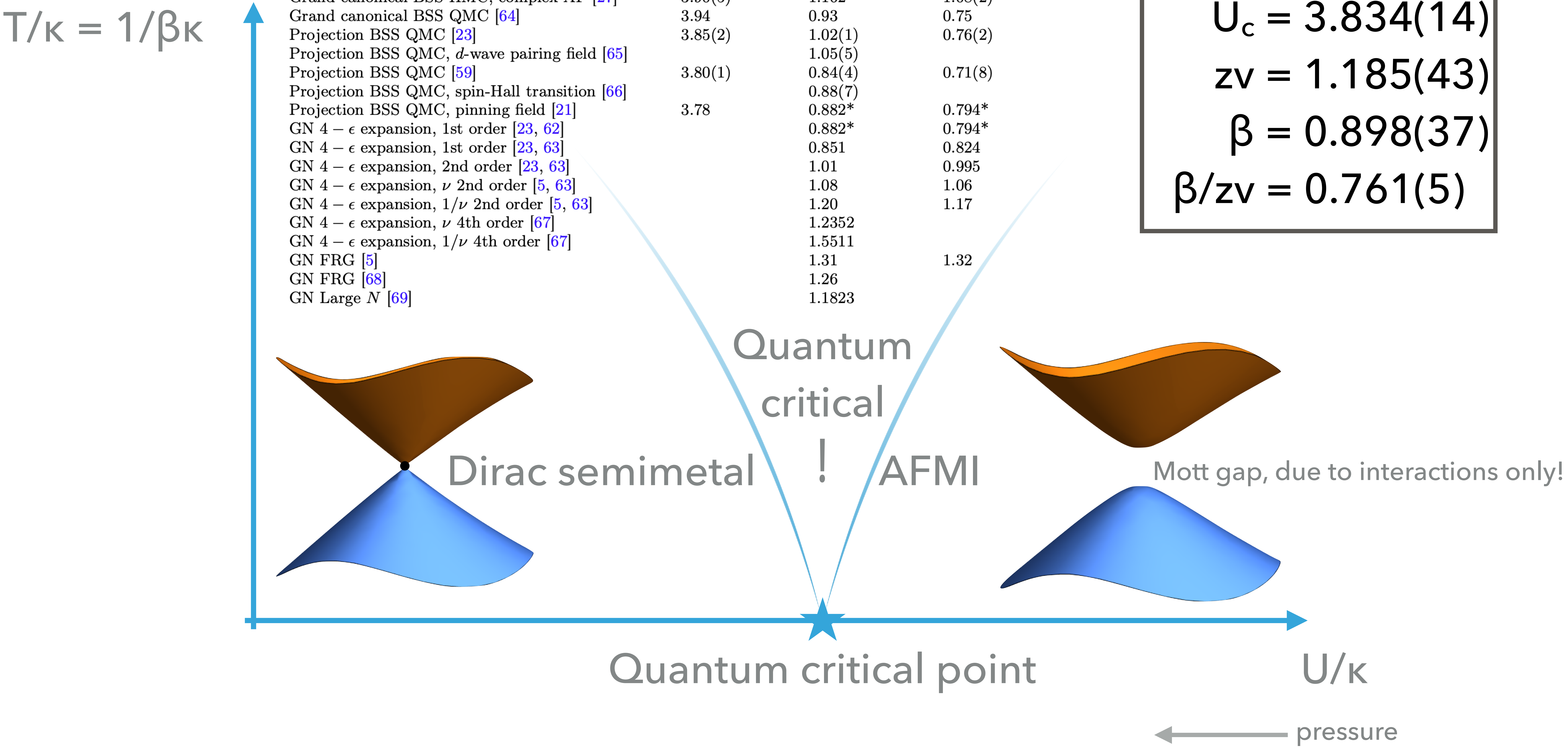
antiferromagnetic

PHASE DIAGRAM

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

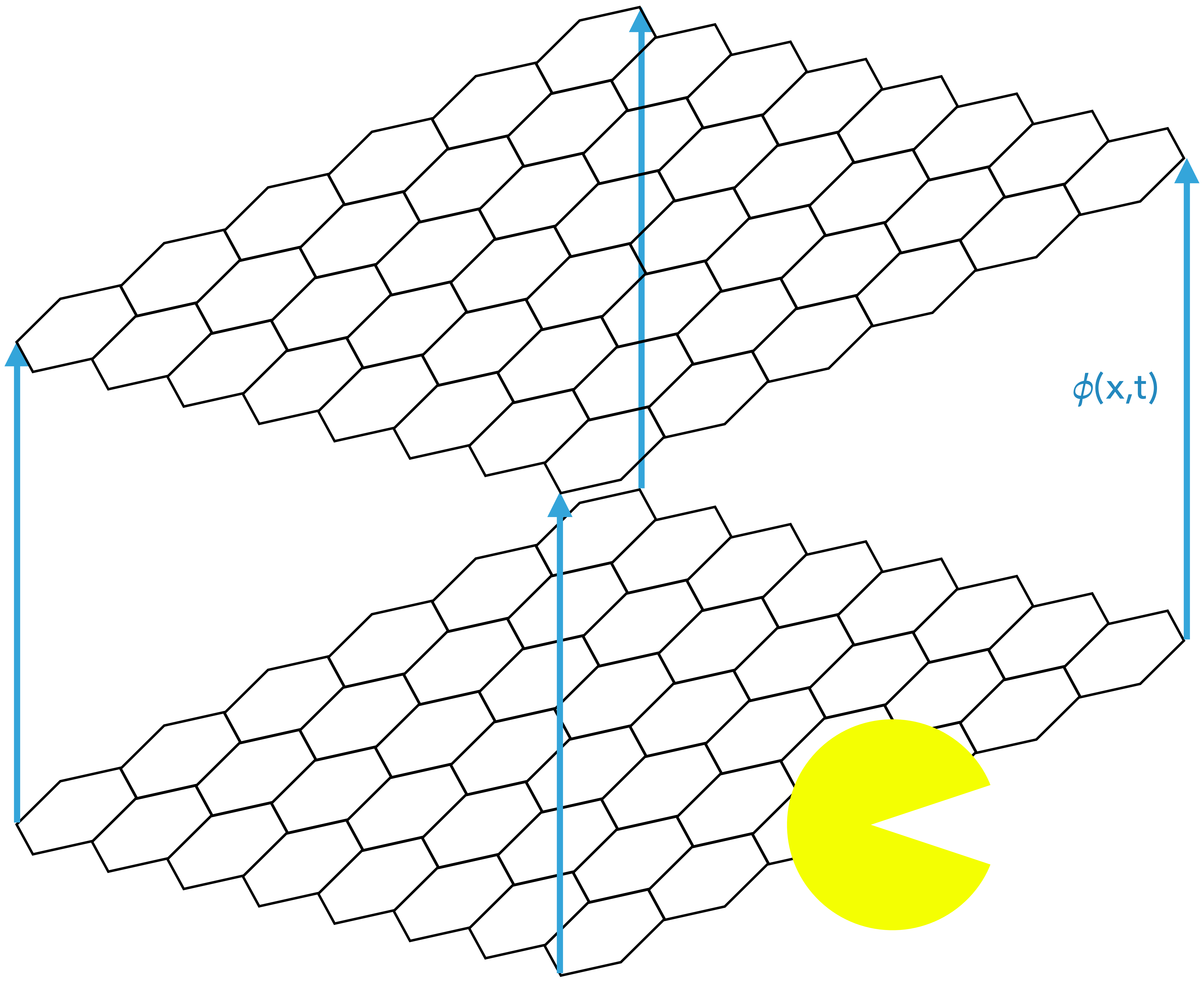
Method	U_c/κ	ν	β
Grand canonical BRS HMC (present work)	3.834(14)	1.185(43)†	1.095(37)‡
Grand canonical BSS HMC, complex AF [27]	3.90(5)	1.162	1.08(2)
Grand canonical BSS QMC [64]	3.94	0.93	0.75
Projection BSS QMC [23]	3.85(2)	1.02(1)	0.76(2)
Projection BSS QMC, *d*-wave pairing field [65]		1.05(5)	
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	

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



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?

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

Trade for M†[+φ, ...]

Flip on a bipartite lattice

No problem in the bipartite μ=0 case.

DISCRETIZATION

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

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

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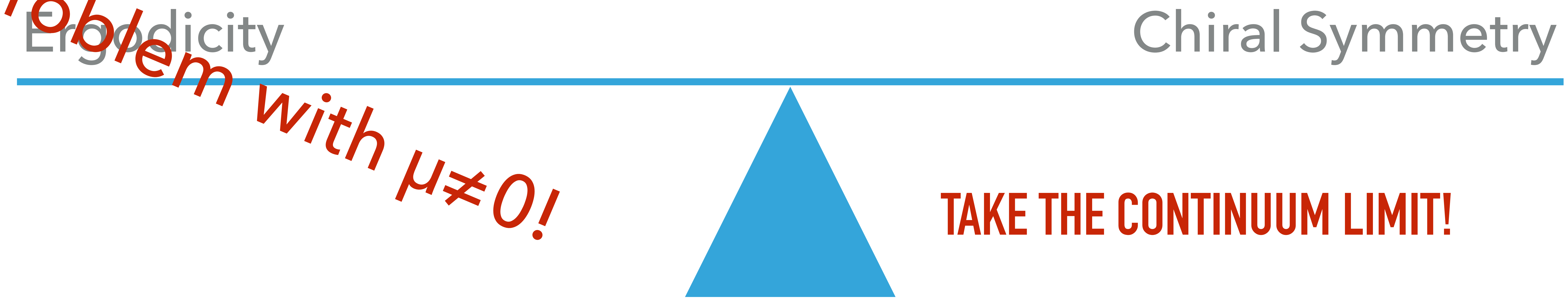
Luu and Lähde, PRB 93, 155106 (2016) 10.1103/PhysRevB.93.155106

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

No problem with $\mu \neq 0$!



TAKE THE CONTINUUM LIMIT!

Beyl, Goth, Assaad (above)

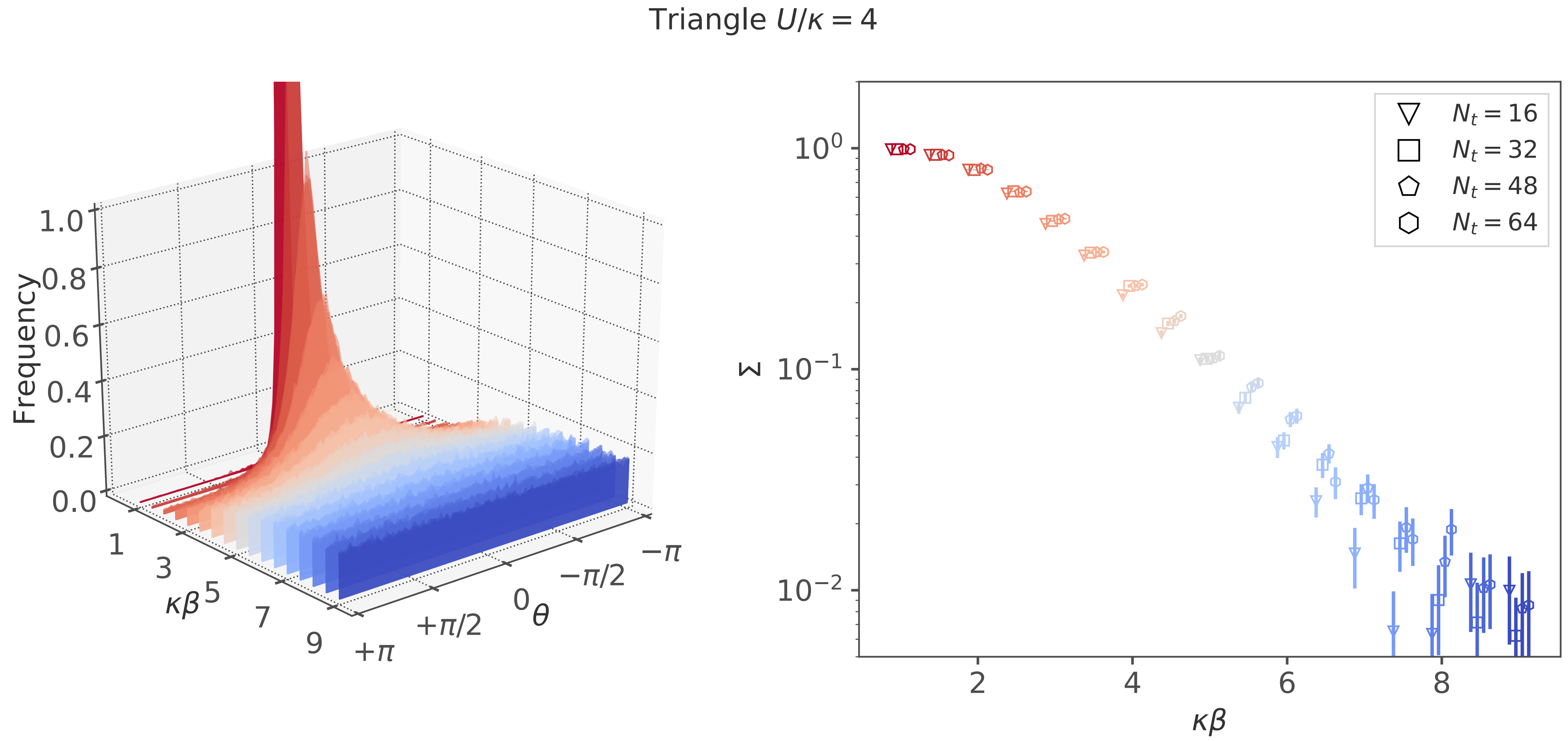
Wynen, EB, Körber, Lähde, Luu PRB 100 075141 10.1103/PhysRevB.100.075141

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

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

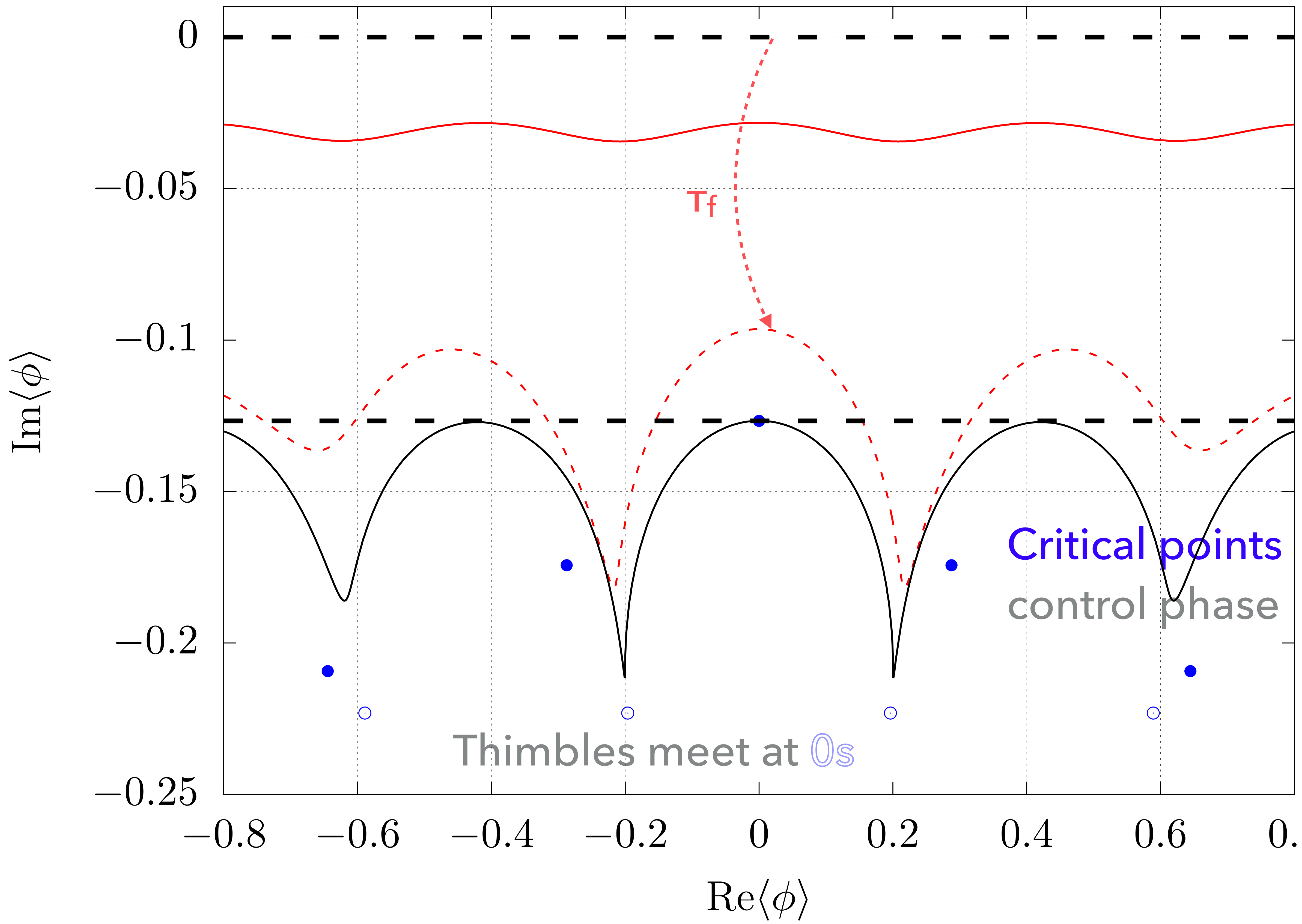
Importance sample according to the real part of the weight

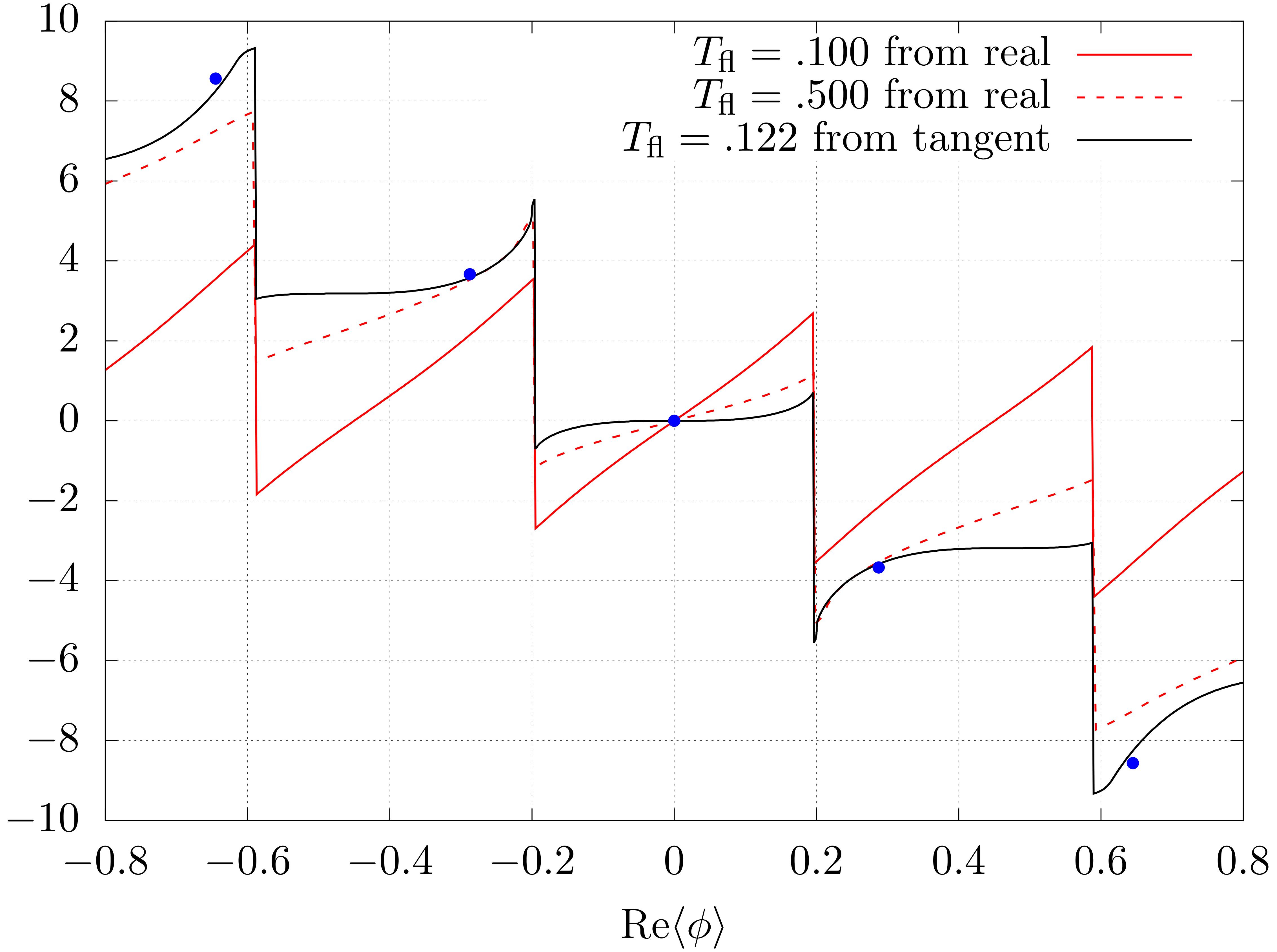
Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221

LEFSCHETZ THIMBLES HAVE CONSTANT SIGN

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

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





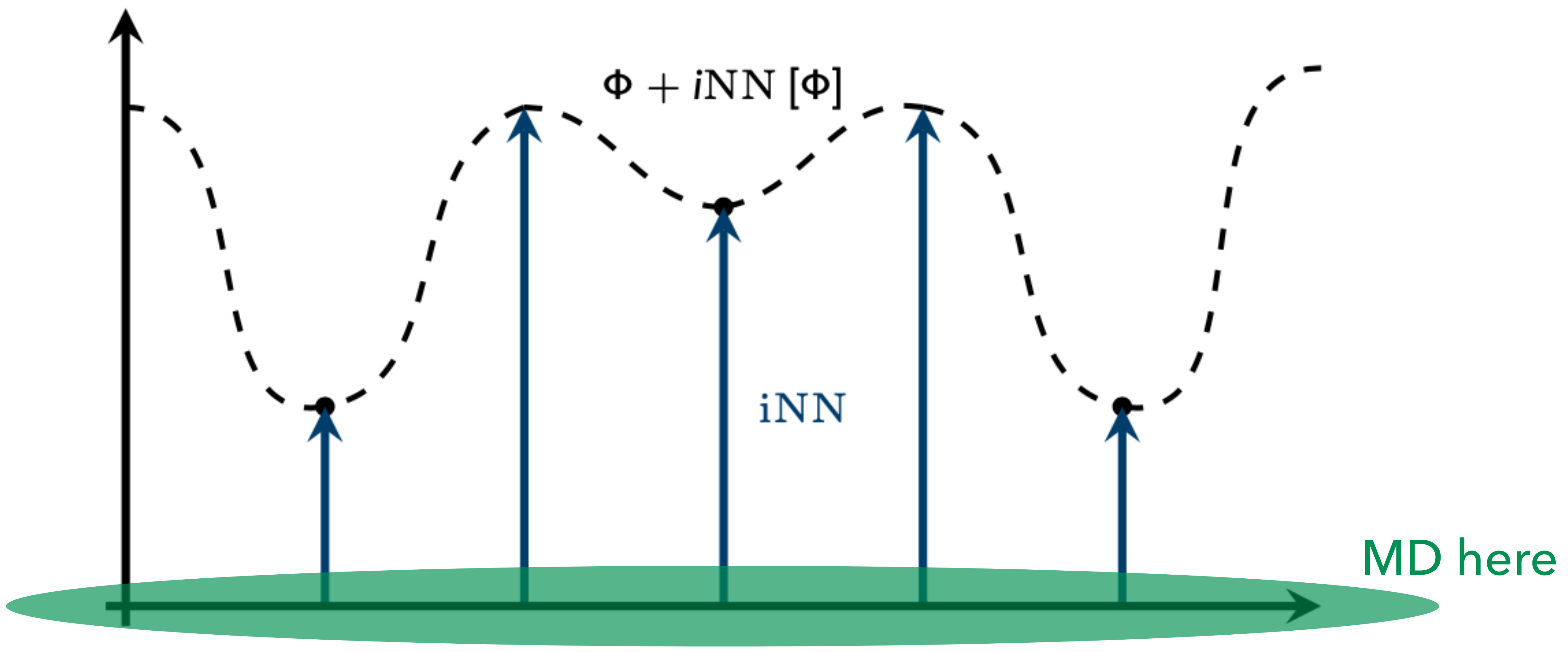
Cristoforetti, Di Renzo, Scorzato PRD 86, 074506 10.1103/PhysRevD.86.074506 1205.3996

Alexandru, Başar, Bedaque, Warrington 2007.05436

NETWORK ARCHITECTURES

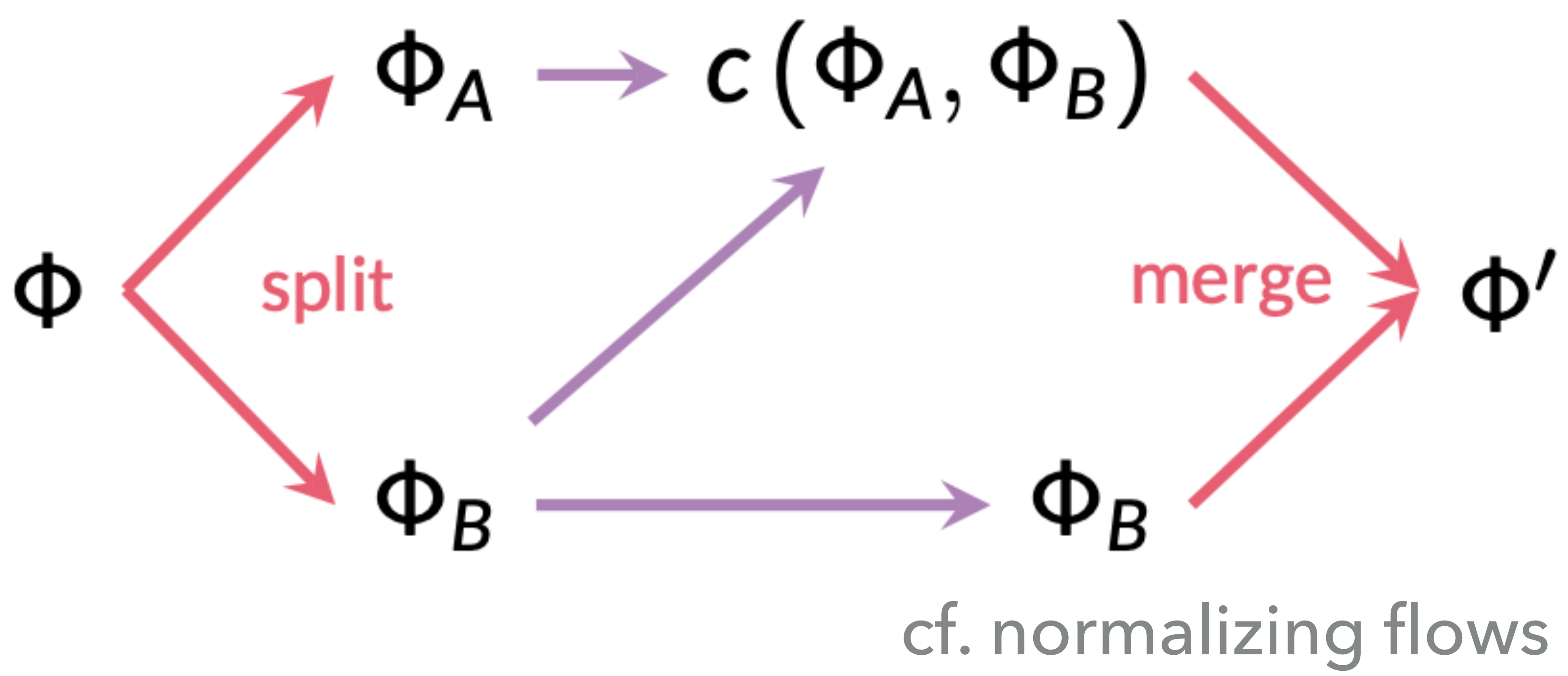
Wynen, EB, Krieg, Luu, Ostmeyer 2006.11221
Rodekamp, EB, Gäntgen, Krieg, Luu, Ostmeyer 2203.00390

$\mathbb{R}$-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



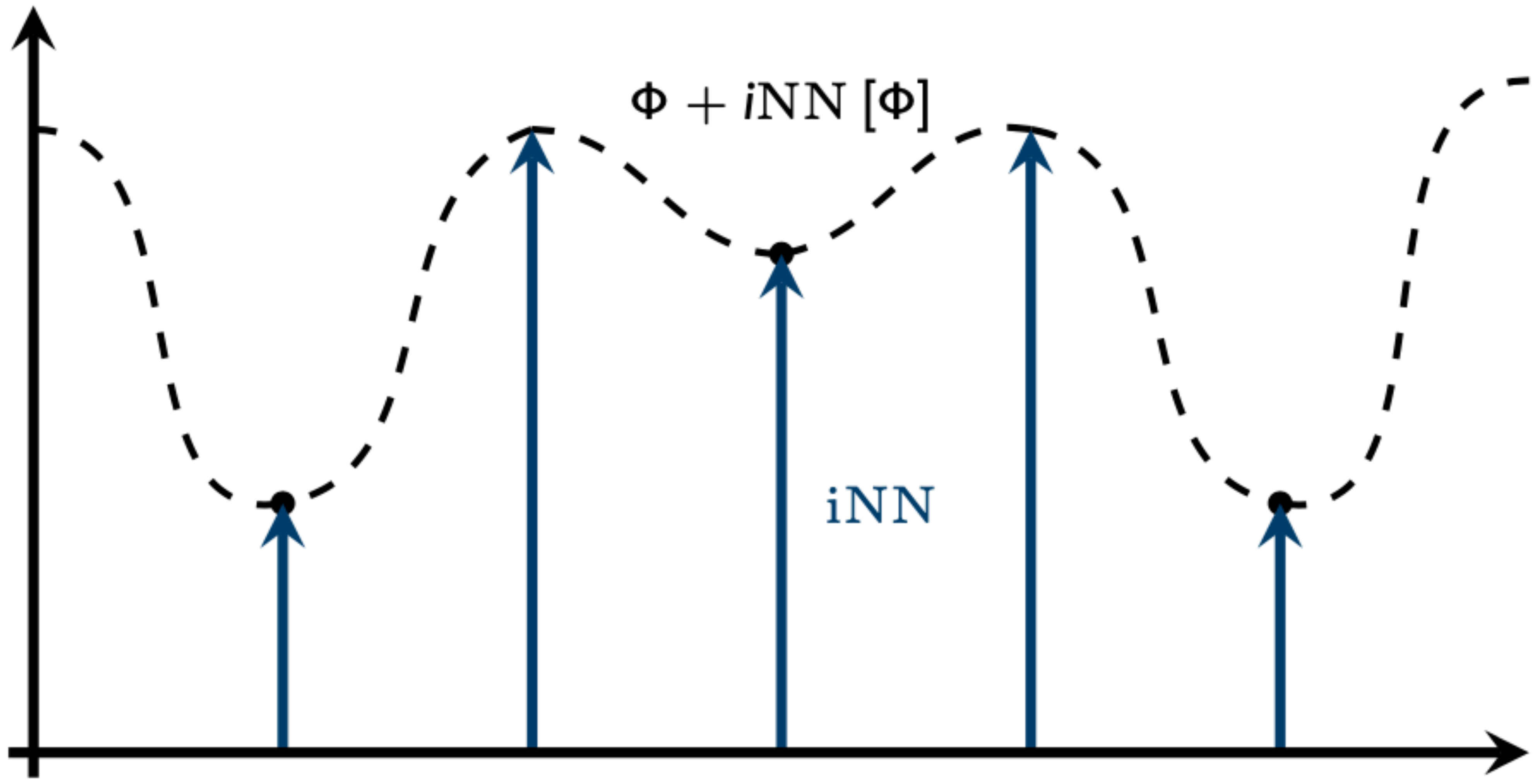
Train the network so that
- Input of the network is Φ at the start of the flow
- Output of the network is Φ at the end of the flow

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

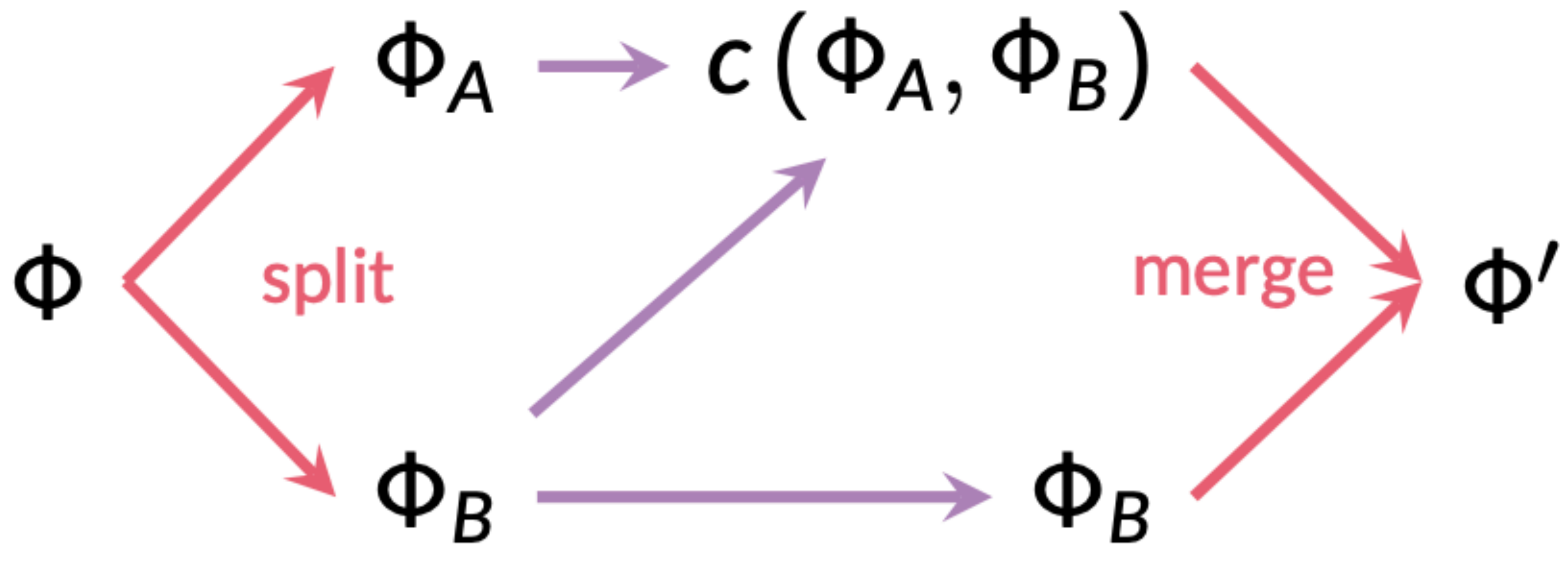
$\mathbb{R}$-Valued Neural Network



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

Jacobian is horrible: V^3

$\mathbb{C}$-Valued Neural Network

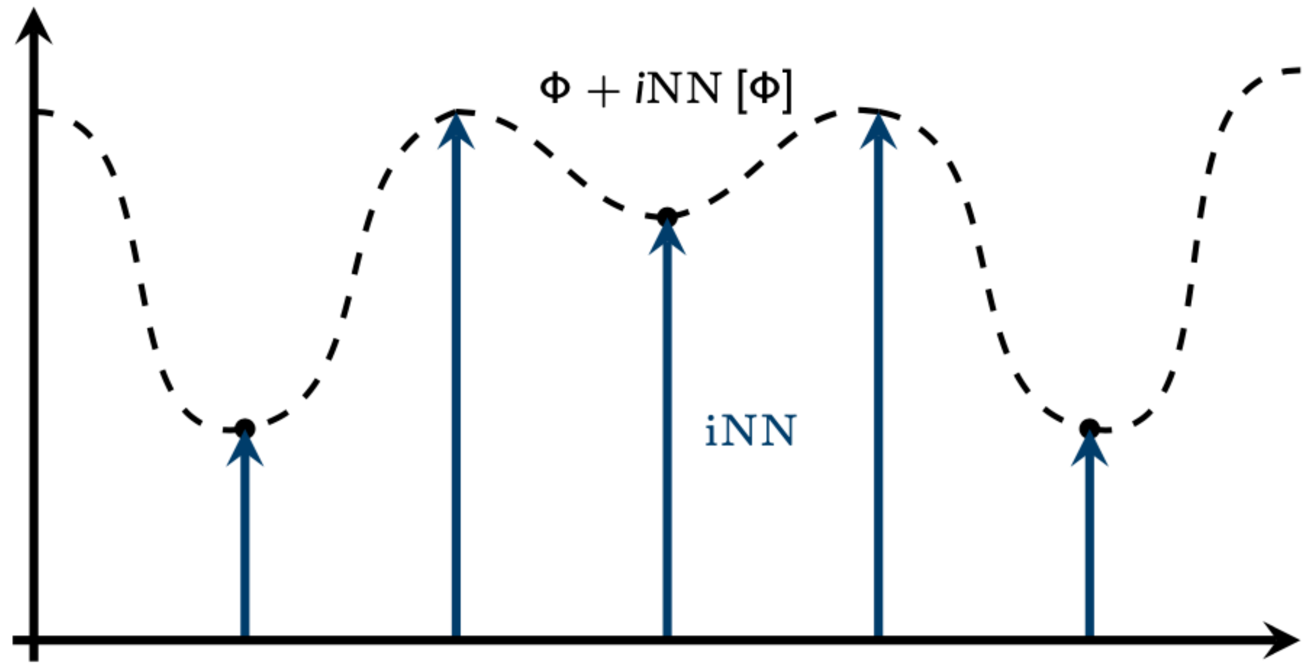


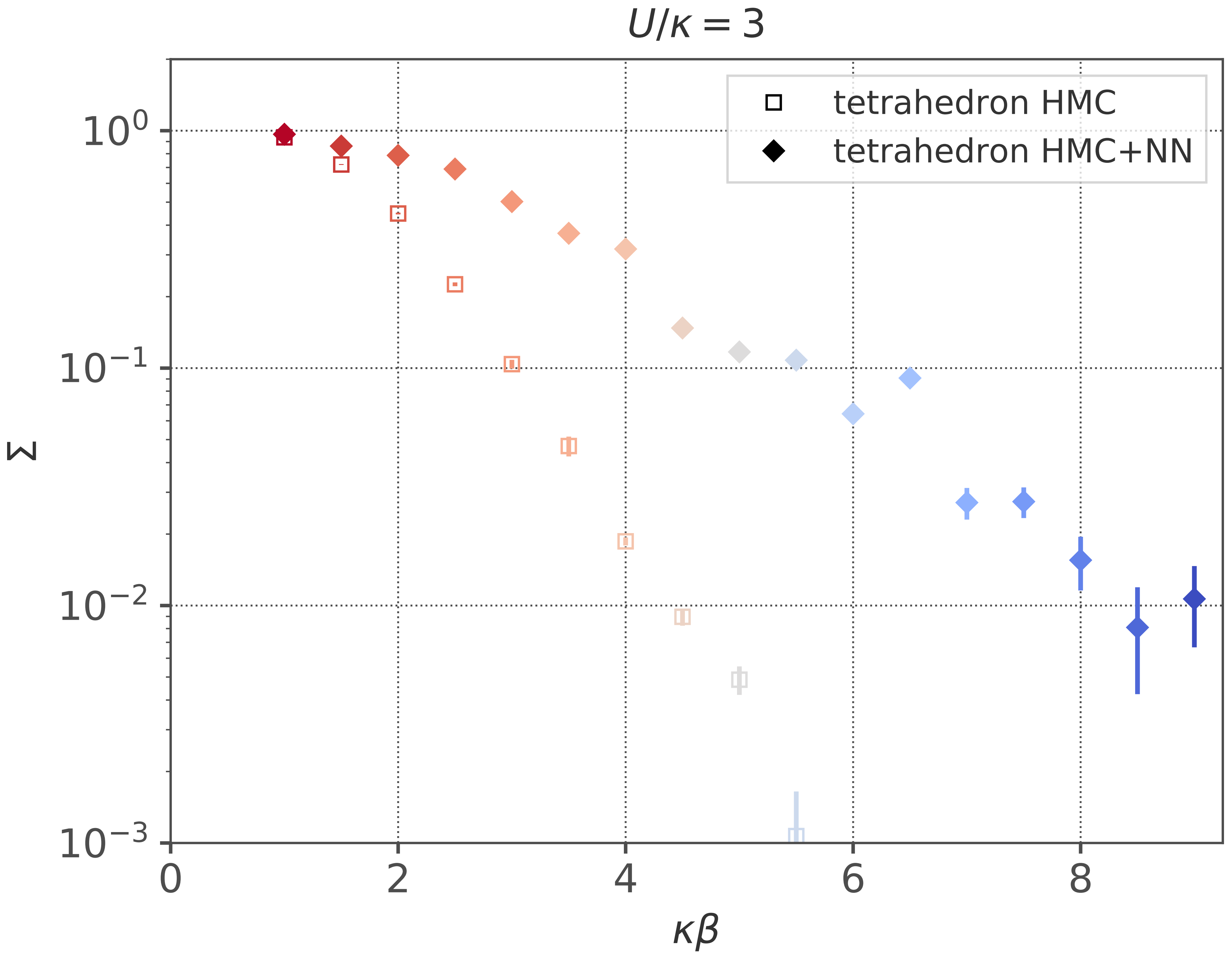
$$\begin{pmatrix} \frac{\partial c(\Phi_A, \Phi_B)}{\partial \Phi_A} & 0 \\ \star & \mathbb{1} \end{pmatrix}$$

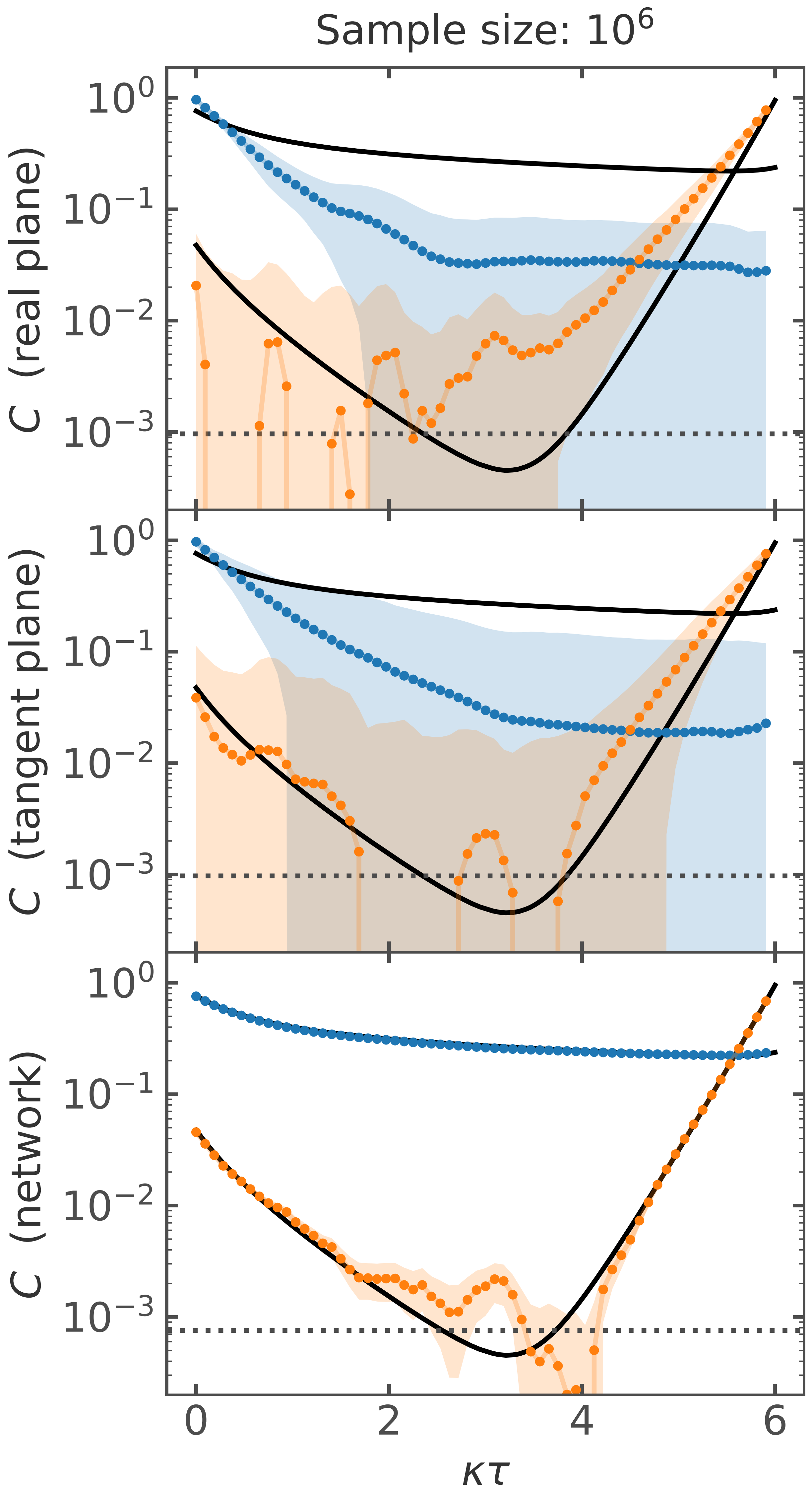
Jacobian is easy: V^1

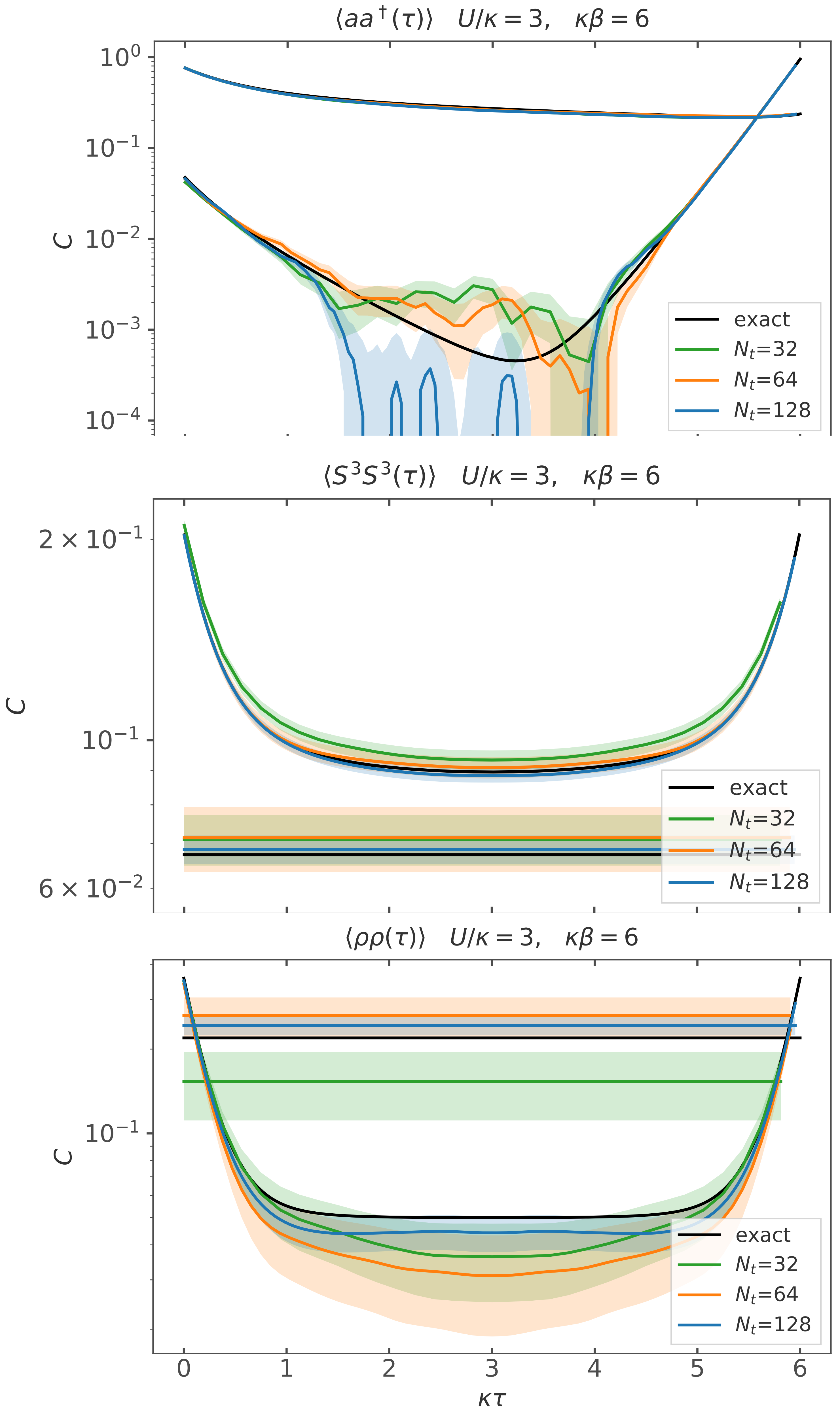
NONBIPARTITE EXAMPLES

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



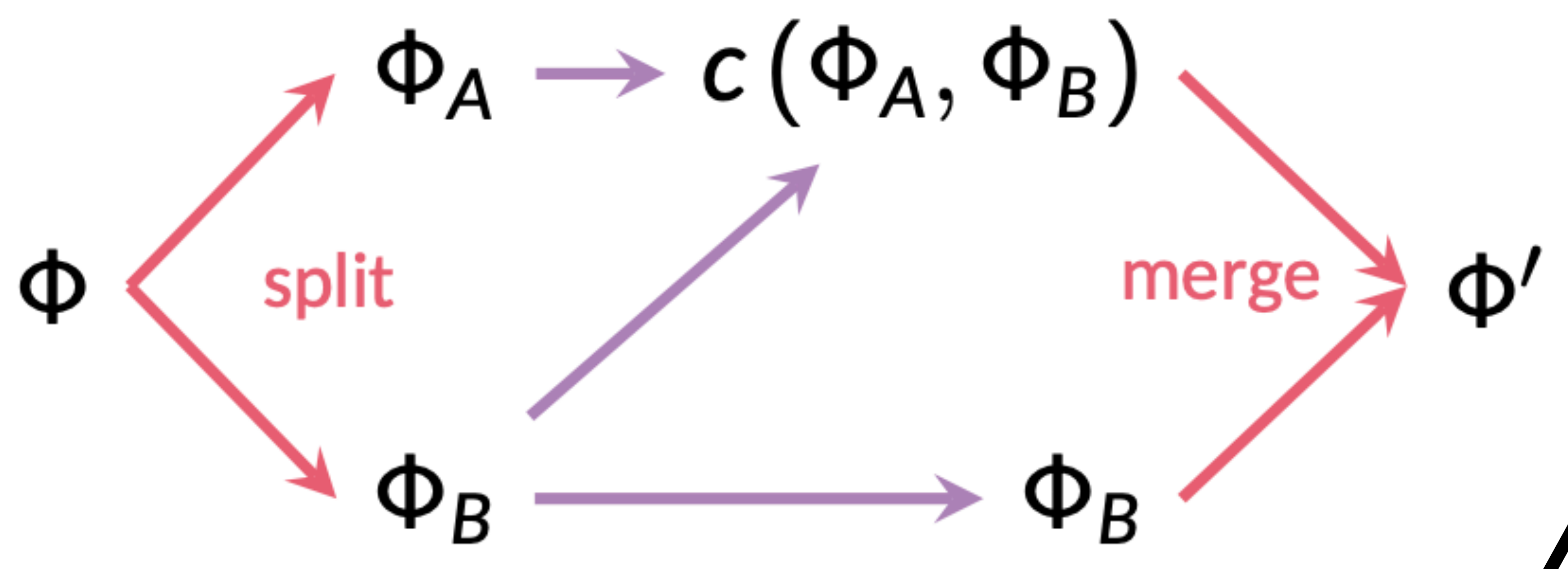


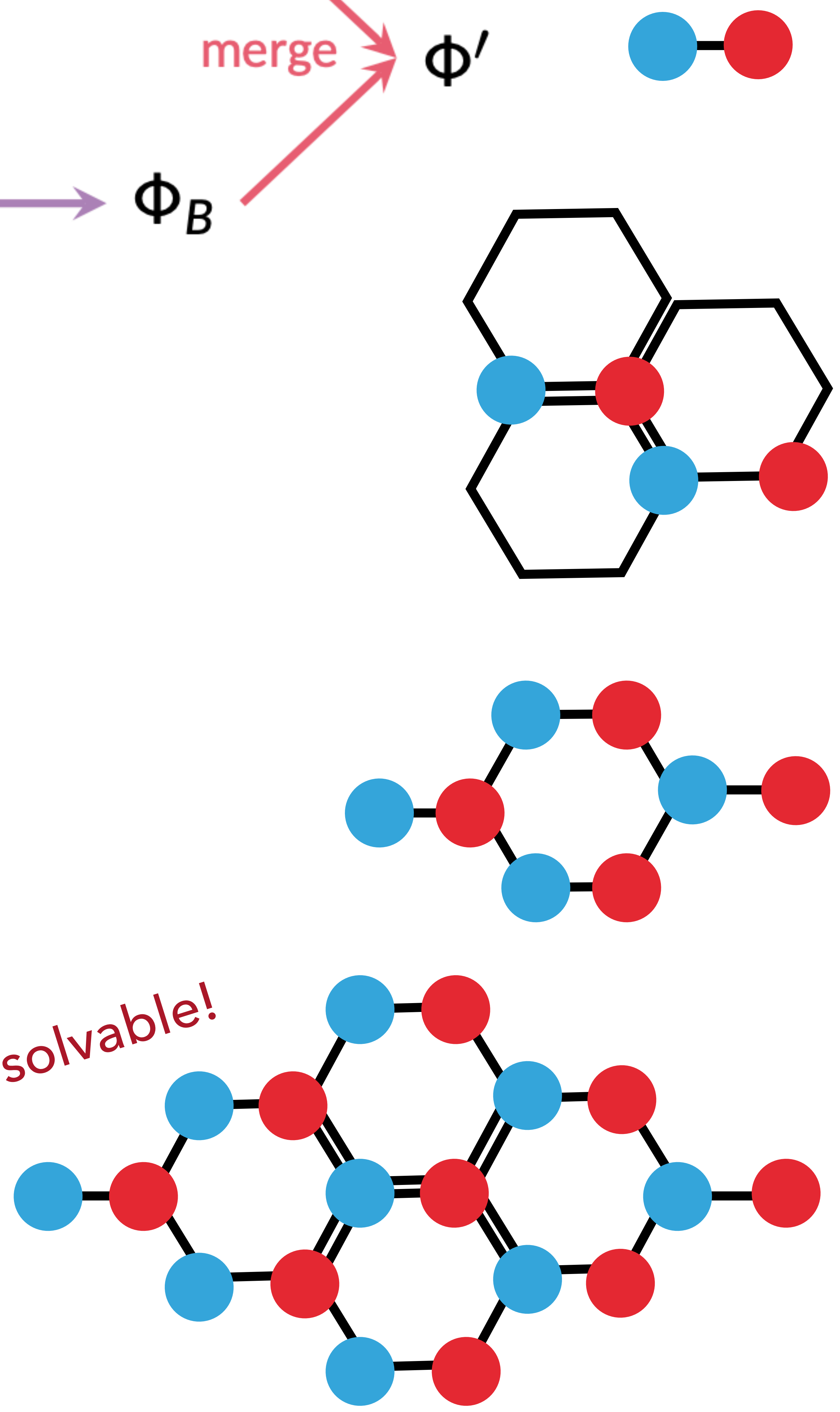




DOPED EXAMPLES

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

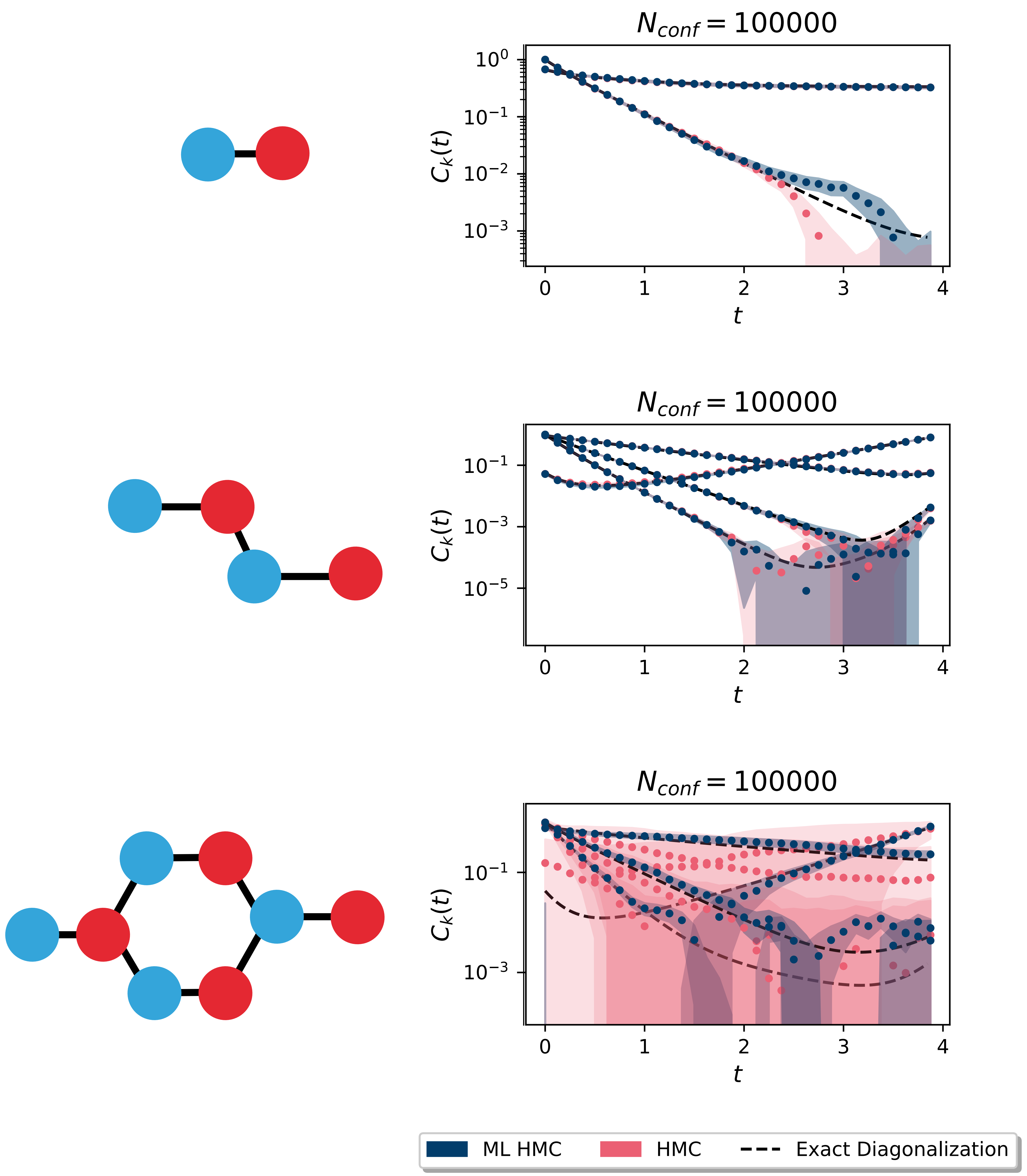


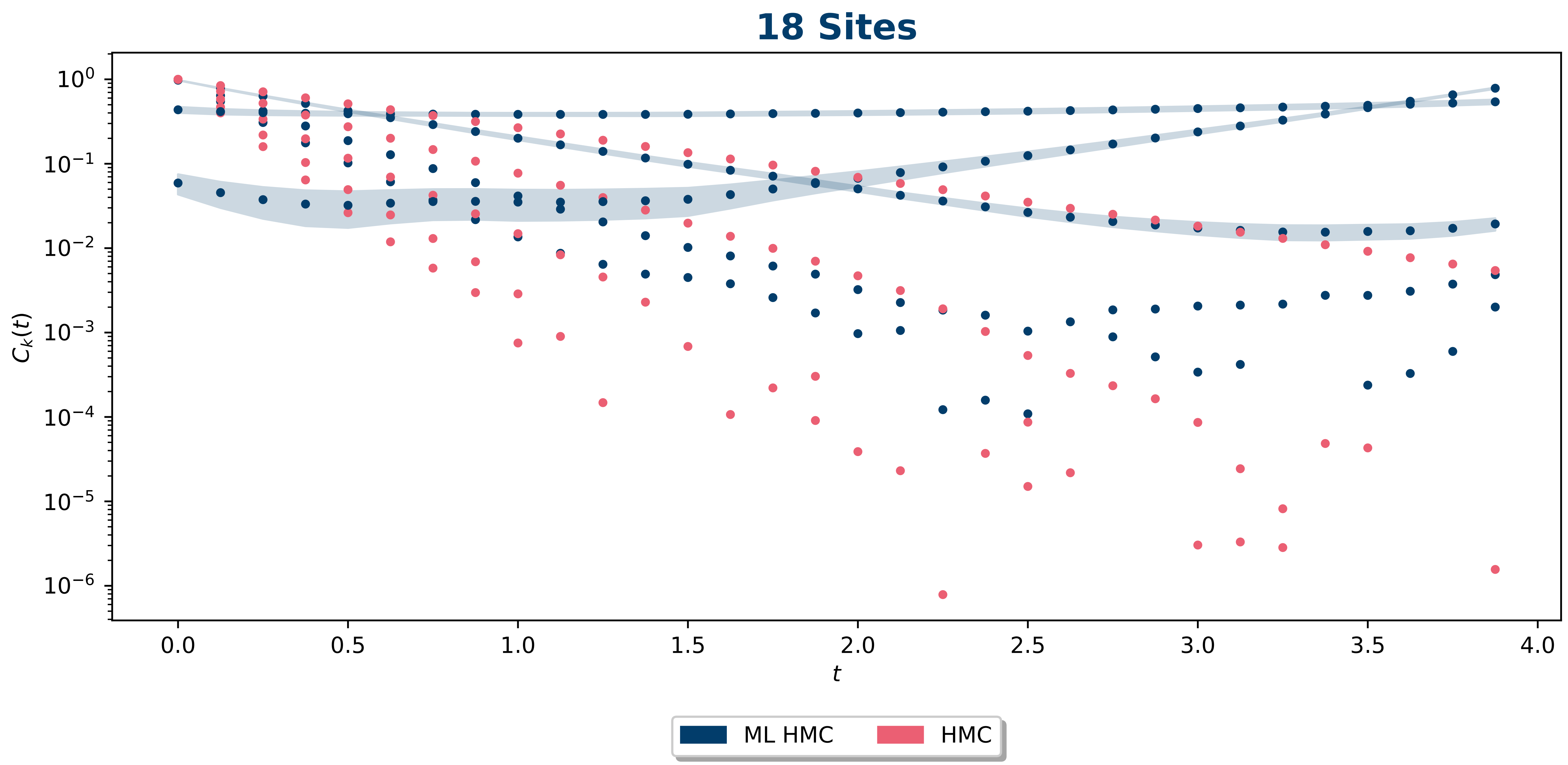


Not exactly solvable!

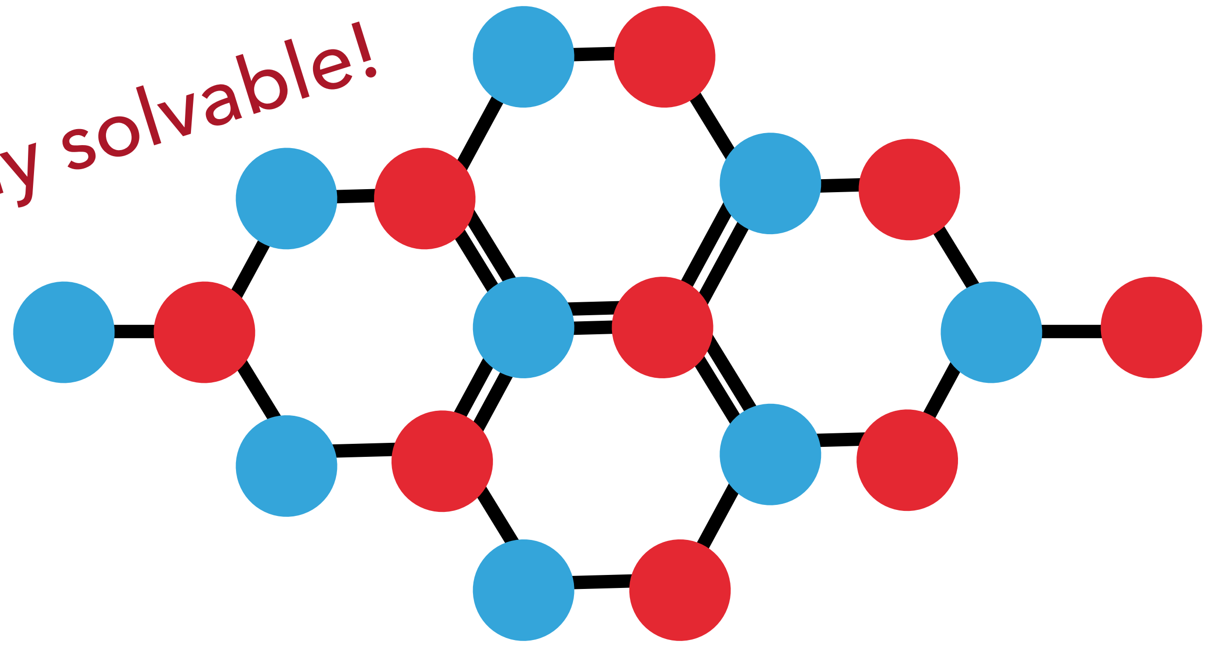
DOPED EXAMPLES

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





Not exactly solvable!

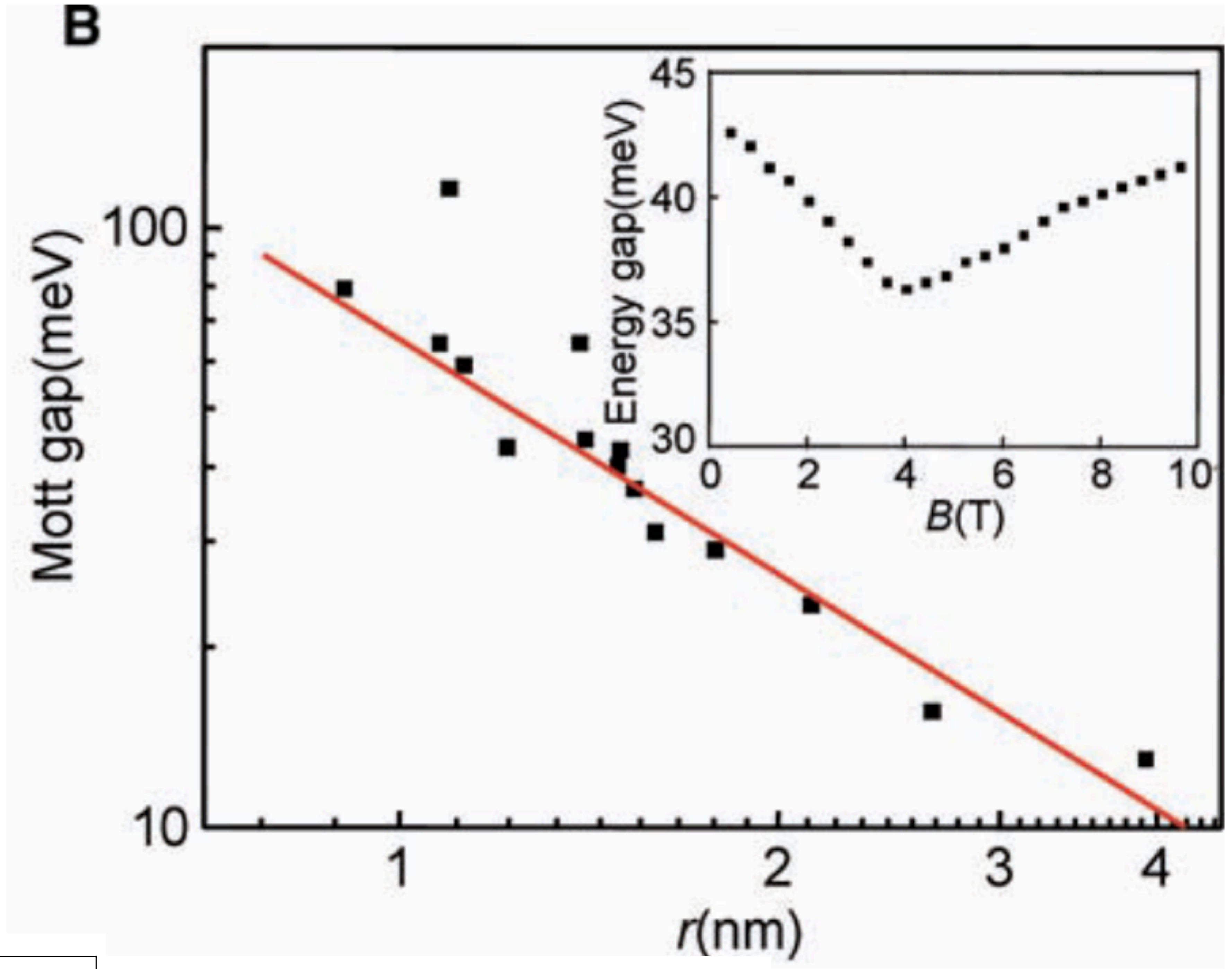


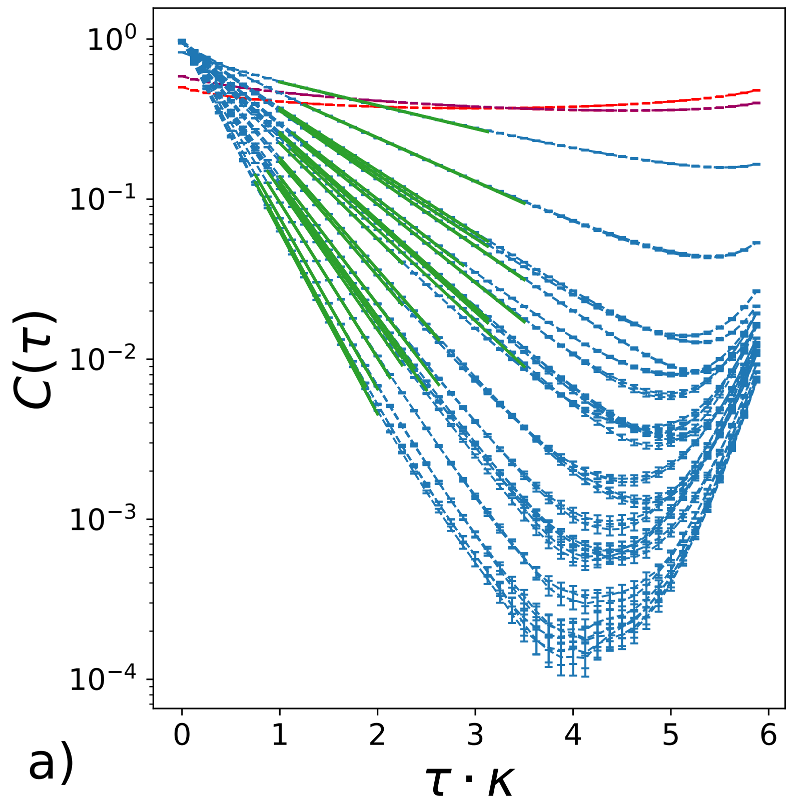
OUTLOOK

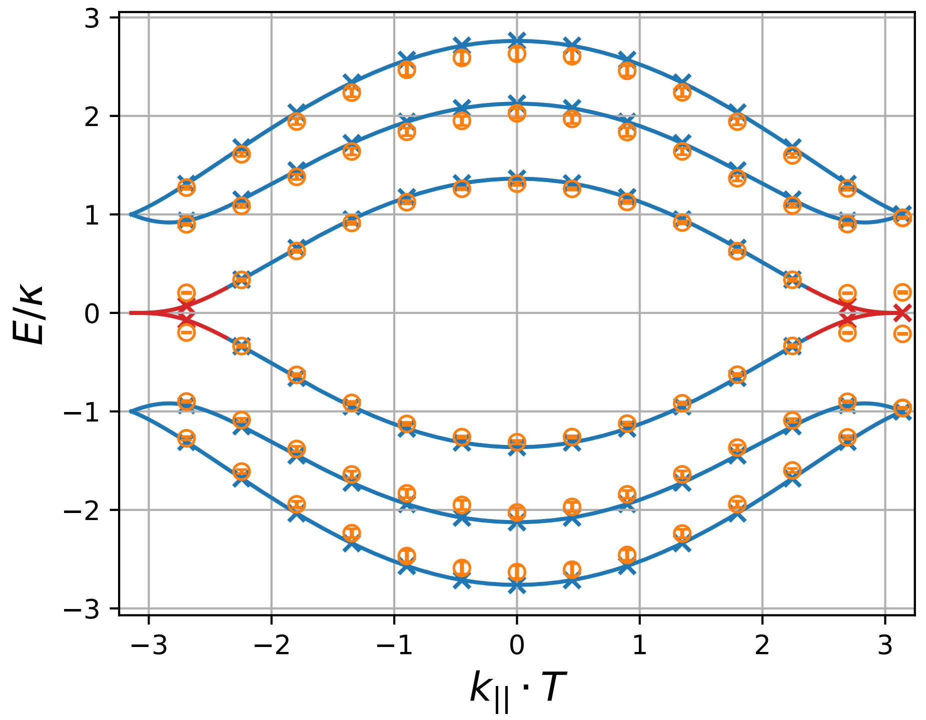
Deshpande et al., Science 323 5910 (2009) 10.1126/science.1165799
EB, Körber, Krieg, Labus, Lähde, Luu Lattice 2017 10.1051/epjconf/201817503009 1710.06213
+ work under way

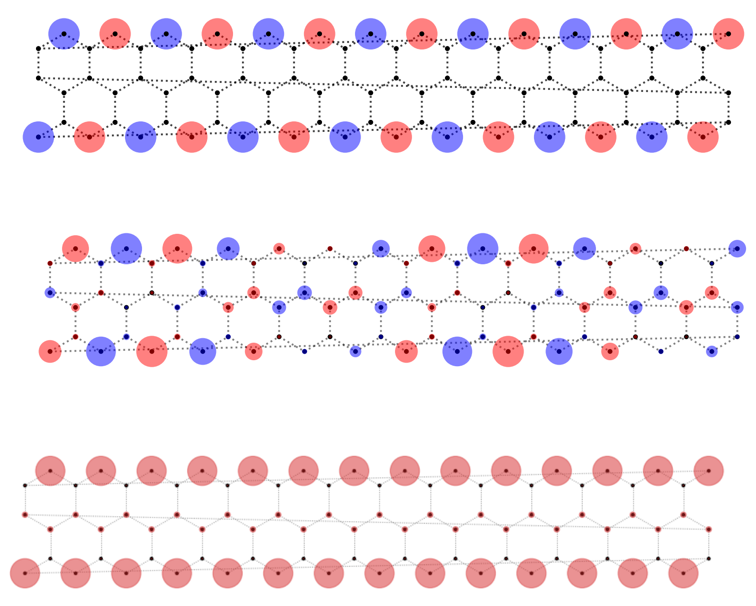
WHAT HUBBARD MODEL BEST DESCRIBES CARBON NANOSTRUCTURES?

- Directly simulate nanotubes and reproduce the experimentally-observed gap's dependence on radius
- Extrapolate to $r = \infty$
- 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!





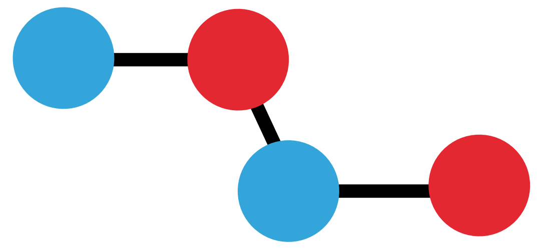




SIGN PROBLEMS AT TRANSITION POINTS

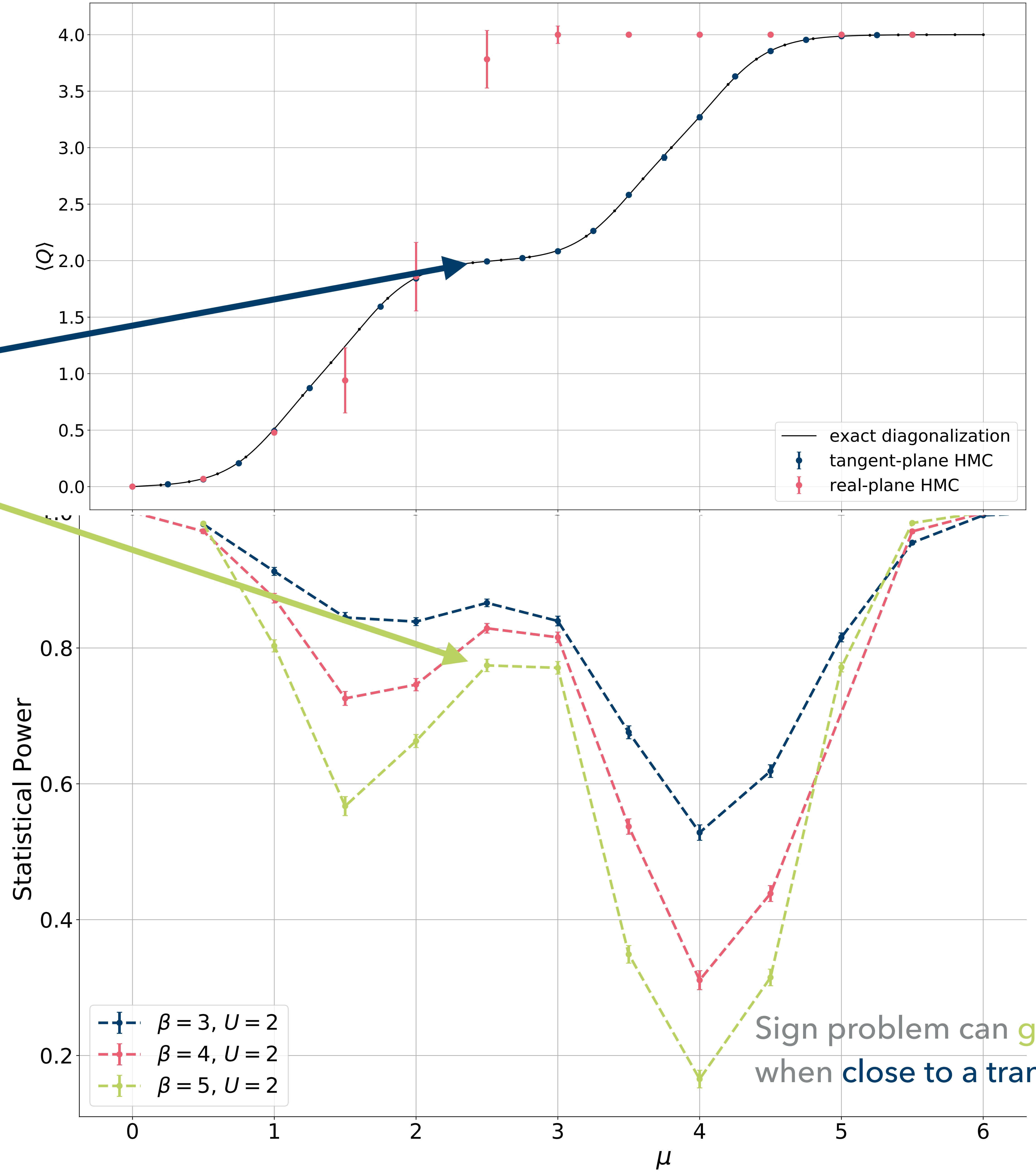
Figures taken from C. Gäntgen's master's thesis

ARE THERE EASY FILLING FRACTIONS?



U=2 β=5

Sign problem can get easier when far from a transition



Sign problem can get worse when close to a transition

Speculation:

- Different thimbles in Φ matter
- Equivariant networks!

SQUARE LATTICE: HIGH T_C SUPERCONDUCTORS?

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