
DUCATI
1098S
brembo

LATTICE QCD ALGORITHMS

Kostas Orginos
William and Mary / JLab

talk number 2

OUTLINE

- Configuration generation
    - Choice of actions
    - Cost estimates
    - Isospin breaking effects
        - Reweighting
- Outlook

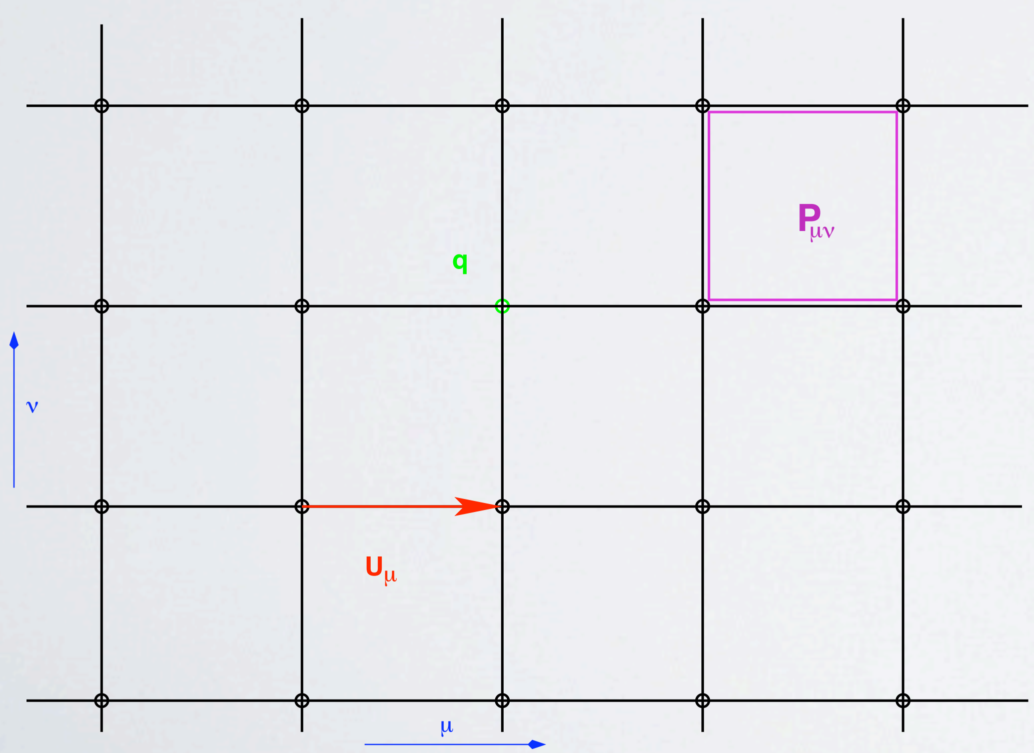
LATTICE QCD

In continuous Euclidian space:

$$\mathcal{Z} = \int \mathcal{D}q\mathcal{D}\bar{q}\mathcal{D}A_\mu \; e^{-S[\bar{q},q,A_\mu]}$$

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}q\mathcal{D}\bar{q}\mathcal{D}A_\mu \; \mathcal{O}(\bar{q}, q, A_\mu) \; e^{-S[\bar{q},q,A_\mu]}$$

Lattice regulator:



Gauge sector:

$$U_\mu(x) = e^{-iaA_\mu(x+\frac{\hat{\mu}}{2})}$$

Fermion sector:

Things get nasty!

Fermion doubling

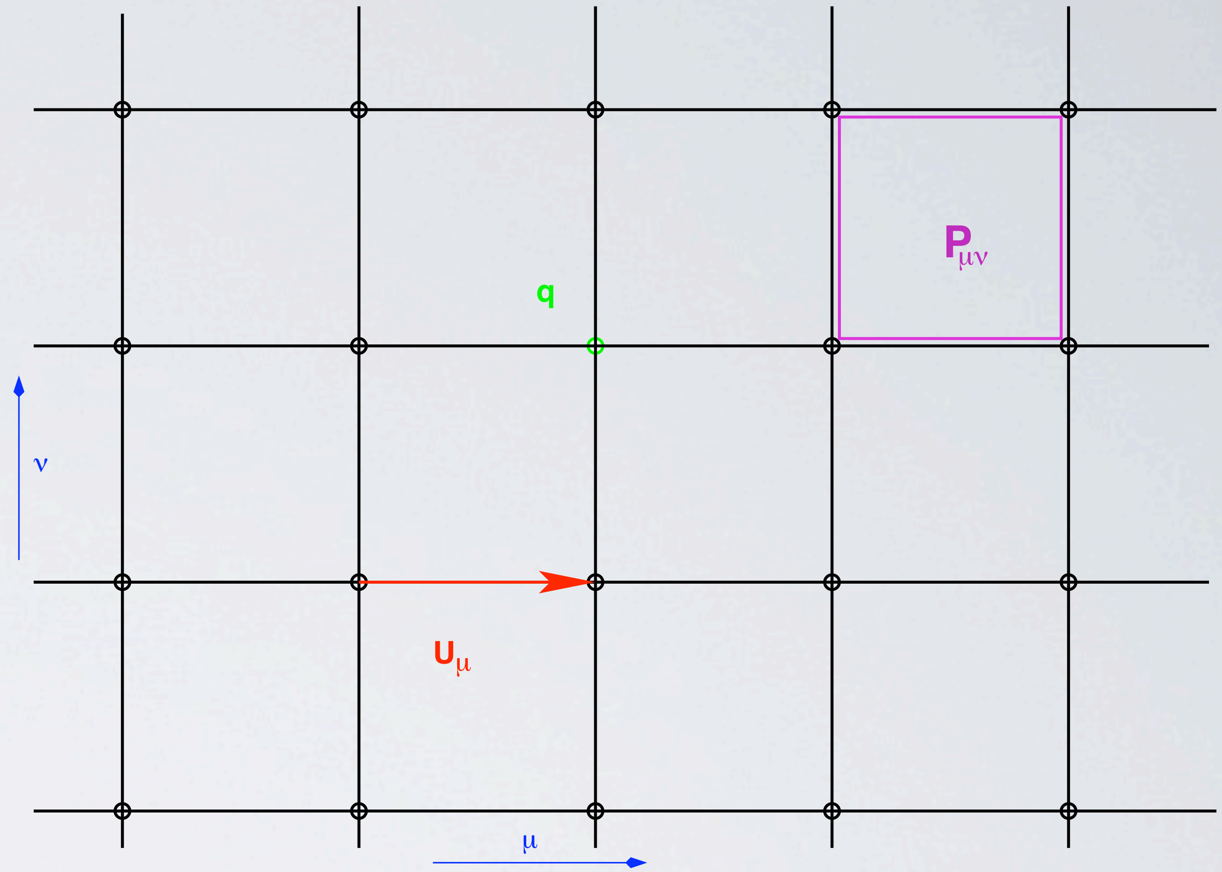
Chiral symmetry breaking

Gauge sector:

$$S_g(U) = \beta \sum_p \left(1 - \frac{1}{3}\mathrm{ReTr}U_p\right) \longrightarrow \frac{1}{4}F_{\mu\nu}^2$$

Fermion sector:

$$S_f(\bar{q}, q, U) = \bar{q}D(U)q$$



- D(U) sparse matrix
- Wilson fermions (Improved)
- Kogut-Susskind fermions
- Domain Wall
- Overlap: Not a sparse matrix

$$\mathcal{Z} = \int \mathcal{D}[U]\ \mathcal{D}[\bar{\psi}]\mathcal{D}[\psi]\ e^{-\bar{\psi}D(U)\psi - S_g(U)}$$

Gauge sector:

$$S_g(U) = \beta \sum_p \left(1 - \frac{1}{3}\mathrm{ReTr}U_p\right) \longrightarrow \frac{1}{4}F_{\mu\nu}^2$$

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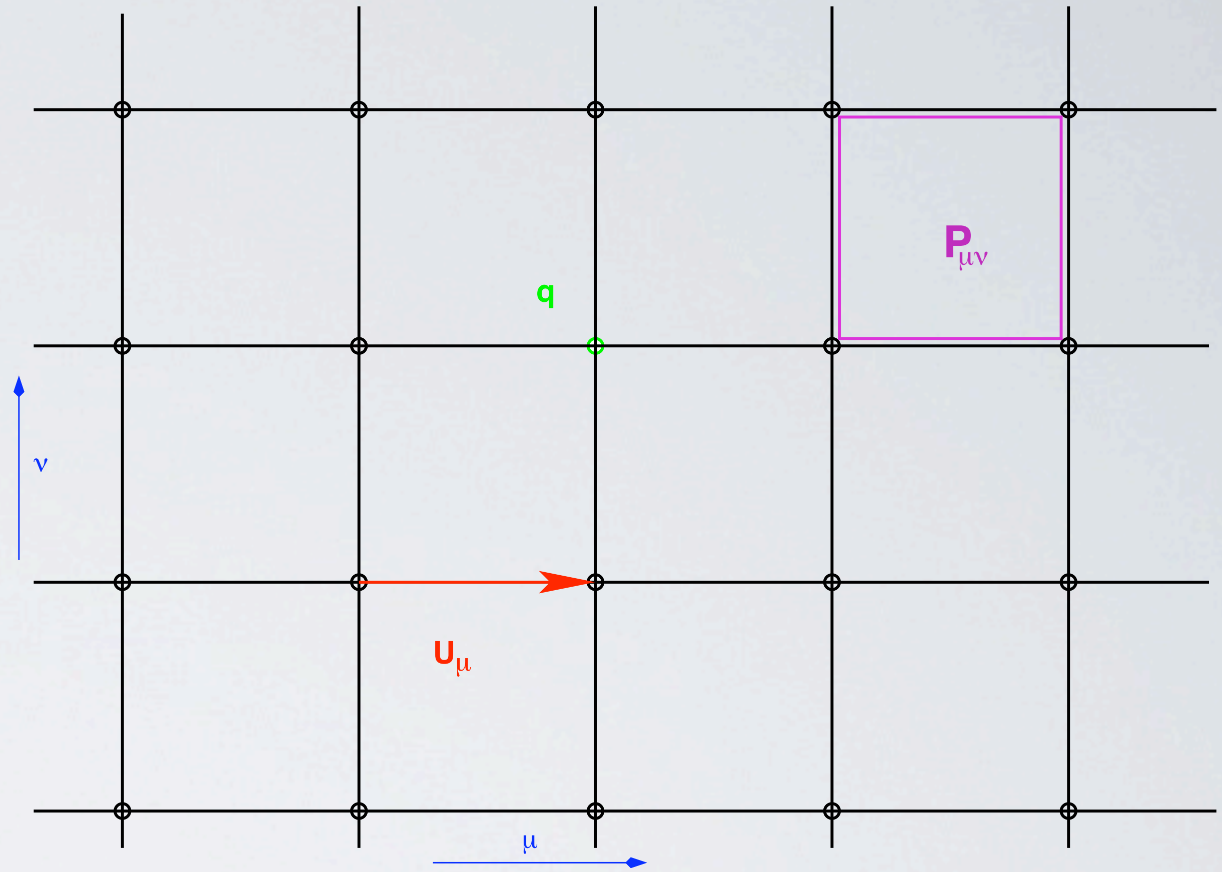
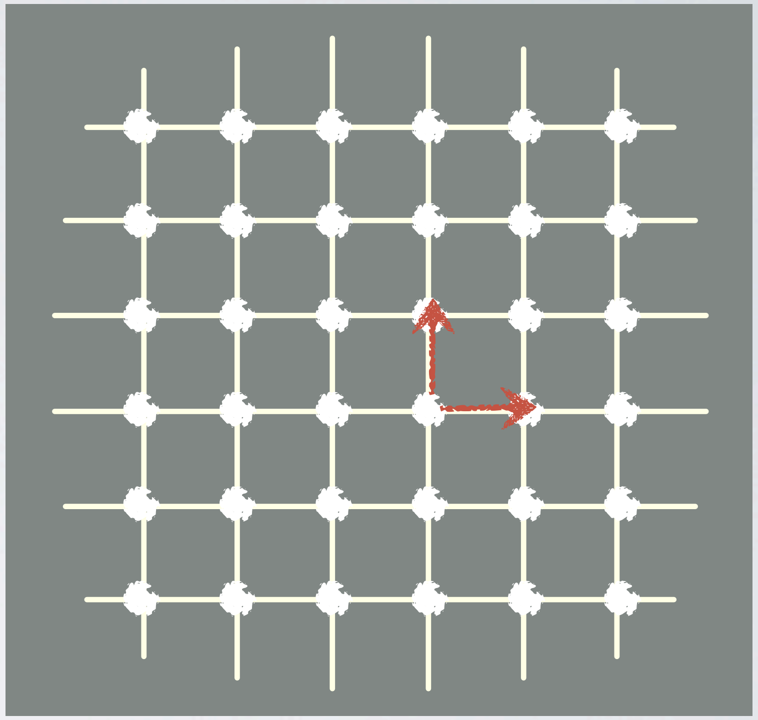


$$\mathcal{Z} = \int \mathcal{D}[U]\ \det(D(U))\ e^{-S_g(U)}$$

WHAT DOES IT TAKE?

- Hadronic Scale: 1fm ~ 1×10^{-13} cm
- Lattice spacing << 1fm
  - take a=0.1fm
- Lattice size La >> 1fm
  - take La = 3fm
- Lattice 32^4
- Gauge degrees of freedom: $8\times4\times32^4 = 3.4\times10^7$



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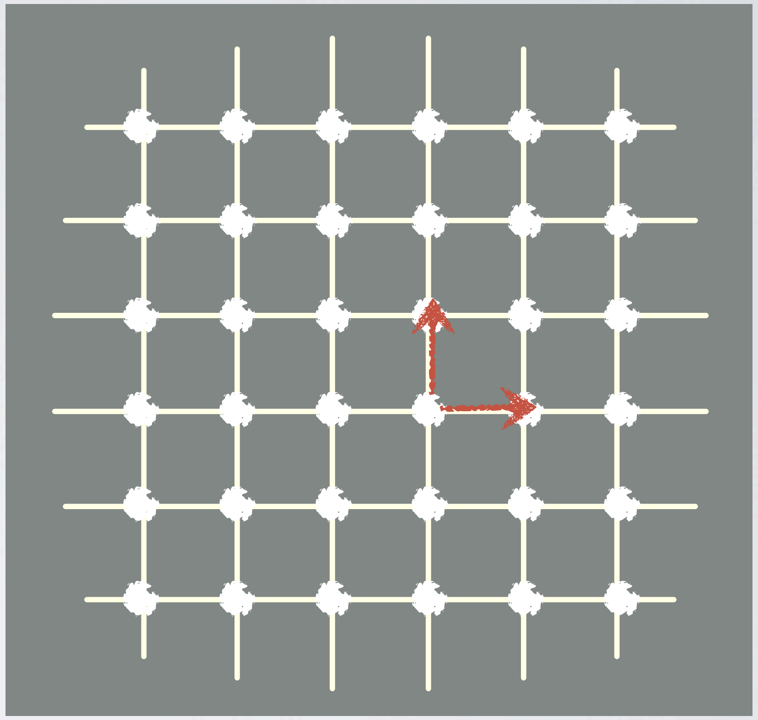

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color

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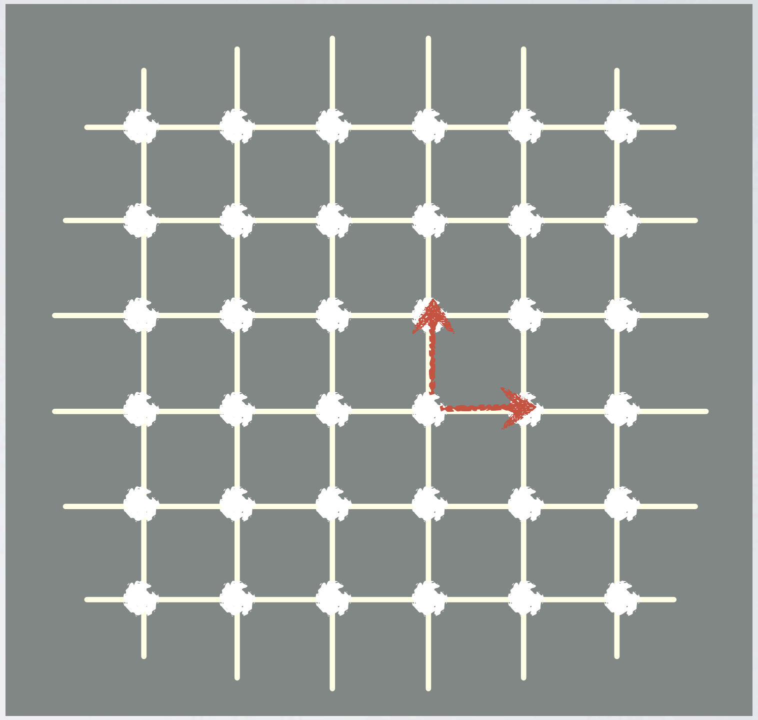

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color   sites

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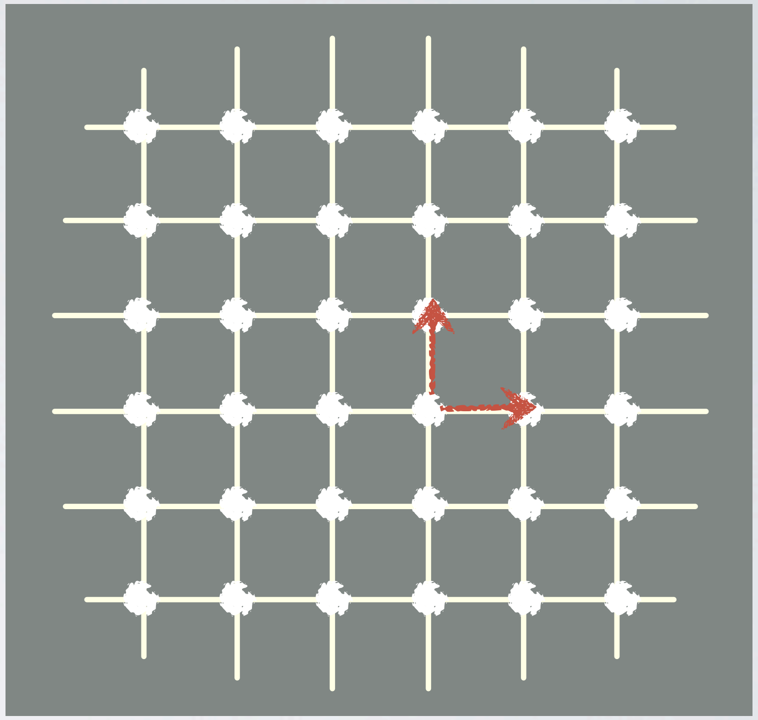

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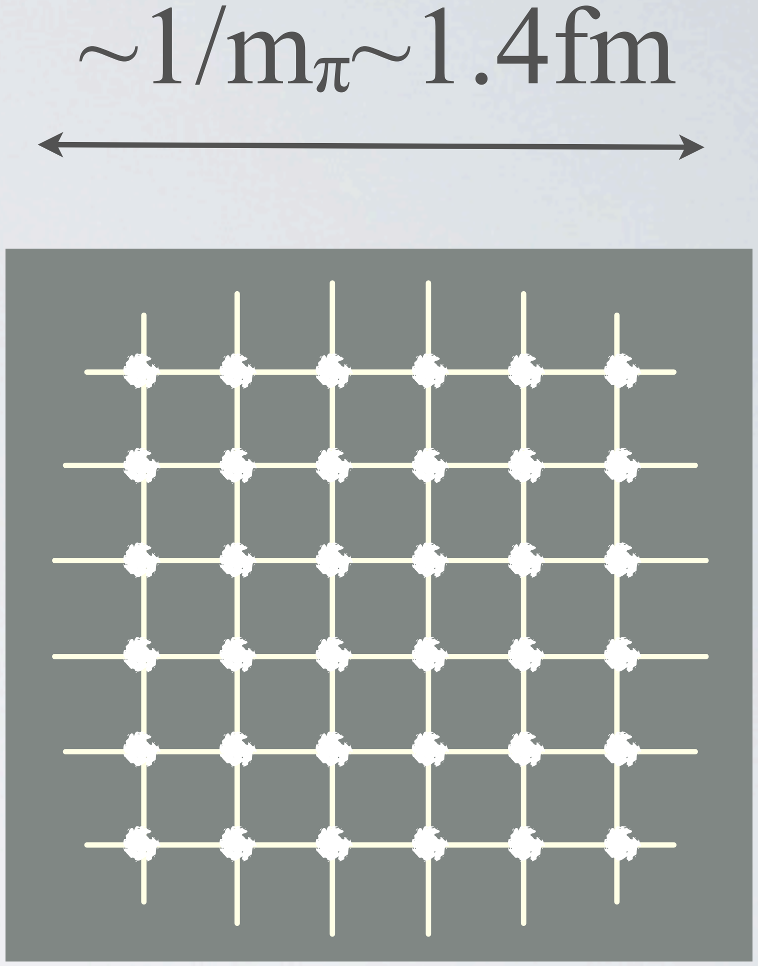
color (8), dimensions (4), sites (32^4)

The pion mass is an additional small scale



Volume corrections $\sim e^{-m_\pi L}$

6 -7 fm boxes might be needed at the physical point

Smaller scale: Binding momentum of the deuteron ~ 40MeV

Nuclear energy level splittings are a few MeV

Box sizes of about 10fm will be needed

REALISTIC CALCULATIONS

- Include the vacuum polarization effects
  - 2 light (up down $O(\sim 3\text{MeV})$) 1 heavy (strange $O(\sim 100\text{MeV})$)
- Finite Volume
  - Compute in multiple and large volume
- Continuum Limit
  - Compute with several lattice spacings
- Chiral Limit
  - Compute with several values for the quark masses
  - Study quark mass dependence of QCD
- Need to work at the physical point $m_\pi \sim 140\text{MeV}$
  - Light quark masses: $m_\pi < 400\text{MeV}$ (?)

TEMPORAL LATTICE SIZE

Temperature $T \sim 1/L_t$

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Use open boundary conditions

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Resolve multiple energy levels using variational methods

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Resolve multiple energy levels using variational methods

Temporal lattice size > 20fm

for a ~ 0.1fm

Typical Lattice volumes should be 128^3 x 512

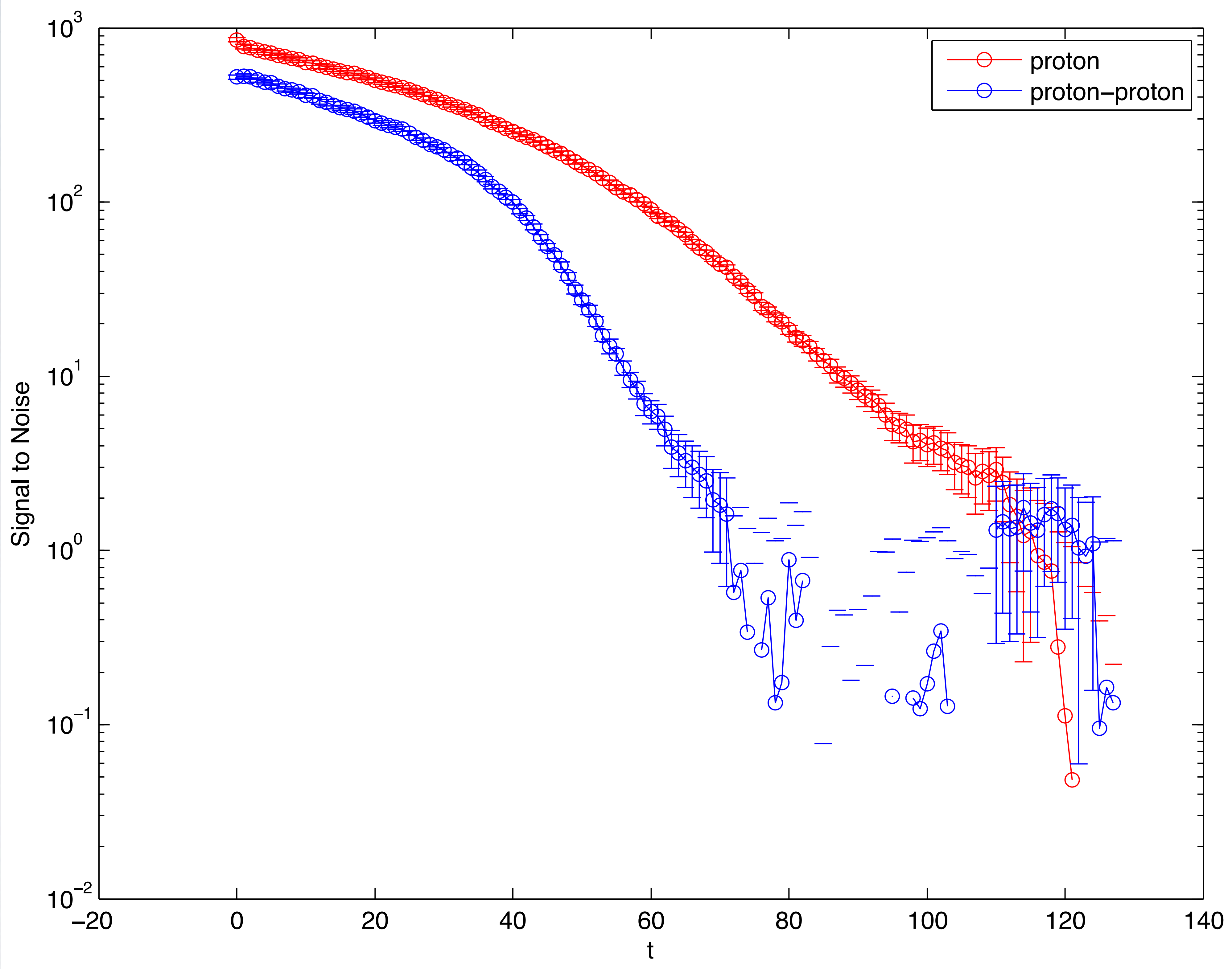
SIGNAL TO NOISE RATIO FOR CORRELATION FUNCTIONS

$$C(t) = \langle N(t)\bar{N}(0)\rangle \sim Ee^{-M_N t}$$

$$var(C(t)) = \langle N\bar{N}(t)N\bar{N}(0)\rangle \sim Ae^{-2M_N t} + Be^{-3m_\pi t}$$

$$StoN = \frac{C(t)}{\sqrt{var(C(t))}} =\sim Ae^{-(M_N - 3/2 m_\pi)t}$$

- The signal to noise ratio drops exponentially with time
- The signal to noise ratio drops exponentially with decreasing pion mass
- For two nucleons: $StoN(2N) = StoN(1N)^2$

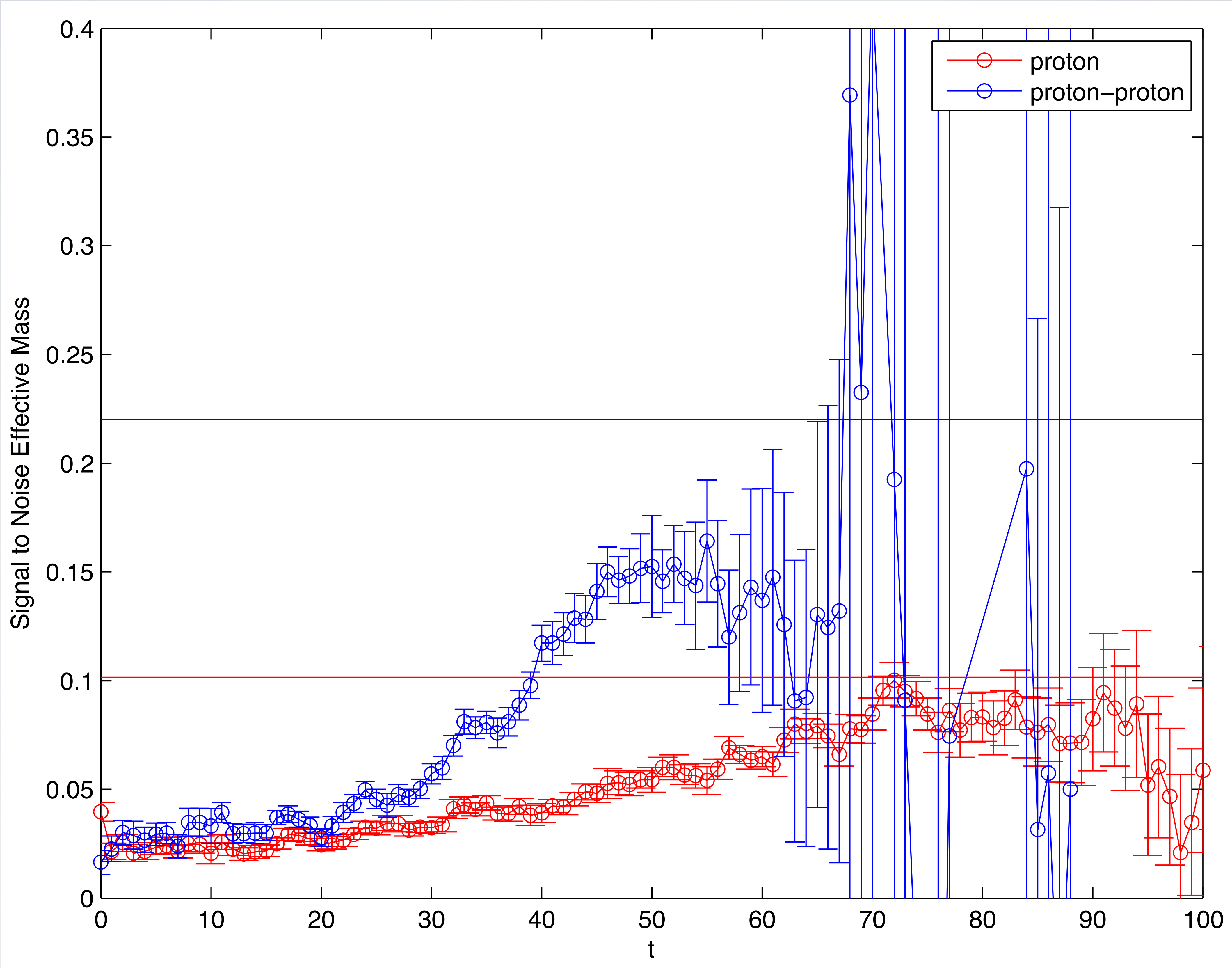


SIGNAL TO NOISE

$32^3 \times 256$
M_π=390MeV

anisotropy factor 3.5

NPLQCD data



SIGNAL TO NOISE EFFECTIVE MASS

$32^3 \times 256$

M_π=390MeV

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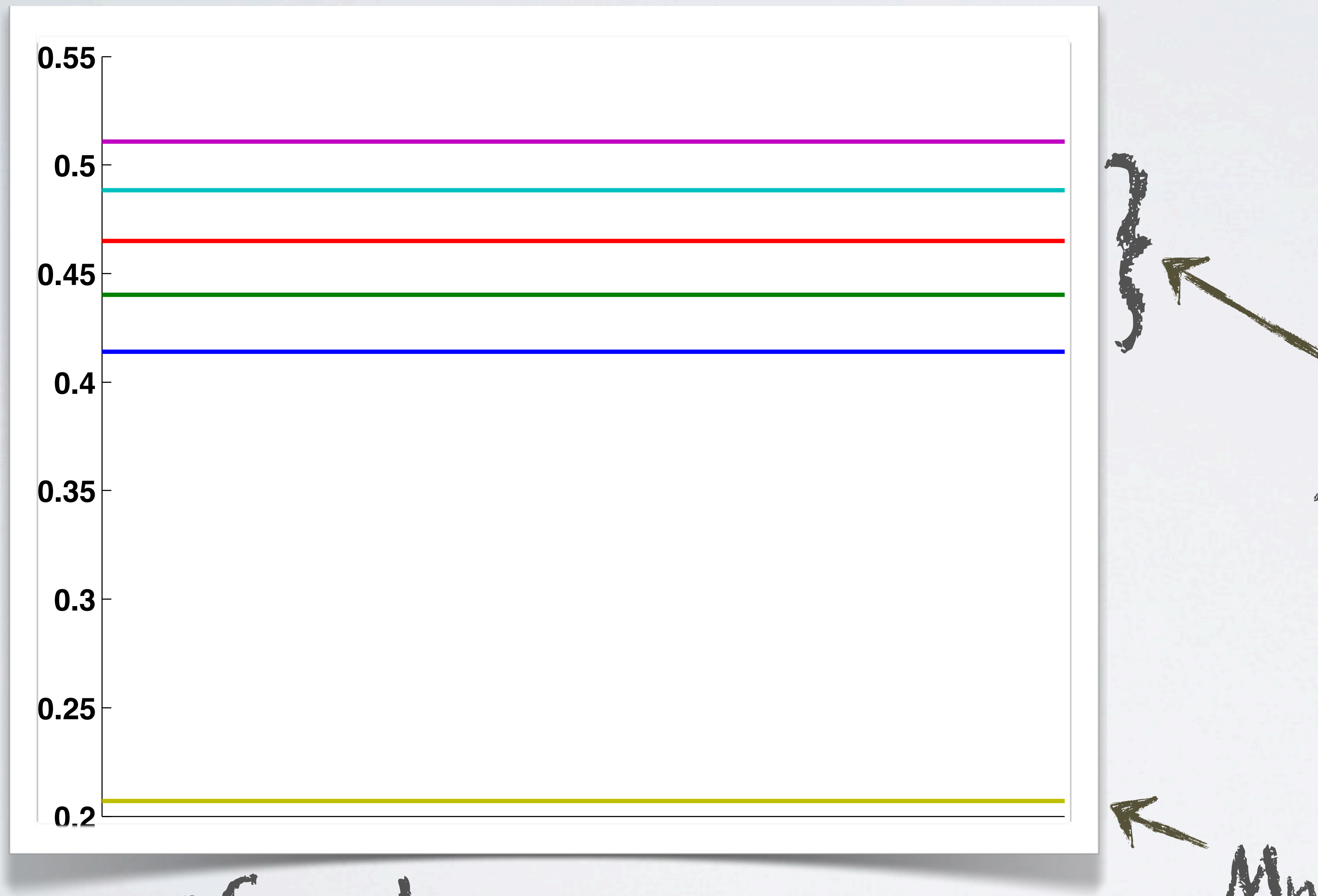
NPLQCD data

TWO NUCLEON SPECTRUM

free nucleons



3fm box

24^3 lattice

anisotropy factor 3.5

M_π=390 MeV

NEEDED TIME SEPARATION

$$e^{-\Delta E \delta t} \approx 10^{-2}$$

3fm box

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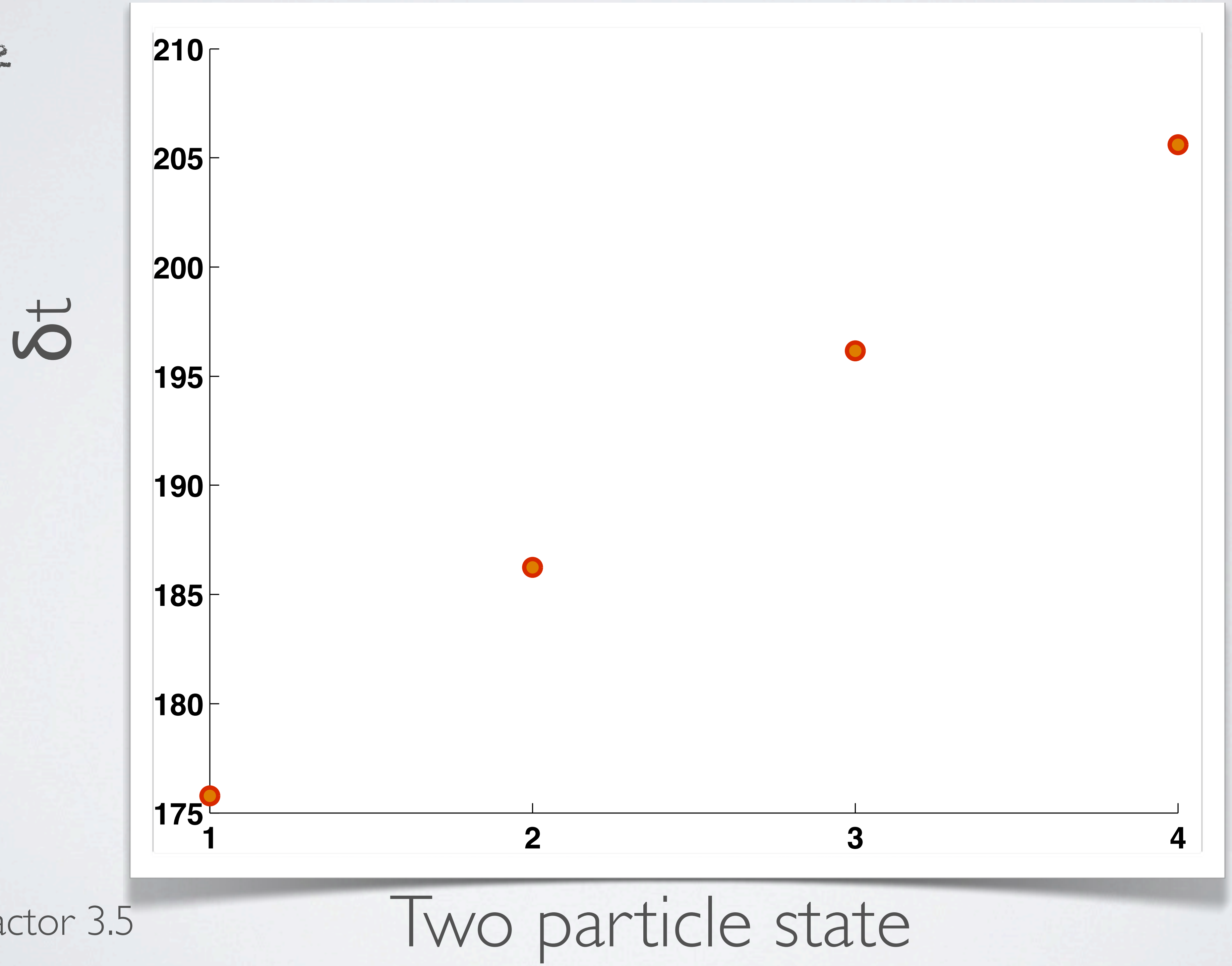

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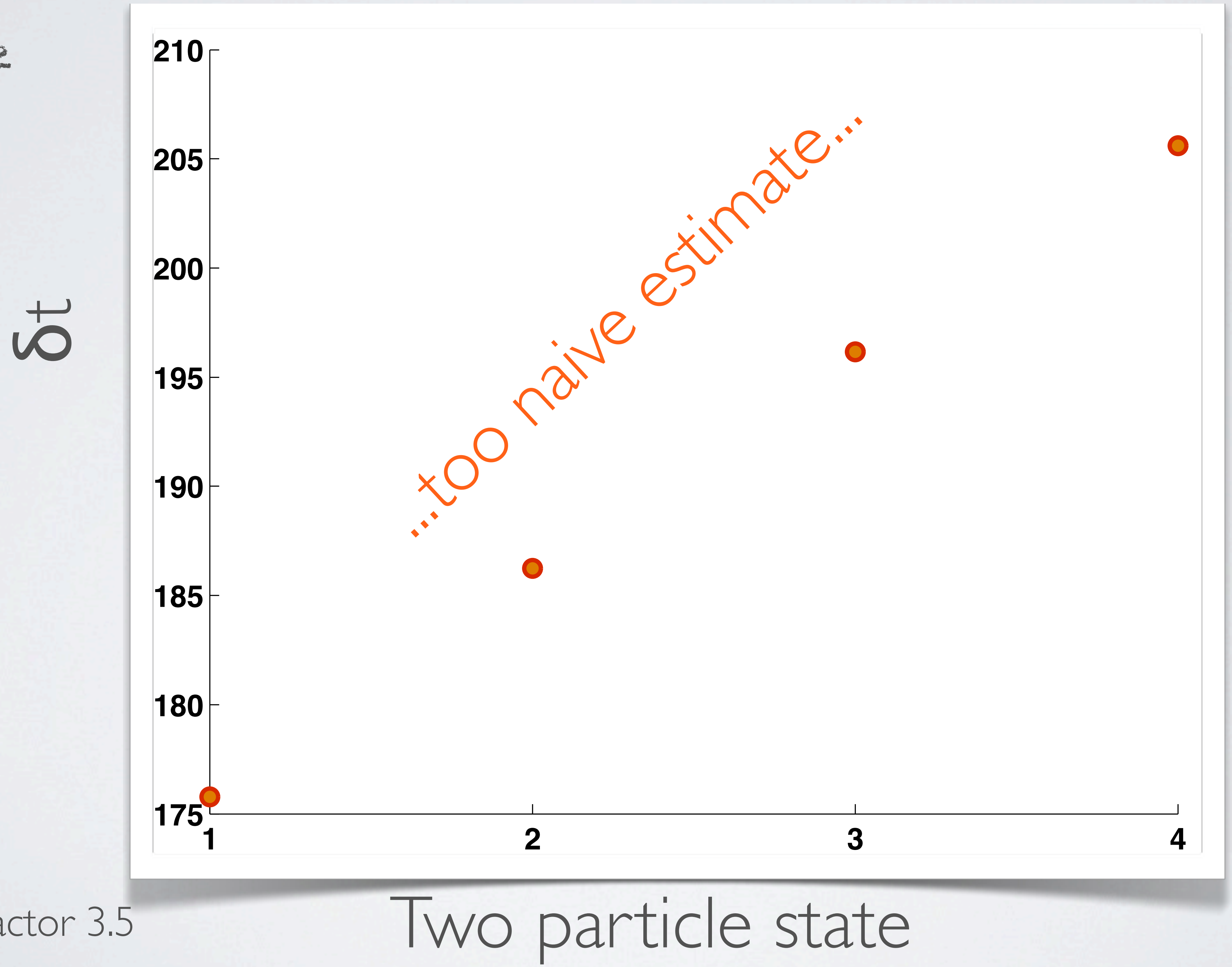

anisotropy factor 3.5

CONCLUSION

- Need exponentially large statistics to resolve the signal at large time separations
- There exists a window at small Euclidean time that things are under control
- However we need to be able to extract multiple energy levels from the correlators at small Euclidean time

FERMION ACTIONS IN THE US

- Kogut-Susskind
  - Asqtad
    - Domain Wall valence (LHPC, NPLQCD, Aubin et.al.)
  - HISQ
- Domain Wall Fermions
  - Overlap Valence (Kentucky group)
- Wilson Fermions
  - Anisotropic Improved Wilson Fermions (JLab, NPLQCD)
  - Isotropic improved Wilson (Just starting at W&M/JLAB)

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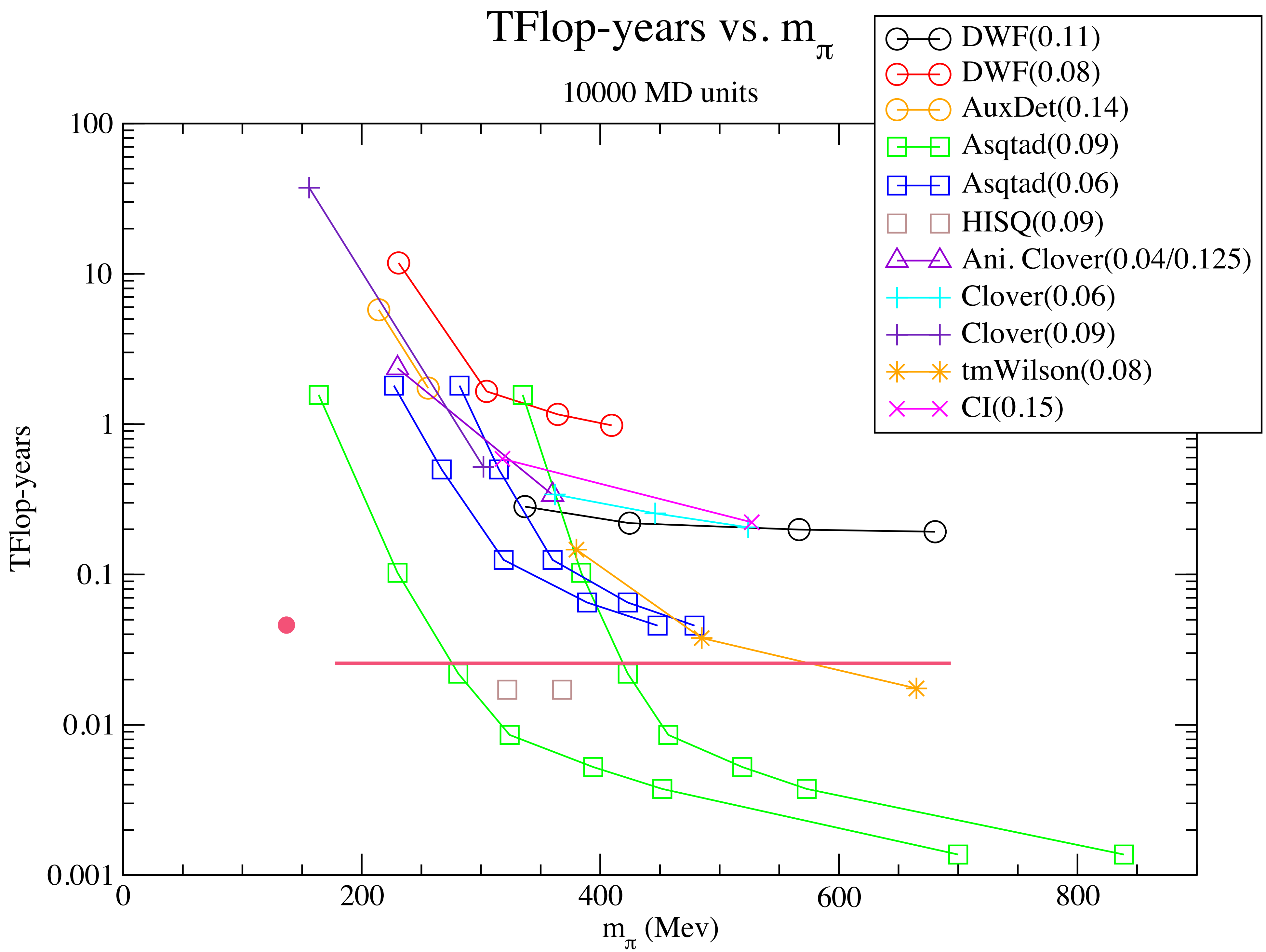
WORLD HMC PERFORMANCE

figure by C. Jung arXiv:001.0941v1



● 2 flavor Clover Defl. - DDHMC arXiv:1002.4232v2

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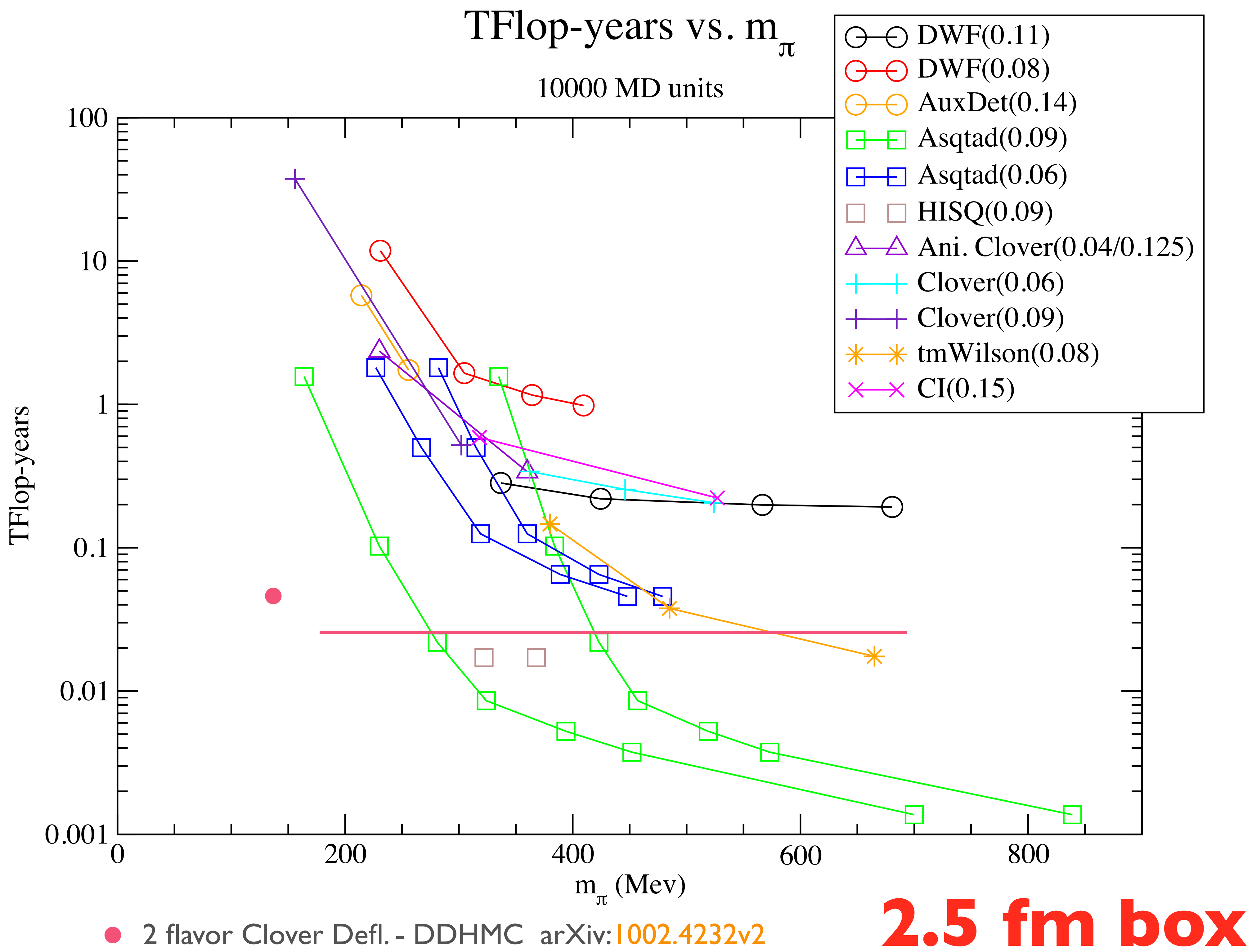


BASIC ALGORITHM

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \prod_{\mu,x} dU_\mu(x) \;\; \mathcal{O}[U, D(U)^{-1}] \;\; \det\left(D(U)^\dagger D(U)\right)^{n_f/2} \;\; e^{-S_g(U)}$$

$$\det(D(U)^\dagger D(U)) = \int d\phi^\dagger d\phi e^{-\phi^\dagger \frac{1}{D^\dagger(U) D(U)} \phi}$$

Add conjugate momenta to the gauge fields with gaussian action:

$$P_\mu(x) \leftrightarrow A_\mu(x)$$

$$U_\mu(x) = e^{-iaA_\mu(x+\frac{\hat{\mu}}{2})}$$

$$S_p = \frac{1}{2} \sum_{\mu,x} P_\mu(x)^2$$

$$\mathcal{H} = \frac{1}{2} \sum_{\mu,x} P_\mu(x)^2 + S_g(U) + \phi^\dagger \frac{1}{D(U)^\dagger D(U)} \phi$$

$$\mathcal{P}(P,\phi,U)dU\,dP\,d\phi \sim e^{-S_g(U)-S_f(U,\phi)-\frac{P^2}{2}}dU\,dP\,d\phi = e^{-\mathcal{H}(P,\phi,U)}dU\,dP\,d\phi$$

In continuous fictitious evolution time:

$$\dot{U} = \frac{\partial \mathcal{H}}{\partial P} \qquad \dot{P} = -\frac{\partial \mathcal{H}}{\partial U}$$

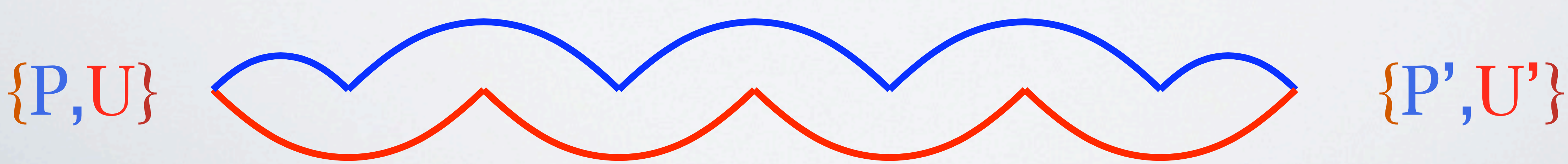
The algorithm satisfies:

- Detailed balance
- Ergodicity

Need numerical reversible integration algorithm

Leapfrog Integrator

Omelyan Integrator [deForcrand and Takaishi Phys.Rev. E73 (2006) 036706]



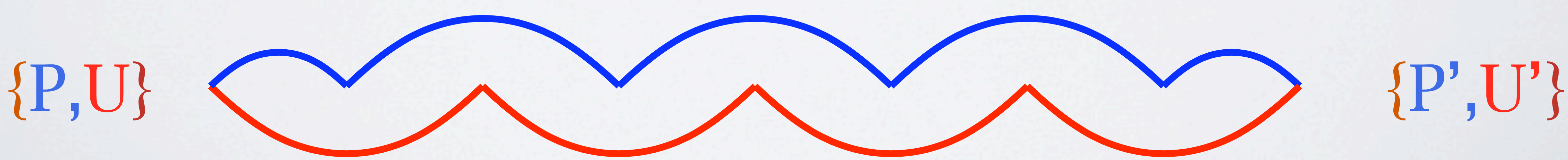
THE FERMION FORCE

Most challenging

$$S_f = \phi^\dagger [D^\dagger D]^{-1} \phi$$

Need to solve: $$\chi = \frac{1}{D^\dagger(U) D(U)} \phi$$

- Harder as the quark mass gets smaller
- Fermion force dominates at small quark masses
- Chronological inversion [Brower, Ivanenko, Levi, KO Nucl.Phys. B484 (1997)]



THE COST OF THE ALGORITHM

$$\mathrm{Cost_{traj}} = \left(\frac{\mathrm{fm}}{a}\right)^6 \cdot \left[\left(\frac{L_s}{\mathrm{fm}}\right)^3 \left(\frac{L_t}{\mathrm{fm}}\right)\right]^{5/4} \cdot \left[B \cdot \left(\frac{140\mathrm{MeV}}{m_\pi}\right)^2 + A\right] \cdot (\mathrm{core\ \ seconds})$$

- Condition number of **D** scales with the quark mass as $1/m_q$ or $1/m^2_\pi$
- Volume scaling $V^{5/4}$ for second order integrators
  - In general the cost is $V^{(1 + 1/2p)}$ for an order p integrator [p=2 for leapfrog]
- Cost associated with strange quark
- This is for fixed physical volume
- Does not include critical slowing down effects
- Improved algorithms could eliminate quark mass dependence (see DD-HMC)

WORLD HMC PERFORMANCE

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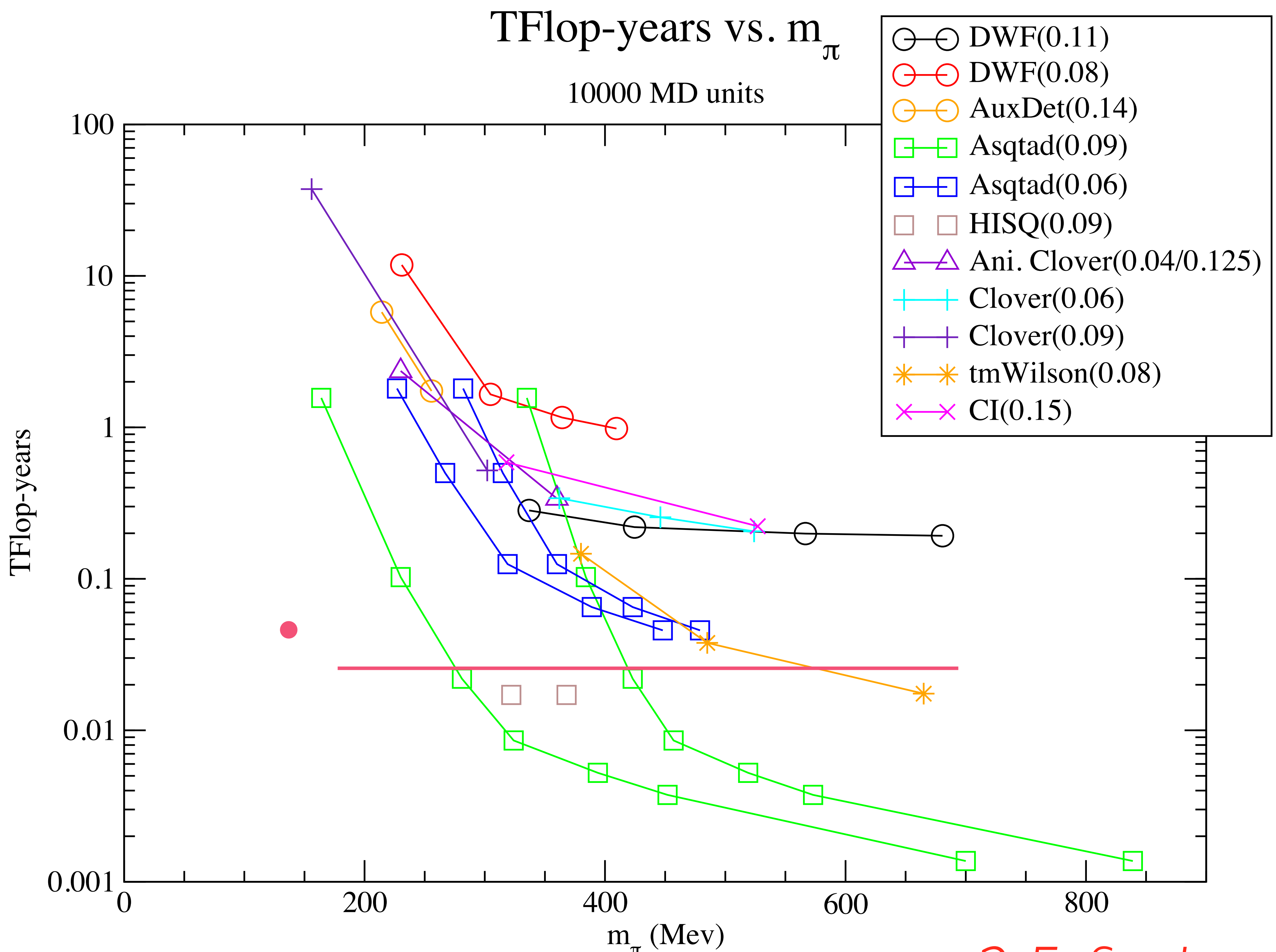


● 2 flavor Clover Defl. - DDHMC a=0.08fm arXiv:1002.4232v2

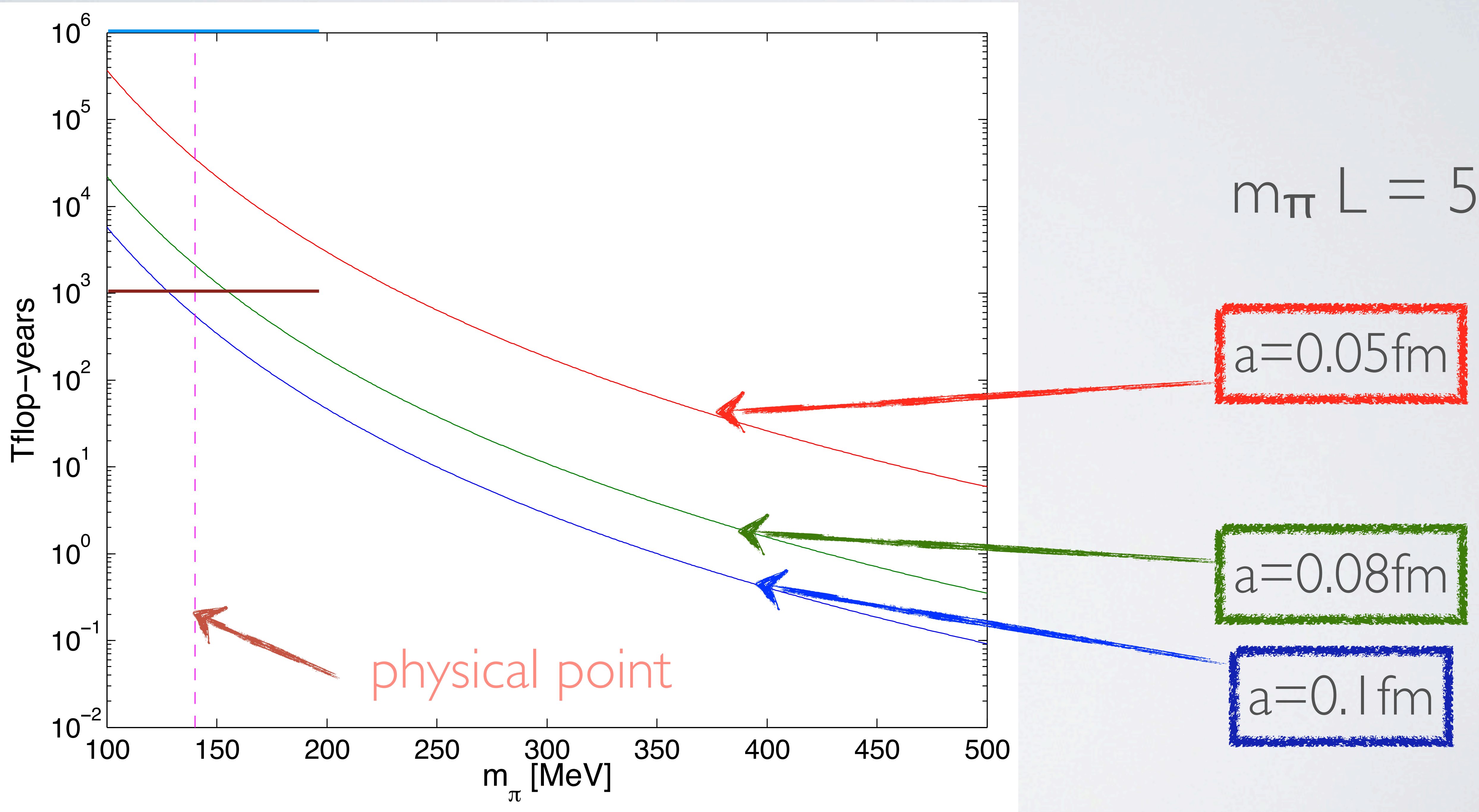
2.5 fm box

WHY CLOVER?

- Isotropic lattices cut down the cost by $(a_s/a_t)^2$
- Flavor symmetry
    - Construction of large class of interpolating fields is easy
- Effective simulation algorithms
- High statistics can be achieved

MONTE CARLO COST ESTIMATE

$$\text{Cost}_{\text{traj}} = \left(\frac{\text{fm}}{a}\right)^6 \cdot \left[\left(\frac{L_s}{\text{fm}}\right)^3 \left(\frac{L_t}{\text{fm}}\right)\right]^{5/4} \cdot \left[B \cdot \left(\frac{140\text{MeV}}{m_\pi}\right)^2 + A\right] \cdot (\text{core seconds})$$



$m_\pi L = 5$

Finite Volume corrections < 1%

10K trajectories

The a~0.1fm problem $128^3 \times 512$

The a~0.1fm problem $128^3 \times 512$

Solution: Get Hopper for a year

ISOTROPIC CLOVER PRODUCTION

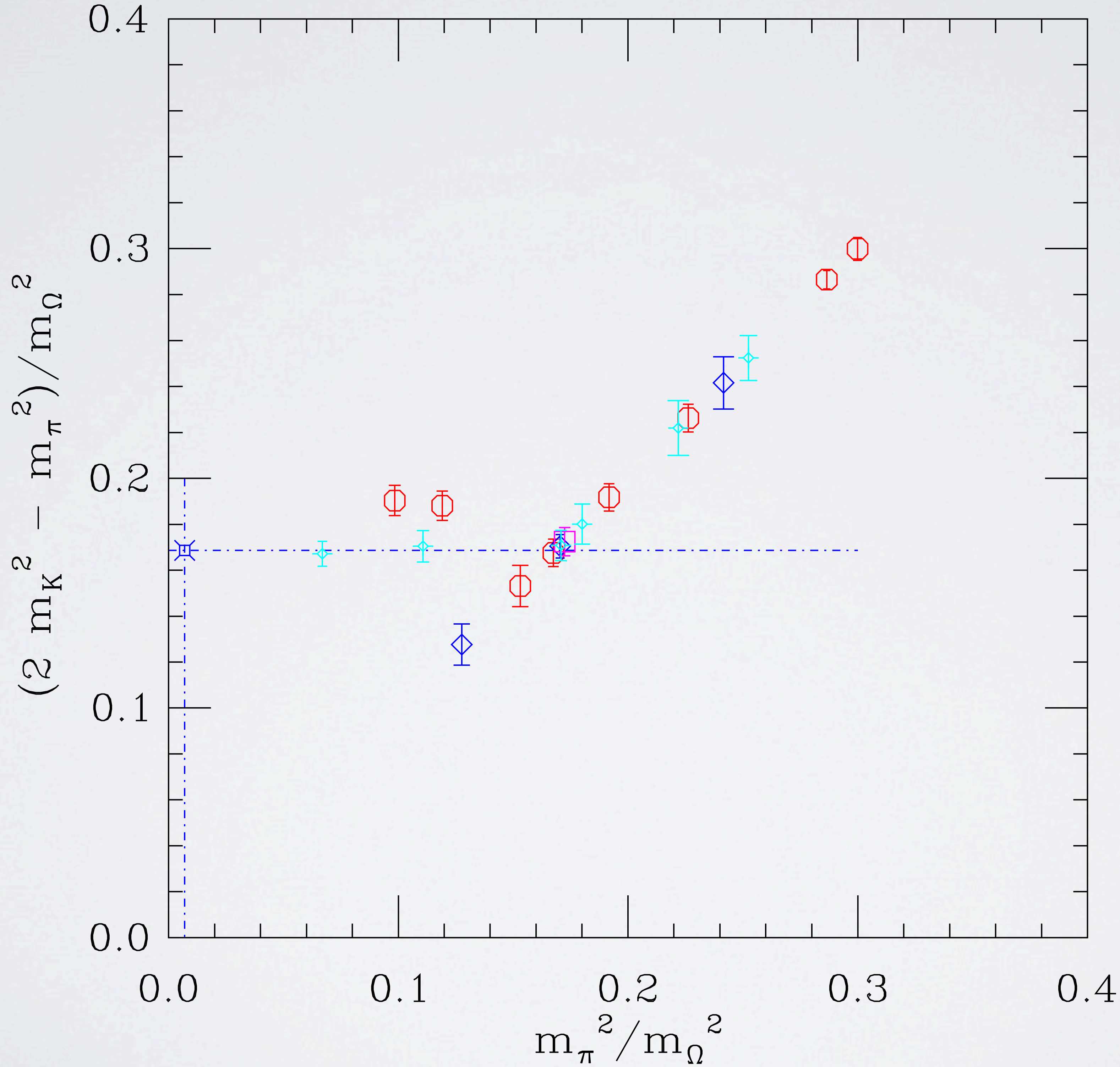
- Gauge action: Luscher Wise with tadpole improvement
- Stout smeared clover improved Wilson fermions
  - One level of stout smearing
  - Tree level clover tadpole improved
  - Checked with Schroedinger functional
- Started work on 4 lattice spacings
- Quark mass tuning
- Need a big machine....

PEOPLE

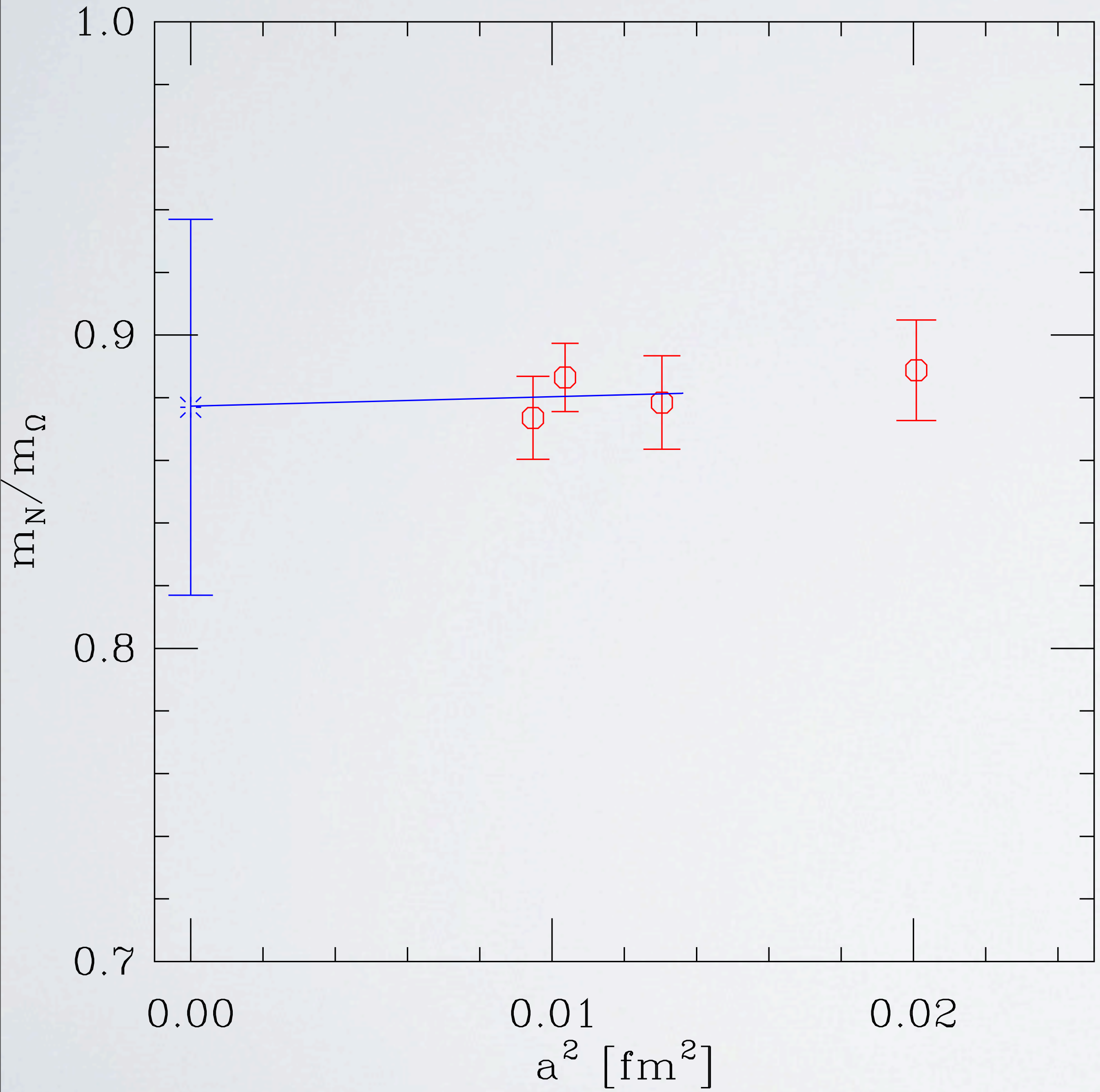
- Robert Edwards
- Balint Joo
- David Richards

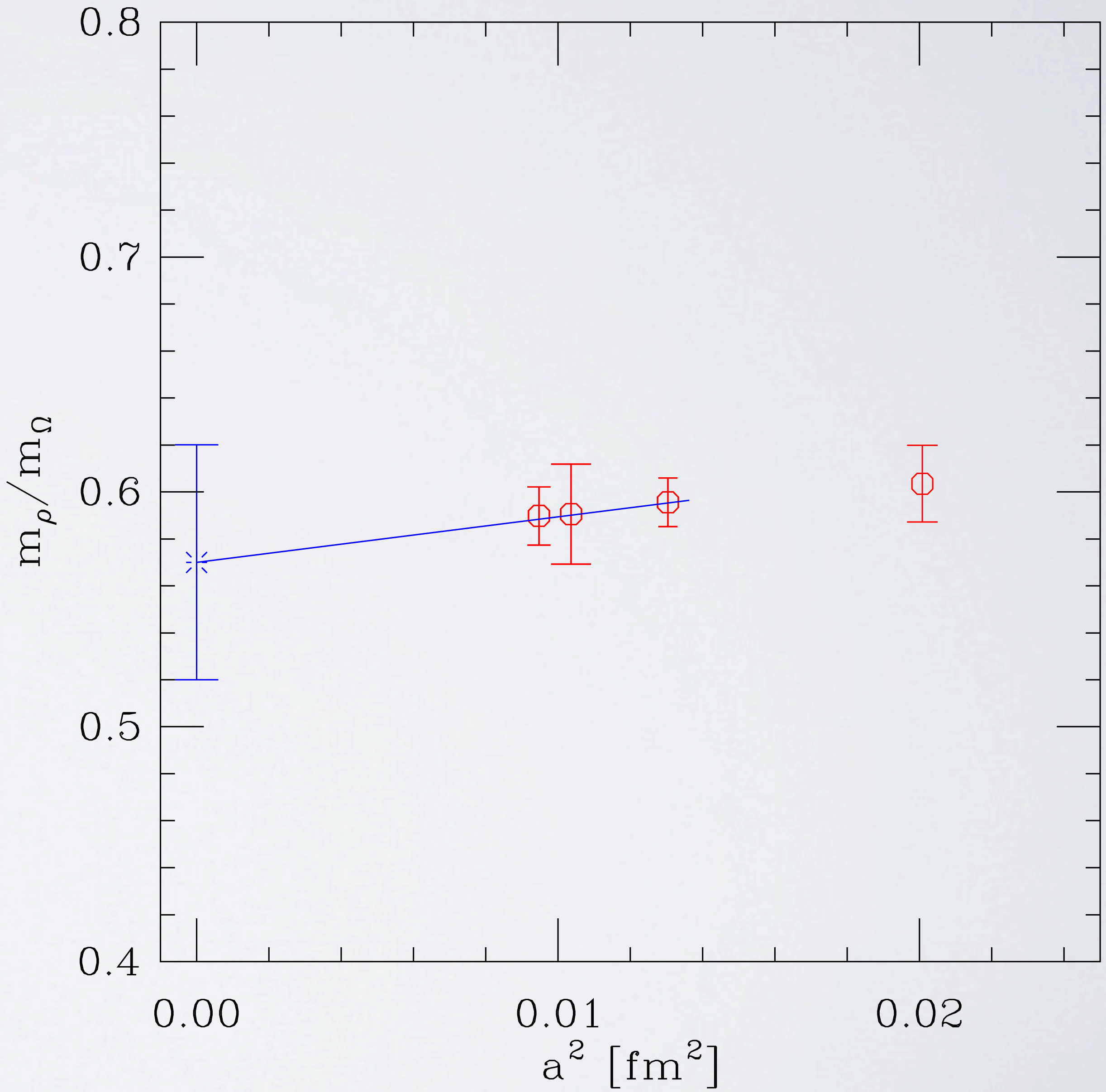
- Will Detmold
- Stefan Meinel
- Abdou Abdel-Rehim

NEWPORT NEWS PLOT



SCALING


1.0
0.9
0.8
0.7
m_N/m_Ω
0.00
0.01
0.02
a^2 [fm^2]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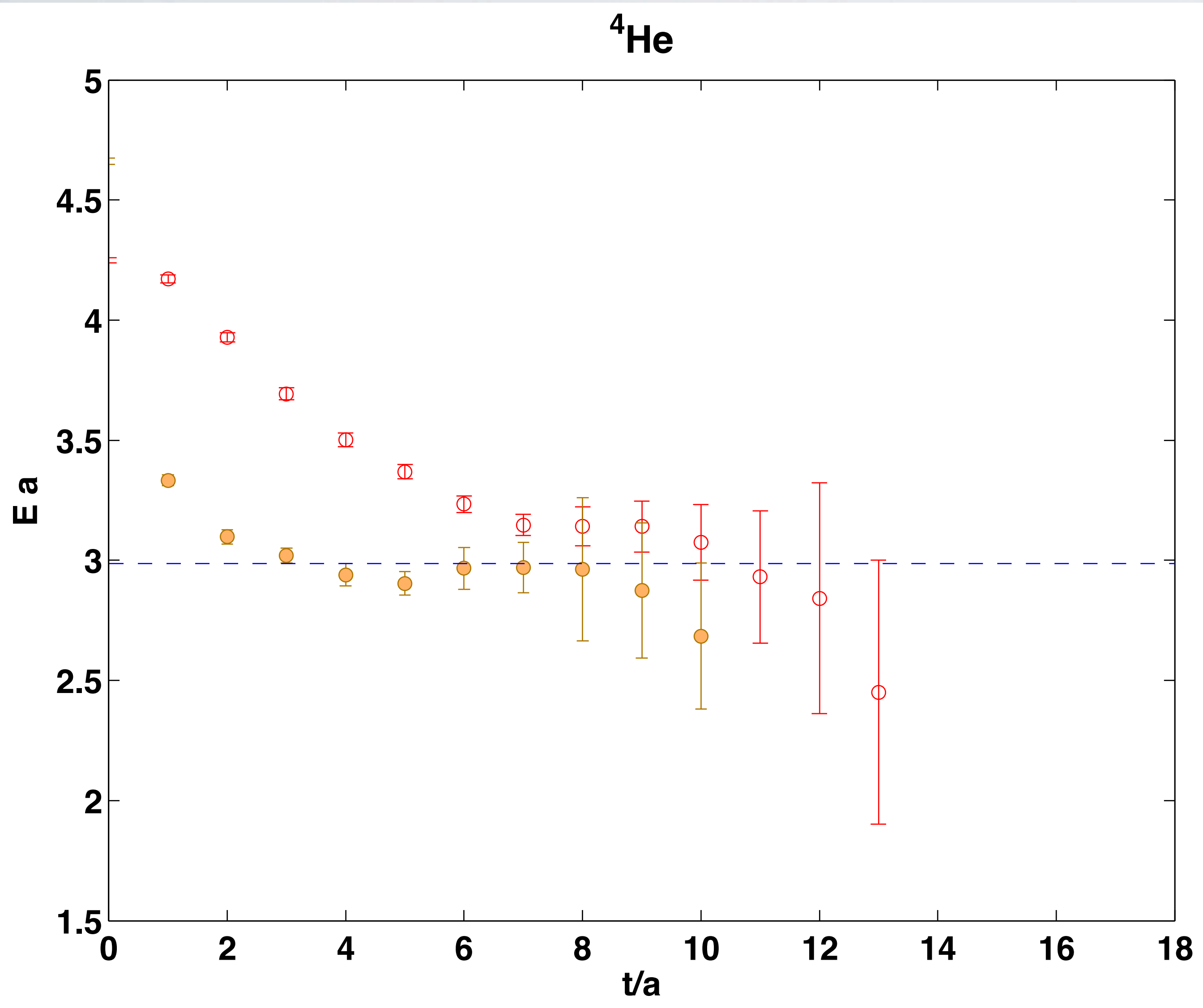
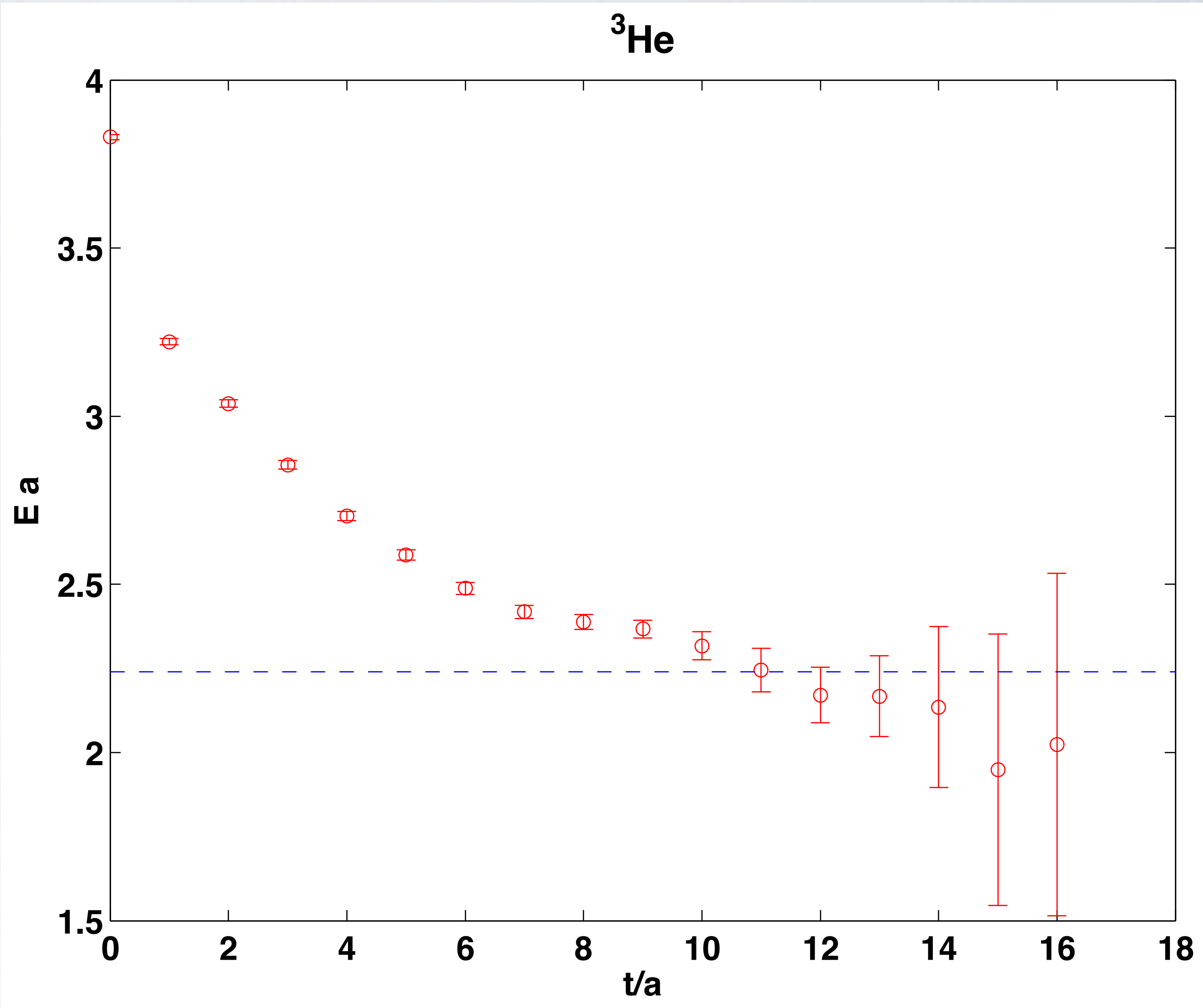


4He
E a
t/a



3He
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t/a

ISOSPIN BREAKING

- Gauge field configurations are generated with the degenerate up and down quark masses
- In nature $m_{up} \sim 2$ MeV and $m_{down} \sim 5$ MeV
- Precision calculations will need to non-degenerate light quark masses
- Nuclear physics: Fine tuned
- We need an efficient way to do calculations to slightly vary parameters in the action

REWEIGHTING

- Reweighting is a method used to perform calculations using an ensemble that does not have the action parameters we want
- Gauge configurations are generated with $m_{up} = m_{down}$
- Observables with $m_{up} \neq m_{down}$ can be calculated

Starting ensemble

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[U] \ \det(D^\dagger(U) D(U))^{N_f/2} \, \mathcal{O}(D(U)^{-1}, U) \ \ e^{-S_g(U)}$$

$$\mathcal{Z} = \int \mathcal{D}[U] \ \det(D(U) D^\dagger(U))^{N_f/2} \ \ e^{-S_g(U)}$$

Target ensemble

$$\langle \mathcal{O} \rangle' = \frac{1}{\mathcal{Z}'} \int \mathcal{D}[U] \ \det(D'^\dagger(U) D'(U))^{N_f/2} \, \mathcal{O}(D'(U)^{-1}, U) \ \ e^{-S_g(U)}$$

$$\mathcal{Z}' = \int \mathcal{D}[U] \ \det(D'(U) D'^\dagger(U))^{N_f/2} \ \ e^{-S_g(U)}$$

Modify the fermion action

$$\langle \mathcal{O} \rangle' = \frac{1}{\mathcal{Z}'} \int \mathcal{D}[U] \, e^{\frac{N_f}{2}\left[Tr \log(D'^{\dagger}(U) D'(U)) - Tr \log(D^{\dagger}(U) D(U))\right]} \, \mathcal{O}(D'(U)^{-1}, U) \;\; e^{-S(U)}$$

$$\mathcal{Z}' = \frac{1}{\mathcal{Z}} \int \mathcal{D}[U] \, e^{\frac{N_f}{2}\left[Tr \log(D'^{\dagger}(U) D'(U)) - Tr \log(D^{\dagger}(U) D(U))\right]} \, e^{-S(U)}$$

Computational task: Evaluate the trace log of a sparse positive definite matrix

- Use pseudofermions just like HMC
  - Compute inverses of the Dirac Matrix

Hassenfratz et. al. arXiv:0805.2369 ;
RBC arXiv:1011.0892 ;
PACS-CS arXiv:0911.2561

- Use Gaussian quadrature [Golub & Meurant '93; Bai, Fahey & Golub '96;]
  - Lanczos iteration
  - Converges faster than solving a linear system (with ex. CG)

Studied in also by Cahill, Irving, Johnson, Sexton '99

GAUSSIAN QUADRATURE

[Golub & Meurant '93; Bai, Fahey & Golub '96]

$$Tr\log(A) \approx \frac{1}{N}\sum_{k=1}^{N} \eta_k^\dagger \log(A)\eta_k$$

η are vectors whose components are random Z_4 noise

Gaussian quadrature evaluates $\eta_k^\dagger \log(A)\eta_k$

$$\eta^\dagger f(A)\eta = \eta^\dagger Q^\dagger f(\Lambda)Q\eta = u^\dagger f(\Lambda)u = \sum_i u_i^* f(\lambda_i)u_i$$

With Q the eigenvector matrix and λ_i the eigenvalues of A

Other method: Pade approximation [C.Thron et.al. hep-lat/9707001]

$$I[f] = \eta^\dagger f(A)\eta = \sum_i u_i^* f(\lambda_i) u_i = \int_a^b d\lambda \sum_{i=1}^n u_i^* u_i \delta(\lambda - \lambda_i) f(\lambda) = \int_a^b d\mu(\lambda) f(\lambda)$$

$$\mu(\lambda) = \begin{cases} 0, & \text{if} \quad \lambda < a = \lambda_1 \\ \sum_j^i u_j^* u_j, & \text{if} \quad \lambda_i \le \lambda < \lambda_{i+1} \\ \sum_j^n u_j^* u_j, & \text{if} \quad b = \lambda_n \le \lambda \end{cases}$$

To calculate the integral use Gaussian Quadrature integration with the orthogonal polynomial defined by the Lanczos recursion relation

$$I[f] \approx \sum_i^k \omega_i^2 f(\theta_i)$$

θ_i are the eigenvalues and ω_i the squares of the first elements of the normalized eigenvectors of the Lanczos matrix T_k

We apply this method to reweighting: [A. Rehim W. Detmold KO]

BIAS

Unbiased estimator of the trace: $Tr\log(A) \approx \frac{1}{N}\sum_{k=1}^{N}\eta_k^\dagger \log(A)\eta_k$

Biased estimator: $e^{TrlogA} \sim e^{\frac{1}{N}\sum_1^N \eta^\dagger log(A)eta}$

Removal of bias:

Jackknife: $f(\langle x\rangle) \approx N\ f(\overline{x}) - (N-1)\ \overline{f^J}$

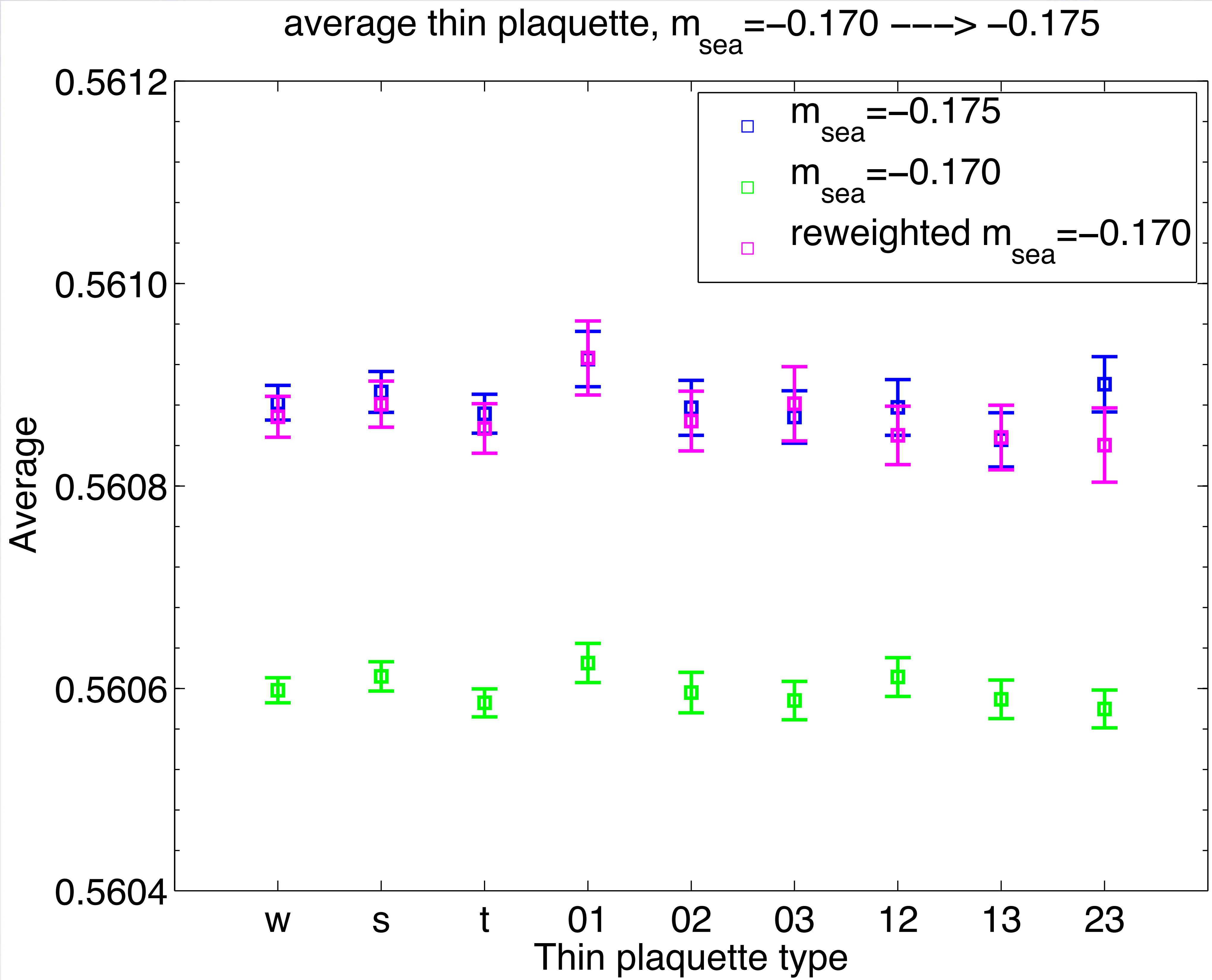
Bootstrap: $f(\langle x\rangle) \approx 2\ f(\overline{x}) - \overline{f^B}$

Stochastic re-summation: [Bahnot-Kennedy Phys. Lett. B 157, 70 ('85)]

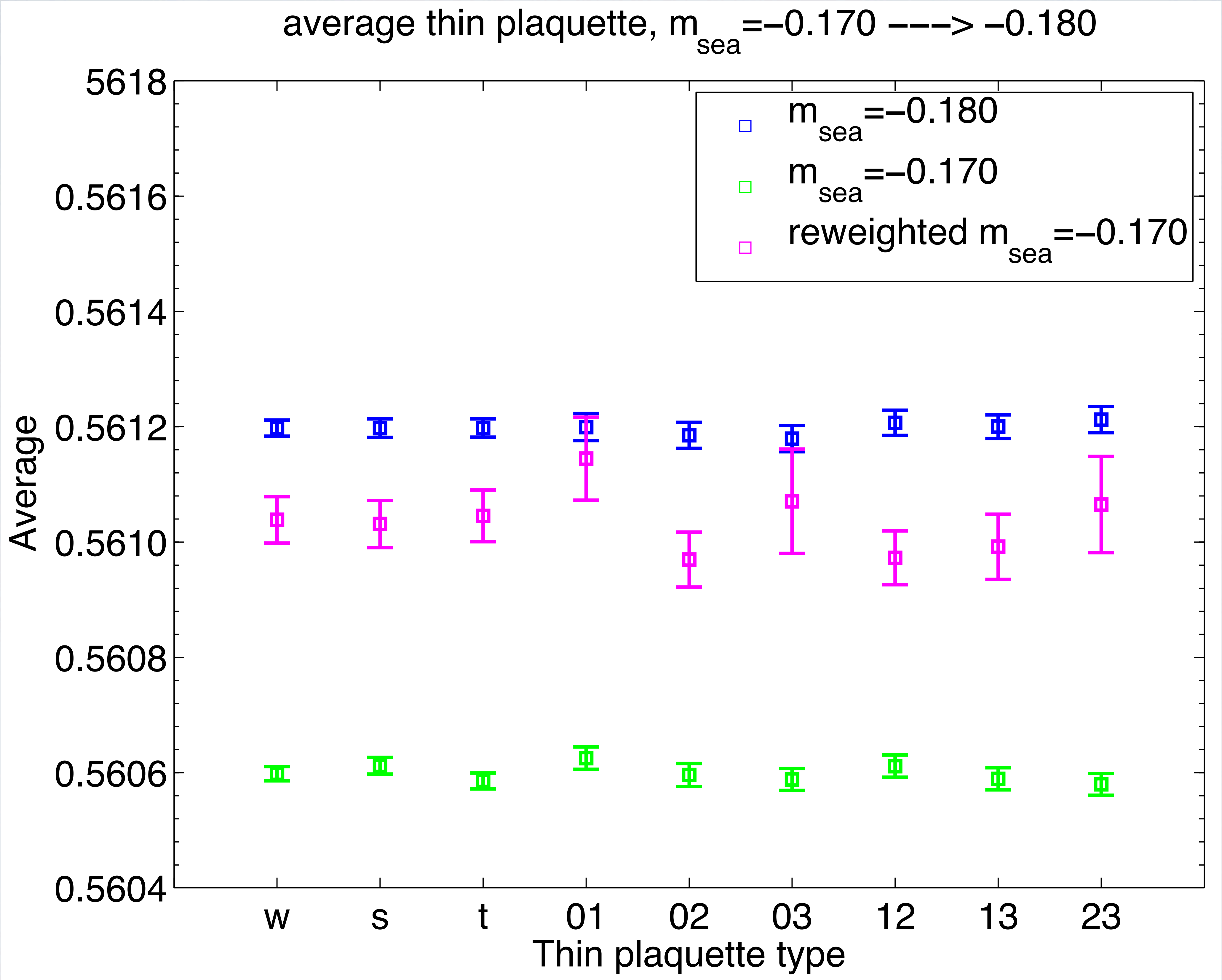
TEST

- Isotropic clover
- Three degenerate flavors at the strange quark mass
- Lattice spacing ~0.09fm
- Shift the quark mass by 50MeV and 100MeV

Work done by Abdou Abdel-Rehim

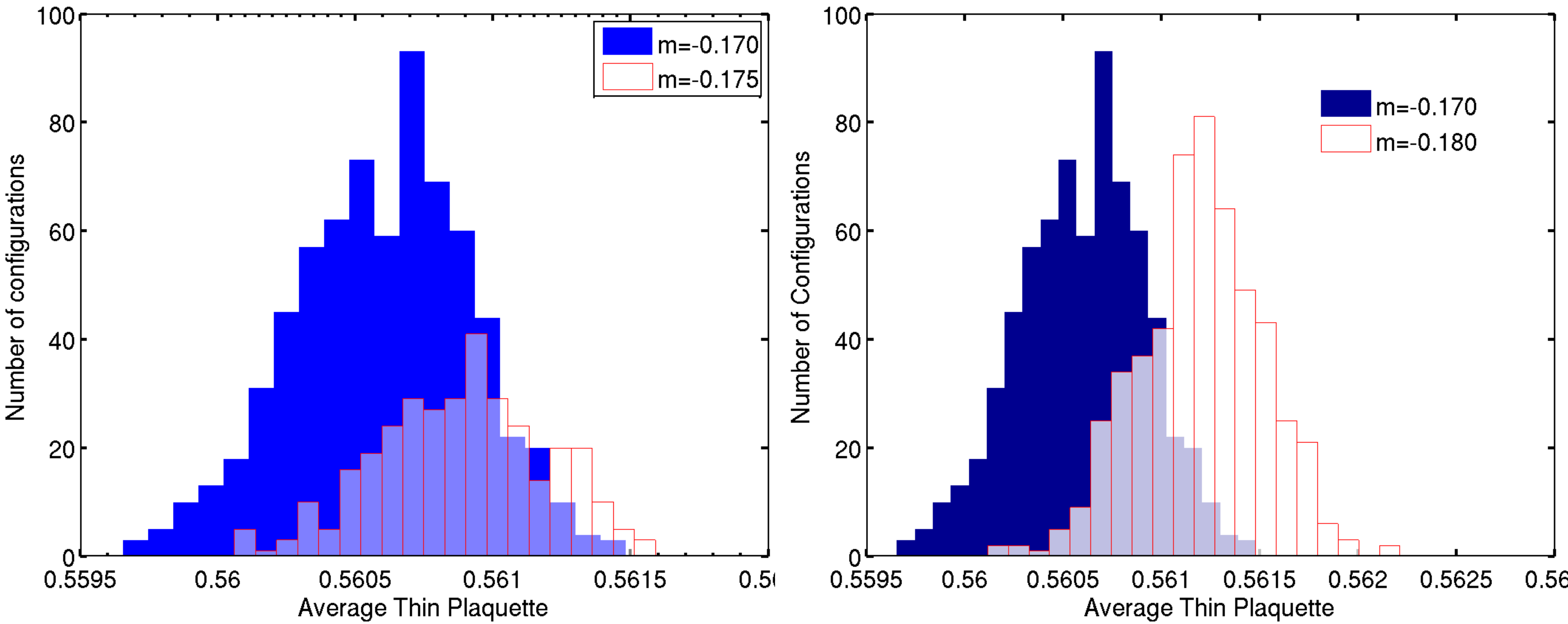


plot by A. Rehim



plot by A. Rehim

ENSEMBLE OVERLAPS



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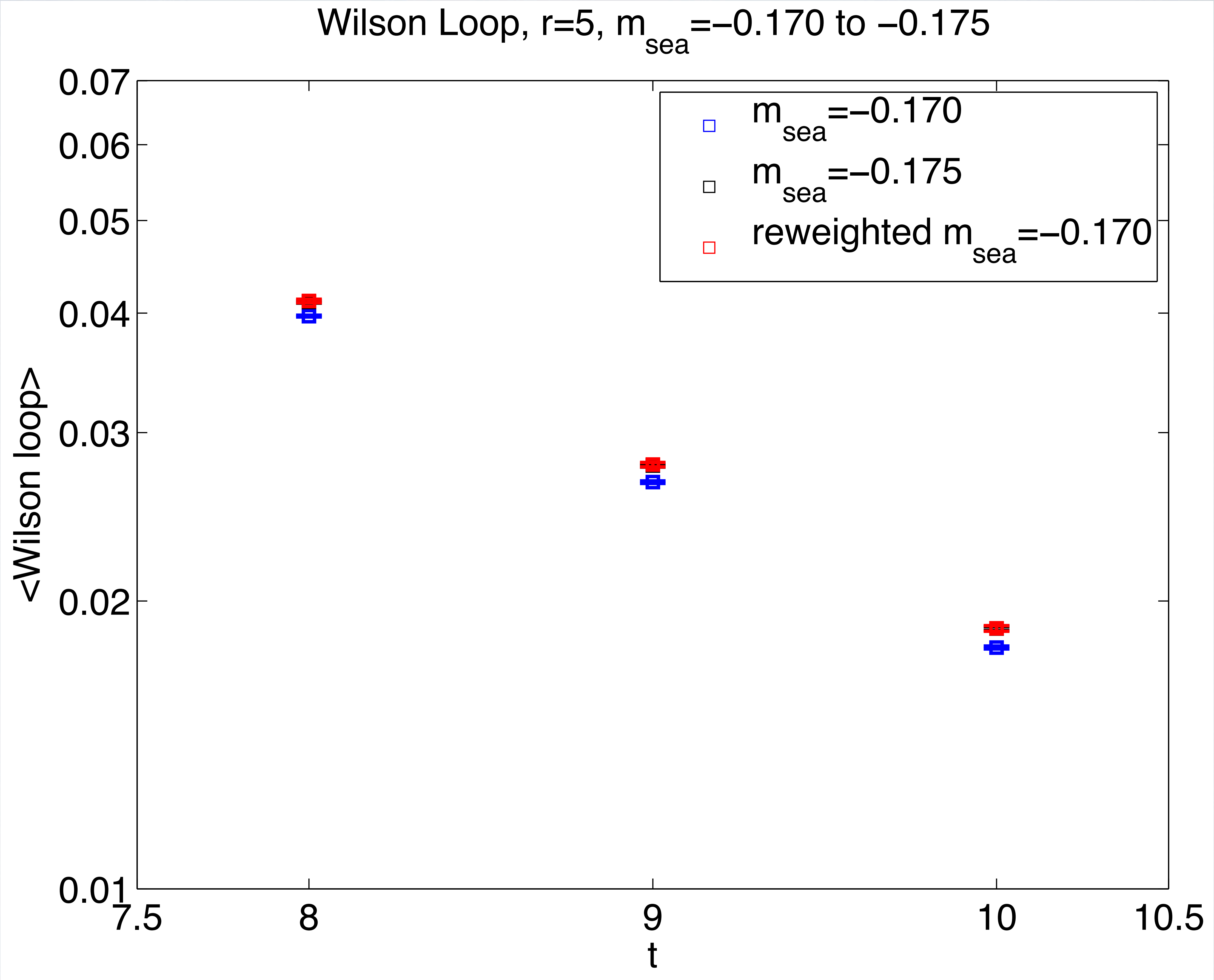

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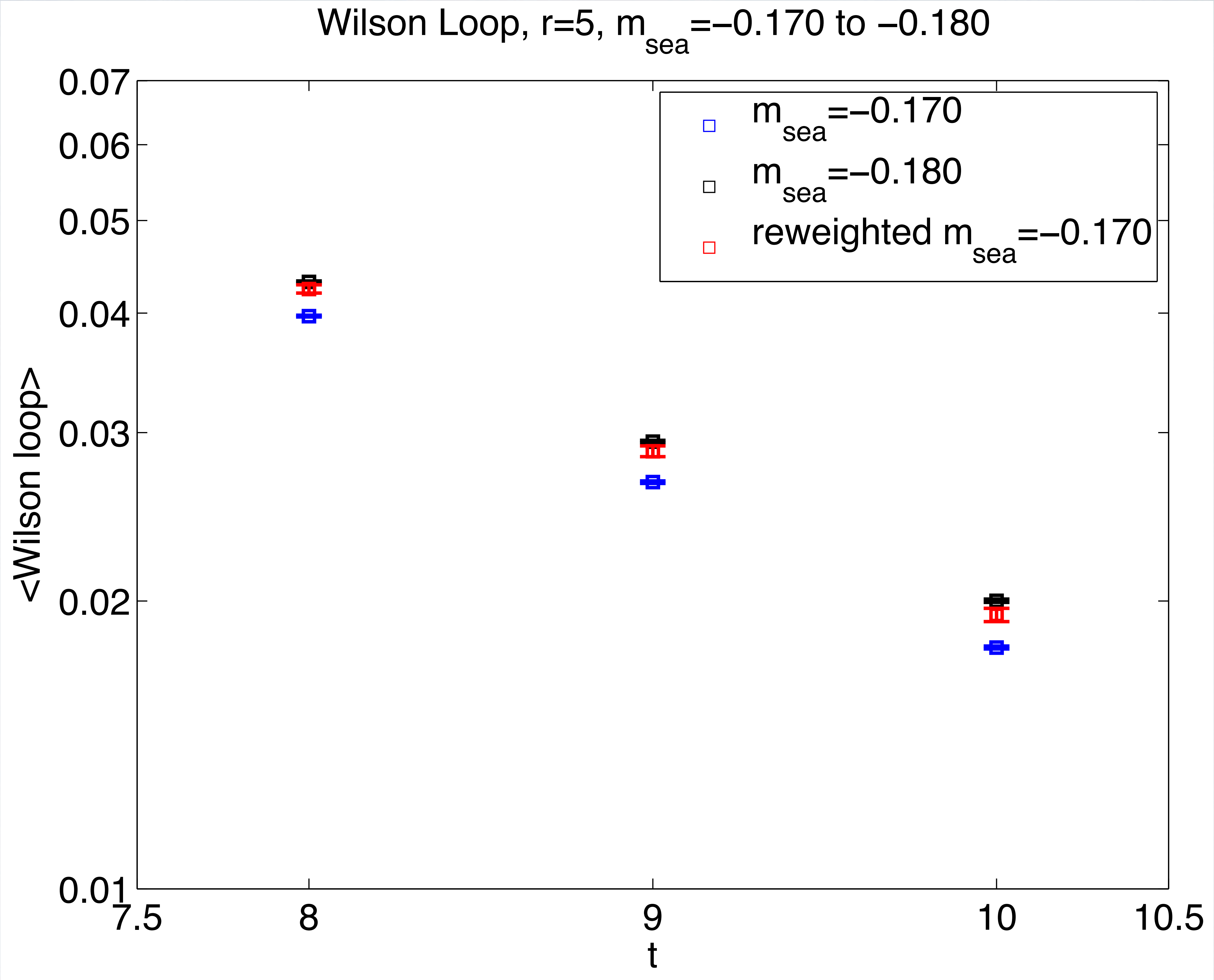

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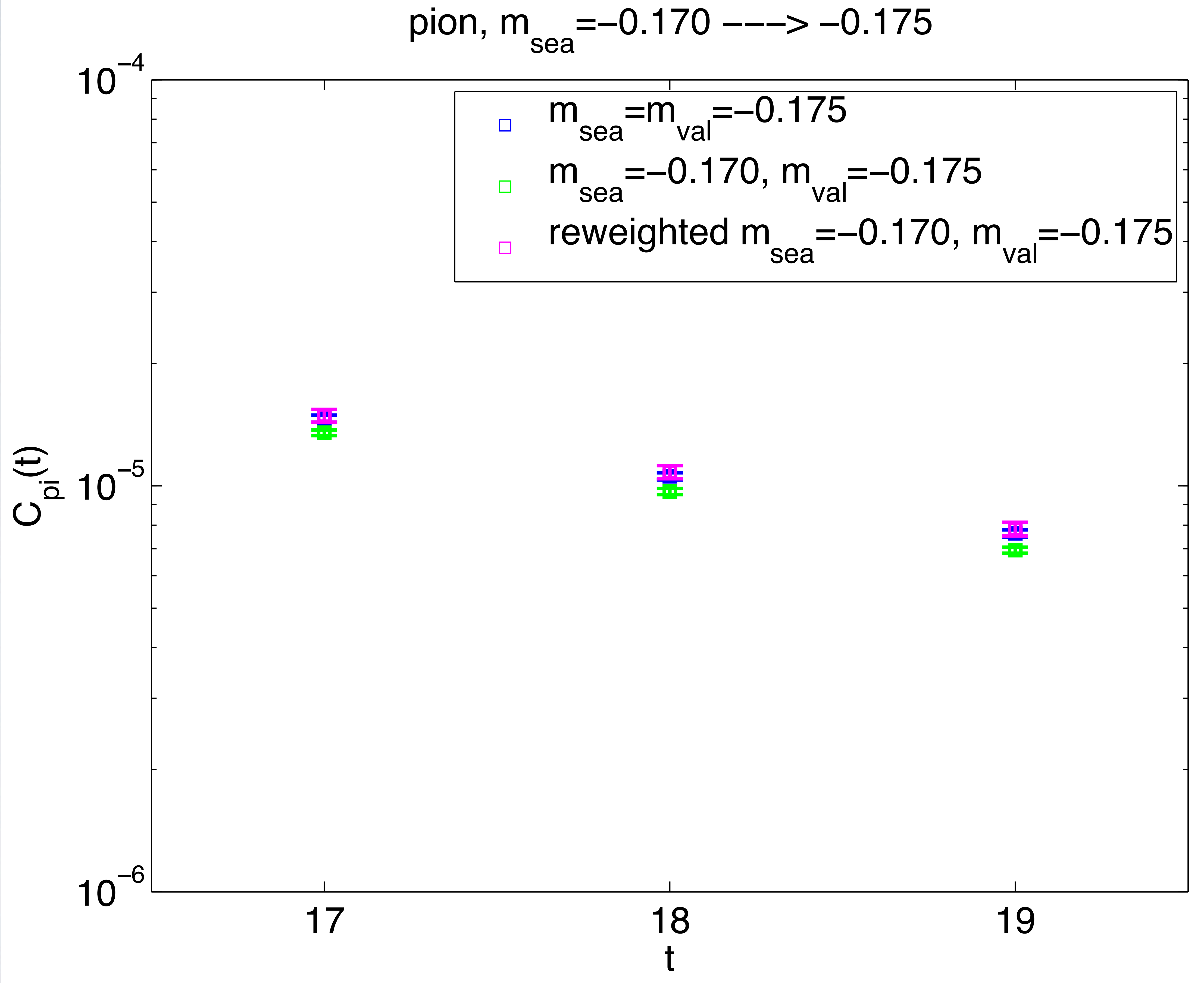

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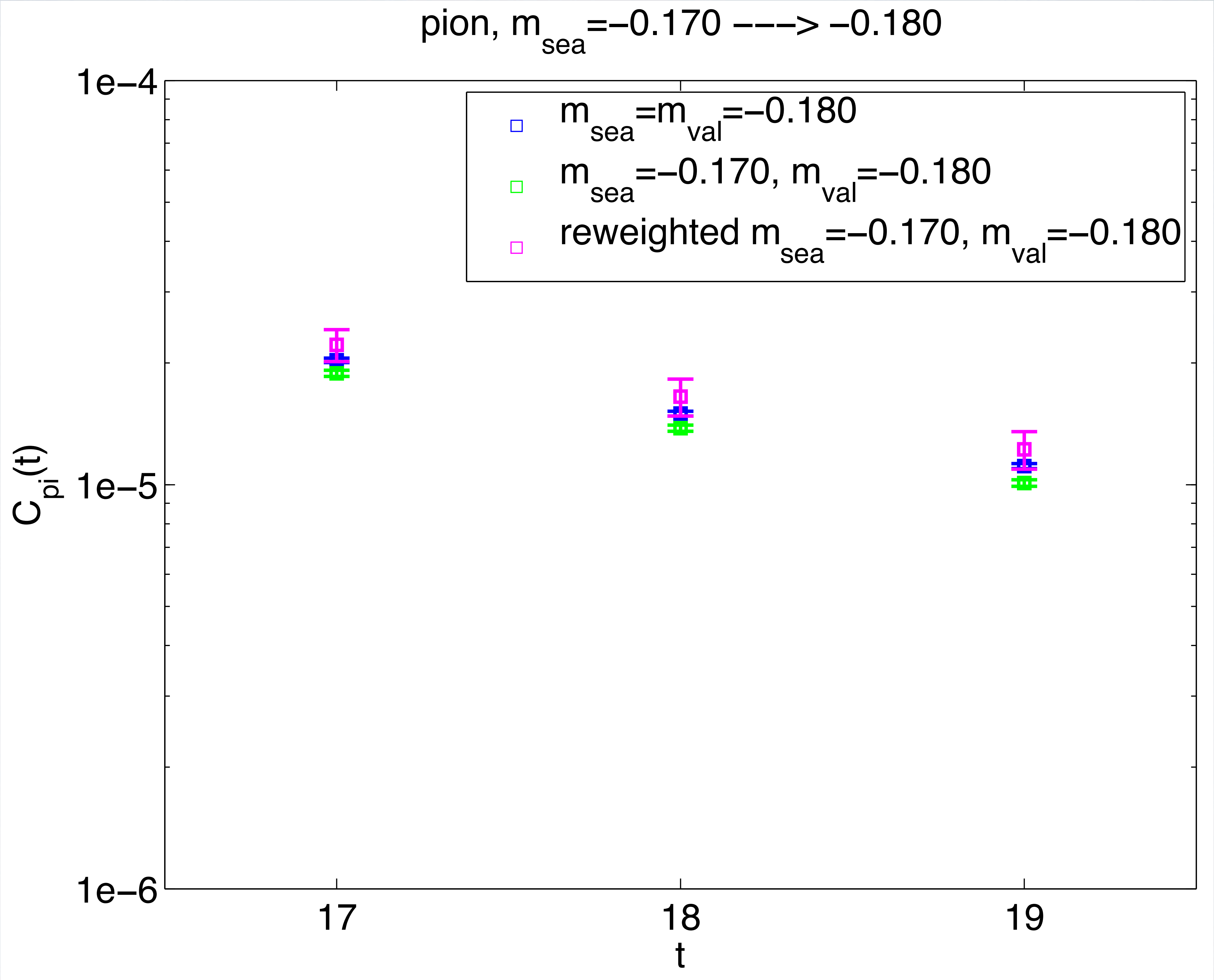

plot by A. Rehim

REWEIGHTING

- Is already very useful and may become even more so in the near future
- Linear algebra methods for determining the reweighting factor works well
- Reweighted observables agree with exact results provided that the shifts in the action parameters are small
    - Isospin breaking seems within the range of applicability
- Can we find further improvements? Do multi-grid like approaches exist?

CONCLUSIONS

- We need computers....