Lattice MC calculations of unitary fermions: *odd-even staggering*

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Phys. Rev. A84 (2011) 043644, Endres, Kaplan, JWL, Nicholson

Phys. Rev. Lett. 107 (2011) 201601, Endres, Kaplan, JWL, Nicholson

Phys. Rev. A87 (2013) 023615, Endres, Kaplan, JWL, Nicholson

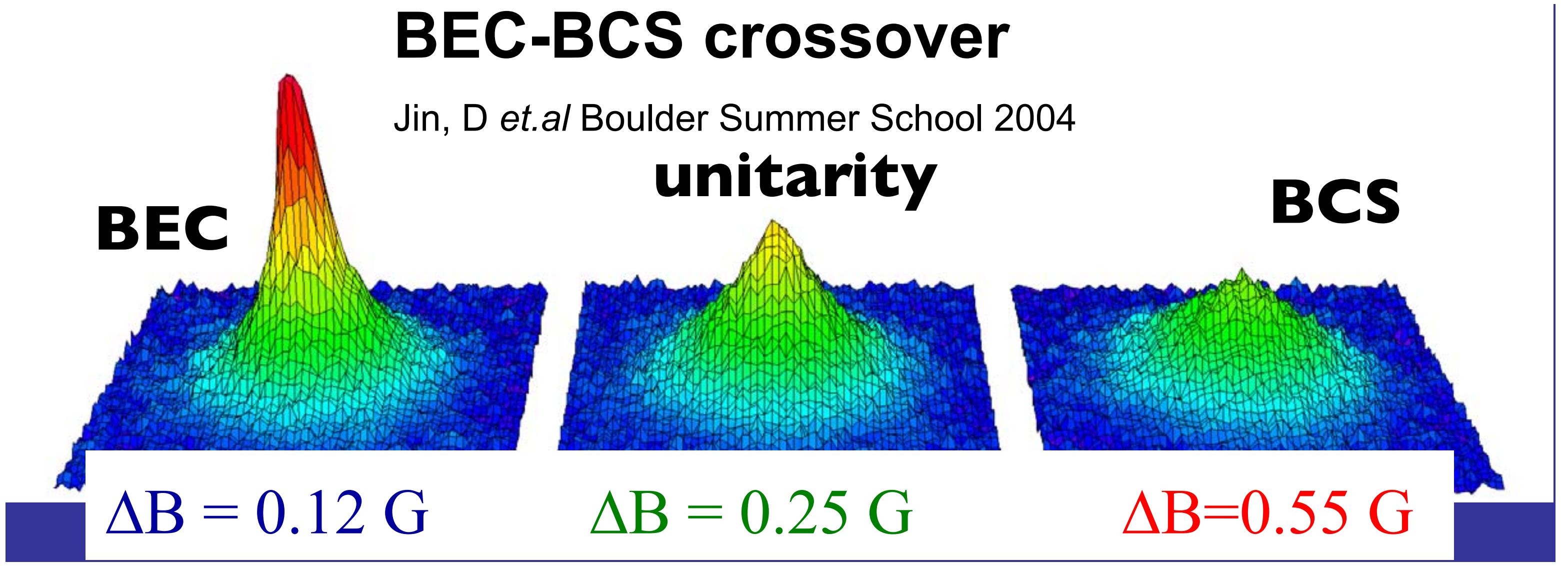
Working in progress (2018), JWL

INT 18-2b

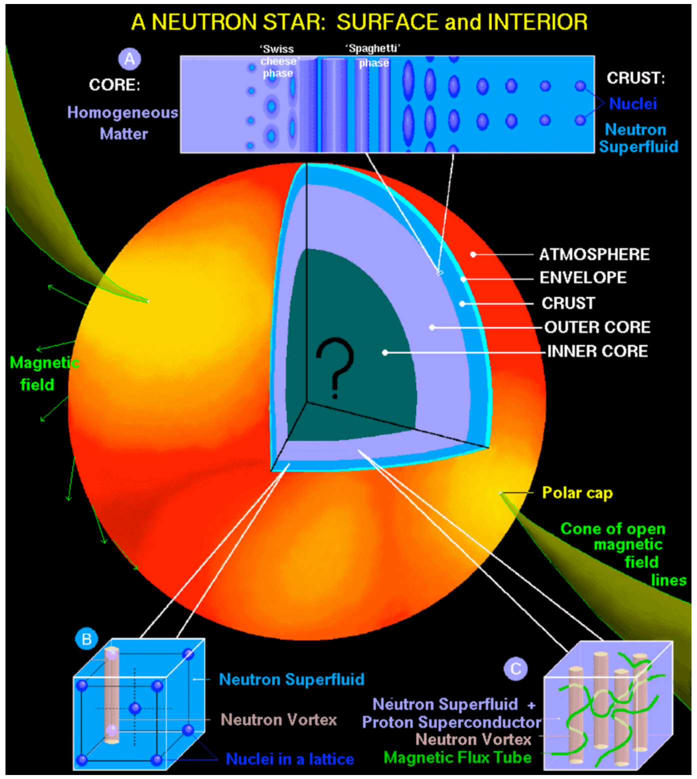
August 6, 2018 @ Seattle, USA

Motivation: unitary fermi gas

- *Cold atom experiments*



- *Approximation to low-density nuclear matter*



Neutron superfluid in crust

$$k_F\, a \sim -10, \;\; a \sim -7 r_e$$

Almost unitary fermi gas

Dany P Page

Fermions at unitarity

- *Definition:* Non-relativistic spin 1/2 fermions with an attractive interaction

$$r_0 \to 0 \quad << \quad n^{-\frac{1}{3}} \quad << \quad |a| \to \infty$$

Range of interaction

Interparticle spacing

S-wave scattering length

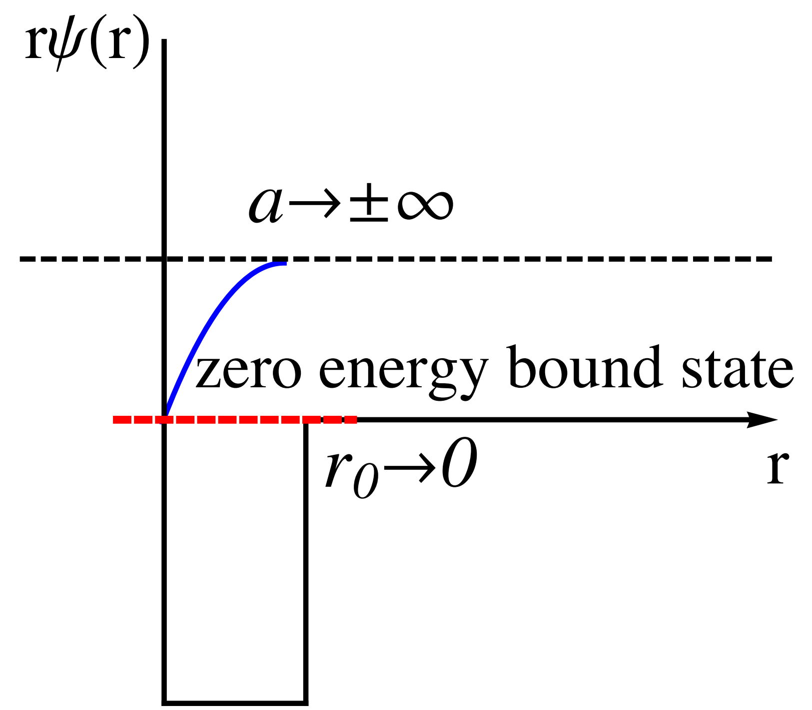
$$p \cot \delta_0 = 0 (\text{or } \delta_0 = \pi/2) \qquad \mathcal{A} = \frac{4\pi}{M} \frac{1}{p \cot \delta_0 - ip}$$

0

Strongly-coupled conformal system

No intrinsic length scales except density

- *Universality:* Physics at low k doesn't care of the details of the interaction.



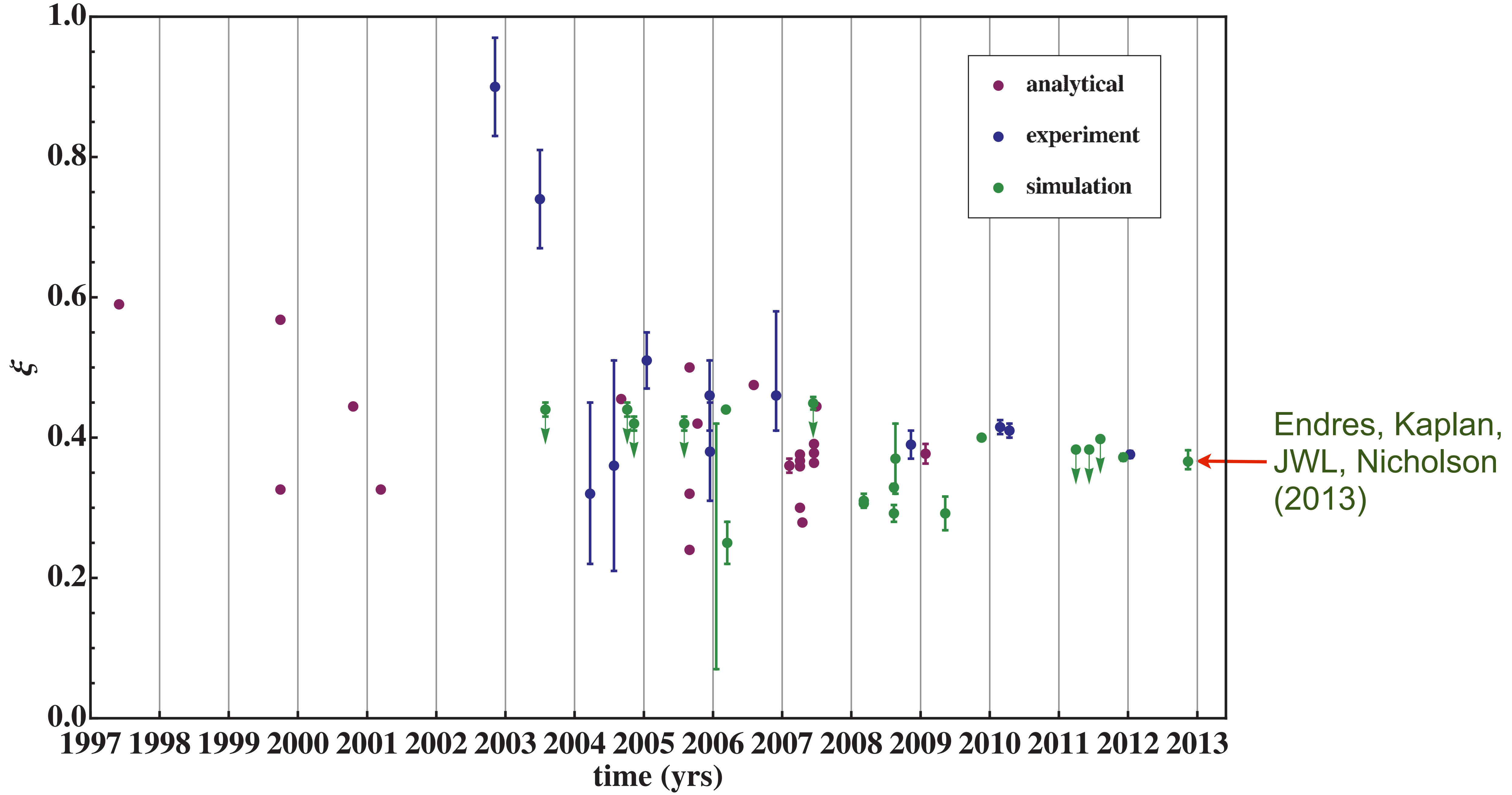
Bertsch parameter

$$E^{\text{unitary}}(n) = \xi E^{\text{free}}(n)$$

Pairing gap

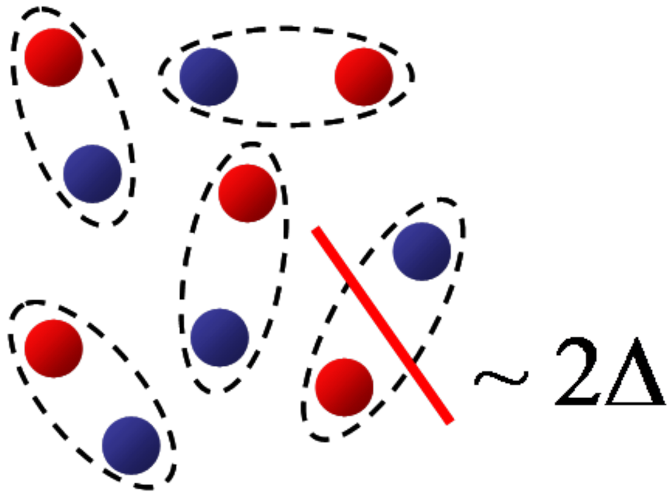
$$\varepsilon^{\text{unitary}}(n) = \Delta \varepsilon_F^{\text{free}}(n)$$

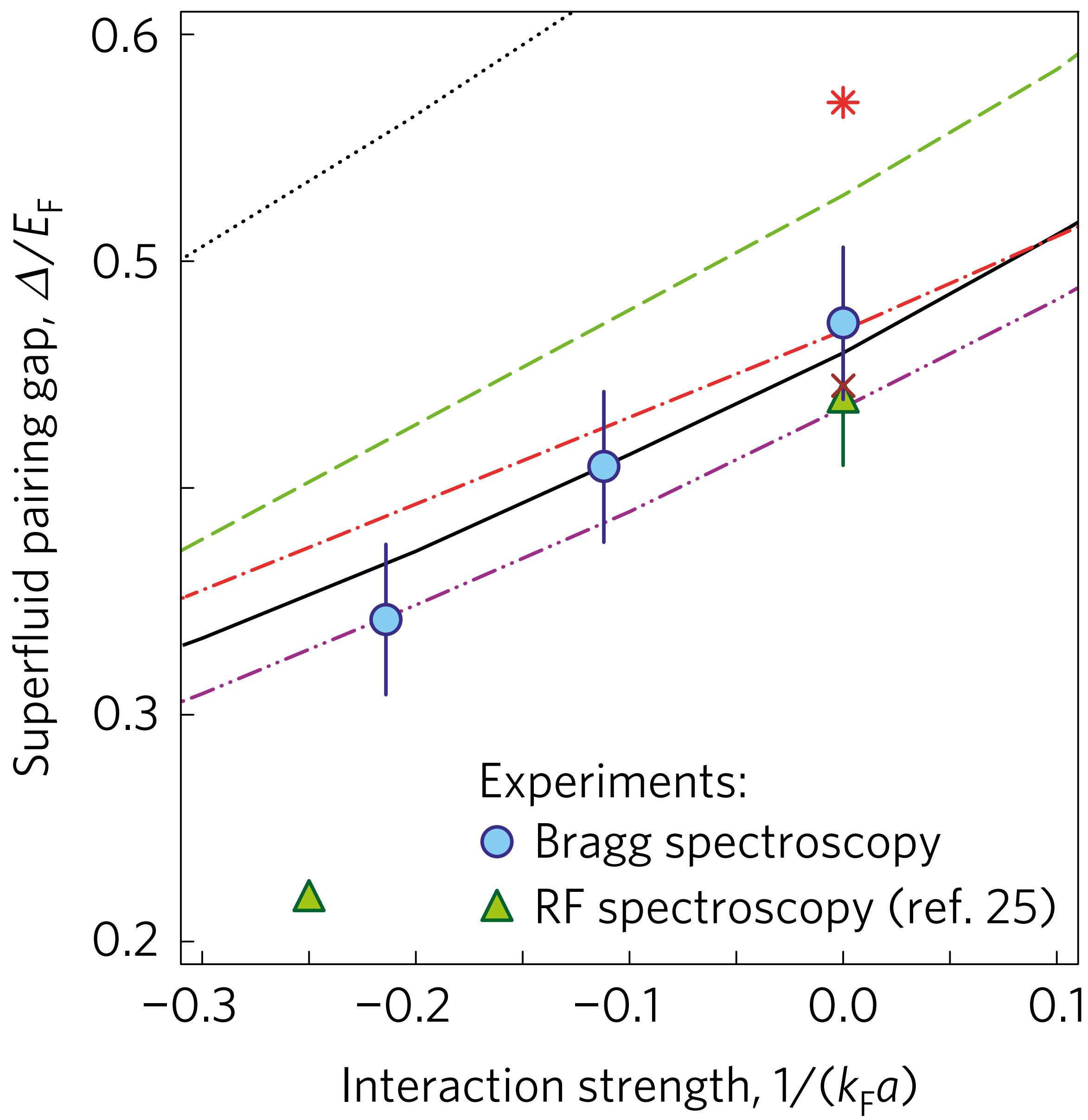
Chronology of the Bertsch parameter



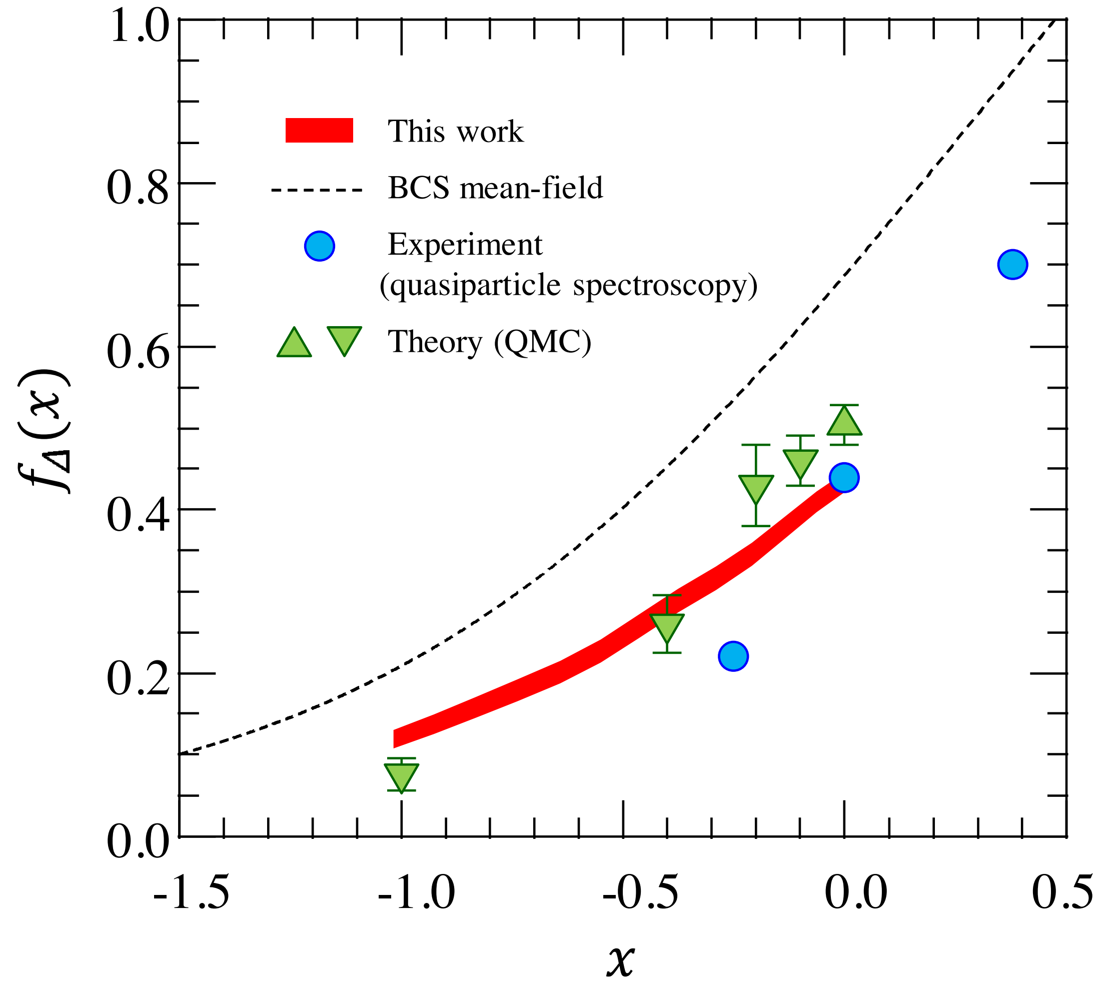
The Bertsch parameter is approaching 0.37 at a few percent level !

Pairing gap from cold atom experiments



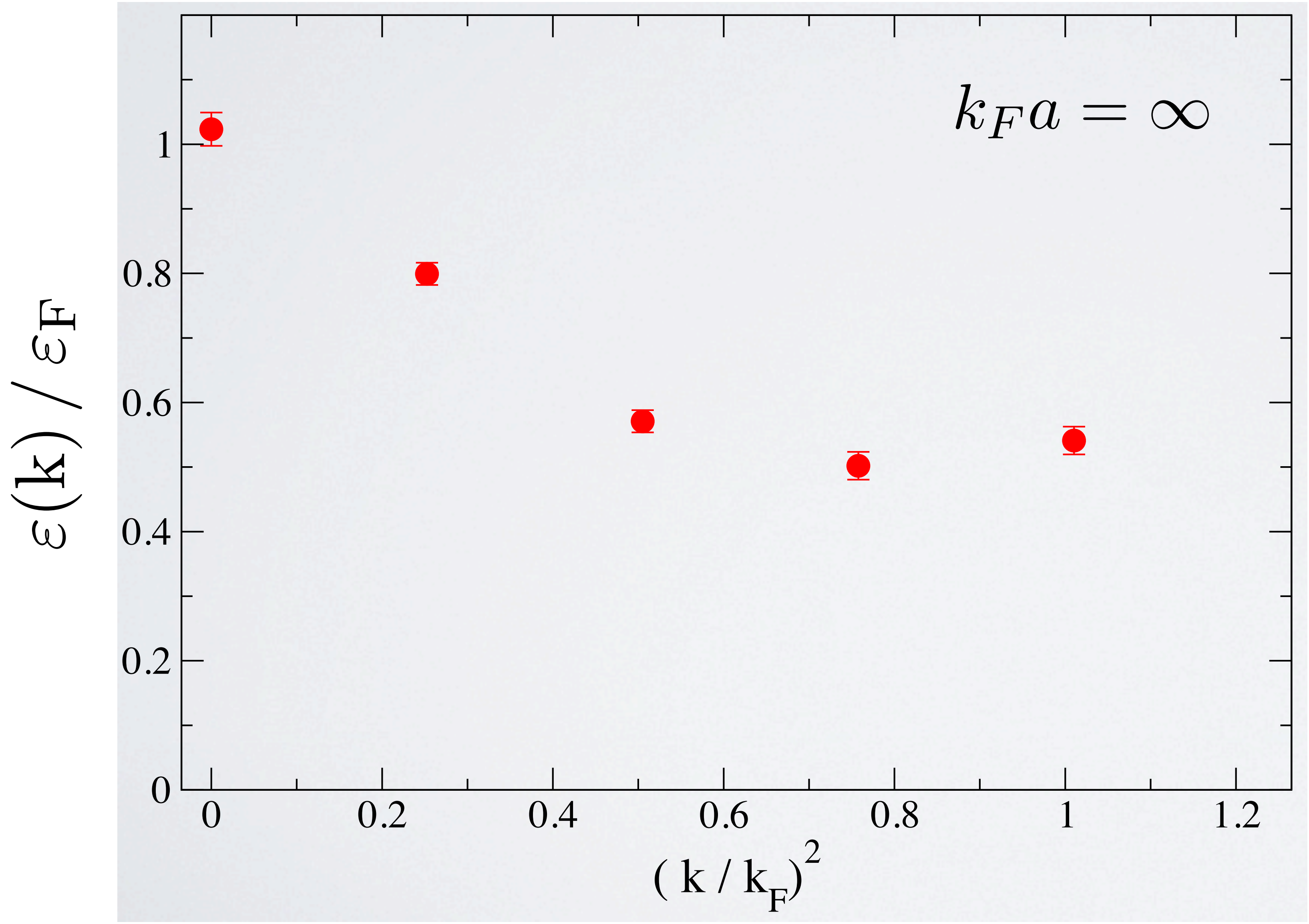


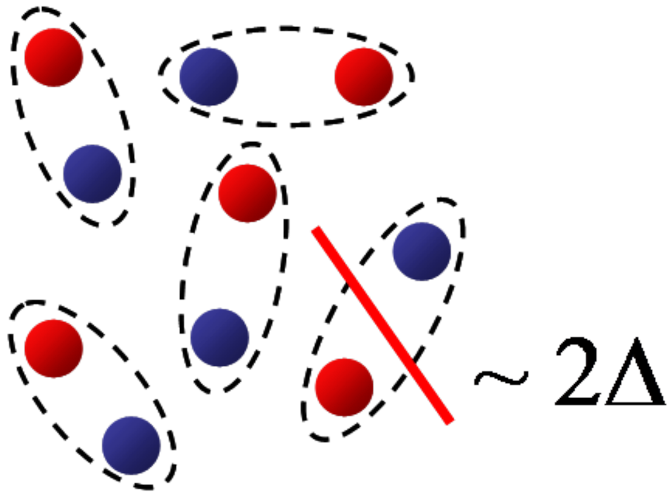
Hoinka et al, Nature 13, 943-946 (2017)



Horikoshi et al, Phys. Rev. X 7, 041004 (2017)

Pairing gap from numerical simulations





$\Delta = 0.504(30)$

Carlson & Reddy (2005)

Any recent update from numerical simulations?

Outline

1) Model

2) Systematics

   I. Unitarity limit and discretization/finite volume effects

   II. Interpolating field overlap

   II. Statistical overlap/noise

   II. Thermodynamic limit

3) Numerical results

4) Summary and Conclusions

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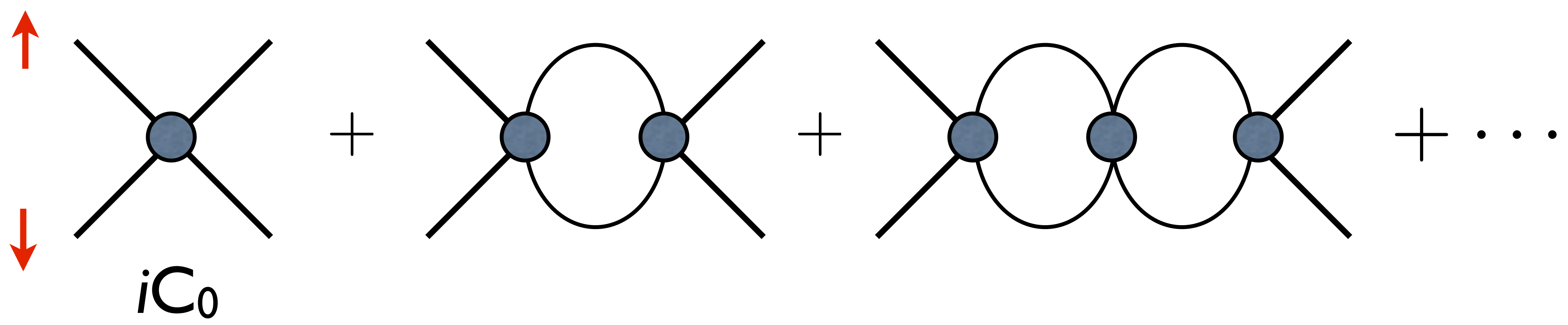
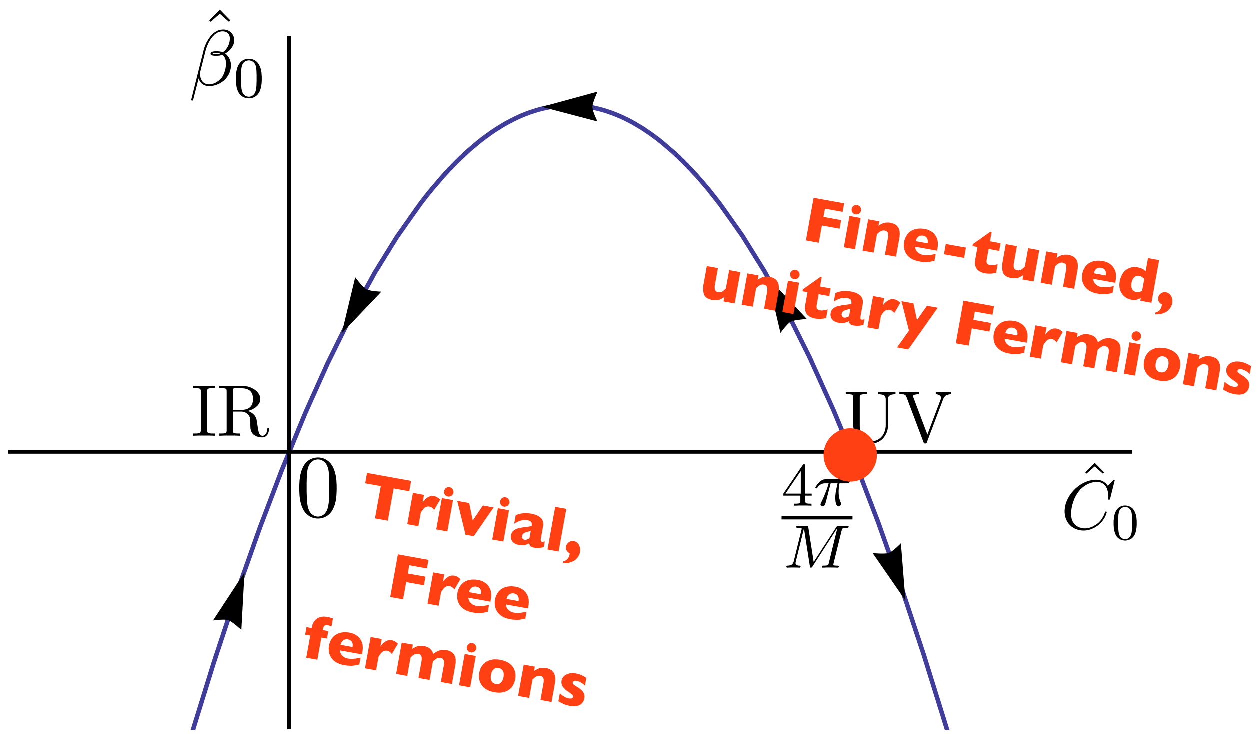
Low energy nuclear EFT - continuum



$$C_0(\mu) = \frac{4\pi}{M}\left(\frac{1}{-\mu + 1/a}\right).$$



Redefine: $\hat{C}_0(\mu) \equiv -\mu C_0(\mu)$

$$\hat{\beta}_0 = \mu \frac{\partial \hat{C}_0}{\partial \mu} = \hat{C}_0 \left(1 - \frac{M}{4\pi}\hat{C}_0\right).$$

D. B. Kaplan, M. Savage, M. Wise (1998)

Lattice construction for non-relativistic fermions

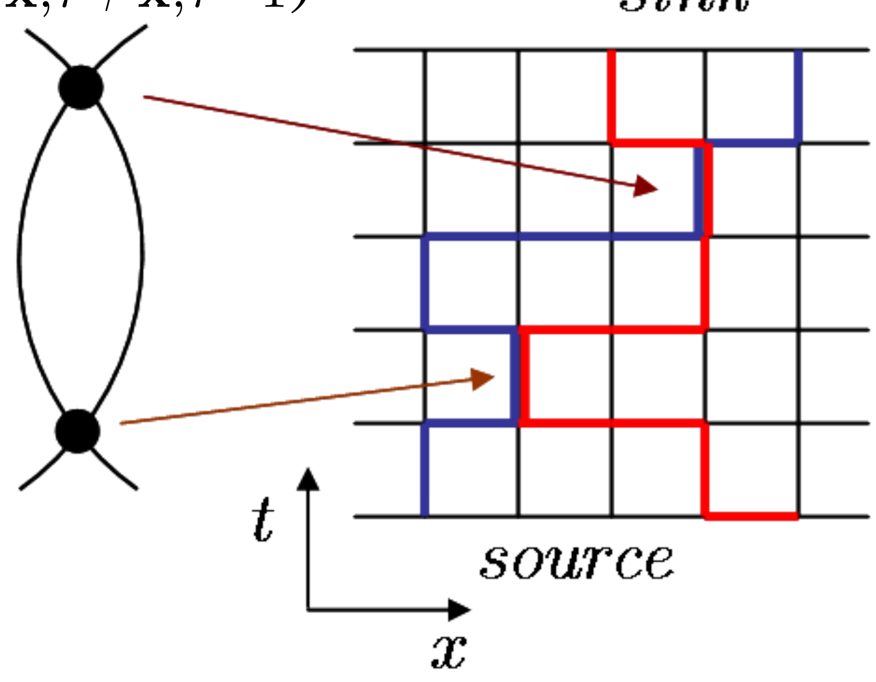
- *Interaction & Lattice action*

J. -W. Chen, D. B. Kaplan (2004)

$$S = b_\tau b_s^3 \sum_{\tau,\mathbf{x}} \left[\bar{\psi}_{\mathbf{x},\tau} (\partial_\tau \psi)_{\mathbf{x},\tau} - \frac{1}{2M} \bar{\psi}_{\mathbf{x},\tau} (\nabla^2 \psi)_{\mathbf{x},\tau} + (\sqrt{C}\phi)_{\mathbf{x},\tau} \bar{\psi}_{\mathbf{x},\tau} \psi_{\mathbf{x},\tau-1} \right]$$

Integrating out

$C(\bar{\psi}_{\mathbf{x},\tau}\psi_{\mathbf{x},\tau-1})^2$



(1) Four-Fermi interaction via auxiliary fields, ϕ=±1 or Gaussian, on time-links

Only fermion loop with forward propagators

$$\langle \phi_{\mathbf{x},\tau} \rangle = 0 \ , \qquad \langle \phi_{\mathbf{x},\tau} \phi_{\mathbf{x}',\tau'} \rangle = \delta_{\mathbf{x},\mathbf{x}'} \delta_{\tau,\tau'}$$

(2) Open B.C. in time and periodic B.C. in space

Restricted to zero temperature

$T \times L^3$ Euclidean Lattice

Lattice construction for non-relativistic fermions

- *Fermion matrix*

$$S = \bar{\psi} K \psi \qquad K = \begin{pmatrix} D & -X(T-1) & 0 & 0 & \dots & 0 \\ 0 & D & -X(T-2) & 0 & \dots & 0 \\ 0 & 0 & D & -X(T-3) & \dots & 0 \\ 0 & 0 & 0 & D & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & -X(0) \\ 0 & 0 & 0 & 0 & \dots & D \end{pmatrix}$$

Open B.C. in time

$$D = 1 - \frac{\nabla^2}{2M}\,, \qquad X(\tau) = 1 - \sqrt{C}\Phi(\tau)$$

$\det K$ is independent of the auxiliary field → *No nontrivial probability measure*
Quenched simulation & sign free

- *Propagator (K^{-1}) & Transfer matrix (T)*

$$K^{-1}(\tau;0) = D^{-1/2}\, T^{\tau}\, D^{-1/2} \qquad T = D^{-1/2} X(\tau) D^{-1/2}$$

Measurement of the ground state energy

$$C_{N\downarrow,N\uparrow}(\tau) = Z_0\, e^{-E_0\,\tau} + Z_1\, e^{-E_1\,\tau} + Z_2\, e^{-E_2\,\tau} + \ldots$$

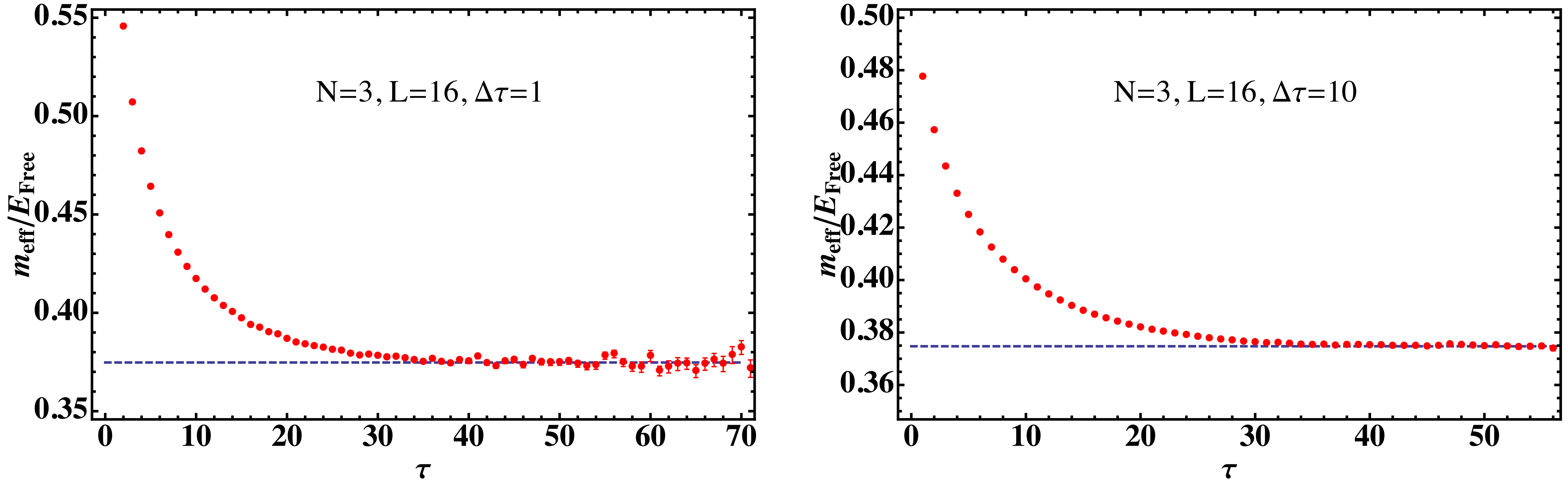
τ is the Euclidean time.

$$m_{eff}(\tau) = \frac{1}{\Delta\tau}\log\left[\frac{C(\tau')}{C(\tau)}\right]$$

effective mass

$$\lim_{\tau\to\infty} m_{eff}(\tau) = E_0$$

energy of ground state



Dashed line: Y. Castin et. al. (2007)

Remarks

1) Canonical approaches on an Euclidean space-time lattice

2) Zero temperature (open b. c.)

3) No trapping potentials

4) Ground state energies of $N_{up}=N_{down}$ and $N_{up}+1=N_{down}$ unitary fermions

5) Numerical results for $N_{up}+1=N_{down}$ unitary fermions are very preliminary (single volume $V=16^3$, selected values of N).

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Improvement: single particle sector

free fermions

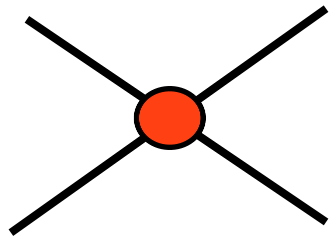
$$D = 1 - \frac{\nabla^2}{2M} \quad \Rightarrow \quad T = D^{-1} \quad \text{and} \quad E = \ln D$$

- *Standard:* $1 + \frac{2\sin^2(\mathbf{p}/2)}{M} \quad \Rightarrow \quad E = \frac{\mathbf{p}^2}{2M}(1 + O(b_s^2))$

- *Perfect:* Separable interaction and FFT algorithm

$$\begin{cases} e^{\mathbf{p}^2/(2M)} & |\mathbf{p}| < \Lambda \\ \infty & |\mathbf{p}| \geq \Lambda \end{cases} \quad \Rightarrow \quad E = \frac{\mathbf{p}^2}{2M}$$

Tuning: four-fermi interaction



$$\sqrt{C(\mathbf{p}^{\downarrow} - \mathbf{q}^{\downarrow})}\sqrt{C(\mathbf{p}^{\uparrow} - \mathbf{q}^{\uparrow})}$$

Discretized & Finite V

Galilean-invariant interaction

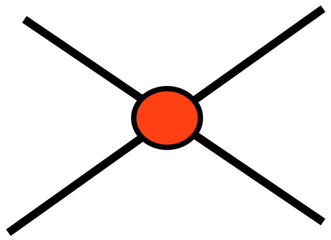
$$\begin{aligned} p \cot \delta_0 &= -\frac{1}{a} + \frac{1}{2} r_0 p^2 + \sum_{i=1}^{\infty} r_i p^{2(i+1)} \\ &= 0 \end{aligned}$$

Continuum & Infinite V

Improvement: two-body sector

M. Luscher (1986, 1991)

Beane, Bedaque, Parreno & Savage (2004)



$$p \cot \delta_0 = \frac{1}{\pi L} S(\eta)$$

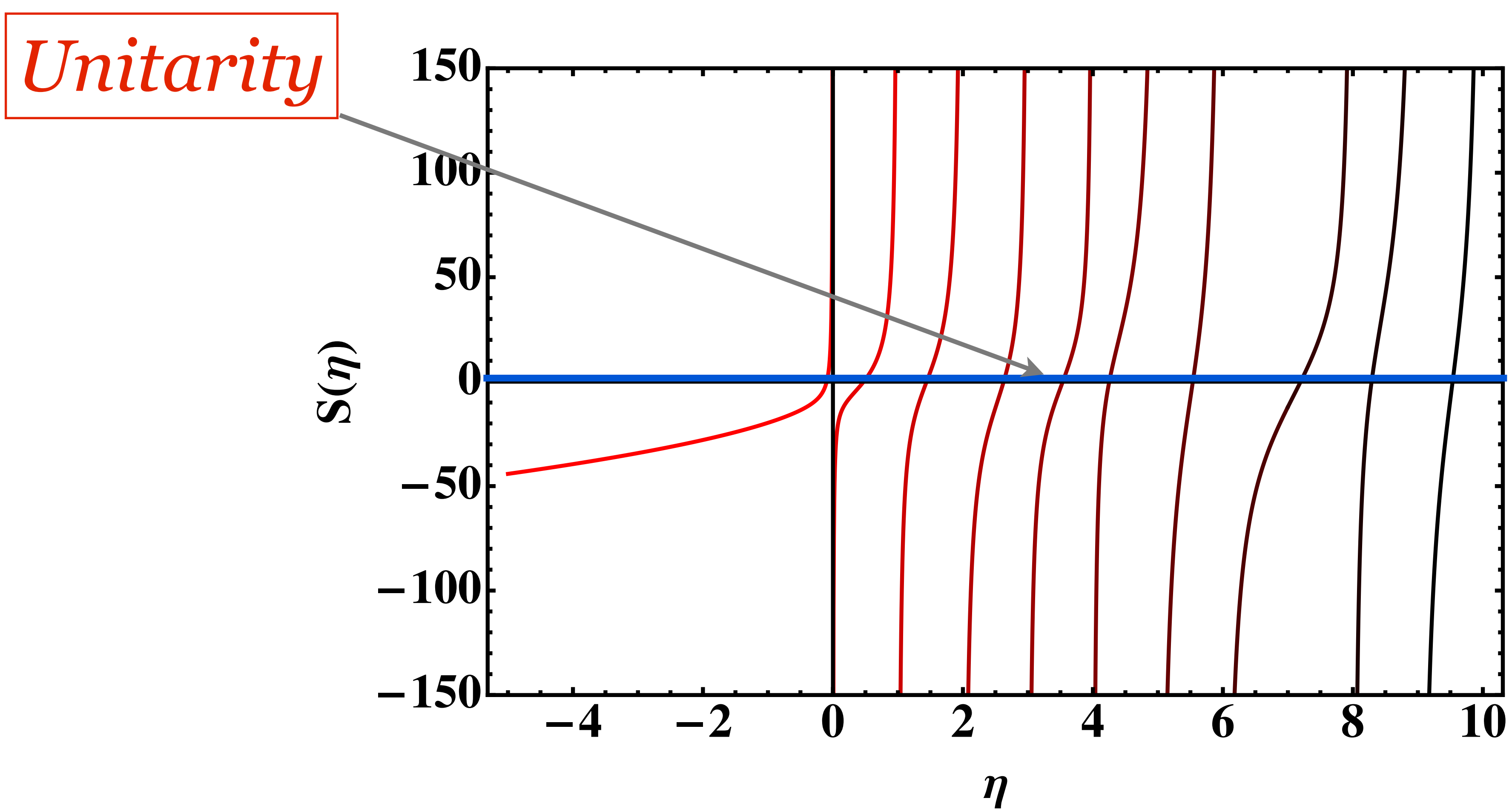
free space

confined in a box

$$C(\mathbf{p}) = \frac{4\pi}{M} \sum_{n=0}^{N_{\mathcal{O}}-1} C_{2n} \mathcal{O}_{2n}(\mathbf{p})$$

$$S(\eta) = \lim_{\Lambda \to \infty} \left[\sum_{|\mathbf{j}|<\Lambda} \frac{1}{\mathbf{j}^2 - \eta} - 4\pi \Lambda \right]$$

$$\eta = (pL/2\pi)^2$$



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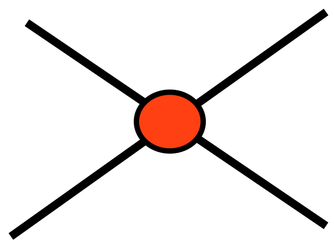

$$C(\mathbf{p}) = \frac{4\pi}{M} \sum_{n=0}^{N_{\mathcal{O}}-1} C_{2n}\mathcal{O}_{2n}(\mathbf{p})$$

$$\mathcal{O}_{2n}(\mathbf{p}) = M_0^n (1 - e^{-\hat{\mathbf{p}}^2/M_0})^n$$

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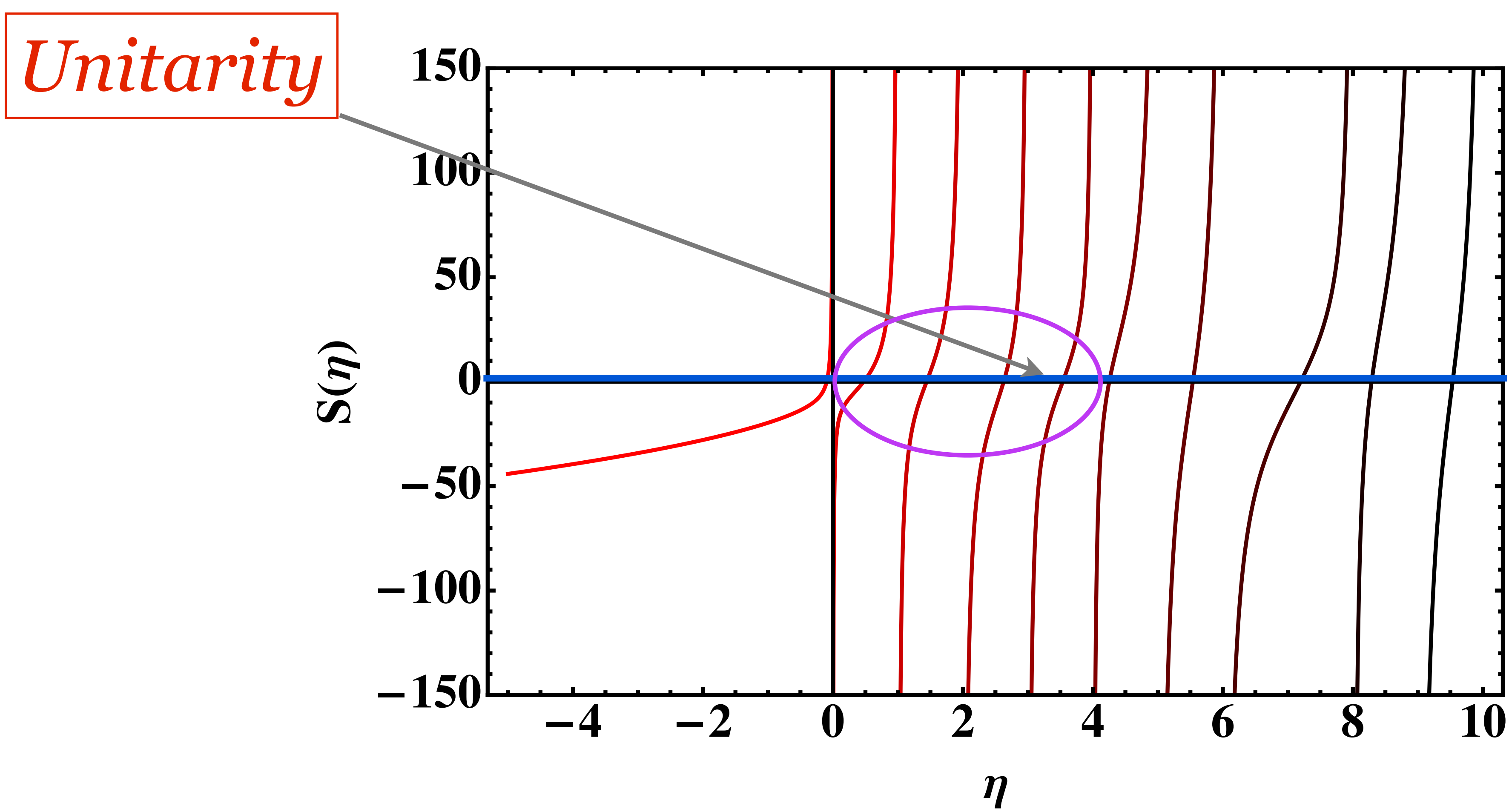
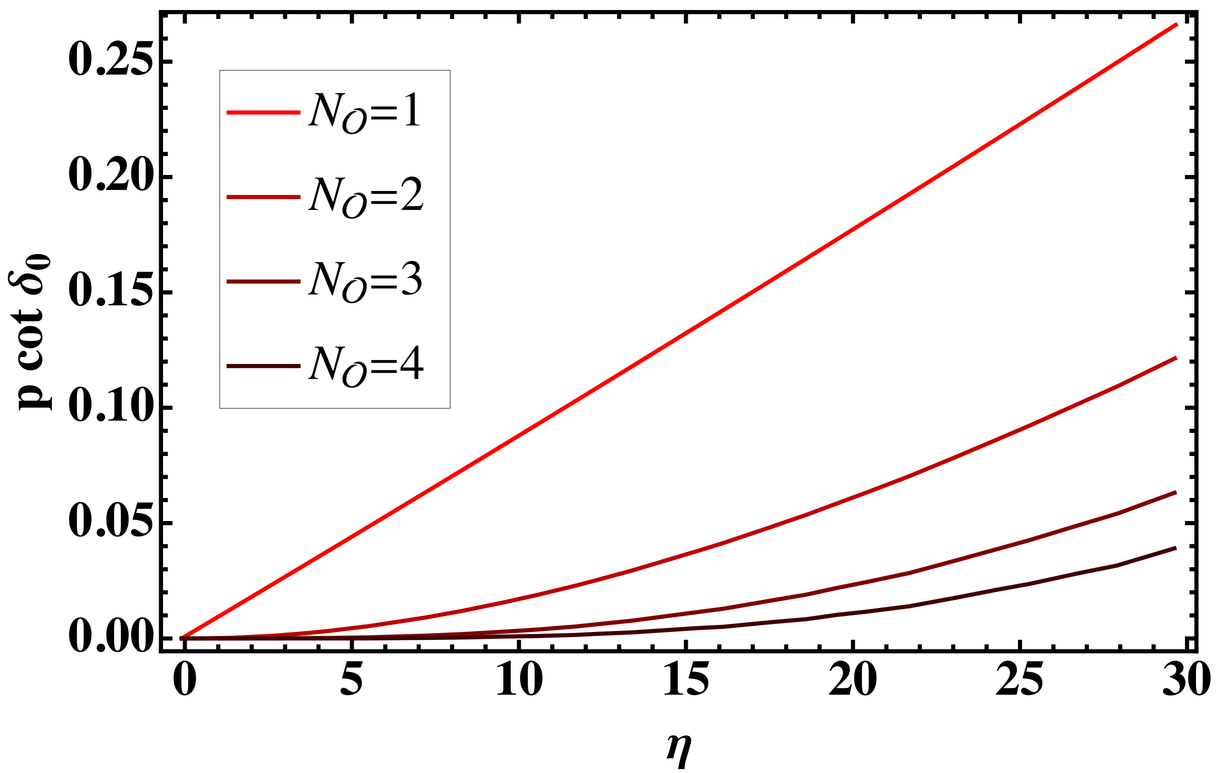
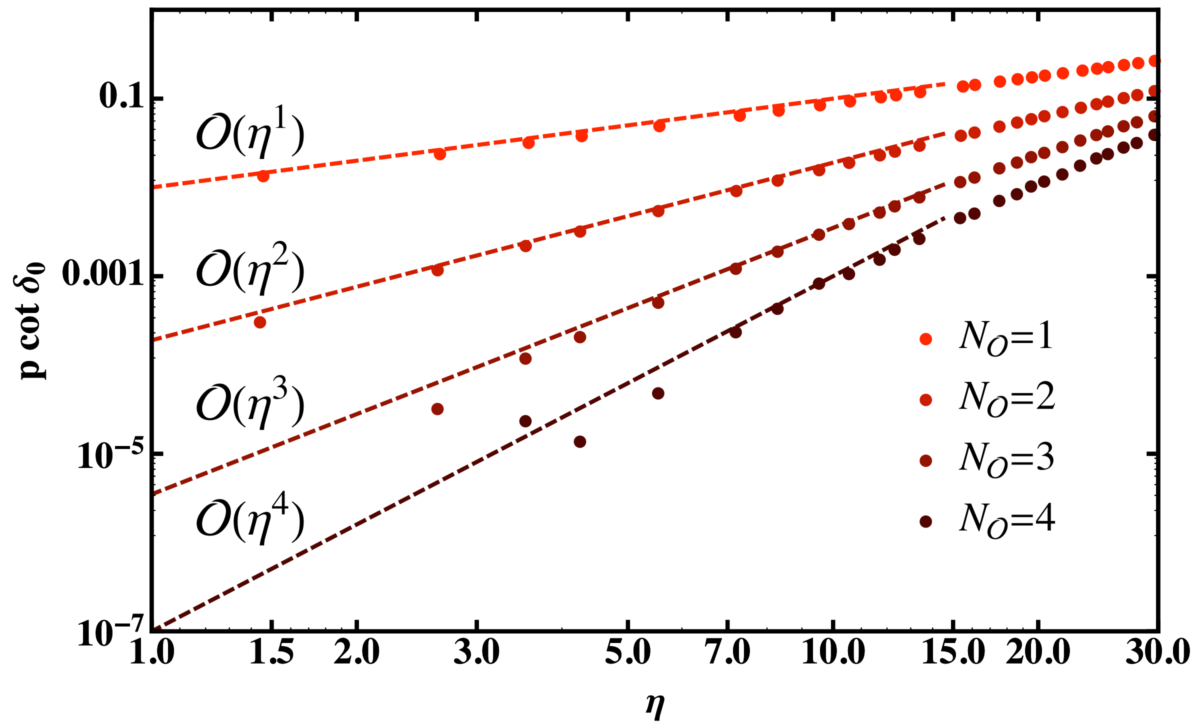


Realization of unitarity

L=32, M=5





- For a few low-lying energy eigenvalues systematically tune the operators $\mathcal{O}_{2n}(\mathbf{p})$ to reproduce

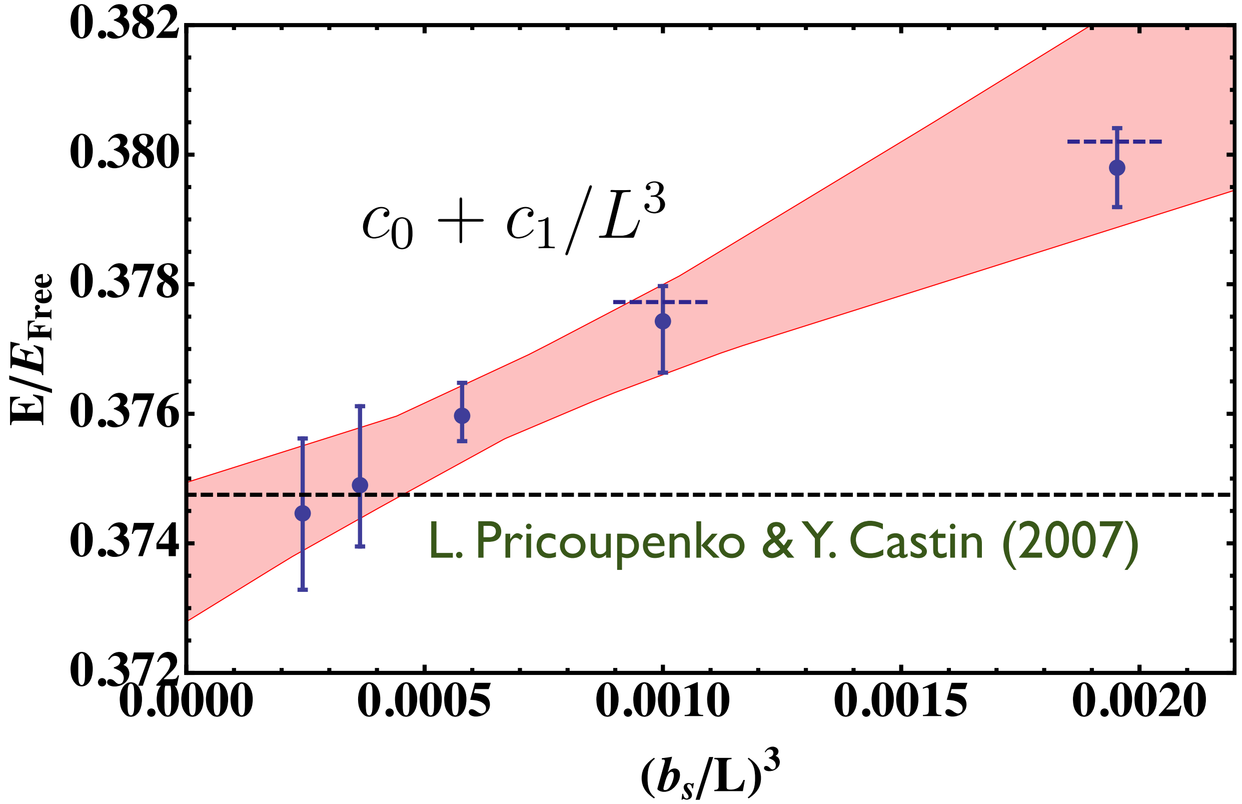
$$p \cot \delta_0 = 0 \quad \text{for sufficiently small } p$$

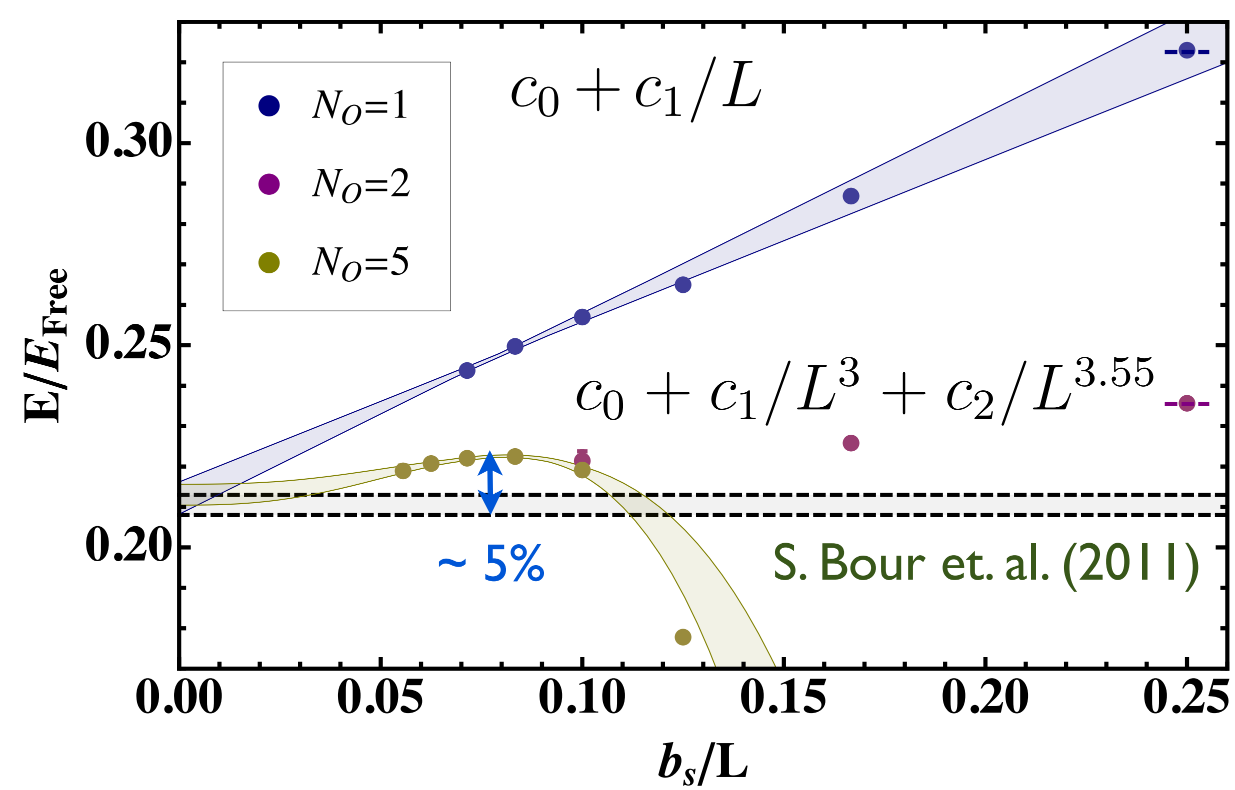
- Found that we are close to unitarity even beyond the exactly tuned states.

- For non-zero net CoM is the tuning affected by the hard momentum cut-off for the single particle?

Gilbreth & Jensen in private conversation

Beyond two-body sector





- Improvement in 2-body sector (S-wave): $1/L^9$ with 5 operators tuned
- No improvement in 2-body sector (P-wave): $1/L^3$
- Contribution of 3-body operators : $L^{-3.55}\,(\ell = 1)$ (N=4) $L^{-4.33}\,(\ell = 0)$ (N=3)

S. Tan (2004) Y. Nishida & D. T. Son (2007)

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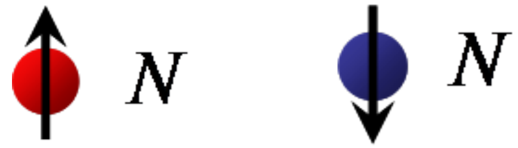
N-body correlators

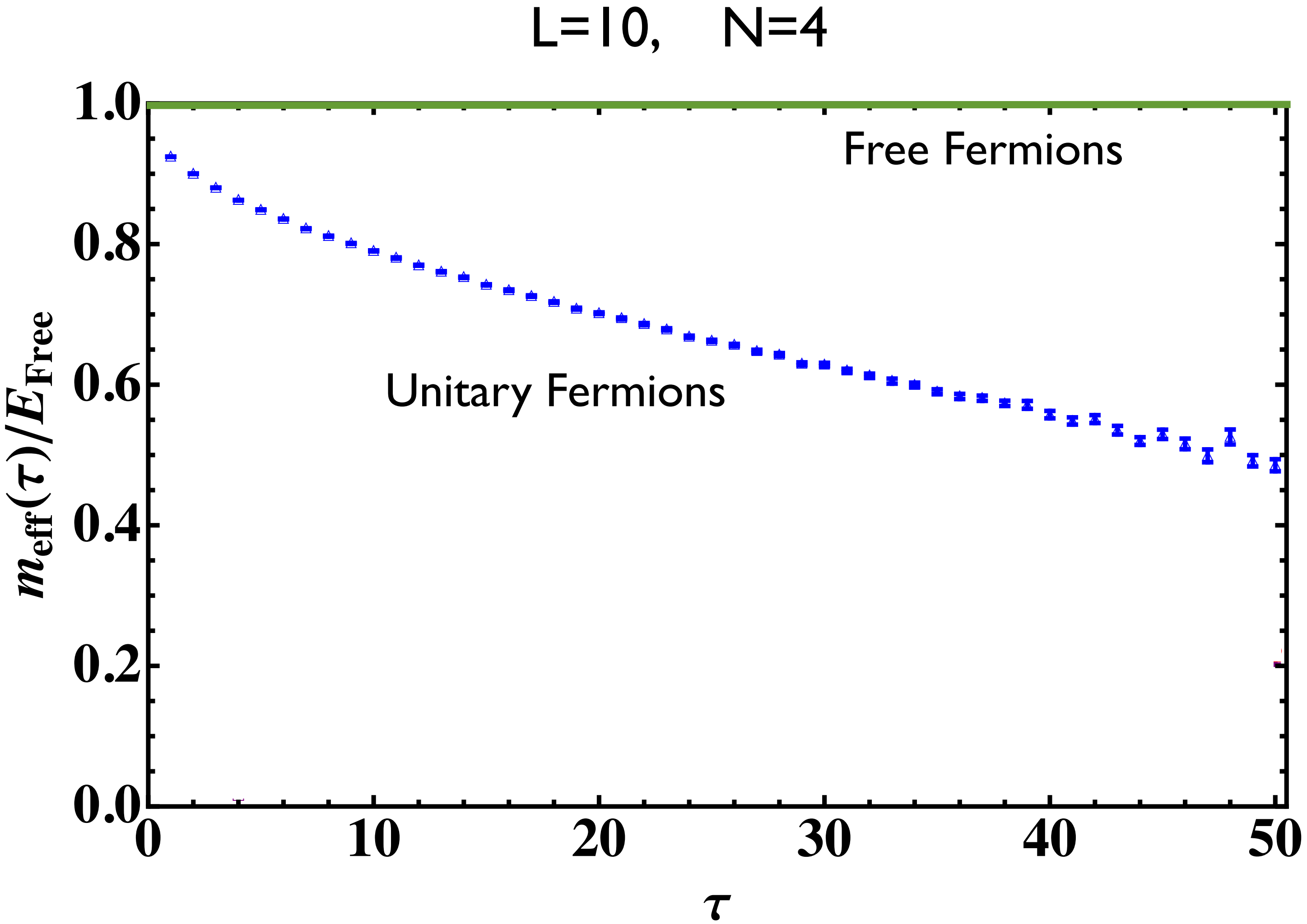


- *Slater-Determinant to take account of Fermi-Dirac Statistics*

$$C_{N_\downarrow,N_\uparrow}(\tau) = \langle \det S^\downarrow(\tau) \det S^\uparrow(\tau) \rangle$$

$$S^\sigma_{i,j}(\tau) = \langle \alpha^\sigma_i | K^{-1}(\tau, 0) | \alpha^\sigma_j \rangle$$

$|\alpha^\sigma_i\rangle$ is a momentum eigenstate of non-interacting fermions



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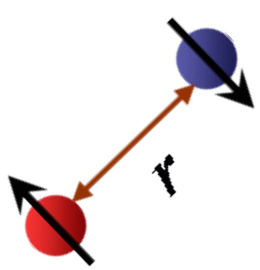
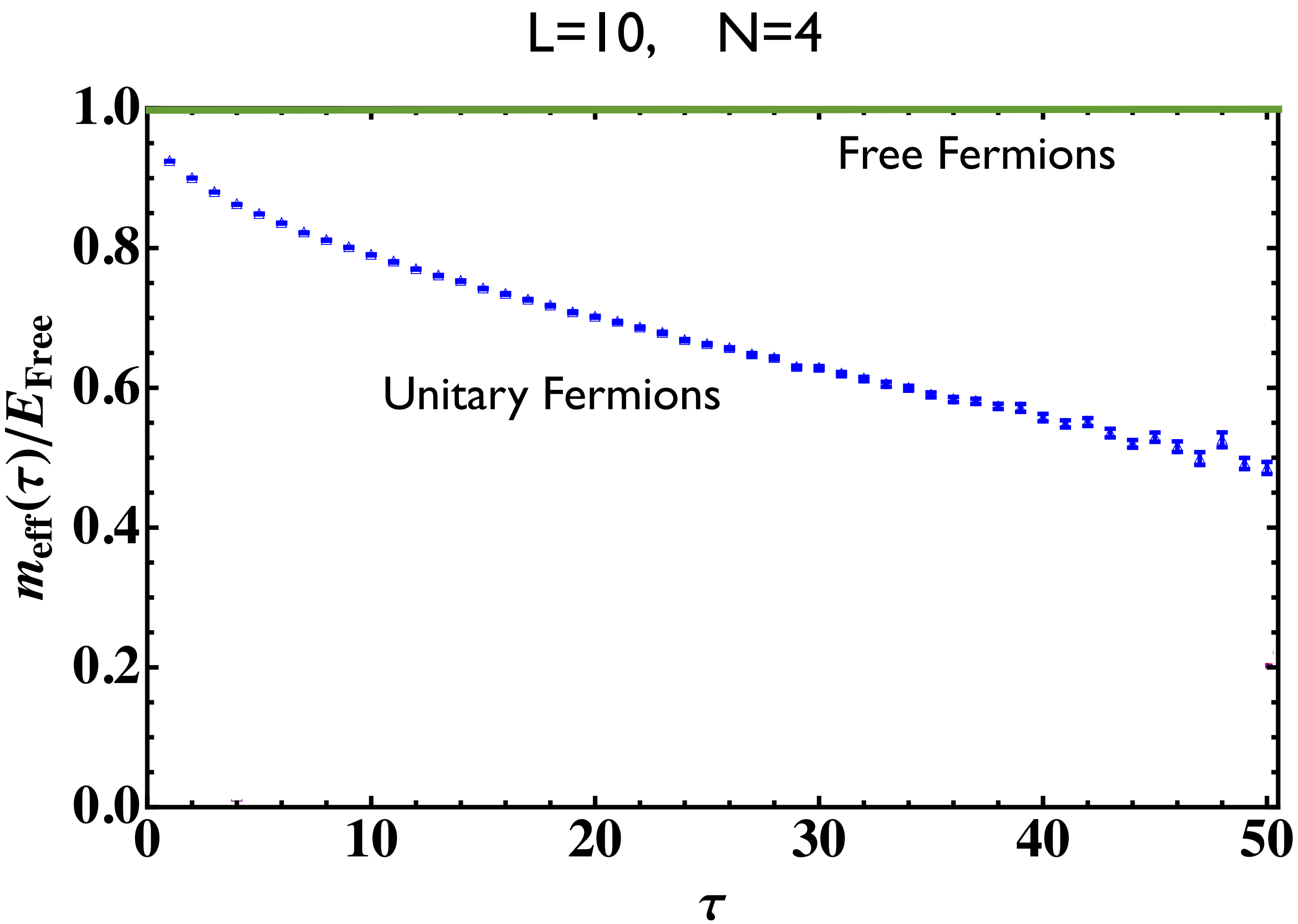


$\Psi_{unitary}(r) \sim 1 / r$

Unitary fermions have small wave function overlap with non-interacting fermions.



Improvement: N-body correlators

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$|\alpha^{\sigma}_i\rangle$ is a momentum eigenstate of non-interacting fermions

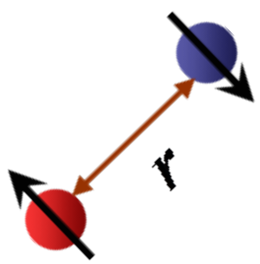
$$C_{N_\downarrow,N_\uparrow}(\tau) = \langle \det S^{\downarrow\uparrow}(\tau) \rangle$$

$$S^{\downarrow\uparrow}_{i,j}(\tau) = \langle \Psi | K^{-1}(\tau,0) \otimes K^{-1}(\tau,0) | \alpha^{\downarrow}_i \alpha^{\uparrow}_j \rangle$$

$|\Psi\rangle$ is a two-fermions state.

For $N_\uparrow = N_\downarrow - 1$, replace j-th row by

$$\langle \alpha^{\downarrow}_j | K^{-1}(\tau,0) | \alpha^{\downarrow}_1 \rangle,\ \langle \alpha^{\downarrow}_j | K^{-1}(\tau,0) | \alpha^{\downarrow}_2 \rangle,\ \cdots,\ \langle \alpha^{\downarrow}_j | K^{-1}(\tau,0) | \alpha^{\downarrow}_{N_\downarrow} \rangle$$



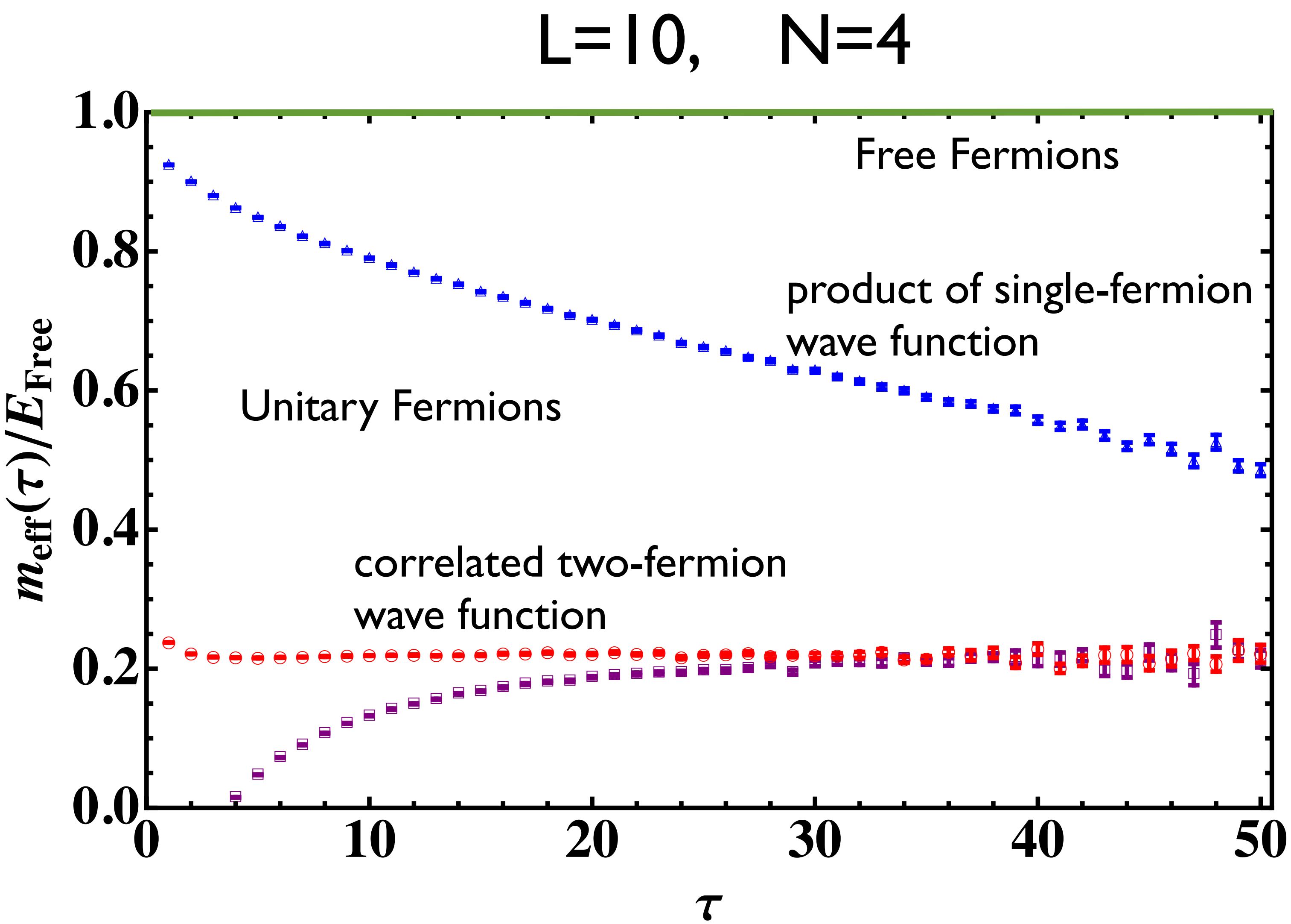
$$\Psi_{unitary}(r) \sim 1/r$$

Unitary fermions have small wave function overlap with non-interacting fermions.

In momentum space

$$\Psi_{untrapped}(\mathbf{p}) = \begin{cases} \frac{e^{-bp}}{p^2}, & p \neq 0 \\ \psi_0, & p = 0 \end{cases}$$

Improvement: N-body correlators



Blue: products of single-fermion wave function (momentum eigenstate)

Red: $\dfrac{e^{-bp}}{p^2}$

Purple: $\dfrac{1}{\lambda\text{-}\mathrm{Exp}[-p^2/M]}$

Large overlap of the wave function significantly improves the results.

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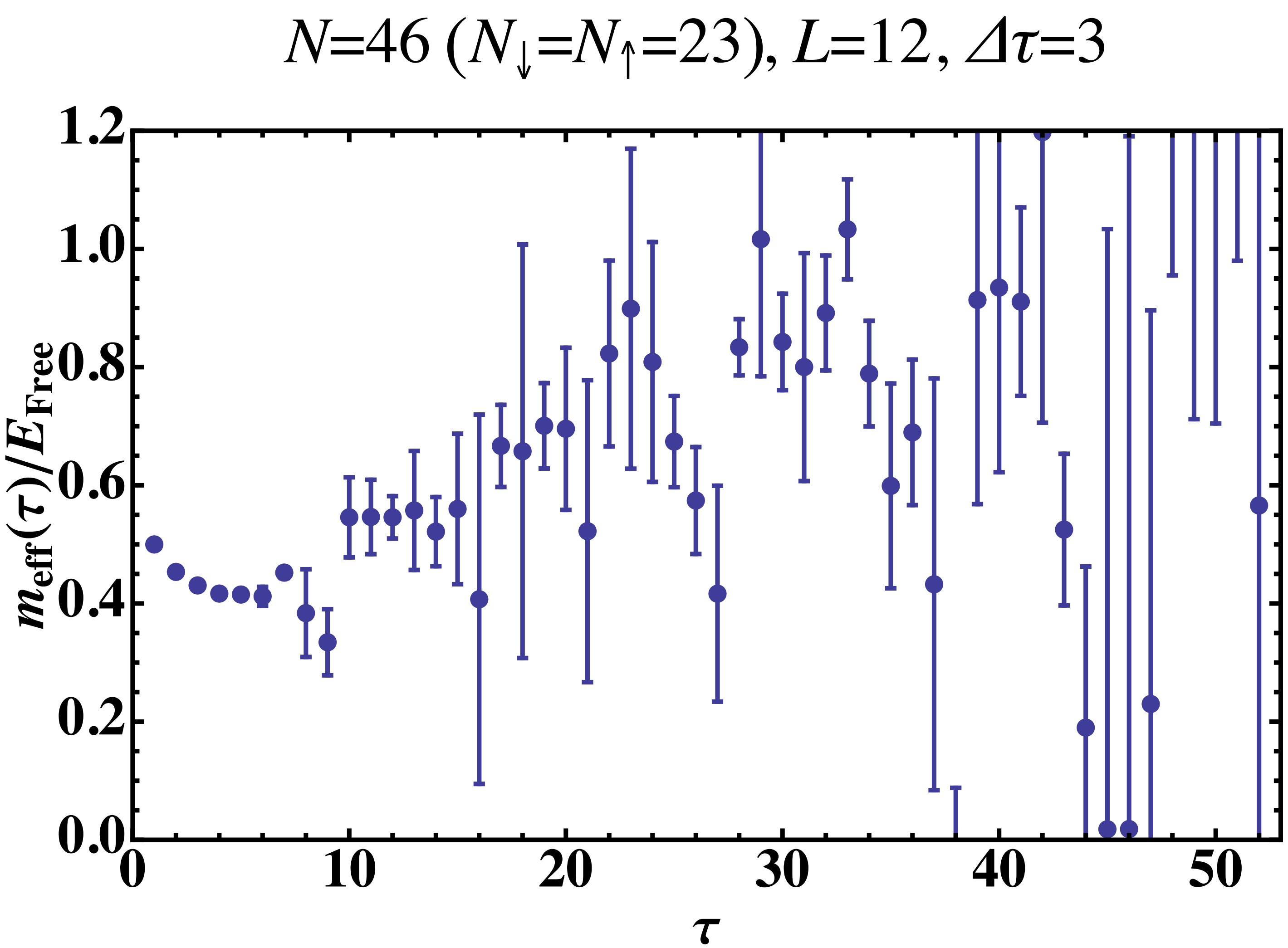
Statistical noise & overlap problems



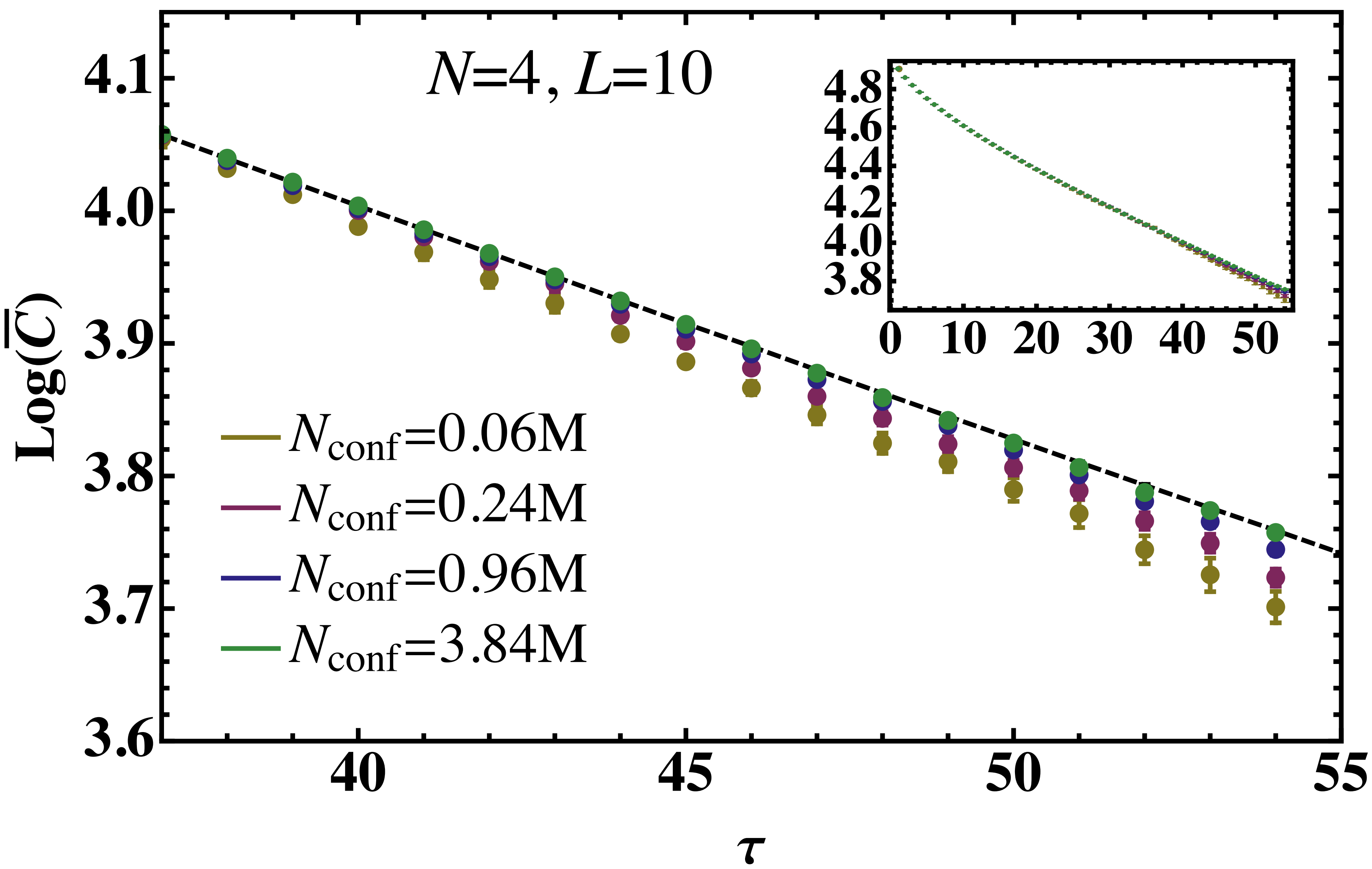
40M configs

- Noise & drifted upward at large Euclidean time

→ ***no plateau***

- Worse for larger number of fermions

Conventional method for small N

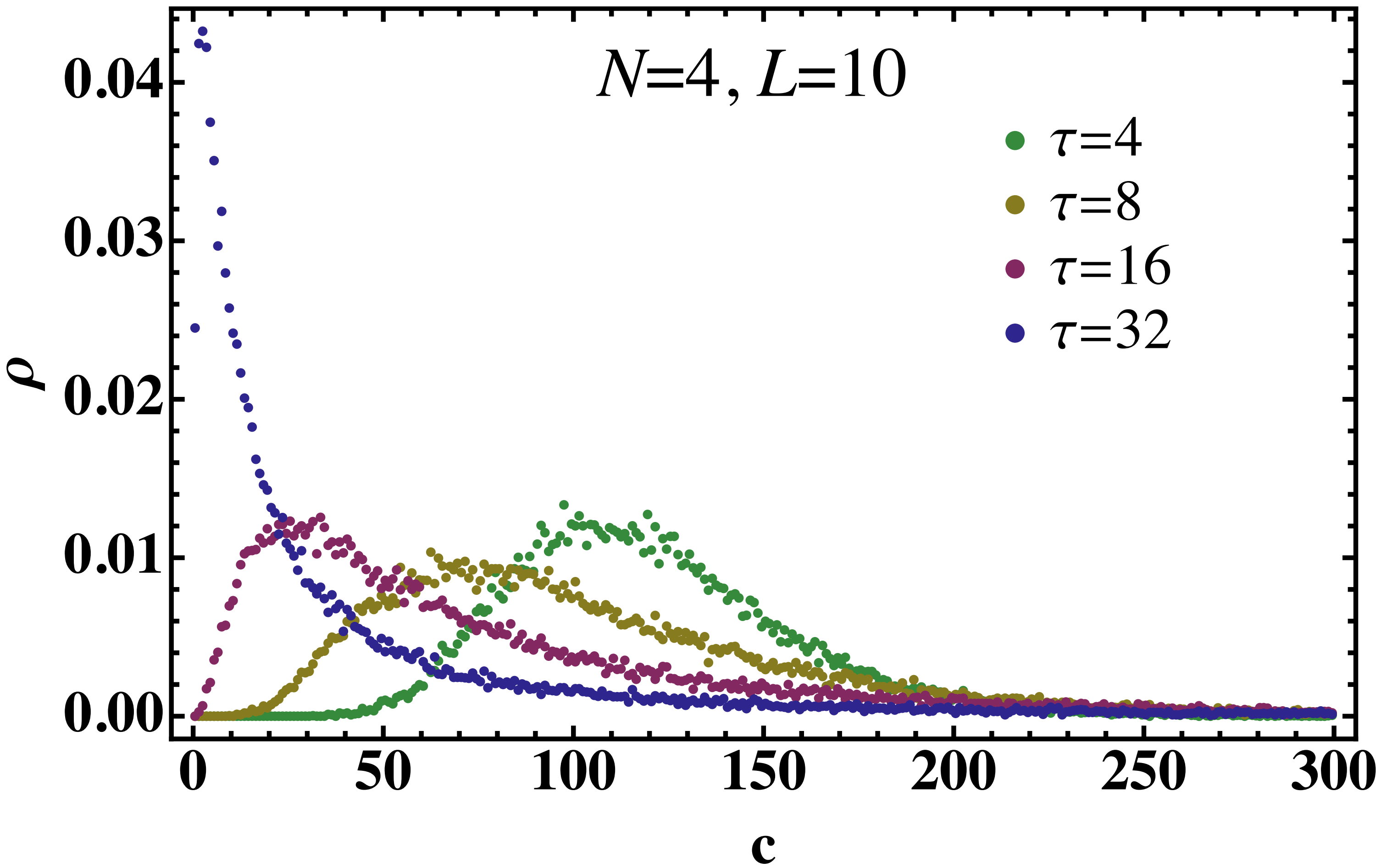


Dashed line: 2 billion configurations

Good agreement for ~4M configurations, but systematically deviated for smaller number of configurations

The error bar doesn't represent the uncertainty of the estimator correctly.

Correlator distribution



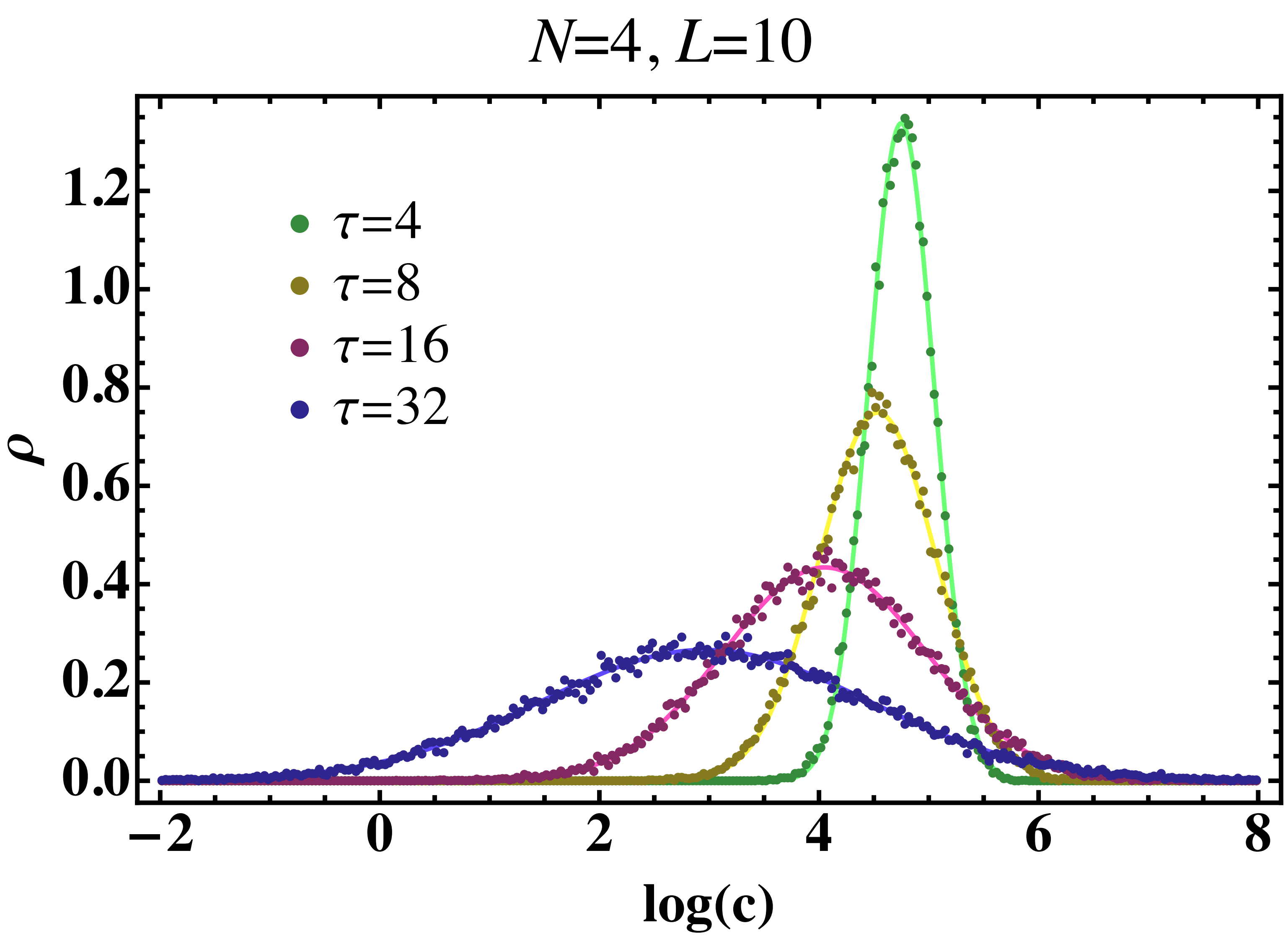
long tails at late times

Most configurations are far off the true ground state.

Insufficient sampling for the long tail leads to the shift in the true ground state energy.

Distribution overlap problem

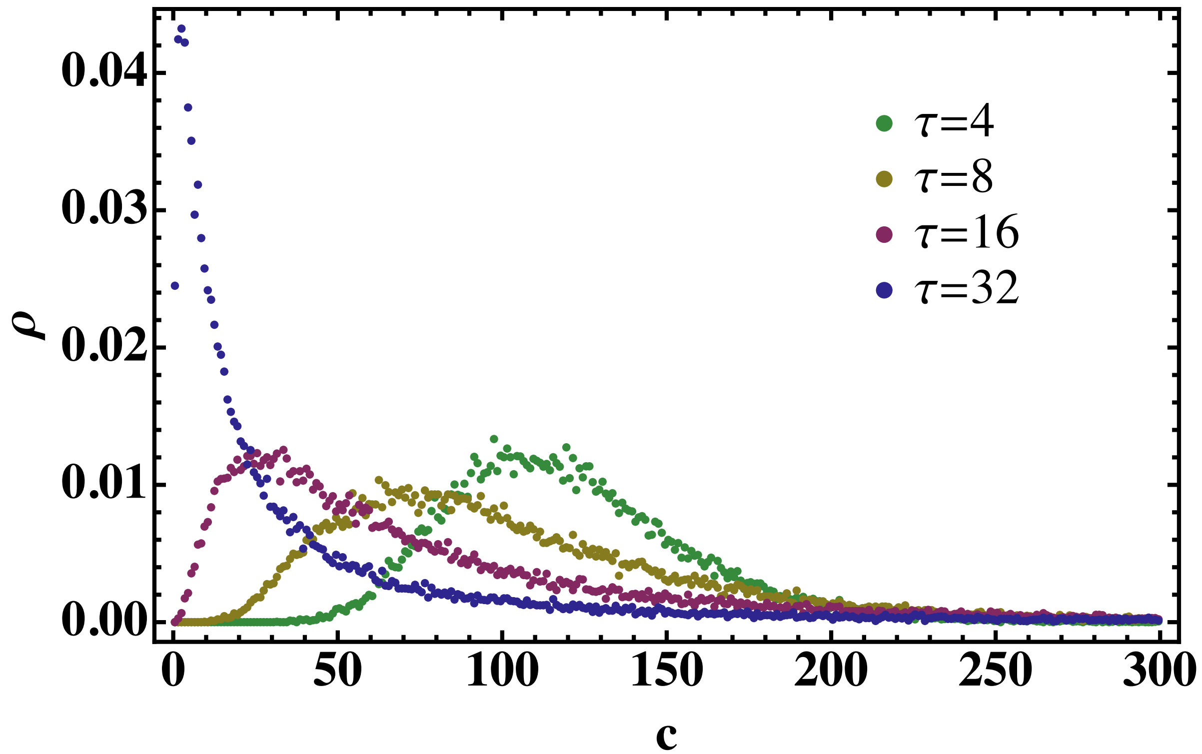
Log-correlator distribution

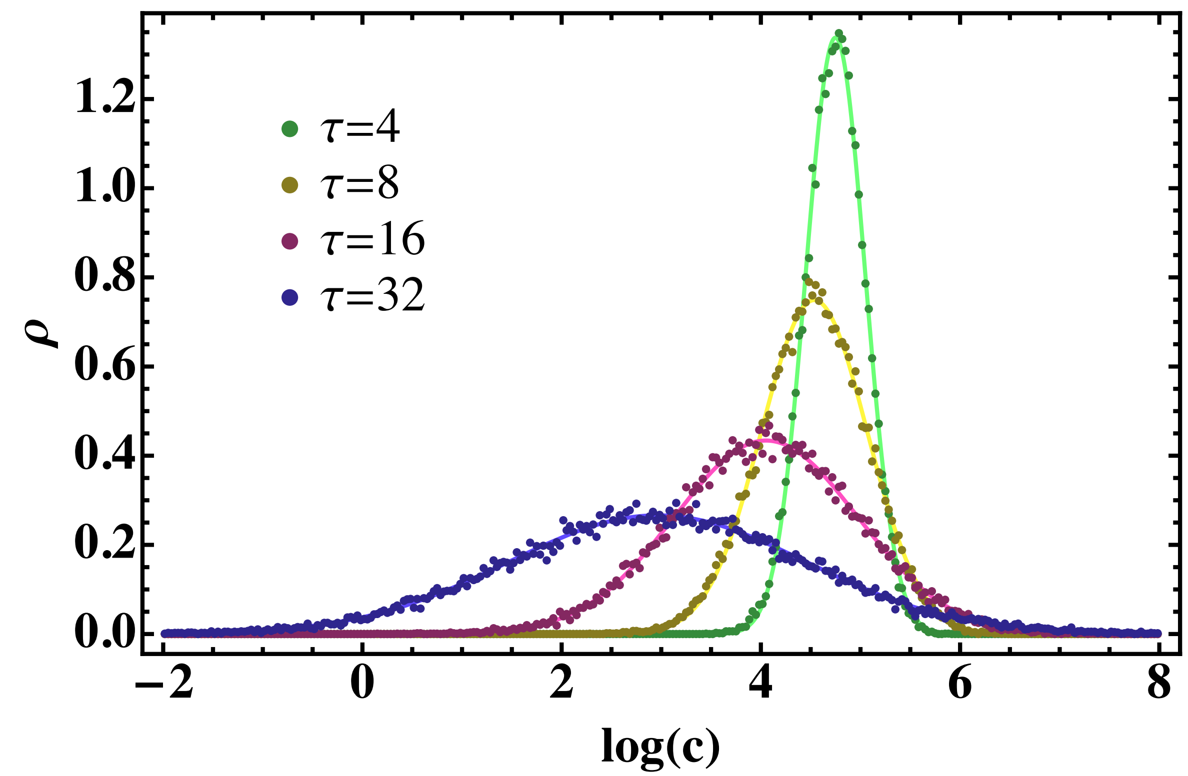


Solid lines: Gaussian fits

Conventional sample average and the estimate of errors by standard deviation work well.

Log-normal distribution?





Log-normal ?

Normal ?

not exactly

cf: Product of random numbers has a log-normal distribution.

Cumulant expansion

- *General relation between* ln<C> *and* <ln C>

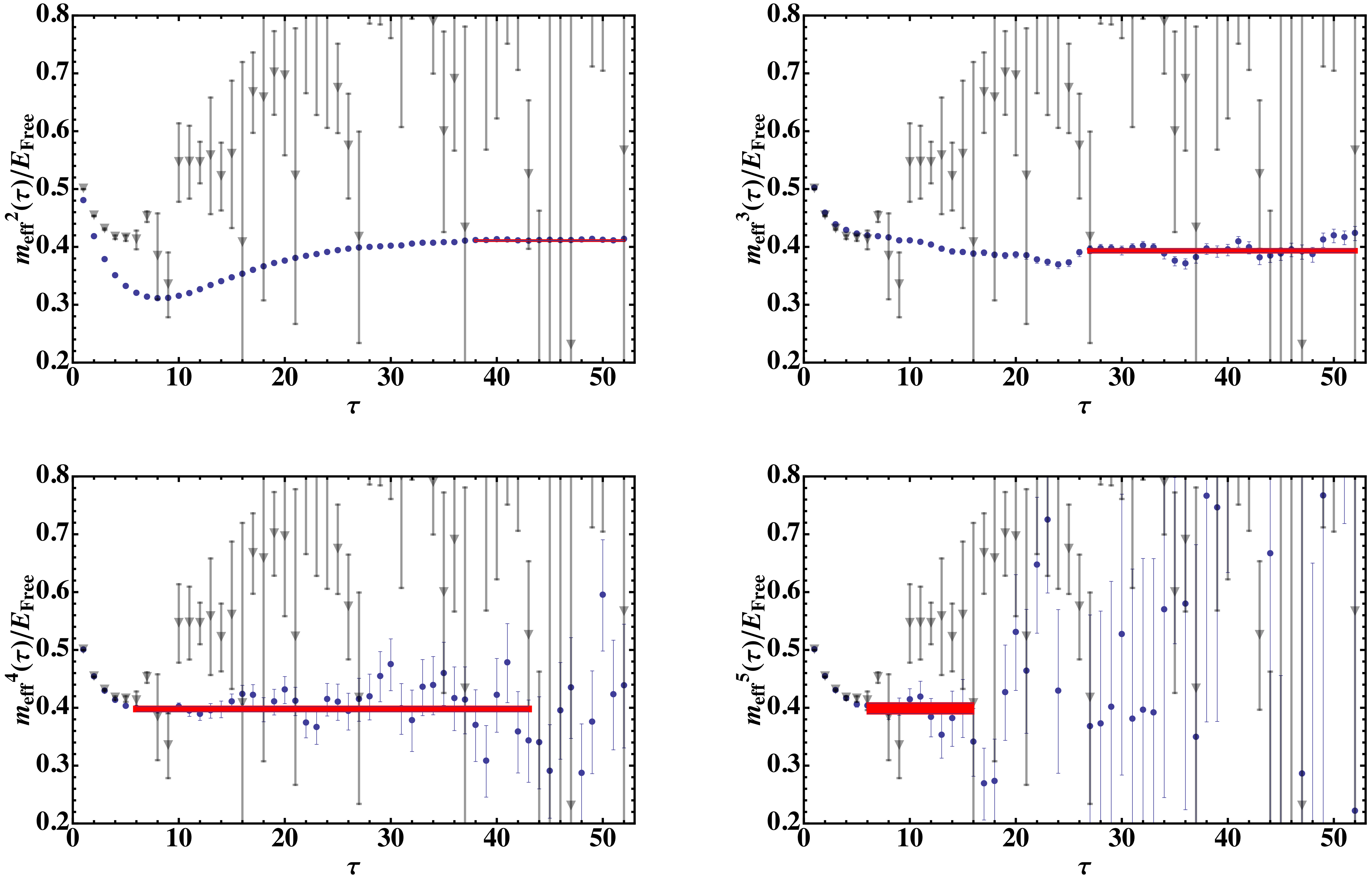
$$\ln\langle C\rangle = \sum_{n=1}^{\infty} \frac{\kappa_n}{n!};$$

where $\kappa_1 = \langle \ln C\rangle, \qquad \kappa_2 = \langle (\ln C)^2\rangle - \langle \ln C\rangle^2, \qquad \text{etc.}$

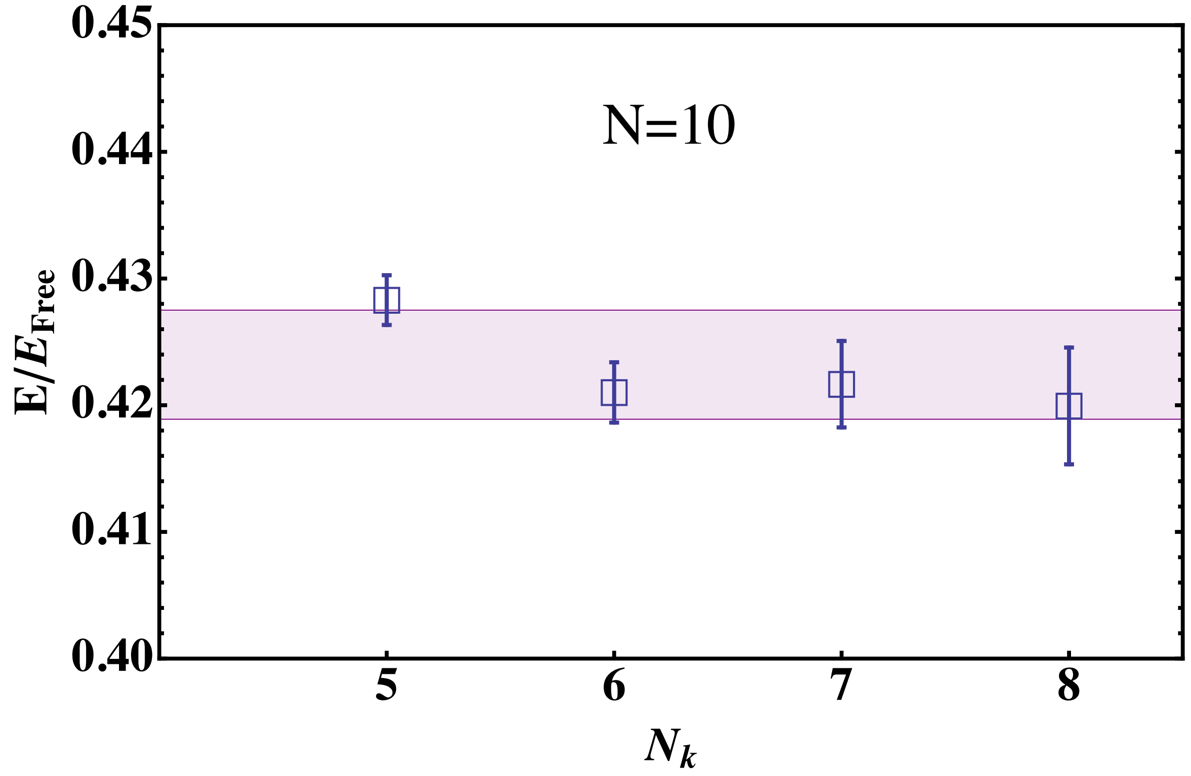
- *Lowest few cumulants don't suffer from the distribution overlap problem & converge quickly.*

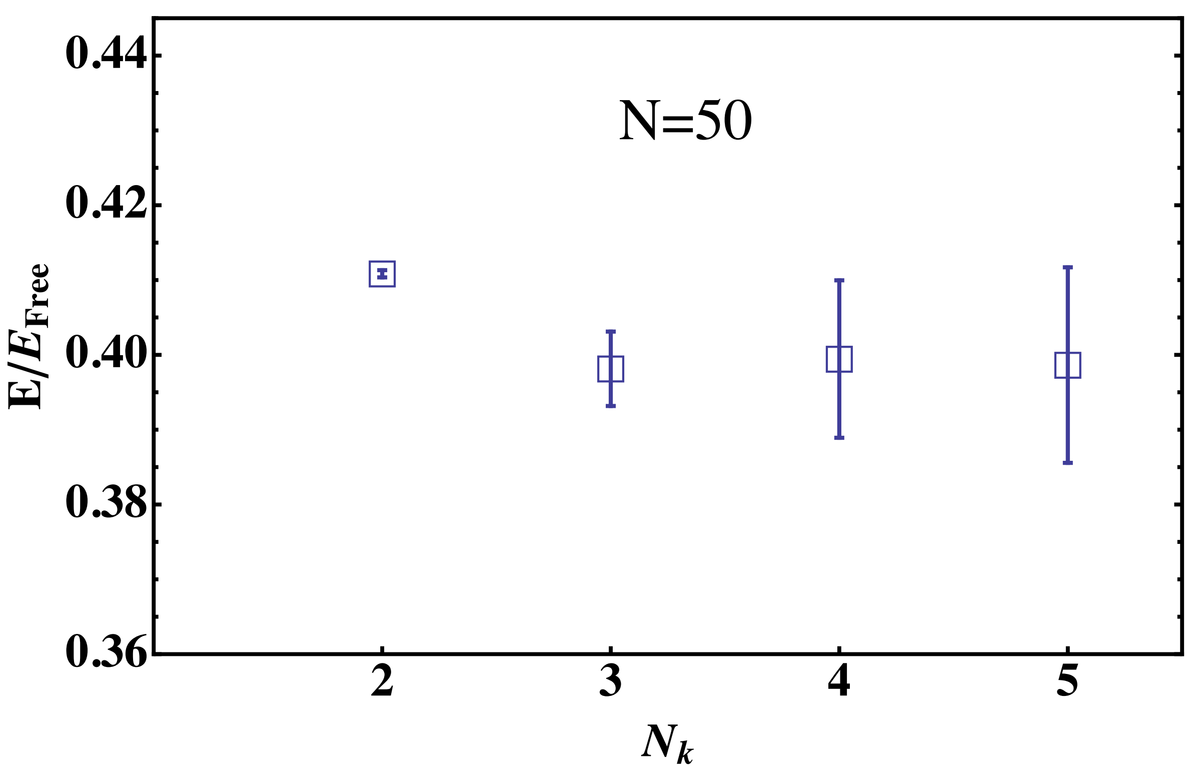
→ *truncate the cumulant expansion at which the statistical error and truncation error are comparable.*

Example: *N=46* unitary fermions



Convergence of cumulant expansion





Purple band represents the energy calculated using conventional method

Ground state energies: (N_{up}+1,N_{down}) unitary fermions

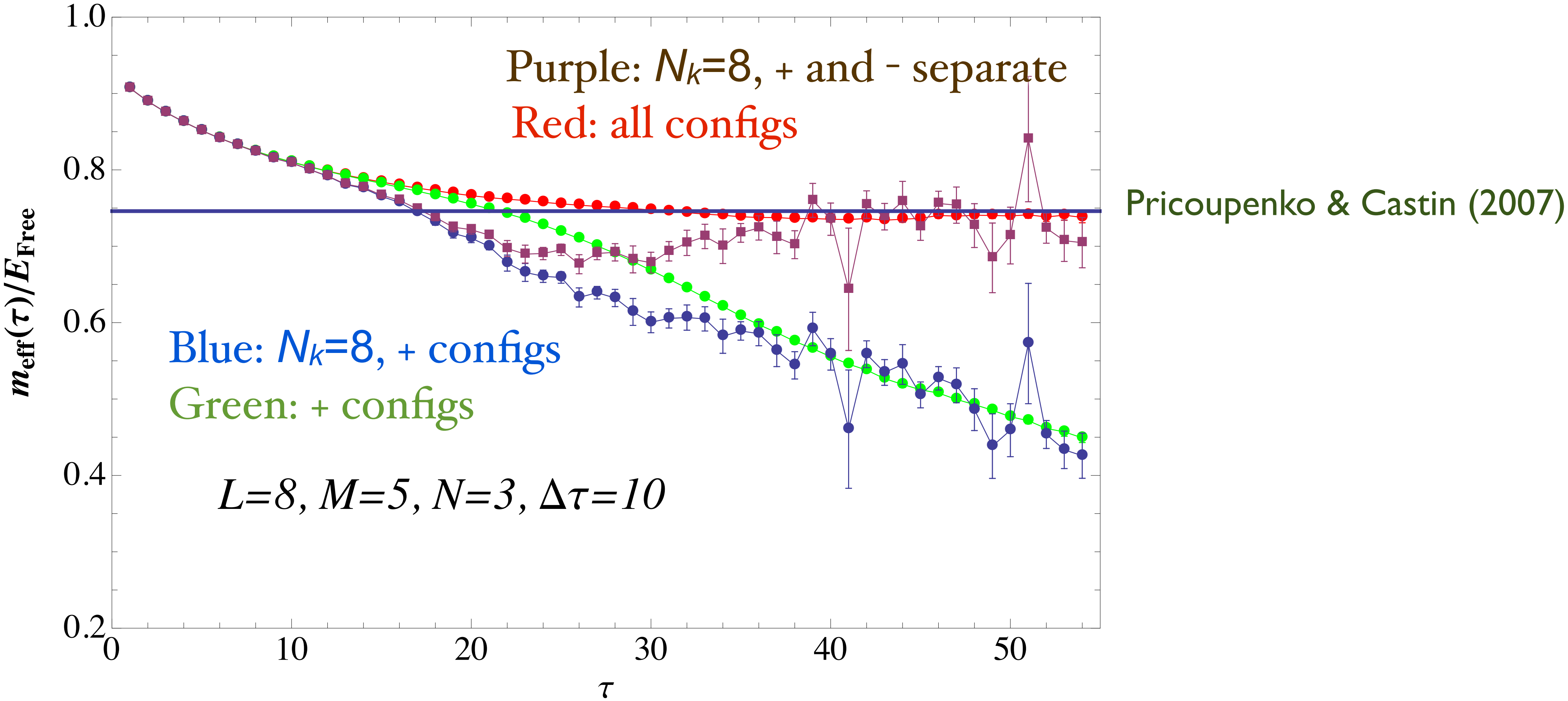
Not all of correlators are positive.

But, the long-tail develops in the distribution for positive correlators.

$$
\begin{aligned}
C_{N_\uparrow,N_\downarrow-1}(\tau) &= \frac{1}{N_\mathrm{c}}\sum_i^{N_c} C_{\phi_i}(\tau) \\
&= \frac{1}{N_\mathrm{c}}\sum_i^{N_\mathrm{c}^-} C^-_{\phi_i}(\tau) + \frac{N_\mathrm{c}^+}{N_\mathrm{c}}\left(\frac{1}{N_\mathrm{c}^+}\sum_i^{N_\mathrm{c}^+} C^+_{\phi_i}(\tau)\right) \\
&= \frac{1}{N_\mathrm{c}}\sum_i^{N_\mathrm{c}^-} C^-_{\phi_i}(\tau) + \frac{N_\mathrm{c}^+}{N_\mathrm{c}}\mathrm{Exp}\left[\sum_n^{\infty}\frac{\kappa_n^+(\tau)}{n!}\right]
\end{aligned}
$$

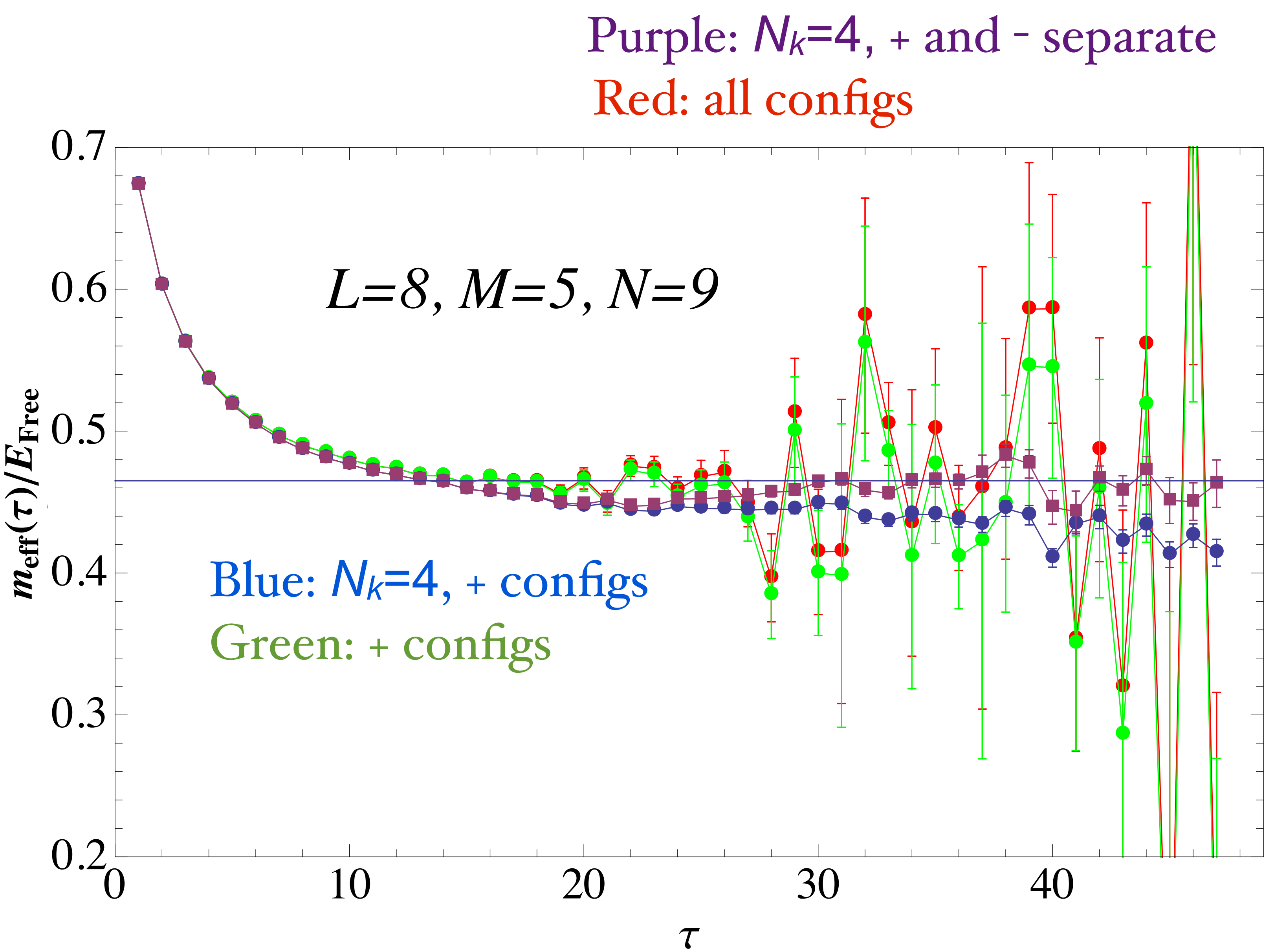
$\kappa_n^+(\tau)$ is the n-th cumulant of the distribution for $\ln C_\phi^+(\tau)$.

Ground state energies: (N_{up}+1,N_{down}) unitary fermions



For positive configurations cumulant expansion method and the conventional approach agree to each other at large Euclidean time, so do for all configurations.

Ground state energies: (N_{up}+1,N_{down}) unitary fermions



A contribution from negative correlators is getting smaller as the number of fermions increases.

Outline

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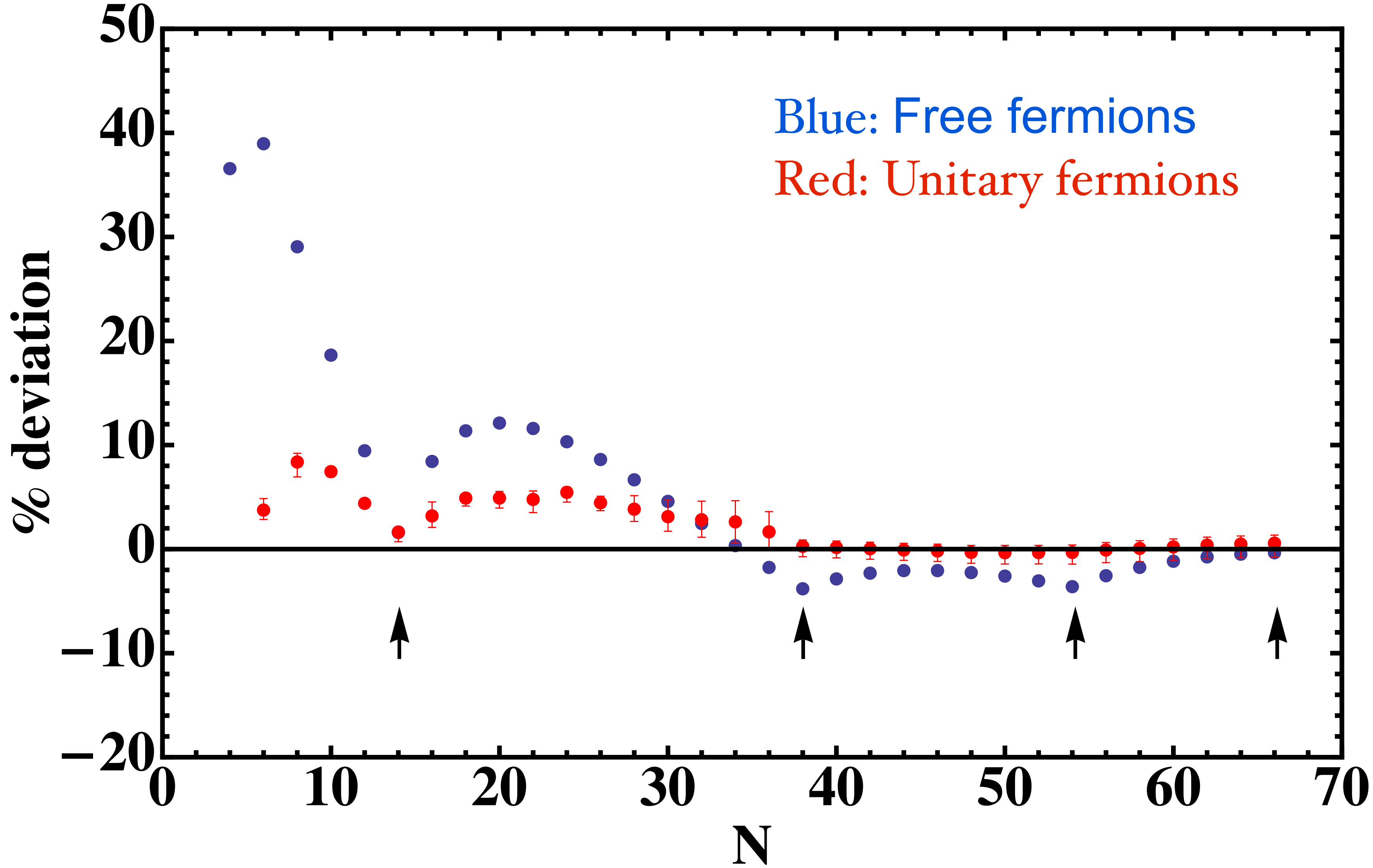
Shell structure at finite N: Bertsch parameter

$$E^{\text{unitary}}(n) = \xi E^{\text{free}}(n)$$

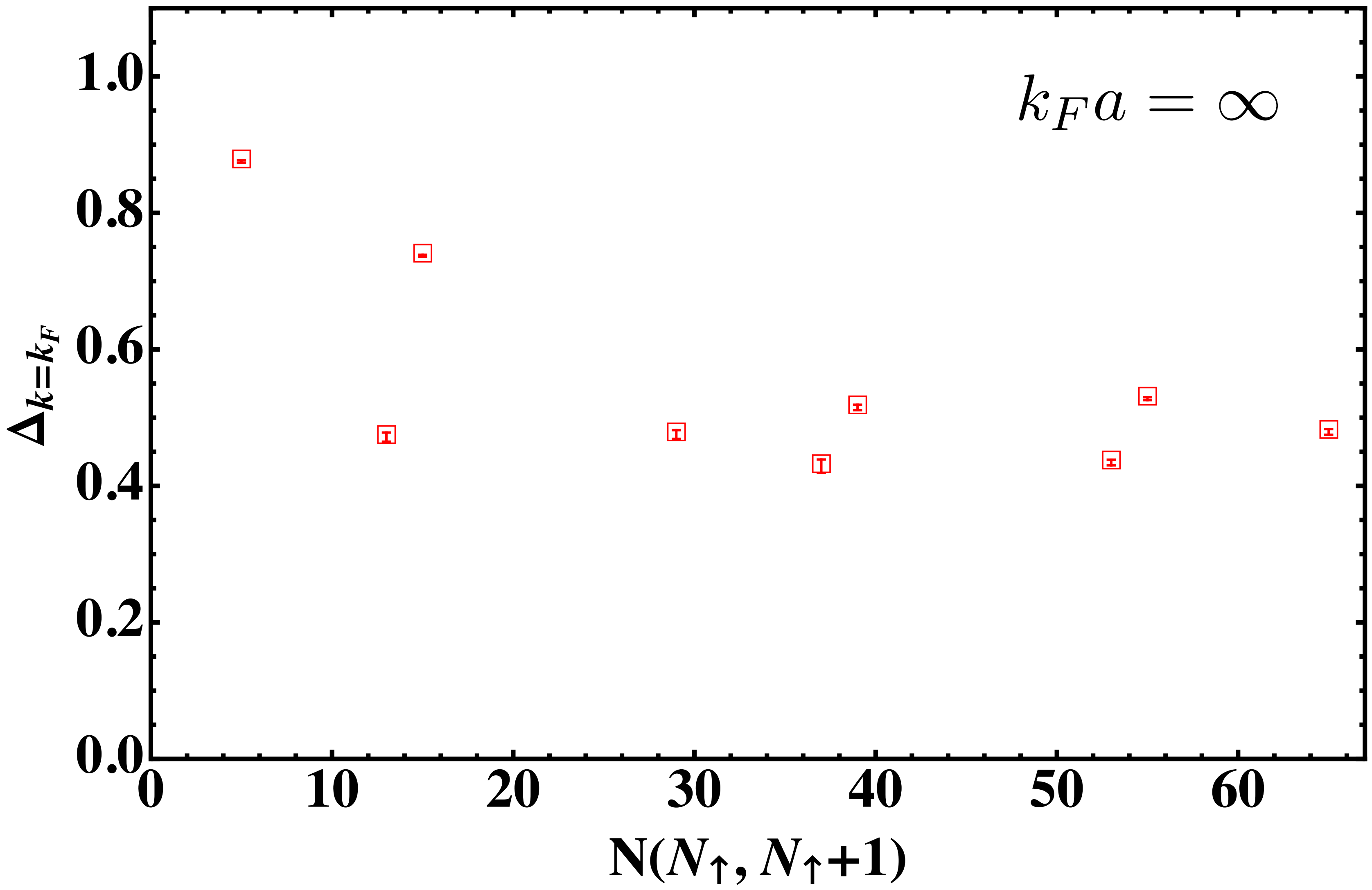


Blue: $\left(1 - \frac{E_F^{\text{finite}}}{E_F^{\text{thermo}}}\right) \times 100$

Red: $\left(1 - \frac{E_{\text{unitary}}^{\text{finite}}}{E_{\text{unitary}}^{\text{thermo}}}\right) \times 100$

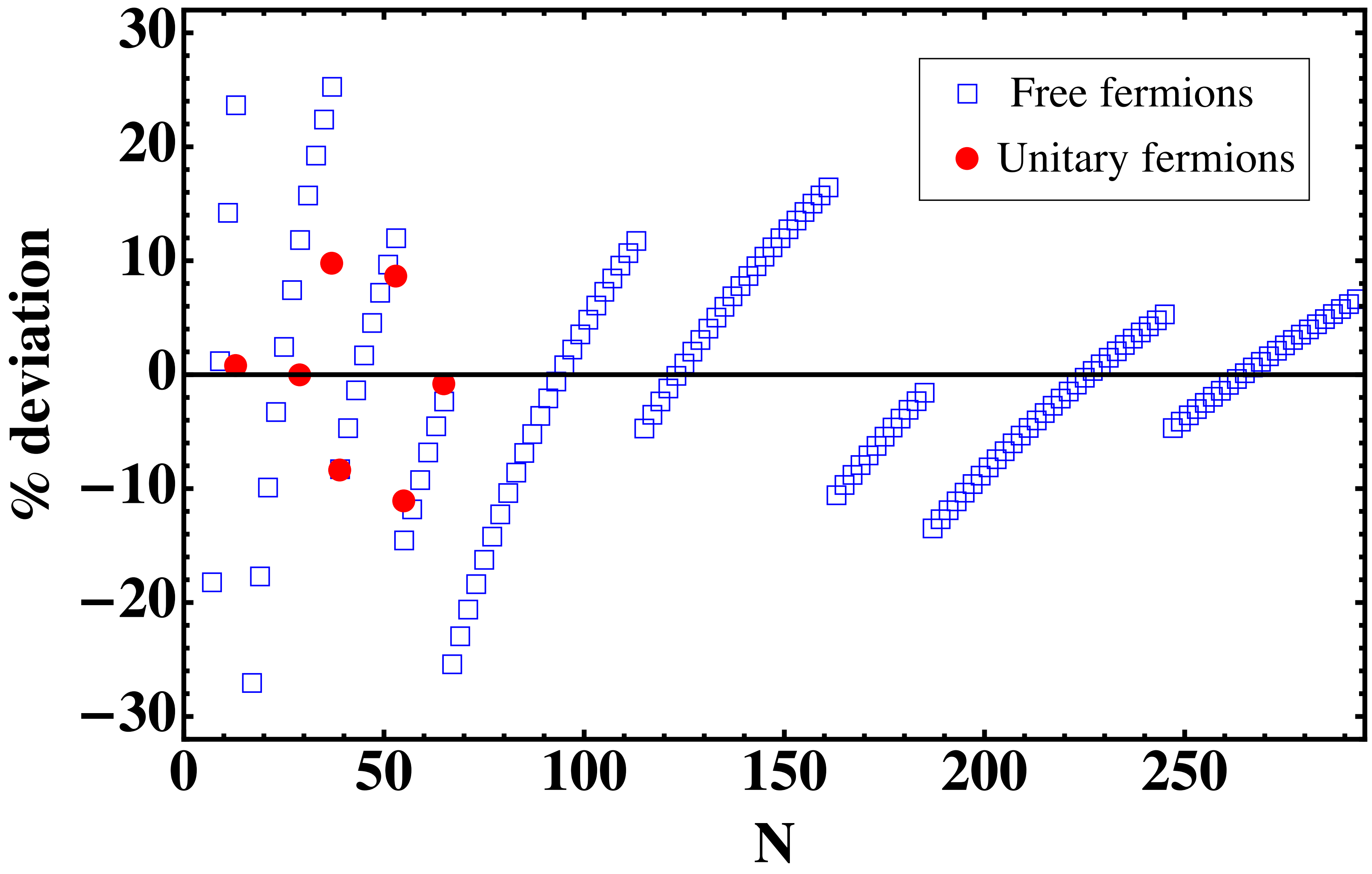
Shell structure at finite N: Pairing gap

$$\varepsilon^{\text{unitary}}(n) = \Delta\varepsilon_F^{\text{free}}(n)$$



$$\varepsilon^{\text{unitary}}(2N_\uparrow + 1) = E(N_\uparrow, N_\uparrow + 1) - \frac{E(N_\uparrow, N_\uparrow) + E(N_\uparrow + 1, N_\uparrow + 1)}{2}$$

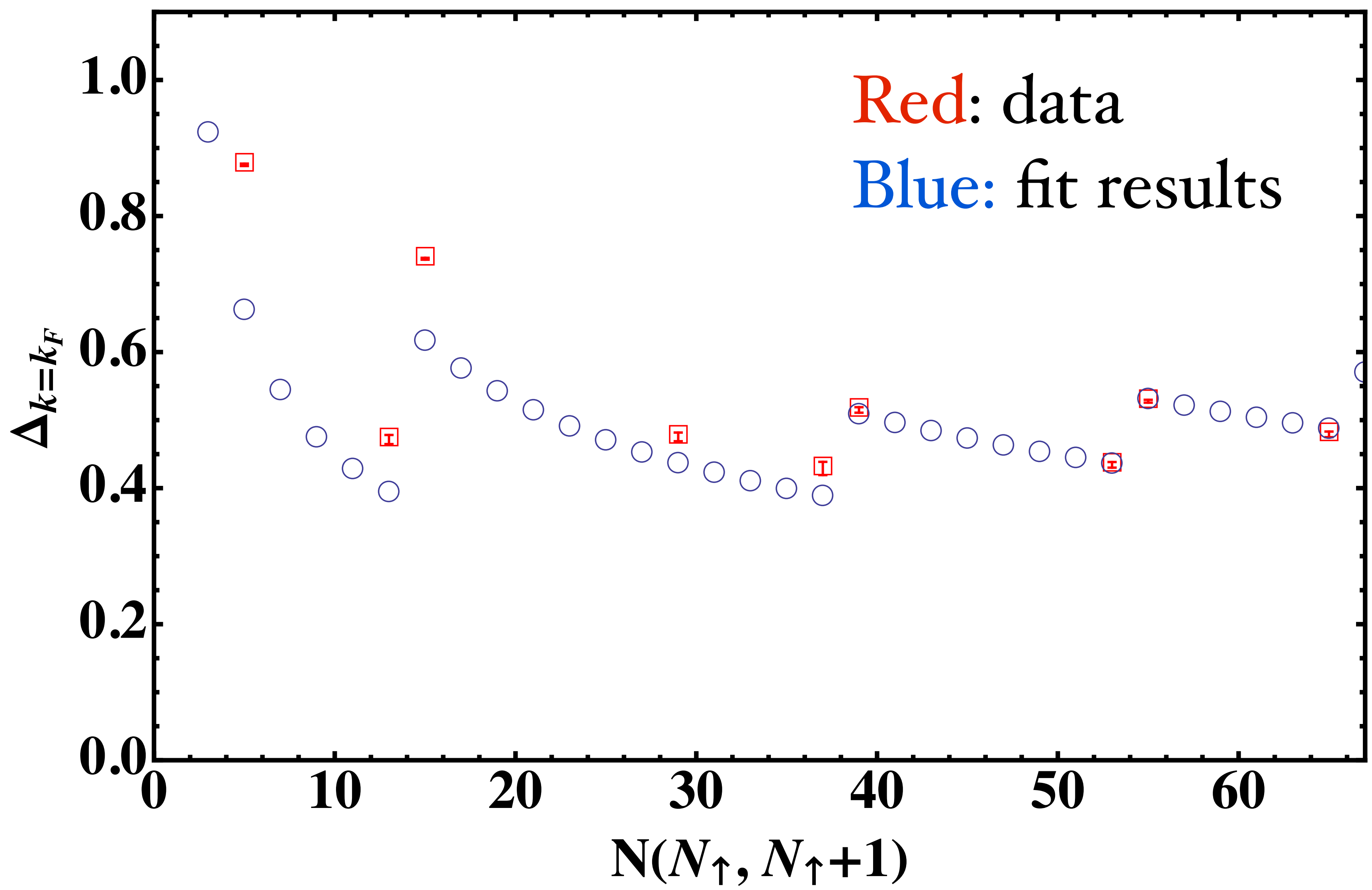
Shell structure at finite N: Pairing gap



Blue: $\left(1 - \frac{\varepsilon_F^{\text{finite}}}{\varepsilon_F^{\text{thermo}}}\right) \times 100$

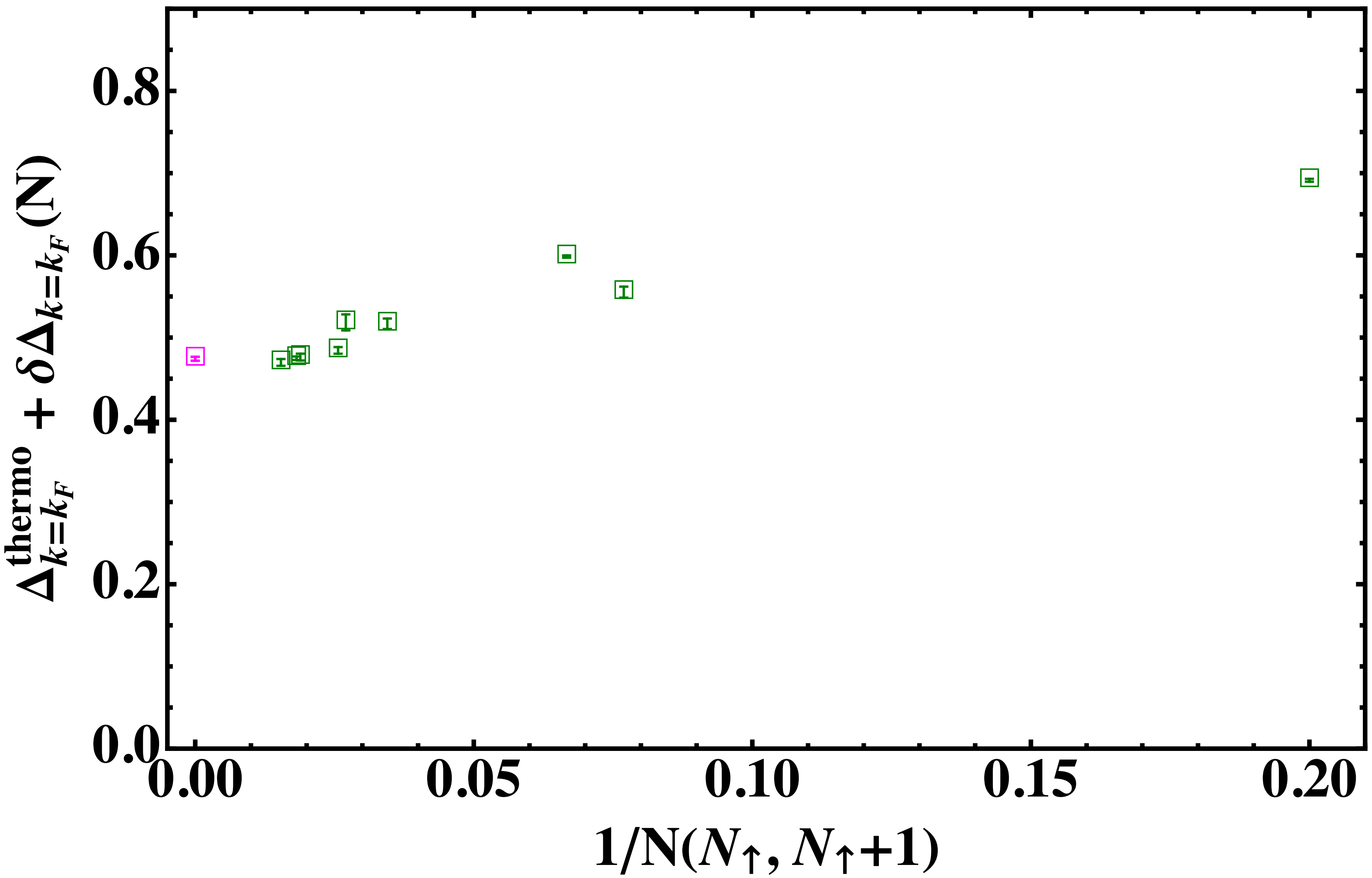
Red: $\left(1 - \frac{\varepsilon_{\text{unitary}}^{\text{finite}}}{\varepsilon_{\text{unitary}}^{\text{thermo}}}\right) \times 100$

Shell structure at finite N: Pairing gap



$$\Delta_{k=k_F}(N) = \Delta_{k=k_F}^{\text{thermo}} + C\left(1 - \frac{\varepsilon_F^{\text{finite}}}{\varepsilon_F^{\text{thermo}}}\right)$$

Finite N correction and thermodynamic limit



$$\delta\Delta_{k=k_F}(N) = \Delta^{\mathrm{Fit}}_{k=k_F}(N) - \Delta^{\mathrm{data}}_{k=k_F}(N)$$

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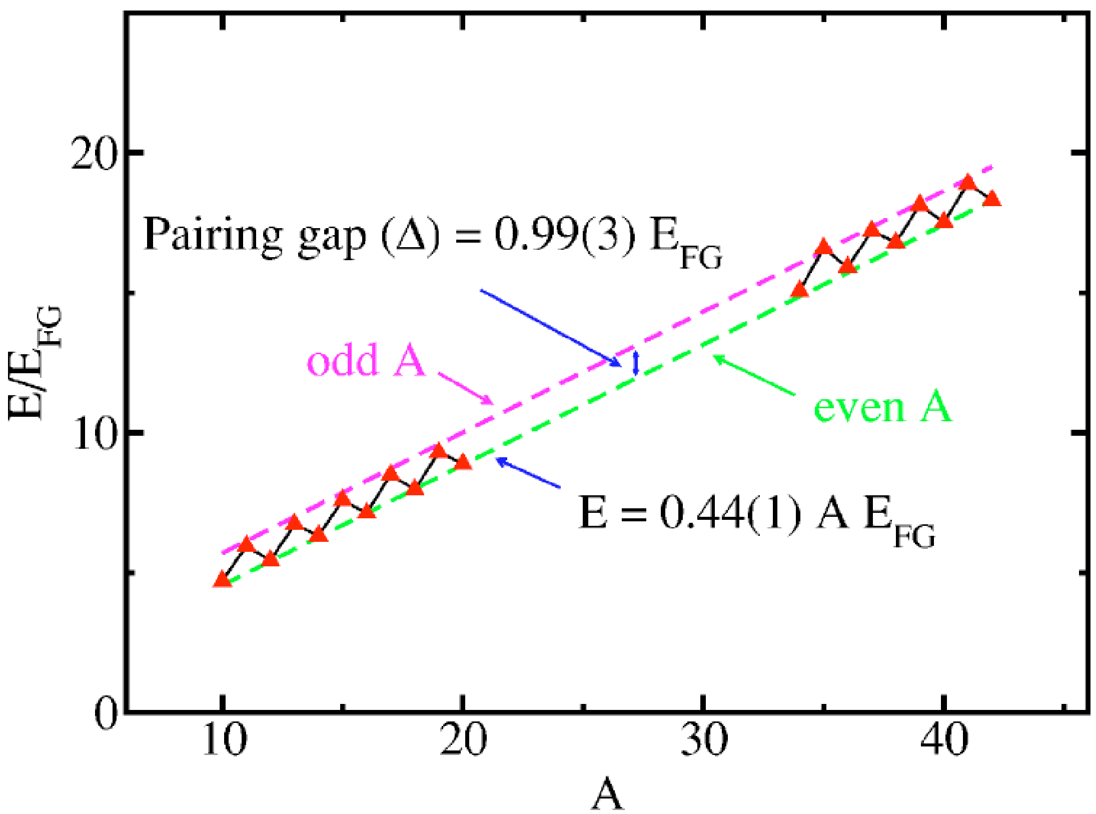
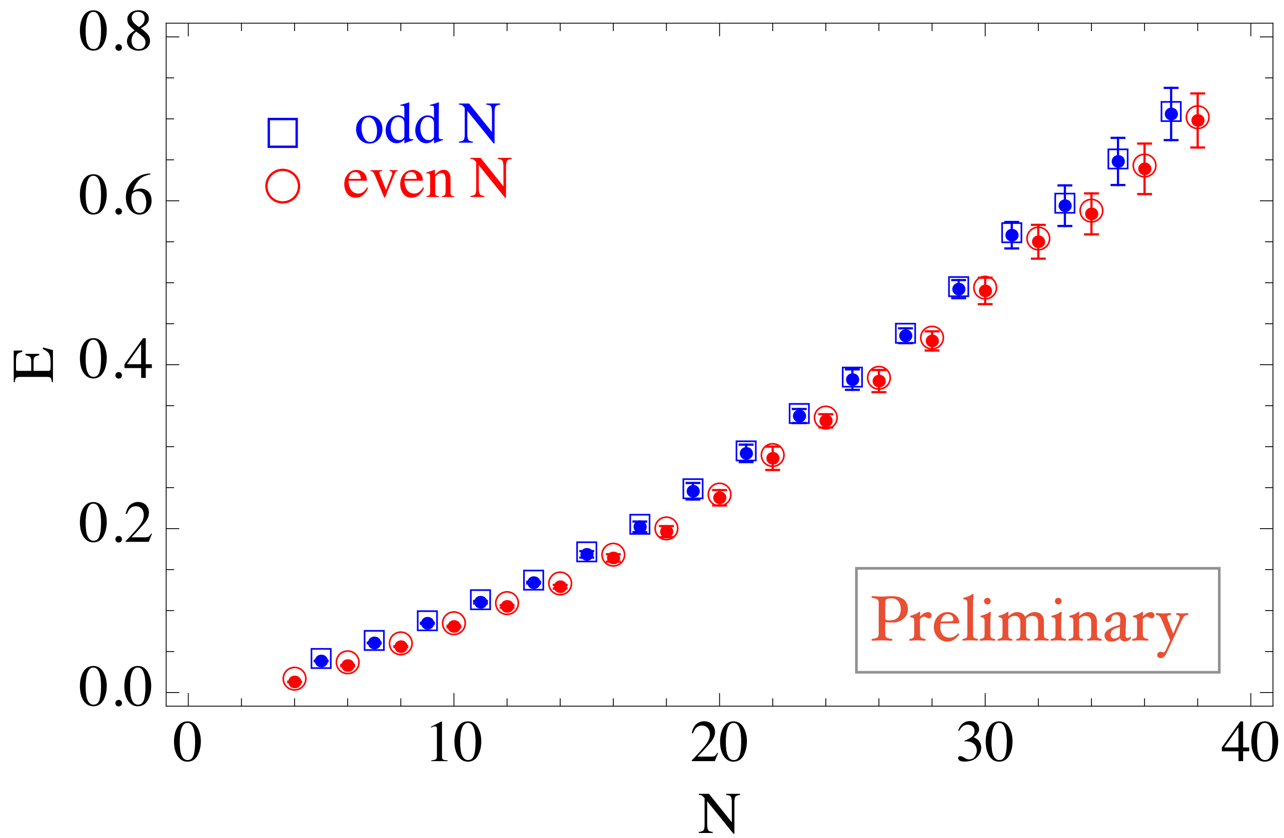
Odd-even Staggering at unitarity



Carlson, Chang, Pandharipande & Schmidt, Phys. Rev. Lett. 91, 050401 (2003)

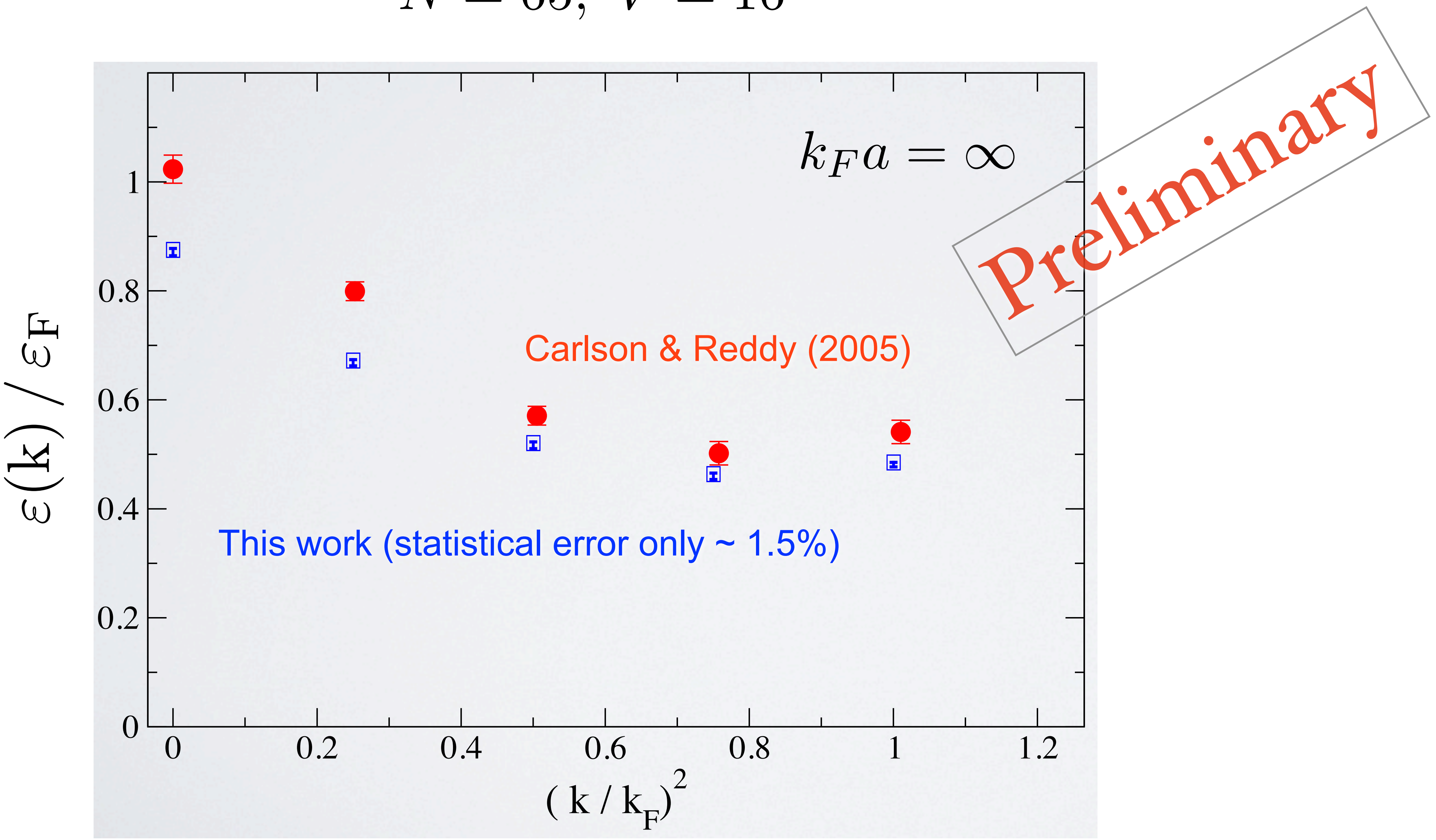


Endres, Kaplan, JWL & Nicholson, PoS Lattice2010 197, (2010)

Odd-even staggering in the ground state energies of unitary fermions has been found both in QMC and Lattice MC calculations.

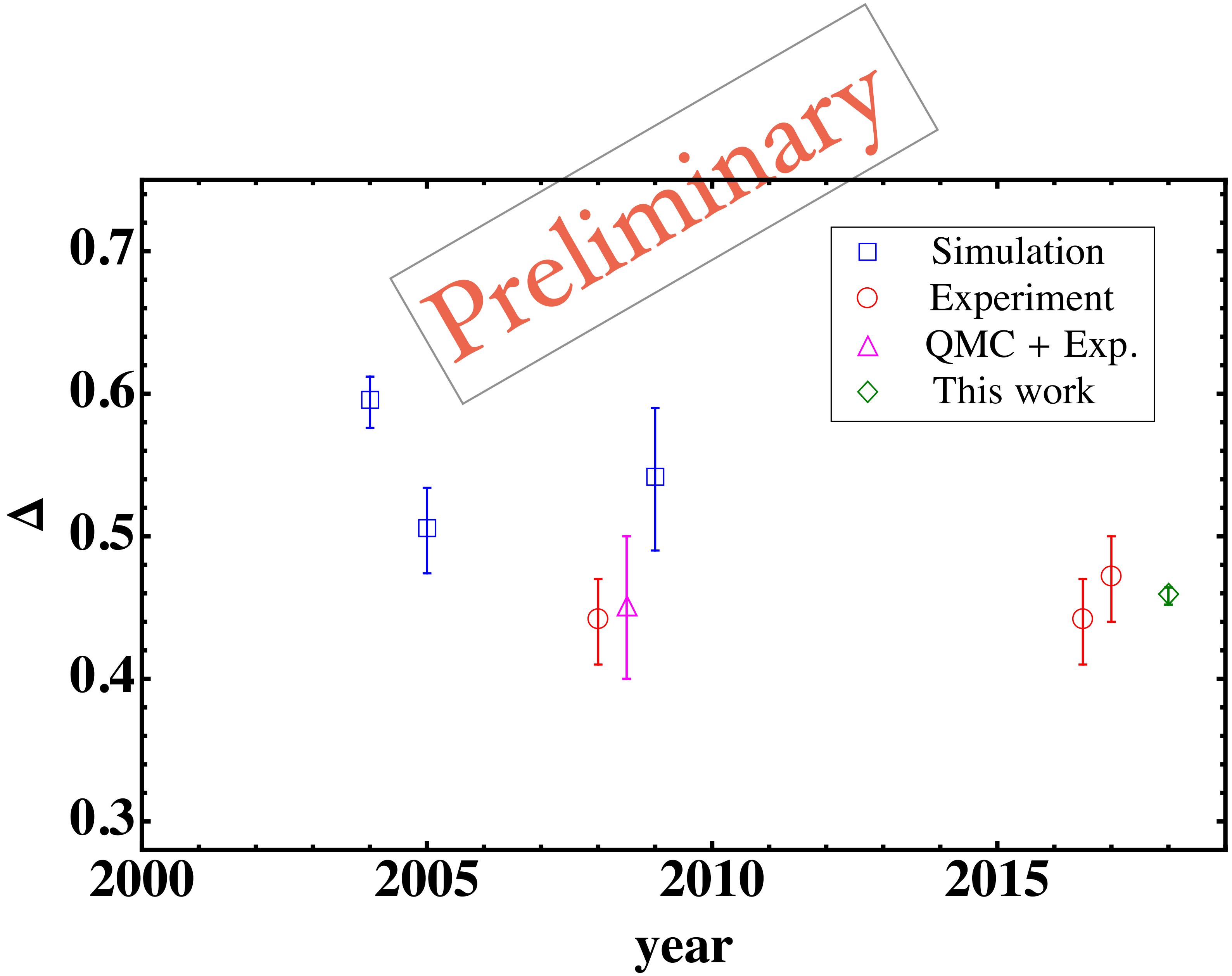
Single particle dispersion relation at unitarity

$$N = 65,\ V = 16^3$$



Preliminary result from the ensemble with largest N and V shows that the pair-breaking energies are lower than QMC results for all *k*.

Chronology of Pairing gap at unitarity



- Carlson, Chang, Pandharipande & Schmidt, Phys. Rev. Lett. 91, 050401 (2003)
- Carlson & Reddy, Phys. Rev. Lett. 95, 060401 (2005)
- Bulgac, Drut, Magierski, & Wlazlowski, Phys. Rev. Lett. 103, 210403 (2009)
- Carlson & Reddy, Phys. Rev. Lett. 100, 150403 (2008)

- Ketterle et al, Phys. Rev. Lett. 101, 140403 (2017)
- Horikoshi et al, Phys. Rev. X 7, 041004 (2017)
- Hoinka et al, Nature 13, 943-946 (2017)

Outline

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Summary and conclusions

- Highly improved lattice technique for strongly interacting non-relativistic fermions at unitarity

  - eliminate finite lattice spacings/finite volume effects systematically

  - improve the overlap of the interpolating field

  - use the cumulant expansion method to calculate the energies of ground states with high precision by improving the statistical overlap

- Results of the pairing gap are still preliminary.

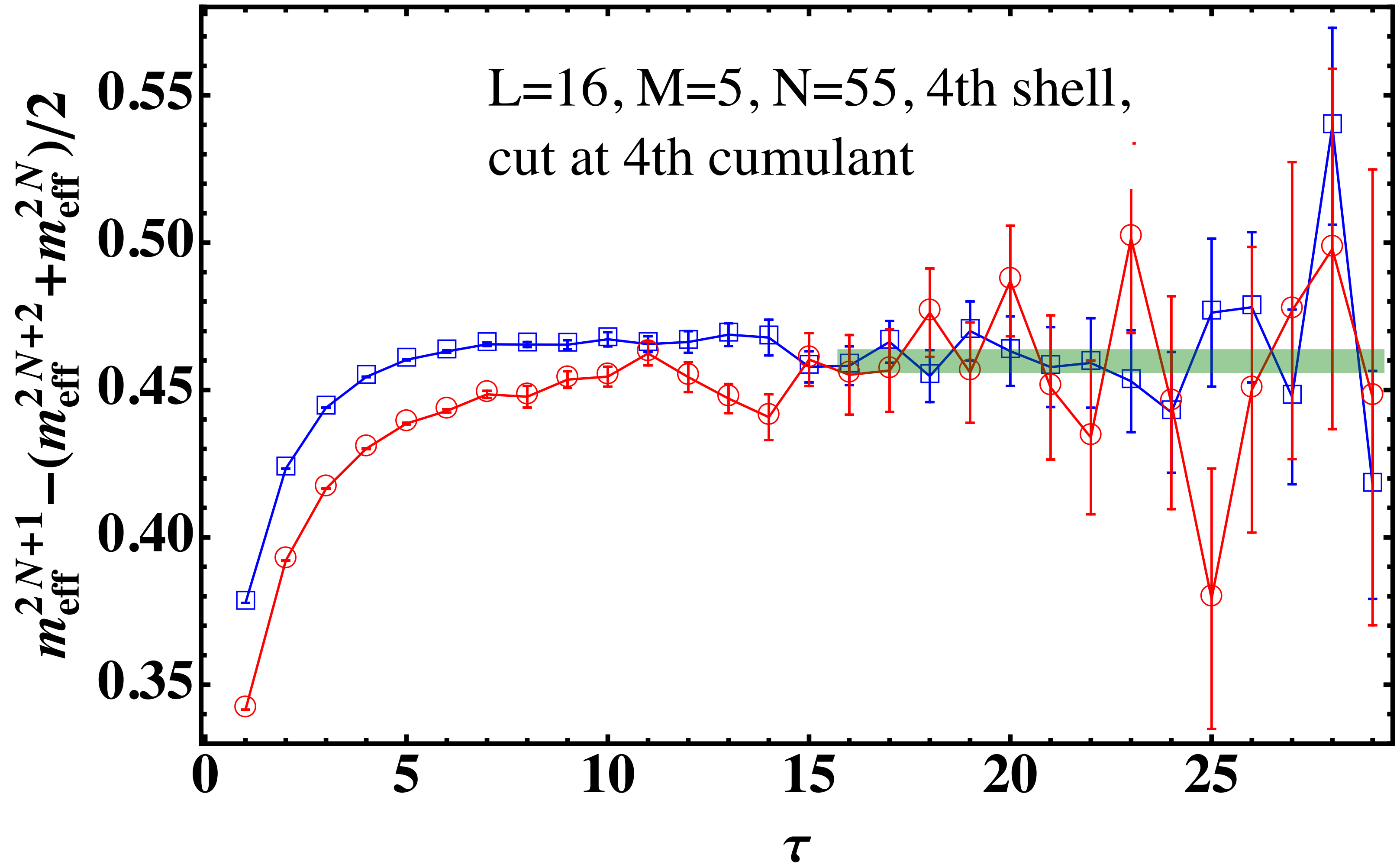
  - agree with the recent cold-atom experiments

  - take account for the finite V and N effects carefully

Thanks!

Backup

Effective mass plot of single particle excitation



Red and blue colors denote two different sinks.

No source dependence at large Euclidean time.

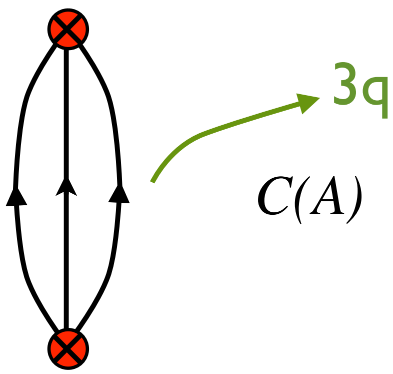
Signal-to-Noise (S/N) problems in numerical simulations of many-body quantum systems

- **Lattice QCD calculation for many baryons (a canonical approach with zero chemical potential)**

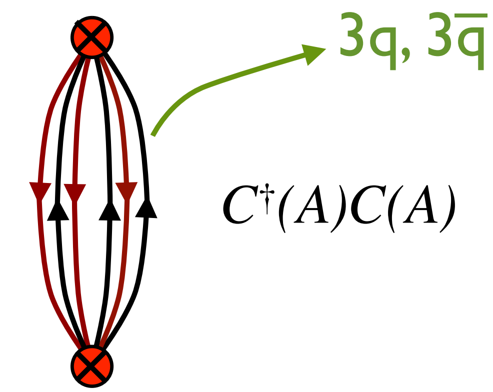
Estimate of A-baryon correlation function:

$$\langle C_A \rangle \sim e^{-M_A \tau} \qquad \sigma^2 = \frac{1}{\mathcal{N}}\left(\langle C_A^\dagger C_A\rangle - \langle C_A^\dagger\rangle\langle C_A\rangle\right) \sim \frac{1}{\mathcal{N}} e^{-3Am_\pi \tau}$$

Mean



Variance



S/N ratio: $$\mathcal{R} = \frac{\langle C_A \rangle}{\sigma} \sim \sqrt{\mathcal{N}} e^{-A(M_A - 3/2 m_\pi)\tau}.$$

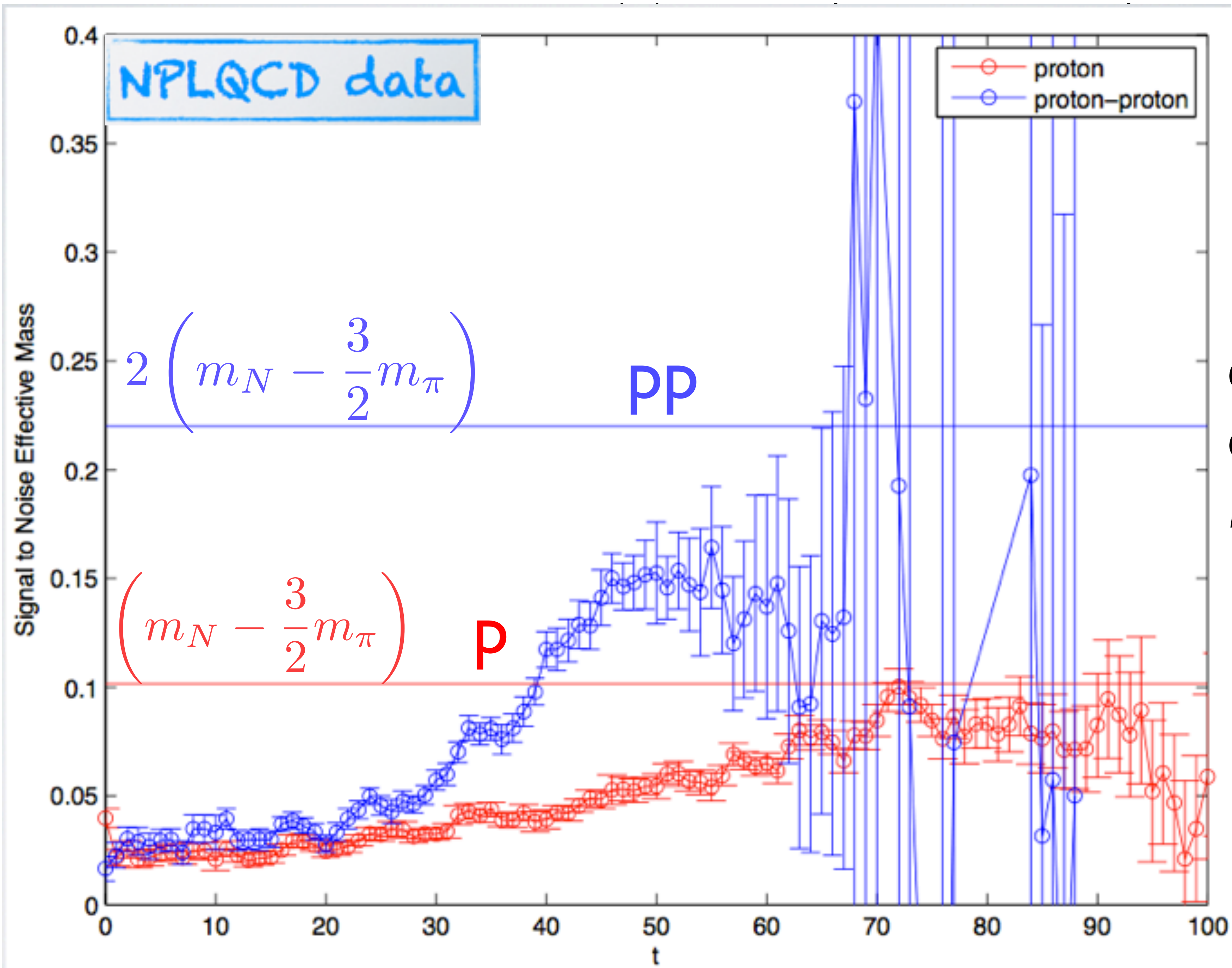
P. Lepage (1989)

closely related to the Sign problem of lattice QCD with a finite chemical potential starting at $\mu = m_\pi/2$

P. E. Gibbs (1986)

Actual QCD data

Signal to noise: $$-\frac{1}{t}\ln\frac{\sigma(t)}{\bar{x}(t)} \sim A\left(m_N - \frac{3}{2}m_\pi\right)$$



qualitatively agrees with Lepage argument

Why do log-normal like distribution arise?

Typically, multiplicative stochastic process

Remember that correlators are products of t and N matrices of the form

constant matrix

$$e^{-K}(1-\sqrt{C}\Phi)e^{-K}$$

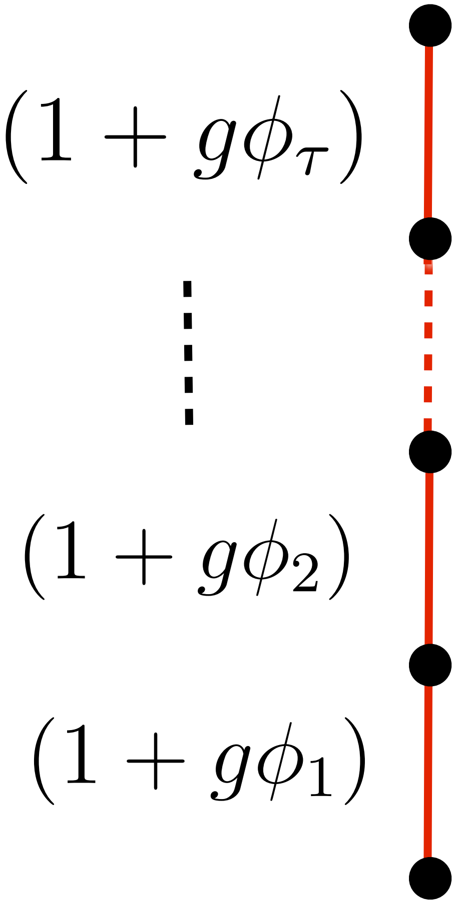
Random diagonal matrix

Little has been known about products of random matrices

⇨ **Toy model - one particle, one spatial site**

Toy model

$$C(\tau) = \prod_{i}^{\tau} (1 + g\phi_i), \quad 0 \le g \le 1$$



Define "Energy" : $\mathcal{E}_\tau = -\frac{1}{\tau} \ln\langle C_\tau \rangle$

- **If** $\phi_i \in [-1, \ 1]$ **,** **then** $\mathcal{E}_\tau = 0$

  Uniform Dist. ***Exact***

- **Analytical result of cumulants of (ln C)**

$$\kappa_1 = \tau \left[\tfrac{1}{2} \log\left(1 - g^2\right) + \frac{\tanh^{-1}(g)}{g} - 1 \right] ,$$

$$\frac{\kappa_n}{n!} = \tau \left(\frac{(-1)^n}{n} - \mathrm{Li}_{1-n}\left(\tfrac{1+g}{1-g}\right) \frac{\left(2\tanh^{-1}(g)\right)^n}{n!} \right) \qquad n > 1$$

Simulation with finite sample size N

- **Measurement of the energy**

conventional method

$$\mathcal{E}_\tau \longrightarrow -\frac{1}{\tau}\left[\frac{1}{N}\sum_{i=1}^{N} C(\tau,\phi_i)\right]$$

truncated cumulant expansion method

$$\mathcal{E}_\tau \longrightarrow -\frac{1}{\tau}\sum_{n=1}^{\infty}\frac{\kappa_n(\tau)}{n!} \qquad \kappa_n(\tau) = \text{cumulants of } \ln C(\tau,\phi)$$

estimate the lowest few cumulants from sample

Then, compare results with exact answers !

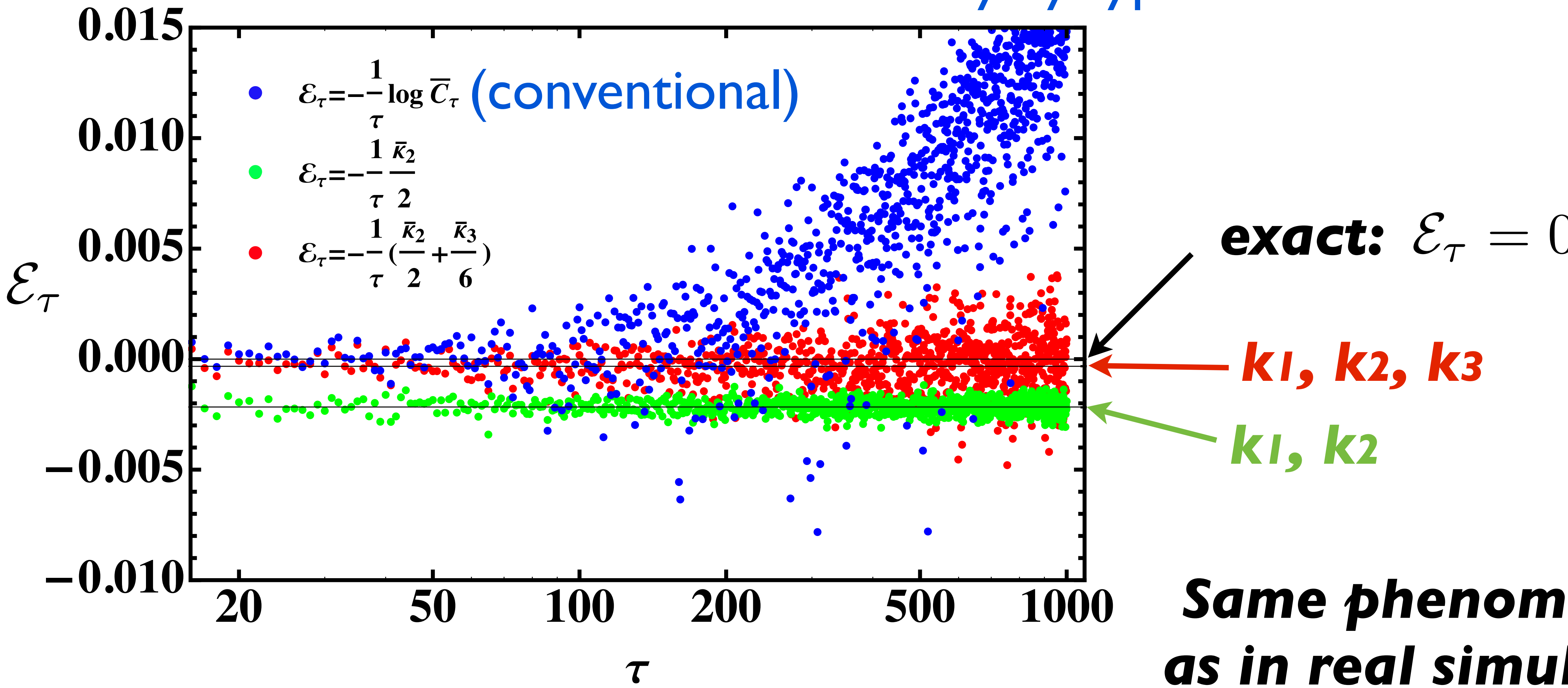
Effective mass plot for toy model

$$C(\tau) = \prod_i^{\tau} (1 + g\phi_i)$$

sample size N=50,000 for each dot

at late t, drift upward & spread

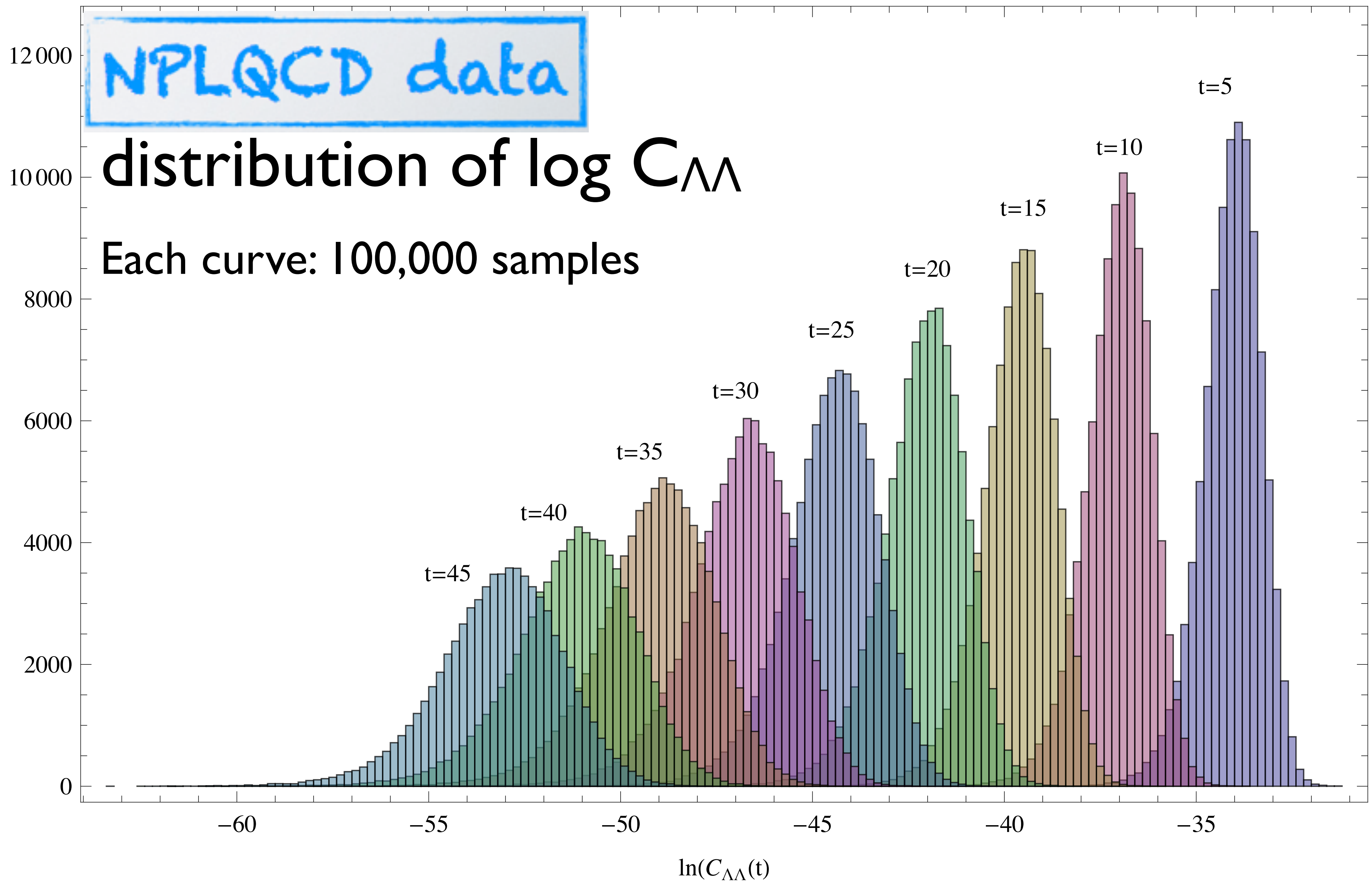
⇨ simulation errors can't be estimated correctly by typical standard deviation



Same phenomenon as in real simulation

Appearance of LN distribution in lattice QCD

Yes, at early time in a Lambda-Lambda correlator



Appearance of LN distribution in lattice QCD

At very late time, however, the distribution of correlator for A baryons presumably goes like a Gaussian with large variance and small mean.

Consider the real part of correlator for A baryons

$$x \equiv Re[C_A(T)]$$

even moments: $\langle x^{2k} \rangle \sim e^{-A3kM_\pi T}$

odd moments: $\langle x^{2k+1} \rangle \sim e^{-AM_N T} e^{-A3km_\pi T}$

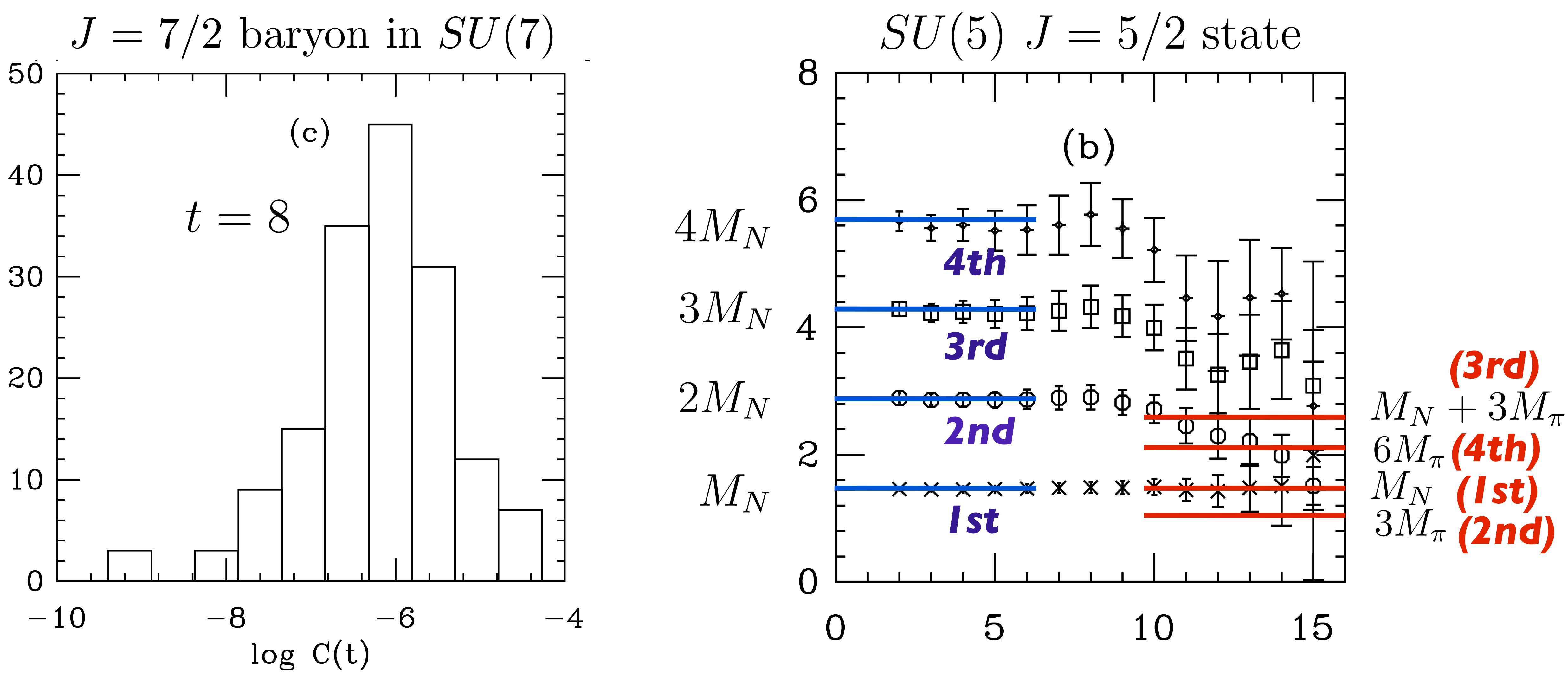
P. Lepage & M. Savage

Since $M_N \gg M_\pi$ **, odd moments die out faster and we expect symmetric distribution at late time.**

Appearance of LN distribution in lattice QCD

Yes, at early time in a SU(N) baryon correlator

T. DeGrand (2012)



Probability dist. ***Mass spectrum of moments***

both k1 and k2 roughly scale ~t

consistent with Lepage argument or just noise?