# Numerical Stochastic Perturbation Theory and The Gradient Flow

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# Motivations

**Goal**: The running coupling of QCD

**Finite-size scaling** techniques provide a general solution to scale-dependent renormalization problems.

(U. Wolff '86; M. Lüscher, P. Weisz, U. Wolff '91)

- The finite-volume scheme i.e. the fields' boundary conditions
  $\rightarrow$ **Schrödinger functional** (K. Symanzik '81; M. Lüscher *et. al.* '92)
- The non-perturbative definition of the coupling
  $\rightarrow$ **gradient flow coupling** (M. Lüscher '10)

**Start:**

- We consider pure $SU(3)$ Yang-Mills theory
- From PT we can obtain important insights into this new tool
  $\rightarrow$ NSPT is a natural framework for the gradient flow!

# The gradient flow coupling

- The **gradient flow** evolves the gauge field as a function of the flow time parameter $t \geq 0$ according to,

$$\boxed{\partial_t B_\mu = D_\nu G_{\nu\mu} + \alpha_0 D_\mu \partial_\nu B_\nu, \quad B_\mu|_{t=0} = A_\mu,}$$

where

$$G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu], \quad D_\mu = \partial_\mu + [B_\mu, \cdot].$$

- Correlation functions of the field $B$ are **automatically finite** for flow times $t > 0$, once the theory in $4d$ is renormalized in the usual way.

(M. Lüscher, P. Weisz '11)

**Energy density**

$$\boxed{\langle E(t) \rangle = -1/2 \, \langle \mathrm{Tr}\, G_{\mu\nu}(t) G_{\mu\nu}(t) \rangle.}$$

- From flow observables one can define a **renormalized coupling**, e.g,

(M. Lüscher '10)

$$\boxed{\bar{g}^2(\mu) \equiv \mathcal{N}^{-1} \langle t^2 E(t) \rangle, \quad \mu = \sqrt{1/8t},}$$

where $\mathcal{N}$ is such that $\bar{g}^2 = g_0^2 + O(g_0^4)$.

# The Schrödinger Functional and $\bar{g}_{\mathrm{GF}}$

- We consider **SF** boundary conditions with **zero boundary fields**, which have to be **maintained** at all flow times $t$.
- To apply **finite-volume scaling**, one has to run the renormalization scale with the size of the finite volume box given by $L$,

$$\boxed{\mu = 1/L,}$$

  and rescale with $L$ all dimensionful parameters, e.g.,

$$\boxed{c = \sqrt{8t}/L, \quad T = L.}$$

(Z. Fodor *et. al.* '12; P. Fritzsch, A. Ramos '13)

- A $c$-family of **running couplings** can be introduced as,

$$\boxed{\bar{g}^2_{\mathrm{GF}}(L) \equiv \mathcal{N}^{-1} \langle t^2 E(t, T/2) \rangle \Big|_{t=c^2L^2/8},}$$

  where $\mathcal{N}$ depends on the specific scheme. (P. Fritzsch, A. Ramos '13)

# The gradient flow on the lattice

- The **gradient flow** can be studied on the lattice as,

$$\boxed{\partial_t V_{x\mu}(t) = -\left\{g_0^2 \nabla_{x\mu} S_G(V(t))\right\} V_{x\mu}(t), \quad V_{x\mu}|_{t=0} = U_{x\mu},}$$

  where $\nabla$ is the Lie-derivative on the gauge group, and $S_G$ is, e.g., the Wilson gauge action $\Longrightarrow$ **Wilson flow!** (M. Lüscher '10)

- The **SF boundary conditions** for zero boundary fields, are realized on the lattice as,

$$V_\mu(x + \hat{k}L, t) = V_\mu(x, t),$$
$$V_k(x, t)|_{x_0=0,T} = \mathbb{I}, \qquad \forall t \geq 0.$$

- We consider the regularized energy density,

$$\boxed{\langle \hat{E}(t, x_0) \rangle = -1/2 \left\langle \mathrm{Tr}\, \hat{G}_{\mu\nu}(t, x_0) \hat{G}_{\mu\nu}(t, x_0) \right\rangle,}$$

  where $\hat{G}$ is the **clover** definition of the field strength tensor corresponding to the lattice flow V.

# Numerical Stochastic Perturbation Theory (D. Hesse's talk)

- Stochastic Quantization introduces a "stochastic time" $t_s$, in which the fundamental fields evolve according to the **Langevin equation**,

$$\boxed{\partial_{t_s} U_{x\mu}(t_s) = -\{\nabla_{x\mu} S_G(U(t_s)) + \eta_{x\mu}(t_s)\} U_{x\mu}(t_s),}$$

  where $\eta$ is a Gaussian distributed noise field. (G. Parisi, Y.S. Wu '81)

- Considering the formal **perturbative expansion**,

$$U(t_s) \to \mathcal{V} + \sum_{k>0} g_0^k U^{(k)}(t_s),$$

  in the Langevin equation, one can obtain an approximate solution by solving the resulting hierarchy of equations order-by-order in $g_0$.

- **Stochastic Perturbation Theory (SPT)**

$$\lim_{t_s \to \infty} \left\langle \mathcal{O}\left[\sum_k g_0^k U^{(k)}(t_s)\right]\right\rangle_\eta = \sum_k g_0^k \mathcal{O}_k[U] = \langle \mathcal{O}[U] \rangle.$$

- **NSPT** considers a **discrete approximation** of the Langevin equation, and performs this program **numerically**! (F. Di Renzo *et. al.* '94)

# NSPT and The Gradient Flow

- In the gradient flow, the noise field is not present and the initial distribution of the fundamental gauge field is taken into account,

$$\boxed{\partial_t V_{x\mu}(t) = -\left\{g_0^2 \nabla_{x\mu} S_G(V(t))\right\} V_{x\mu}(t), \quad V_{x\mu}|_{t=0} = U_{x\mu}(t_s).}$$

- Analogously to the Langevin equation, considering the formal **perturbative expansion**,

$$V(t;t_s) \to \mathcal{V} + \sum_{k>0} g_0^k V^{(k)}(t;t_s), \quad V^{(k)}|_{t=0} = U^{(k)}(t_s), \forall k,$$

  one can obtain an approximate solution for the gradient flow!

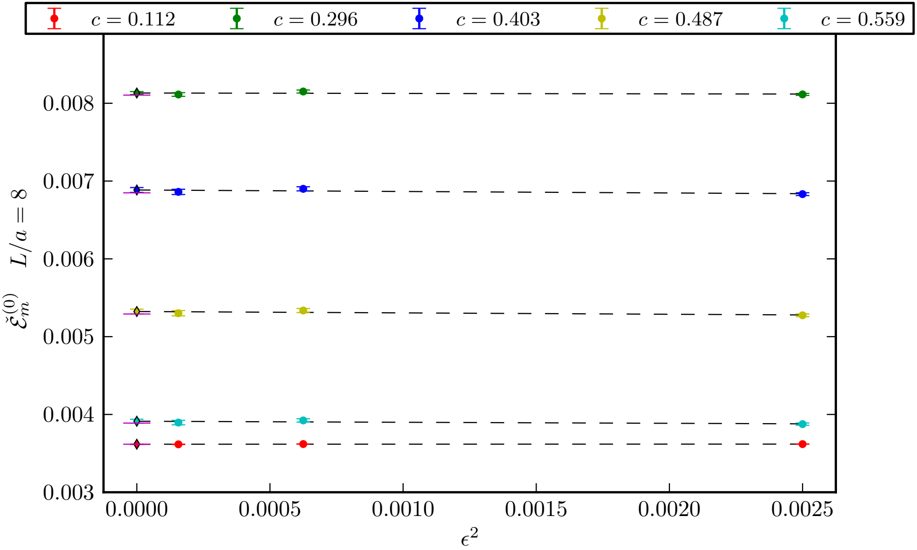
- **SPT for The Gradient Flow**

$$\lim_{t_s \to \infty} \left\langle \mathcal{O}\Big[\sum_k g_0^k V^{(k)}(t;t_s)\Big]\right\rangle_\eta = \sum_k g_0^k \mathcal{O}_k[V(t)] = \langle \mathcal{O}[V(t)] \rangle.$$

- Using the machinery of NSPT this program can be implemented **numerically**!
- **No gauge fixing step** is needed along the flow.

## Determination of $\langle t^2 \hat{E}(t, T/2)\rangle = \check{\mathcal{E}}^{(0)} g_0^2 + \check{\mathcal{E}}^{(1)} g_0^4 + \check{\mathcal{E}}^{(2)} g_0^6 + \ldots$

(P. Fritzsch, A. Ramos '13)



## Determination of $\langle t^2 \hat{E}(t, T/2)\rangle = \check{\mathcal{E}}^{(0)} g_0^2 + \check{\mathcal{E}}^{(1)} g_0^4 + \check{\mathcal{E}}^{(2)} g_0^6 + \ldots$

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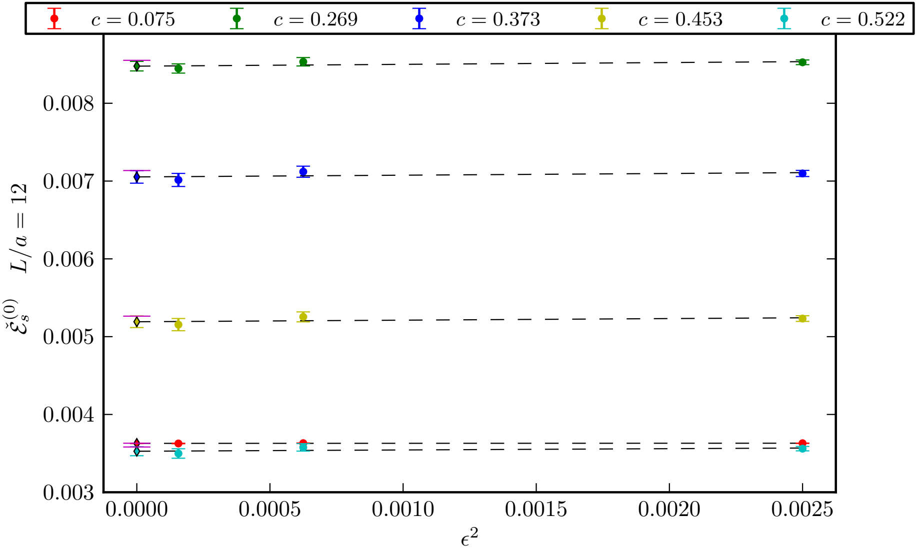

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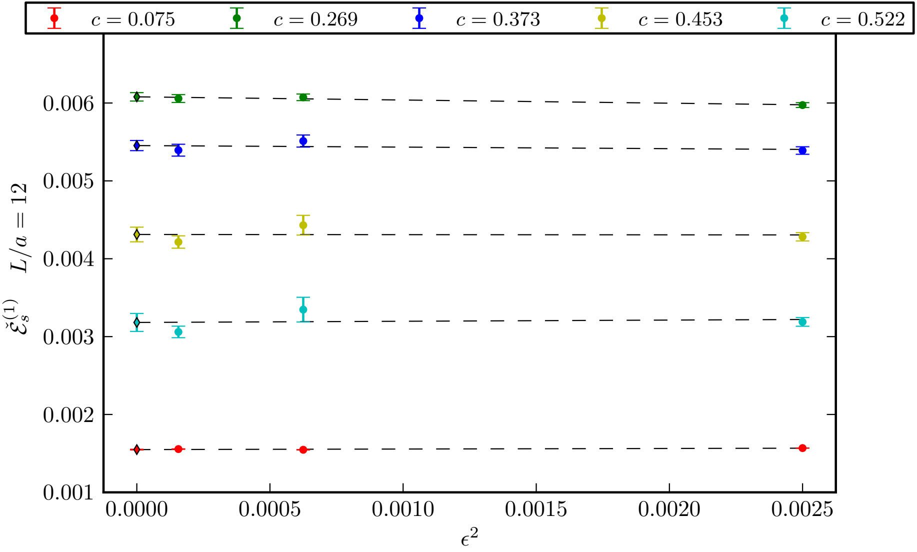
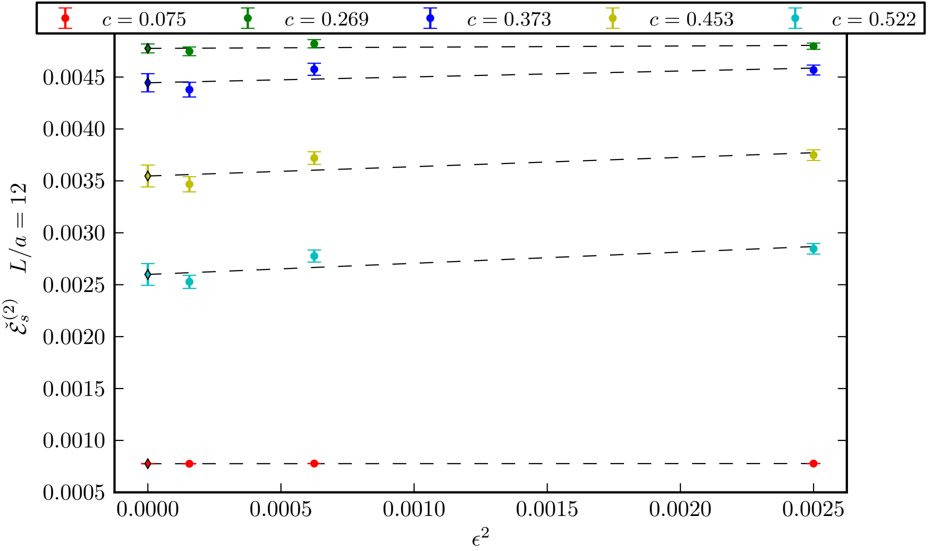
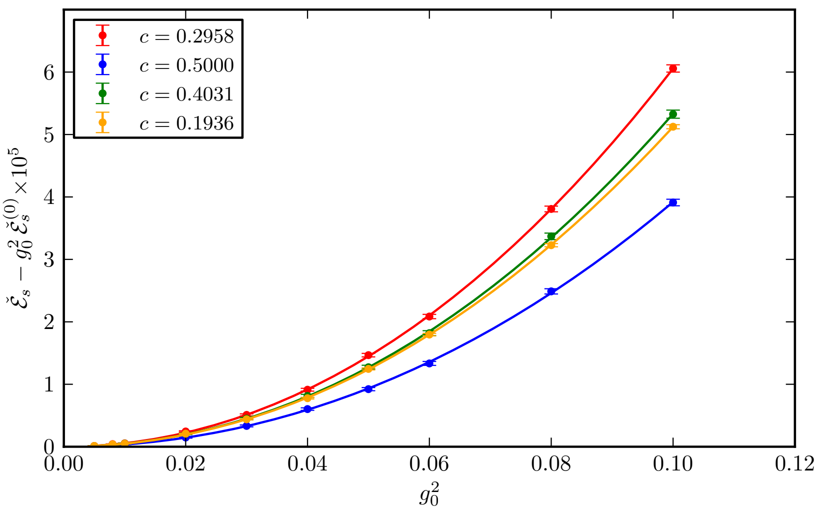


# Determination of $\langle t^2 \hat{E}(t, T/2)\rangle = \check{\mathcal{E}}^{(0)} g_0^2 + \check{\mathcal{E}}^{(1)} g_0^4 + \check{\mathcal{E}}^{(2)} g_0^6 + \ldots$



# Comparison with Monte Carlo data

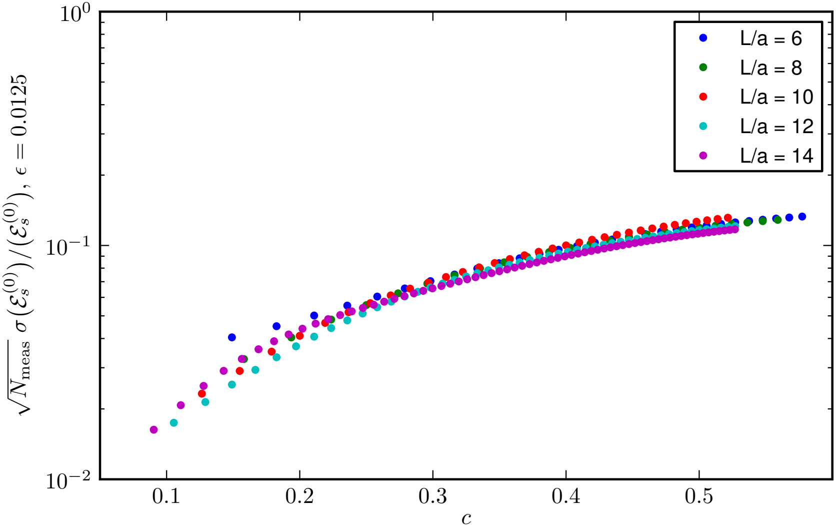


# Comparison with Monte Carlo data

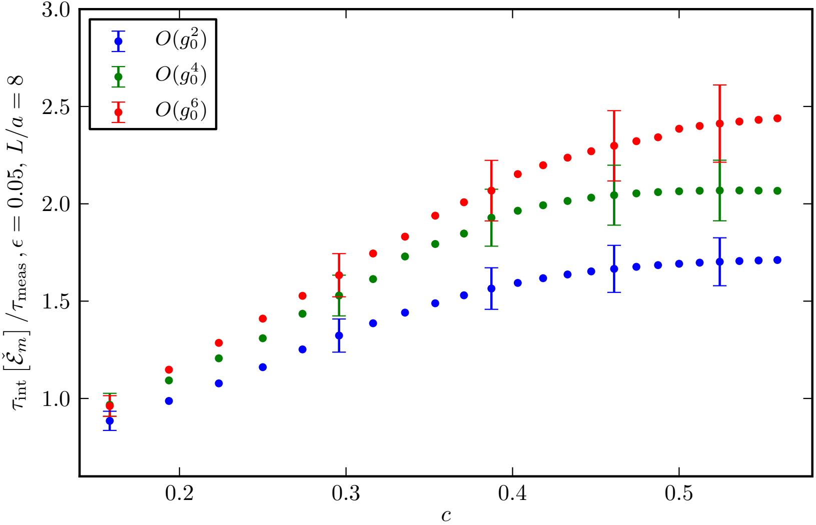
| | $O(g_0^4)$ | | $O(g_0^6)$ | |
|---|---|---|---|---|
| $c$ | MC | NSPT | MC | NSPT |
| $\langle t^2 \hat{E}_s \rangle$ | | | | |
| 0.1936 | 0.004780(86) | 0.004631(22) | 0.0034(11) | 0.0031669(96) |
| 0.2958 | 0.00552(15) | 0.005464(49) | 0.0054(19) | 0.004095(29) |
| 0.4031 | 0.00483(18) | 0.004776(64) | 0.0050(21) | 0.003744(44) |
| 0.5000 | 0.00355(14) | 0.003489(64) | 0.0037(17) | 0.002785(44) |
| $\langle t^2 \hat{E}_m \rangle$ | | | | |
| 0.1936 | 0.004859(90) | 0.004615(23) | 0.0020(11) | 0.003151(10) |
| 0.2958 | 0.00557(17) | 0.005407(52) | 0.0036(21) | 0.004031(31) |
| 0.4031 | 0.00479(22) | 0.004715(66) | 0.0041(27) | 0.003663(46) |
| 0.5000 | 0.00351(21) | 0.003499(63) | 0.0039(25) | 0.002779(47) |

MC data obtained with a customized MILC code, results are for $L/a = 8$.

# Noise to signal ratio vs $c$



# Autocorrelation time vs $c$



## Conclusions

- Mild extrapolations, and good statistical behavior for the flow observables we have considered.
- NPST provides a natural setup for a (numerical) perturbative solution of the gradient flow.
- The setup is flexible: different action regularizations, boundary conditions, and observables can be implemented easily.

## Outlook

- Continuum limit extrapolations
  - Cut-off effects in the step-scaling function
  - $\Lambda_{\mathrm{GF}}$ and PT relation to other schemes

  $\rightarrow$ require bigger lattices (n.b. cost $\propto (L/a)^6$)
- Inclusion of fermions and QCD


Thanks

# Numerical precision

The most expensive simulations were performed at $L/a = 12$.
The results of the extrapolations are,

| $c$ | $\check{\mathcal{E}}_s^{(0)}$ | $\frac{\delta\check{\mathcal{E}}_s^{(0)}}{\check{\mathcal{E}}_s^{(0)}}$ | $\check{\mathcal{E}}_s^{(1)}$ | $\frac{\delta\check{\mathcal{E}}_s^{(1)}}{\check{\mathcal{E}}_s^{(1)}}$ |
|---|---|---|---|---|
| 0.2 | 0.008656(38) | 0.5% | 0.005827(37) | 0.6% |
| 0.3 | 0.008231(66) | 0.8% | 0.005958(45) | 0.8% |
| 0.4 | 0.006413(78) | 1.2% | 0.005004(85) | 1.7% |
| 0.5 | 0.004026(62) | 1.5% | 0.00345(11) | 3.2% |

Autocorrelation $\tau_{\rm int}$ $(\tau_{\rm int}/10\,\mathrm{LDU})$ and $N_{\rm eff} = N_{\rm meas}/(2\,\tau_{\rm int})$,

| | $\epsilon$ | 0.0125 | 0.025 | 0.05 |
|---|---|---|---|---|
| $\check{\mathcal{E}}_s^{(0)}$ | $\tau_{\rm int}\|_{c=0.22}$ | 4.43(94) | 4.10(87) | 2.07(24) |
| | $\tau_{\rm int}\|_{c=0.50}$ | 8.2(22) | 5.1(12) | 2.66(33) |
| | $N_{\rm eff}\|_{c=0.22}$ | 109(24) | 112(24) | 550(63) |
| | $N_{\rm eff}\|_{c=0.50}$ | 61(16) | 89(21) | 429(53) |

| | $\epsilon$ | 0.0125 | 0.025 | 0.05 |
|---|---|---|---|---|
| $\check{\mathcal{E}}_s^{(1)}$ | $\tau_{\rm int}\|_{c=0.22}$ | 5.8(14) | 3.54(70) | 2.54(32) |
| | $\tau_{\rm int}\|_{c=0.50}$ | 9.9(28) | 21.3(75) | 4.85(78) |
| | $N_{\rm eff}\|_{c=0.22}$ | 87(20) | 130(26) | 448(56) |
| | $N_{\rm eff}\|_{c=0.50}$ | 51(14) | 21.6(76) | 235(38) |

# Numerical effort

| $\check{\mathcal{E}}_s^{(0)}$ | $\epsilon$ | 0.0125 | 0.025 | 0.05 |
|---|---|---|---|---|
| $L=4$ | $\tau_{\rm int}\|_{c=0.22}$ | 1.117(28) | 0.677(19) | 0.541(14) |
| | $\tau_{\rm int}\|_{c=0.50}$ | 1.567(48) | 0.837(25) | 0.567(14) |
| | $N_{\rm eff}\|_{c=0.22}$ | 17880(45) | 24980 | 24980 |
| | $N_{\rm eff}\|_{c=0.50}$ | 12750(38) | 24980 | 24980 |
| $L/a=6$ | $\tau_{\rm int}\|_{c=0.21}$ | 1.955(78) | 0.981(30) | 0.663(19) |
| | $\tau_{\rm int}\|_{c=0.50}$ | 3.27(17) | 1.651(64) | 0.842(26) |
| | $N_{\rm eff}\|_{c=0.21}$ | 6100(24) | 23940 | 23960 |
| | $N_{\rm eff}\|_{c=0.50}$ | 3660(18) | 7250(28) | 23960 |
| $L/a=8$ | $\tau_{\rm int}\|_{c=0.22}$ | 3.22(29) | 1.66(12) | 0.919(51) |
| | $\tau_{\rm int}\|_{c=0.50}$ | 4.89(54) | 2.61(22) | 1.390(89) |
| | $N_{\rm eff}\|_{c=0.22}$ | 917(84) | 1810(12) | 5960 |
| | $N_{\rm eff}\|_{c=0.50}$ | 603(66) | 1133(97) | 2140(14) |
| $L/a=12$ | $\tau_{\rm int}\|_{c=0.22}$ | 4.43(94) | 4.10(87) | 2.07(24) |
| | $\tau_{\rm int}\|_{c=0.50}$ | 8.2(22) | 5.1(12) | 2.66(33) |
| | $N_{\rm eff}\|_{c=0.22}$ | 109(24) | 112(24) | 550(63) |
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| $\check{\mathcal{E}}_s^{(1)}$ | $\epsilon$ | 0.0125 | 0.025 | 0.05 |
|---|---|---|---|---|
| $L=4$ | $\tau_{\rm int}\|_{c=0.22}$ | 1.717(54) | 0.921(28) | 0.636(16) |
| | $\tau_{\rm int}\|_{c=0.50}$ | 4.00(17) | 2.030(83) | 1.144(37) |
| | $N_{\rm eff}\|_{c=0.22}$ | 11630(36) | 24980 | 24980 |
| | $N_{\rm eff}\|_{c=0.50}$ | 5000(22) | 6150(25) | 10910(35) |
| $L/a=6$ | $\tau_{\rm int}\|_{c=0.21}$ | 2.38(10) | 1.273(44) | 0.762(21) |
| | $\tau_{\rm int}\|_{c=0.50}$ | 7.96(58) | 4.20(23) | 2.32(10) |
| | $N_{\rm eff}\|_{c=0.21}$ | 5020(22) | 9400(33) | 23960 |
| | $N_{\rm eff}\|_{c=0.50}$ | 1500(11) | 2850(16) | 5170(22) |
| $L/a=8$ | $\tau_{\rm int}\|_{c=0.22}$ | 4.42(46) | 1.99(15) | 1.143(69) |
| | $\tau_{\rm int}\|_{c=0.50}$ | 14.1(23) | 6.00(69) | 2.99(26) |
| | $N_{\rm eff}\|_{c=0.22}$ | 667(70) | 1490(11) | 2610(16) |
| | $N_{\rm eff}\|_{c=0.50}$ | 209(34) | 493(57) | 995(87) |
| $L/a=12$ | $\tau_{\rm int}\|_{c=0.22}$ | 5.8(14) | 3.54(70) | 2.54(32) |
| | $\tau_{\rm int}\|_{c=0.50}$ | 9.9(28) | 21.3(75) | 4.85(78) |
| | $N_{\rm eff}\|_{c=0.22}$ | 87(20) | 130(26) | 448(56) |
| | $N_{\rm eff}\|_{c=0.50}$ | 51(14) | 21.6(76) | 235(38) |

$$\boxed{N_{\rm eff} = \frac{N_{\rm meas}}{2\,\tau_{\rm int}}}$$

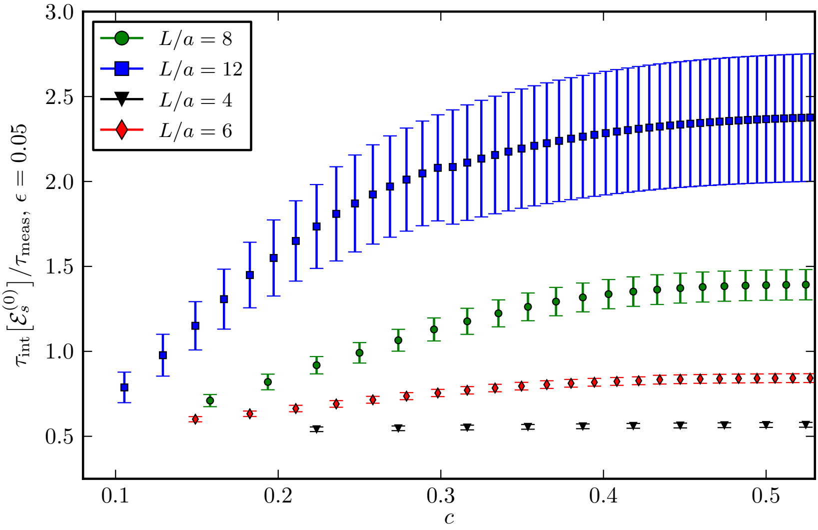
## Determination of $\langle t^2 \hat{E}(t, T/2)\rangle = \check{\mathcal{E}}^{(0)} g_0^2 + \check{\mathcal{E}}^{(1)} g_0^4 + \check{\mathcal{E}}^{(2)} g_0^6 + \ldots$

(P. Fritzsch, A. Ramos '13)

| | | | | | | |
|---|---|---|---|---|---|---|
| $L=4$ | $c$ | 0.1581 | 0.3162 | 0.4183 | 0.5000 | 0.5701 |
| | $\delta\check{\mathcal{E}}_s^{(0)}$ | 0.0001(23) | 0.0004(26) | 0.0002(31) | 0.0000(30) | 0.0002(28) |
| | $\delta\check{\mathcal{E}}_m^{(0)}$ | 0.0001(23) | 0.0006(25) | 0.0006(30) | 0.0005(28) | 0.0005(26) |
| $L/a=6$ | $c$ | 0.1054 | 0.2981 | 0.4082 | 0.4944 | 0.5676 |
| | $\delta\check{\mathcal{E}}_s^{(0)}$ | 0.0003(22) | 0.0007(18) | 0.0018(14) | 0.0025(17) | 0.0029(20) |
| | $\delta\check{\mathcal{E}}_m^{(0)}$ | 0.0002(19) | 0.0010(24) | 0.0012(22) | 0.0014(22) | 0.0015(23) |
| $L/a=8$ | $c$ | 0.1118 | 0.2958 | 0.4031 | 0.4873 | 0.5590 |
| | $\delta\check{\mathcal{E}}_s^{(0)}$ | 0.00056(63) | 0.0016(27) | 0.0023(36) | 0.0028(43) | 0.0031(48) |
| | $\delta\check{\mathcal{E}}_m^{(0)}$ | 0.00003(59) | 0.0032(23) | 0.0051(45) | 0.0057(57) | 0.0057(64) |
| $L/a=12$ | $c$ | 0.0745 | 0.2687 | 0.3727 | 0.4534 | 0.5217 |
| | $\delta\check{\mathcal{E}}_s^{(0)}$ | 0.00021(68) | 0.0083(68) | 0.011(11) | 0.014(14) | 0.015(16) |
| | $\delta\check{\mathcal{E}}_m^{(0)}$ | 0.00045(80) | 0.0062(87) | 0.007(14) | 0.009(18) | 0.011(21) |

$$\boxed{\delta\check{\mathcal{E}}_{s,m}^{(0)} = \frac{\check{\mathcal{E}}_{s,m}^{(0)}}{\hat{\mathcal{N}}_{s,m}} - 1}$$

# Autocorrelation time vs $c$



# Autocorrelation time vs $L$