Numerical Stochastic Perturbation Theory in the Schrödinger Functional: Opportunities & Challenges

Dirk Hesse
in collaboration with
Michele Brambilla & Francesco Di Renzo

STRONGnet Workshop Madrid 2012

Overview

- What is NSPT and what is it useful for?
- Teaming up NSPT and the Schrödinger Functional.

The Schrödinger Functional

	Fermions	**Gluons**
Dirichlet boundary conditions in **time**.	$\zeta(\mathbf{x}) = \sum_y \tilde{K}(\mathbf{x}, y)\psi(y)$ $\overline{\zeta}(\mathbf{x}) = \sum_y \overline{\psi}(y) K(y, \mathbf{x})$ $P_+\psi(x)\|_{x_0=0} = \overline{\psi}(x)P_-\big\|_{x_0=0} = 0$	$U_k(x)\|_{x_0=0} = e^{C(\mathbf{x})}$ $U_k(x)\|_{x_0=T} = e^{C'(\mathbf{x})}$
Periodic boundary conditions in **space**.	$\psi(x + \hat{k}L) = e^{i\theta_k}\psi(x)$	$U_\mu(x + \hat{k}L) = U_\mu(x)$

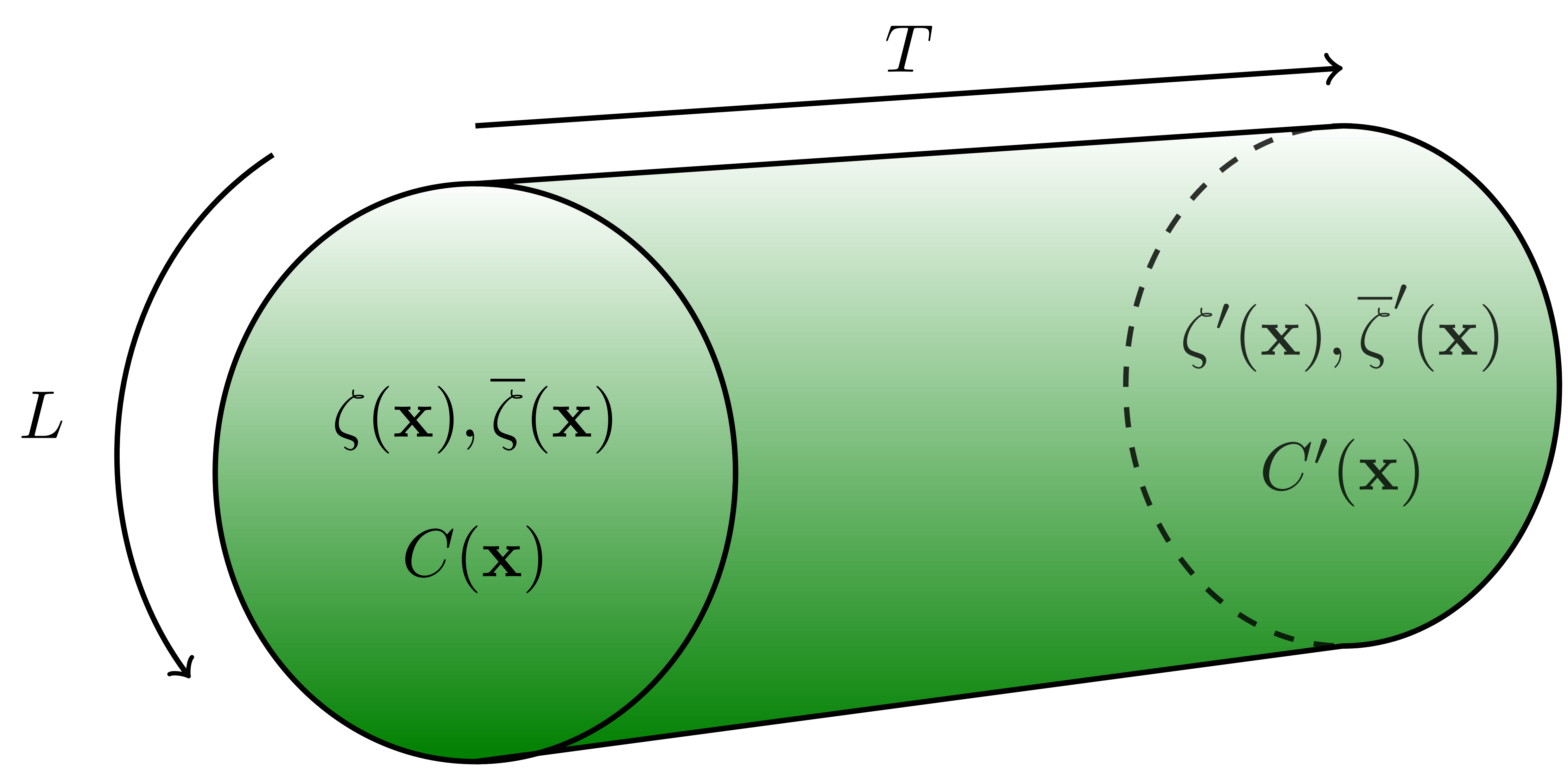
M. Lüscher, P. Weisz, R. Narayanan, U. Wolff, 1992. S. Sint, 1996, M. Lüscher 2006.

The Schrödinger Functional

	Fermions	Gluons
Dirichlet boundary conditions in **time**.	$\zeta'(\mathbf{x}) = \sum_y \tilde{K}'(\mathbf{x}, y)\psi(y)$ $\bar{\zeta}'(\mathbf{x}) = \sum_y \overline{\psi}(y)K'(y, \mathbf{x})$ $P_-\psi(x)\vert_{x_0=T} = \overline{\psi}(x)P_+\vert_{x_0=T} = 0$	$U_k(x)\vert_{x_0=0} = e^{C(\mathbf{x})}$ $U_k(x)\vert_{x_0=T} = e^{C'(\mathbf{x})}$
Periodic boundary conditions in **space**.	$\psi(x + \hat{k}L) = e^{i\theta_k}\psi(x)$	$U_\mu(x + \hat{k}L) = U_\mu(x)$

M. Lüscher, P. Weisz, R. Narayanan, U. Wolff, 1992. S. Sint, 1996, M. Lüscher 2006.

The Schrödinger Functional

	Fermions	**Gluons**
Dirichlet boundary conditions in **time**.		
Periodic boundary conditions in **space**.		

M. Lüscher, P. Weisz, R. Narayanan, U. Wolff, 1992. S. Sint, 1996, M. Lüscher 2006.

Perturbation Theory

In **perturbation theory**, we want to obtain **expansions** like this one:

$$\langle O[\phi] \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, O[\phi] \, \exp\{S_0[\phi] + \alpha \, S_1[\phi] + \ldots\} = O^{(0)} + \alpha \, O^{(1)} + \ldots$$

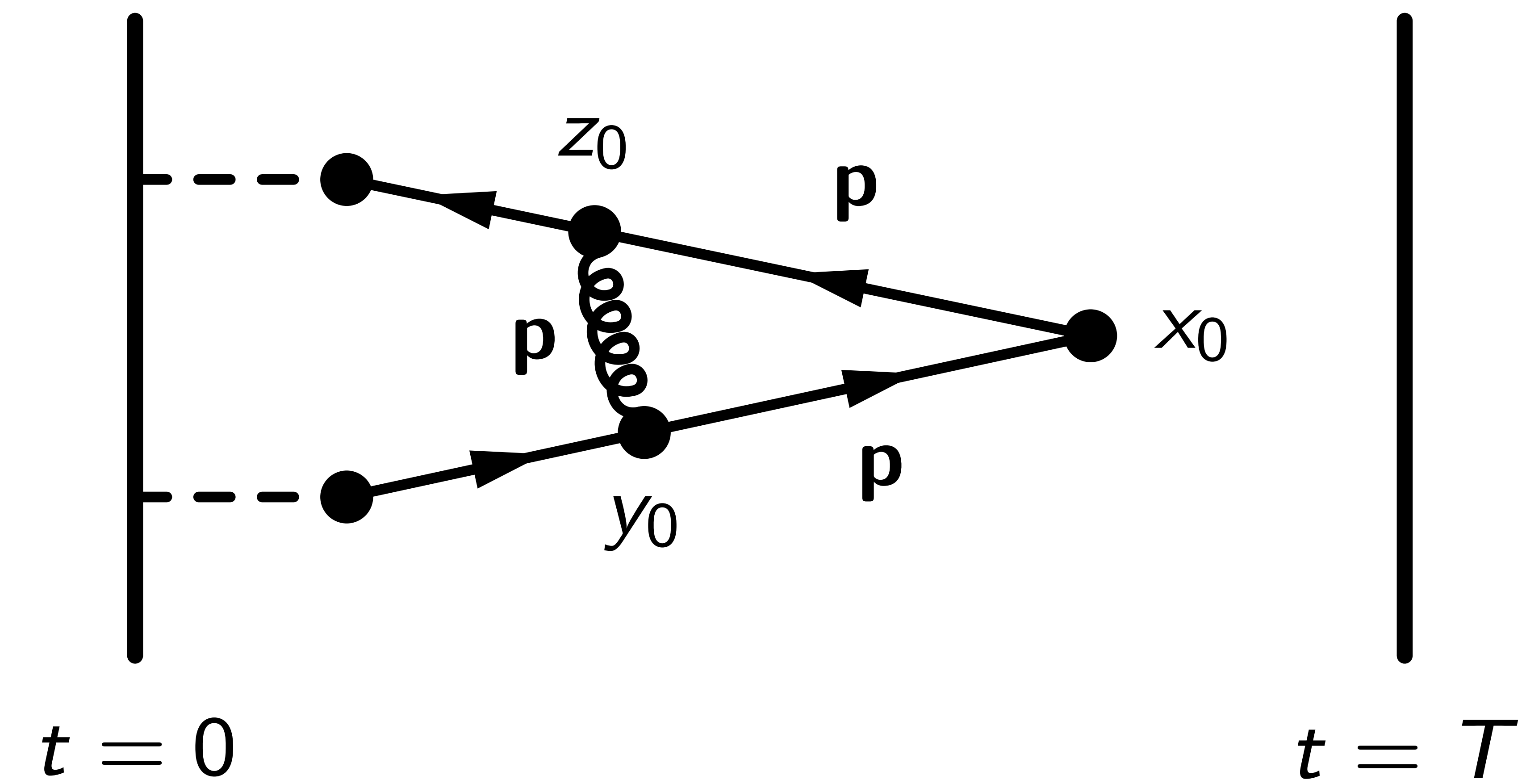
Usually, one calculates $O^{(i)}$ using **Feynman diagrams** and **rules** extracted from

$$S[\phi] = S_0[\phi] + \alpha S_1[\phi] + \ldots$$

PT in the SF

In the Schrödinger Functional one would like to **avoid** PT!

$$\sum_{\mathbf{p},y_0,z_0} \mathrm{tr} \left\{ \quad \right\}$$



- Big number of diagrams even at low orders
- Background field makes Feynman rules complicated

Numerical Stochastic PT avoids both!

Stochastic Quantization I

We want to calculate an **expectation value**

$$\langle O[\phi] \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, O[\phi] \, e^{-S[\phi]}$$

Introduce a new d.o.f., the **stochastic time** t.

The evolution in stochastic time is given by the **Langevin Equation**,

$$\dot{\phi}_\eta(x;t) = -\partial_{\phi_\eta(x;t)} S[\phi] + \eta(x;t)$$

With **Gaussian noise** η.

Parisi, Wu, 1981

Stochastic Quantization 2

Defining the **'noise average'**

$$\langle O \rangle_\eta = \frac{1}{Z'} \int \mathcal{D}\eta \, O \, e^{-\frac{1}{4} \int \mathrm{d}[z,\tau] \; \eta^2(z,\tau)},$$

One asserts that the **functional integral** can be calculated using

$$\langle O[\phi_\eta(x_1;t), \ldots, \phi_\eta(x_n;t)] \rangle_\eta \xrightarrow{t \to \infty} \langle O[\phi(x_1), \ldots, \phi(x_n)] \rangle$$

Stochastic Perturbation Theory

Split up the action into free and interacting parts

$$S[\phi] = S_0[\phi] + gS_1[\phi] + \dots$$

and formally write $\phi(x;t) = \sum_{i=0}^{\infty} g^i \phi^{(i)}(x;t)$

Using the Langevin equation one may now obtain $\langle O \rangle_\eta = \sum_{i=0}^{\infty} g^i \langle O \rangle_\eta^{(i)}$

By defining $(\phi + \varphi)^{(r)} = \phi^{(r)} + \varphi^{(r)}, \qquad (\phi\varphi)^{(r)} = \sum_{i=0}^{r} \phi^{(i)} \varphi^{(r-i)}$

Numerical Stochastic Perturbation Theory

- In NSPT, one integrates the perturbative Langevin Equation numerically.
- This is similar to hybrid MC methods c.f. Stefan's talk.
- However, there is no perturbative expression for an accept/reject step.
- Hence, one is stuck with a finite integration time τ

  and has to extrapolate $\tau \to 0$.

Di Renzo, 2004

Stochastic Gauge Fixing

Zwanziger, 1981

In principle no GF is need. However, if one looks at the Langevin eqn.,

$$\frac{\partial}{\partial t} A_\mu^a(\eta, x; t) \;=\; D_\nu^{ab} F_{\nu\mu}^b(\eta, x; t) + \eta_\mu^a(x; t)$$

One finds that for a solution in Fourier space

$$A_\mu^{(n)a}(k; t) \;=\; T_{\mu\nu}^{ab} \int_0^t ds\, e^{-k^2(t-s)} f_\nu^{(n)b}(k, s) + L_{\mu\nu}^{ab} \int_0^t ds\, f_\nu^{(n)b}(k, s)$$

The longitudinal component will diverge like a random walk.
GF introduces a damping factor and stabilizes the simulation.

A similar statement holds for the gauge zero modes.

Gauge Fixing Pitfalls

The gauge fixing function in the SF **at the boundary** reads

$$[d^* q(x)]_{ij} = \begin{cases} (a^2/L^3) \sum_{\mathbf{y}} [q_0(0,\mathbf{y})]_{ij} & \text{if} \quad x_0 = 0, i = j \\ 0 & \text{else} \end{cases}$$

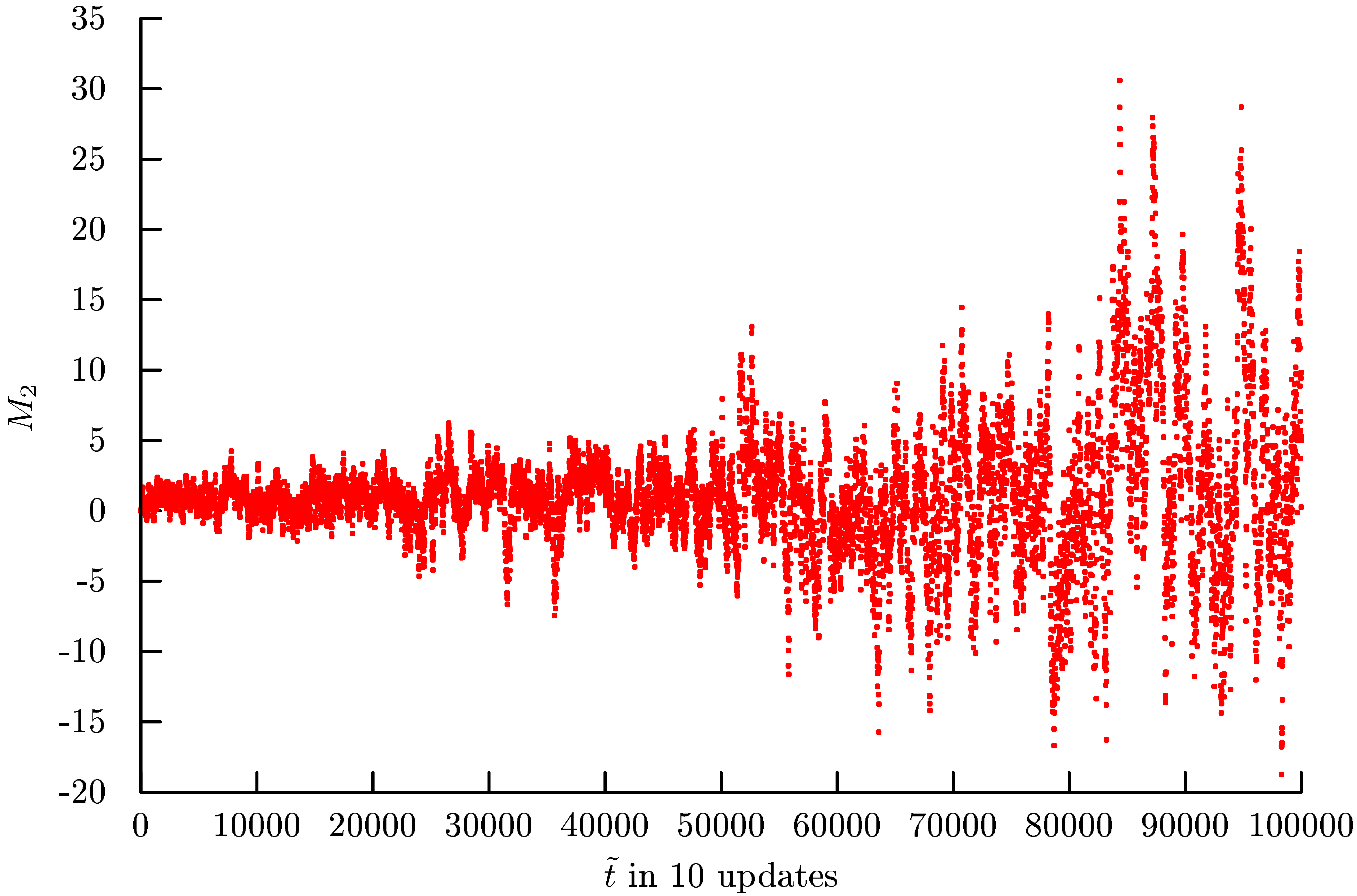
It acts on the fluctuation field, writing

$$U_\mu(x) = \exp\{g_0\, a\, q_\mu(x)\} V_\mu(x)$$

This amounts to suppressing **spatial zero modes** at the boundary.

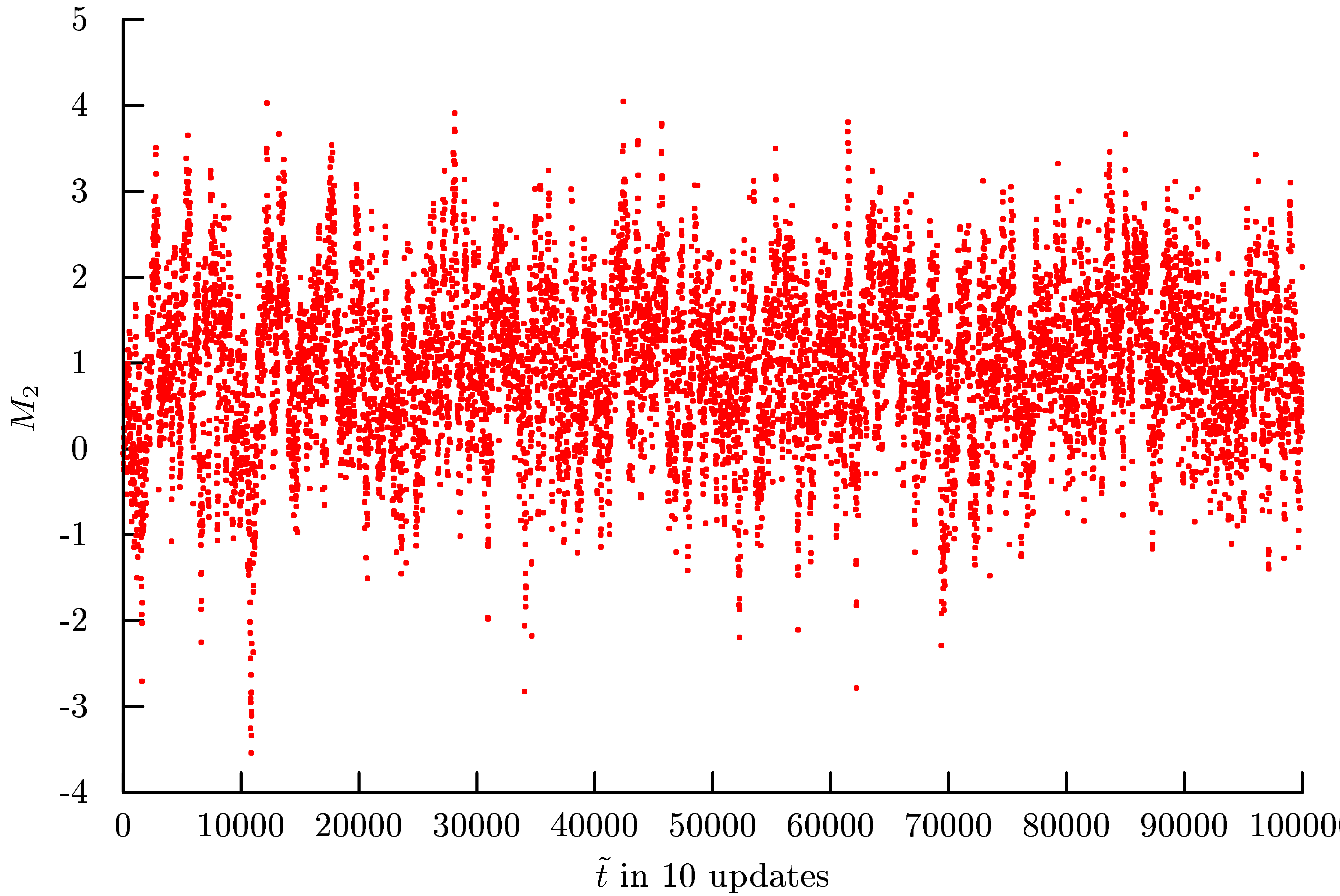
Lüscher, Narayanan, Weisz, Wolff, 1992

Bad History



Incorrect gauge fixing leads to a slow increase of noise (which can be confusing).

Good History



Correct gauge fixing leads to a drastic decrease of the noise.

Advantages of NSPT

- No Feynman Rules, i.e. easier to implement various actions.
- No Feynman Diagrams, i.e. higher order are only a matter of CPU time.
- NSPT codes can benefit from non-perturbative ones ...
- ... and vice versa!

No Free Lunch

- Way more numerical effort than common PT.
- Stochastic noise makes extraction of logs difficult.

But NSPT has many applications, e.g. improvement:

$$\mathcal{O}_{\mathrm{I}}(a/L) = \frac{\mathcal{O}(a/L)}{1+\delta(a/L)}$$

$$\delta(a/L) = \frac{\mathcal{O}(a/L) - \mathcal{O}(0)}{\mathcal{O}(0)} = \delta^{(0)}(a/L) + g_0^2 \delta^{(1)}(a/L) + \dots$$

de Divitiis et al. Nucl. Phys. B437

The SF coupling

The SF introduces an external scale T = cL (usually c = 1).

This enables us to give a precise definition for a coupling

$$\overline{g}(\mu = 1/L)$$

Furthermore one can calculate a discrete beta-function

$$u = \overline{g}^2(L), \quad u' = \overline{g}^2(sL), \quad \sigma(s,u) = u'$$

On the lattice: $\Sigma(s,u,a/L) = u'$

Lüscher, Narayanan, Weisz, Wolff, 1992

Defining the SF coupling

The usual choice for the background field is 'defined' by setting

$$C = i/L\,\mathrm{diag}(\phi_1, \phi_2, \phi_3), \quad C' = i/L\,\mathrm{diag}(\phi'_1, \phi'_2, \phi'_3)$$

Where ϕ_i, ϕ'_i depend on two parameters, ν and η.

Defining as usual $e^{-\Gamma} = \int D[u] e^{-S[U]}$

one can define a coupling through $\left.\frac{\partial \Gamma}{\partial \eta}\right|_{\eta=\nu=0} = \frac{k}{\overline{g}^2}$

Lüscher, Sommer, Weisz, Wolff, 1993

O(a) improvement

To implement O(a) improvement, one defines

$$S[U] = \frac{1}{g^2} \sum_p w(p)\ \mathrm{tr}[1 - U(p)]$$

For plaquettes at the boundary, containing a spatial link, one sets

$$w(p) = c_t(g_0) = 1 + c_t^{(1)} g^2 + \ldots \qquad \text{else} \qquad w(p) = 1$$

Lüscher, Sommer, Weisz, Wolff, 1993

The Coupling Order by Order

We then write the coupling order by order,

$$\bar{g}^2(L) = g_0^2 + m_1(L/a)g_0^4 + m_2(L/a)g_0^6 + \dots$$

with

$$\begin{aligned} m_1 &= m_1^a + c_t^{(1)} m_1^b, \\ m_2 - m_1^2 &= m_2^a + c_t^{(1)} m_2^b + \left[c_t^{(1)}\right]^2 m_2^c + c_t^{(2)} m_2^d \end{aligned}$$

We use this as a check for our quenched code!

Bode, Weisz, Wolff, 1997

Data Analysis

- We use a custom implementation of the method presented by Ulli Wolff (CPC 156, 2004) to control autocorrelation and determine the errors.
- The extrapolation $\tau \to 0$ was done using a bootstrap analysis.
- We performed a cross check using binned Jackknife samples.

Our Data

- Did **test runs** on L/a = 4,8,12
- Coupling is known to be hard to measure
- We experience
  - Lots of **noise**
  - Slow **thermalization**
  - Long **autocorrelation** times

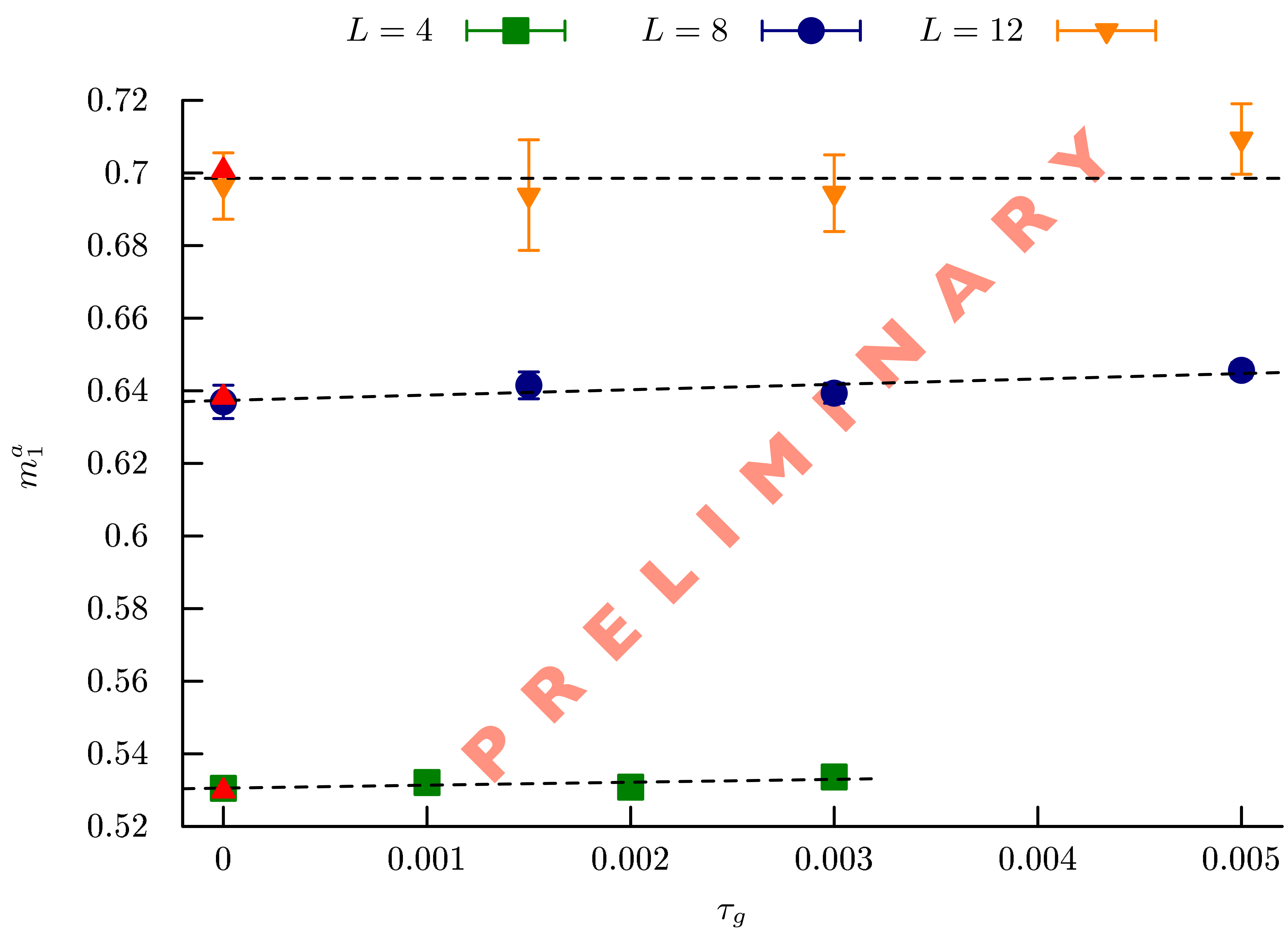
Simulation Details

- L = 4 on TURING (Univ. of Milan Bicocca)
- L = 8,12 on FERMI (CINECA)

This is an ideal test case to **check core performances**!

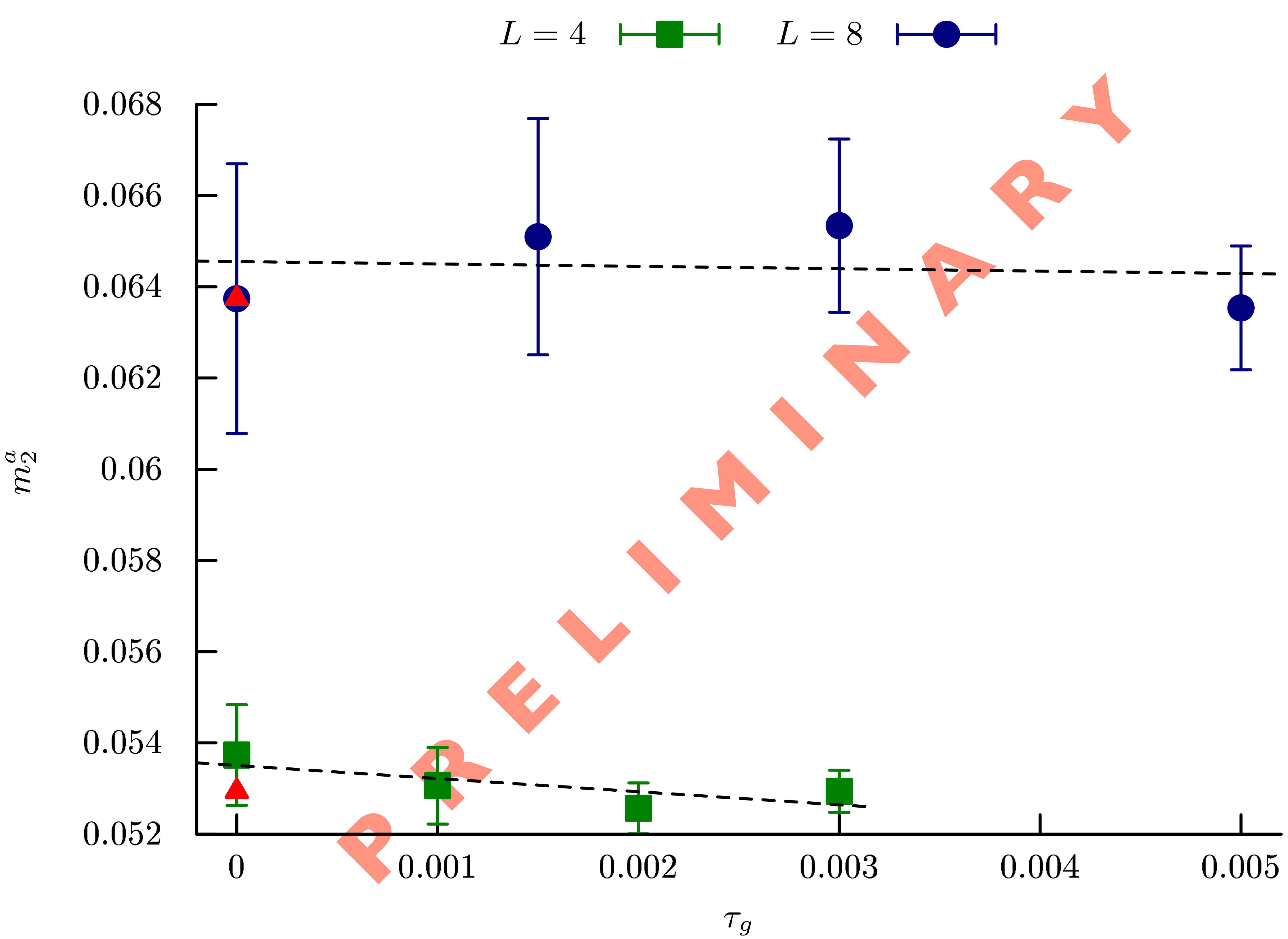
	$L=12$			$L=8$			$L=4$		
τ	0.0015	0.003	0.005	0.0015	0.003	0.005	0.001	0.002	0.003
$N_{\rm eff}$	270(50)	540(80)	800(100)	1.6(2)k	3.3(2)k	6.3(3)k	6.6(3)k	14.9(5)k	21.8(6)k
CORE-H	2k			1.6k			33		

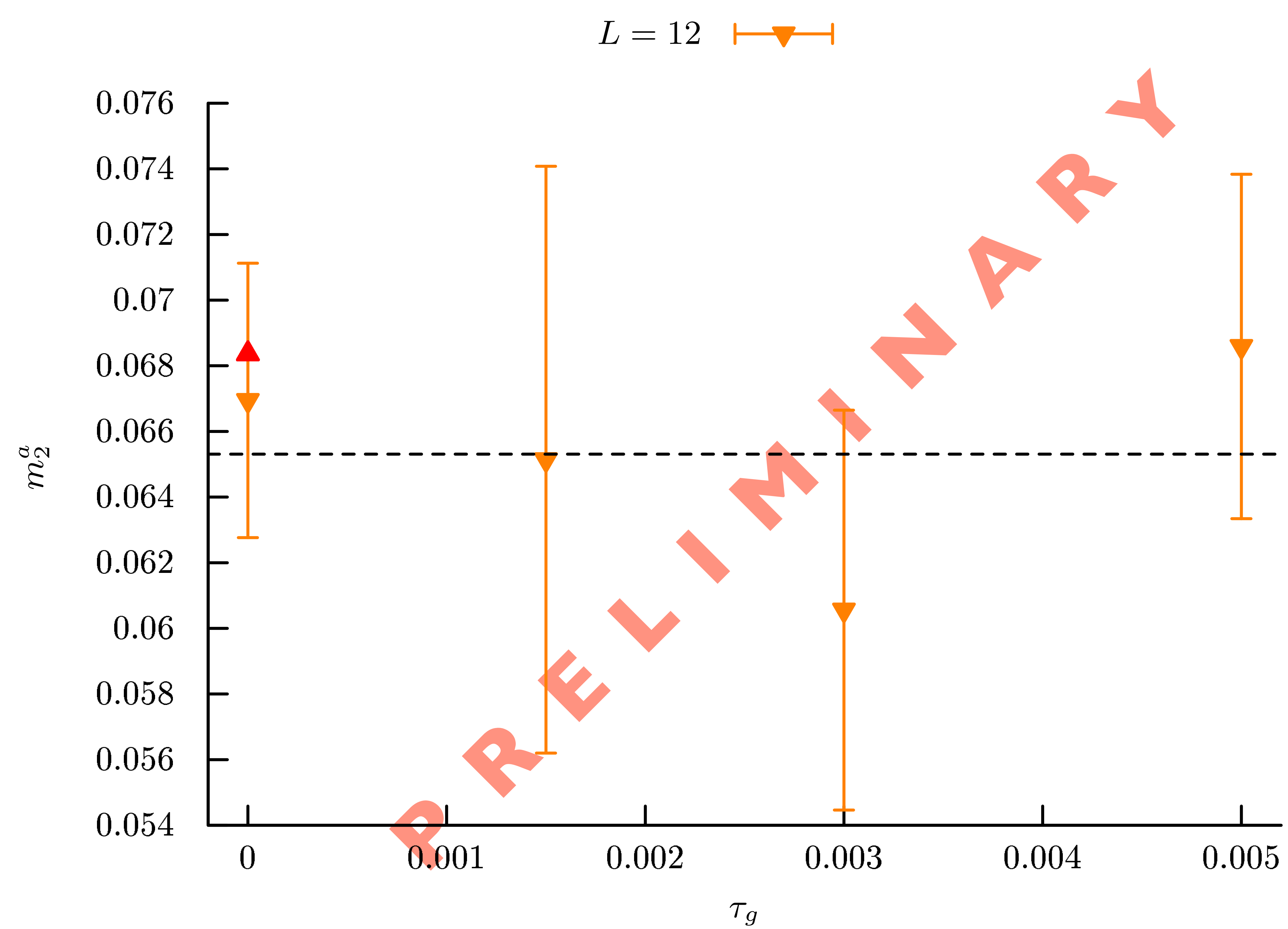
Results - One Loop



Known results (red) form: Bode, Weisz, Wolff: hep-lat/9809175

Results - Two Loops





Known results (red) form: Bode, Weisz, Wolff: hep-lat/9809175

Conclusions

- Quenched NSPT for the SF is implemented.
- Applications: Cut-off effects.
- Next Step: Fermions!

A word about logs.

An observable with at most a logarithmic divergence looks like this

$$f(I) = \sum_{n=0}^{\infty} \frac{a_n + b_n \log I}{I^n} \qquad I = L/a$$

M. Lüscher, P. Weisz, 1996,

One can extract the coefficients using successive fits.

A. Bode, P. Weisz, U. Wolff, 2000.

But: One requires many data points with high precision.