

# Algorithmic advances in NSPT

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*Based on work done in collaboration with  
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*Frontiers in Lattice Quantum Field Theory*

1<sup>st</sup> of June 2018, IFT, Madrid, Spain

# Motivation

Why perturbation theory?

## Renormalization

$$\text{Ex.: } O(q) \stackrel{q \rightarrow M_Z}{\approx} \alpha_{\overline{\text{MS}}}(q) + \textcolor{red}{k}_1 \alpha_{\overline{\text{MS}}}(q)^2 + \textcolor{red}{k}_2 \alpha_{\overline{\text{MS}}}(q)^3 + \dots \quad \left[ \alpha_{\overline{\text{MS}}}(M_Z) \approx 0.12 \right]$$

$\approx 10\% \qquad \qquad \approx 1\%$

but also

- ▶ quark-masses
- ▶ effective electro-weak Hamiltonians
- ▶ small-flow time expansions
- ▶ quasi-PDF
- ▶ ...

## Improvement

$$\text{Ex.: } \tilde{g}_0^2 = g_0^2 \left[ 1 + \frac{1}{3} \textcolor{blue}{b}_g(g_0) \text{tr}\{aM_q\} \right], \quad b_g = \mathcal{O}(g_0^2)$$

or in general

$$\frac{\Sigma(g^2, a/L) - \sigma(g^2)}{\sigma(g^2)} \stackrel{g^2 \rightarrow 0}{\approx} g^2 \textcolor{blue}{\delta}_1(a/L) + g^4 \textcolor{blue}{\delta}_2(a/L) + \dots$$

# Motivation

## Lattice: a tool for automation

Perturbative lattice calculations, however, can too easily become difficult, tedious, and (human) time consuming ...

### Why?

- ▶ Feynman rules can be very complicated
- ▶ In gauge-theories new vertices appear at each order  
⇒ the number of diagrams grows very rapidly
- ▶ Requires numerical evaluation even for simple diagrams  
⇒ naive computational cost  $\propto V^N$  @  $N$  loops

... a lot of additional troubles for some cutoff effects

A possible **solution** ...

## Numerical stochastic perturbation theory (NSPT)

- ✓ Fully automated
- ✓ Easy to set-up and very flexible tool
- ✓ Allows for high-order computations
- ✗ Systematic and statistical errors

Ultimately the lattice is introduced as a **technical tool** for automation: what we want are **continuum results!**

# Introduction

The Parisi and Wu way

(Parisi, Wu '81)

Ex.: Lattice  $\varphi^4$ -theory

$$S(\varphi) = \sum_x \left\{ \frac{1}{2} \partial_\mu \varphi(x) \partial_\mu \varphi(x) + \frac{1}{2} (m^2 + \delta m^2) \varphi(x)^2 + \frac{g_0}{4!} \varphi(x)^4 \right\}$$

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int d\varphi \mathcal{O}(\varphi) e^{-S(\varphi)}$$

Langevin equation

$$\partial_t \phi(t, x) = - \frac{\delta S(\phi)}{\delta \phi(t, x)} + \eta(t, x)$$

$$\langle \eta(t, x) \eta(s, y) \rangle_\eta = 2 \delta_{xy} \delta(t - s)$$

Stochastic quantization

$$\lim_{t \rightarrow \infty} \langle \phi(t, x_1) \dots \phi(t, x_n) \rangle_\eta = \langle \varphi(x_1) \dots \varphi(x_n) \rangle$$

$$\lim_{t \rightarrow \infty} P(t, \phi) = P_{\text{eq}}(\phi) \propto e^{-S(\phi)}$$

# Introduction

## Stochastic perturbation theory

(Parisi, Wu '81)

### Perturbative field

$$\phi = \phi_0 + g_0 \phi_1 + g_0^2 \phi_2 + \dots$$

### Forces & c.t.

$$\frac{\delta S(\phi)}{\delta \phi} = F_0(\phi_0) + g_0 F_1(\phi_0, \phi_1) + \dots$$

$$\delta m^2 = g_0 \delta m_1^2 + g_0^2 \delta m_2^2 + \dots$$

### Dynamics

$$\partial_t \phi_0 = -\Delta \phi_0 + \eta$$

$$[\Delta = -\partial_\mu^* \partial_\mu + m^2]$$

$$\partial_t \phi_1 = -\Delta \phi_1 - \delta m_1^2 \phi_0 - \frac{1}{3!} \phi_0^3$$

...

$$\partial_t \phi_r = -F_r(\phi_0, \dots, \phi_r) + \delta_{r0} \eta$$

$$[F_r(\phi) = \Delta \phi_r + V_r(\phi_0, \dots, \phi_{r-1})]$$

### Observables

$$\mathcal{O}(\phi) = \mathcal{O}_0(\phi_0) + g_0 \mathcal{O}_1(\phi_0, \phi_1) + \dots \quad \text{Ex.:} \quad \phi^2 = \phi_0^2 + g_0 2\phi_0 \phi_1 + \dots$$

$$\lim_{t \rightarrow \infty} \langle \mathcal{O}_r(\phi_0, \dots, \phi_r) \rangle_\eta = k_r^\mathcal{O} \quad \text{where} \quad \langle \mathcal{O} \rangle = k_0^\mathcal{O} + g_0 k_1^\mathcal{O} + \dots$$

# Numerical stochastic perturbation theory

Go numerical!

(Di Renzo et. al. '94)

Computerize

$$t \rightarrow t_n = n\varepsilon, \quad n \in \mathbb{N} \quad \text{and} \quad r = 0, 1, \dots, N$$

Discrete dynamics

$$\text{Ex.:} \quad \phi_0(t_{n+1}) = -\varepsilon \Delta \phi_0(t_n) + \sqrt{\varepsilon} \eta(t_n)$$

$$\phi_1(t_{n+1}) = -\varepsilon \Delta \phi_1(t_n) - \varepsilon \delta m_1^2 \phi_0(t_n) - \frac{\varepsilon}{3!} \phi_0(t_n)^3$$

...

$$\phi_r(t_{n+1}) = -\varepsilon F_r(\phi_0(t_n), \dots, \phi_r(t_n)) + \delta_{r0} \sqrt{\varepsilon} \eta(t_n)$$

Order-by-order ops.

$$\phi = \{\phi_0, \dots, \phi_N\} \quad \text{Ex.:} \quad \phi + \chi \rightarrow \phi_r + \chi_r, \quad \phi^2 \rightarrow \phi_r^2 = \sum_{s=0}^r \phi_{r-s} \cdot \phi_s$$

Stochastic estimates

$$\overline{\mathcal{O}}_r = \frac{1}{N_{\text{cnfg}}} \sum_{n=0}^{N_{\text{cnfg}}} \mathcal{O}_r(\phi_0(t_n), \dots, \phi_r(t_n)) \quad \text{Ex.:} \quad \phi^2 = \{\phi_0^2, 2\phi_0\phi_1, \dots\}$$

# Langevin based NSPT

Some known (and proven) facts

## [Statistical errors]

$$\sigma(\overline{\mathcal{O}}_r)^2 = N_{\text{cnfg}}^{-1} \times \tau_{\text{int}}(\mathcal{O}_r) \times \text{var}(\mathcal{O}_r) \quad [\mathcal{O} \equiv \text{multiplicatively ren.}]$$

### ► Autocorrelations

(Zinn-Justin '86; Zinn-Justin, Zwanziger '88)

$$\tau_{\text{int}}(\mathcal{O}_r) \stackrel{a \rightarrow 0}{\propto} 1/a^2$$

### ► Variances

(Lüscher '15)

$$\text{var}(\mathcal{O}_r) = \overline{\mathcal{O}_r^2} - (\overline{\mathcal{O}_r})^2 \stackrel{a \rightarrow 0}{\propto} \ln(a)$$

**IMPORTANT:**  $\text{var}(\mathcal{O}_r) \neq 2r\text{-order of } \langle \mathcal{O}^2 \rangle - \langle \mathcal{O} \rangle^2 \quad [r \neq 0]$

$\Rightarrow$  they are **NOT** given by the theory **ALONE!**

## [Systematic errors]

(Parisi '81; Batrouni et. al. '85)

$$\text{► } \lim_{N_{\text{cnfg}} \rightarrow \infty} \overline{\mathcal{O}}_r = k_r^{\mathcal{O}} + \mathcal{O}(\varepsilon^p) \quad [p \equiv \text{order integration scheme}]$$

**IMPORTANT: NO** accept-reject step: **NOT** smooth in  $g_0$ !

$\Rightarrow$  inexact algorithm and step-size errors

## CONCLUSION

A good NSPT algorithm must give small: autocorrelations, **variances**, and systematic errors!

# Stochastic molecular dynamics algorithm

The Horowitz way

(Horowitz '85, '87, '91; Jansen, Liu '95)

## Stochastic molecular dynamics (SMD)

$$\partial_t \phi(t, x) = \pi(t, x)$$

$$\partial_t \pi(t, x) = -\frac{\delta S(\phi)}{\delta \phi(t, x)} - \gamma \pi(t, x) + \eta(t, x)$$

$$\langle \eta(t, x) \eta(s, y) \rangle_\eta = 2\gamma \delta_{xy} \delta(t - s)$$

- ▶ Adjustable “friction” parameter  $\gamma > 0$
- ▶ Coincides with Langevin equation for  $\gamma \rightarrow \infty$
- ▶ On the lattice this limit is also reached if  $\gamma \equiv a\gamma = \text{const.}$

(Lüscher, Schaefer '11)

In this case:

(MDB, Garofalo, Kennedy '17; MDB, Lüscher '17)

- ▶ **Autocorrelations:**  $\tau_{\text{int}}(\mathcal{O}_r) \stackrel{a \rightarrow 0}{\approx} c_{\mathcal{O}_r}(\gamma)/a^2$
- ▶ **Variances:**  $\text{var}(\mathcal{O}_r) \stackrel{a \rightarrow 0}{\approx} d_{\mathcal{O}_r}(\gamma) \ln(a)$

## Phase-space stochastic quantization

$$\lim_{t \rightarrow \infty} \langle \phi(t, x_1) \dots \phi(t, x_n) \rangle_\eta = \langle \varphi(x_1) \dots \varphi(x_n) \rangle$$

$$P_{\text{eq}}(\pi, \phi) \propto e^{-H(\pi, \phi)}, \quad H(\pi, \phi) = \frac{1}{2}(\pi, \pi) + S(\phi)$$



# SMD based NSPT

## The algorithm in a nutshell

(MDB, Garofalo, Kennedy '17; MDB, Lüscher '17)

### Start:

$$t \rightarrow t_n = n\epsilon, \quad n \in \mathbb{N}, \quad \text{and} \quad \phi = \{\phi_0, \dots, \phi_N\}, \quad \pi = \{\pi_0, \dots, \pi_N\}$$

### Step 1: Momentum rotation

$$\pi_r \rightarrow c_1 \pi_r + c_2 \delta_{r0} v, \quad c_1 = e^{-\gamma\epsilon}, \quad c_1^2 + c_2^2 = 1$$

$$\langle v(x)v(y) \rangle_v = \delta_{xy},$$

### Step 2: Molecular dynamics step

$$\left. \begin{aligned} I_{\pi_r, h} : \pi_r &\rightarrow \pi_r - h F_r(\phi) \\ I_{\phi_r, h} : \phi_r &\rightarrow \phi_r + h \pi_r \end{aligned} \right\} \begin{array}{l} \text{Symplectic reversible int.} \\ t_n \rightarrow t_{n+1} \end{array}$$

$$\text{Ex. LPF: } I_\epsilon = I_{\phi, \epsilon/2} I_{\pi, \epsilon} I_{\phi, \epsilon/2}$$

Step 1  $\rightarrow$  Step 2  $\rightarrow$  Step 1  $\rightarrow \dots \rightarrow$  Step 2

### Step 3: Do not forget to measure

$$\overline{\mathcal{O}}_r = \frac{1}{N_{\text{cnfg}}} \sum_{n=0}^{N_{\text{cnfg}}} \mathcal{O}_r(\phi_0(t_n), \dots, \phi_r(t_n))$$

# SMD based NSPT

## Convergence to a unique and stationary distribution

(MDB, Lüscher '17)

The discrete stochastic processes  $\{\phi_r(t_n), \pi_r(t_n)\}_{r=0,1,\dots,N}$ , all converge for  $t_n \rightarrow \infty$  to a **unique** and **stationary** distribution iff:

1.  $\Delta > 0$
2.  $\epsilon^2 \|\Delta\| < \kappa$

$$S_0(\phi_0) = \frac{1}{2}(\phi_0, \Delta \phi_0)$$

$$\|\Delta\| \equiv \lambda_{\max} \approx 16$$

## Leading-order distros [ $r = 0$ - free theory]

$$\hat{P}_{\text{eq}}(\pi_0, \phi_0) \propto e^{-\hat{H}_0(\pi_0, \phi_0)}, \quad \hat{H}_0 \equiv \text{Shade Hamiltonian}$$

$$\hat{H}_0(\pi_0, \phi_0) = \frac{1}{2}(\pi_0, \pi_0) + \hat{S}_0(\phi_0), \quad \hat{S}_0(\phi_0) = \frac{1}{2}(\phi_0, \hat{\Delta} \phi_0)$$

## Examples

(Omelyan, Mryglod, Folk '03)

- |  |  |
|--|--|
| ▶ $\hat{\Delta}_{\text{LPPF}} = \Delta(1 + a_0 \epsilon^2 \Delta)$           | $a_0 = -2.5 \times 10^{-1}, \quad \hat{\Delta} > 0 \Rightarrow \kappa = 4$ |
| ▶ $\hat{\Delta}_{\text{OMF2}} = \Delta(1 + a_1 \epsilon^2 \Delta + \dots)$   | $a_1 \approx -2.5 \times 10^{-3}, \quad \kappa = 6.51$                     |
| ▶ $\hat{\Delta}_{\text{OMF4}} = \Delta(1 + a_2 \epsilon^4 \Delta^2 + \dots)$ | $a_2 \approx -2.6 \times 10^{-5}, \quad \kappa = 9.87$                     |

## Effectiveness

$$\|1 - \hat{\Delta}_{\text{LPPF}}/\Delta\| \approx 25 \|1 - \hat{\Delta}_{\text{OMF2}}/\Delta\| \approx 300 \|1 - \hat{\Delta}_{\text{OMF4}}/\Delta\| \quad [\text{@ fixed cost per MDU}]$$

# NSPT in lattice QCD

SU(3) Yang-Mills theory

(MDB, Lüscher '17)

SMD equations

$$\partial_t U_t(x, \mu) = g_0 \pi_t(x, \mu) U_t(x, \mu)$$

$$\partial_t \pi_t(x, \mu) = -g_0 (\partial_{x,\mu}^a S_G)(U_t) T^a - \gamma \pi_t(x, \mu) + \eta_t(x, \mu)$$

$$\langle \eta_t^a(x, \mu) \eta_s^b(y, \nu) \rangle = 2\gamma \delta^{ab} \delta_{\mu\nu} \delta_{xy} \delta(t-s)$$

Perturbative fields (  $U_k \notin \mathfrak{su}(3)$ ,  $\pi_k \in \mathfrak{su}(3)$  )

$$U = e^{g_0 A} = 1 + g_0 U_0 + g_0^2 U_1 + \dots, \quad \pi = \pi_0 + g_0 \pi_1 + \dots$$

Step 1. Momentum rotation

$$\pi \rightarrow c_1 \pi + c_2 v$$

Step 2. Molecular dynamics step

$$\left. \begin{aligned} I_{\pi,h} : \pi &\rightarrow \pi - h g_0 \partial S_G(U) \\ I_{U,h} : U &\rightarrow e^{h g_0 \pi} U \end{aligned} \right\} \begin{array}{l} \text{Symplectic reversible int.} \\ t_n \rightarrow t_{n+1} \end{array}$$

Step 3. Gauge damping ...

**NOTE:** Convergence to a unique and stationary distribution requires care due to **gauge and other zero modes**, but it can **rigorously** be guaranteed!

# NSPT in lattice QCD

Inclusion of quarks

(MDB, Lüscher '17)

Action [Ex.:  $N_f = 2$  Wilson-fermions]

$$S = S_G + S_{\text{pf}}, \quad S_{\text{pf}} = (D^{-1}[U]\phi, D^{-1}[U]\phi), \quad \phi \equiv \text{pseudo-fermions}$$

Step 1. Momentum and pseudo-fermions rotation

$$\pi \rightarrow c_1 \pi + c_2 v, \quad \phi \rightarrow c_1 \phi + c_2 (D[U]\eta), \quad v, \eta \equiv \text{Gaussian random fields}$$

$$\text{with} \quad \phi = \phi_0 + g_0 \phi_1 + \dots \quad \eta = \eta_0$$

Step 2. Molecular dynamics step

$$\left. \begin{aligned} I_{\pi,h} : \pi &\rightarrow \pi - hg_0 \partial S(U) \\ I_{U,h} : U &\rightarrow e^{hg_0 \pi} U \end{aligned} \right\} \begin{array}{l} \text{Symplectic reversible int.} \\ t_n \rightarrow t_{n+1} \end{array}$$

Step 3. Gauge damping ...

**KNOWN-ISSUE:** The integration of the MD eqs. requires solving

Dirac equation

$$D[U]\chi = \phi$$

...but it cannot be too hard in PTh!

# NSPT in lattice QCD

## Inclusion of quarks (cont.)

### Dirac op.

$$D[U] = D_0 + g_0 D_1[U_0] + g_0^2 D_2[U_0, U_1] + \dots$$

### Inverse Dirac op.

$$D^{-1} = D_0^{-1} + g_0 (D^{-1})_1 + g_0^2 (D^{-1})_2 + \dots$$

with

$$(D^{-1})_1 = -D_0^{-1} D_1 D_0^{-1}$$

$$(D^{-1})_2 = -D_0^{-1} D_2 D_0^{-1} - D_0^{-1} D_1 (D^{-1})_1, \text{ etc.}$$

### Solution Dirac eq.

$$\chi = \chi_0 + g_0 \chi_1 + g_0^2 \chi_2 + \dots$$

with

$$\chi_0 = D_0^{-1} \phi_0$$

$$\chi_1 = (D^{-1})_1 \phi_0 + D_0^{-1} \phi_1 = -D_0^{-1} [D_1 \chi_0 - \phi_1], \text{ etc.}$$

### Remarks

- ▶ Only  $D_0^{-1}$  is needed: we can use a FFT! (Di Renzo, Scorzato '04)
- ▶  $D_0 \equiv D_0(m_R)$ : we shall use an automated mass-renormalization (MDB, Garofalo, Kennedy '17)
- ▶ Quarks do **NOT** add more constraints on the convergence to equilibrium (MDB, Lüscher '17)

# The gradient flow coupling in SU(3) Yang-Mills

## A non-trivial case study

### Gradient flow

$$\partial_t B_\mu(t, x) = D_\nu G_{\nu\mu}(t, x) \quad [t \equiv \text{flow time}]$$

$$G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu], \quad B_\mu(0, x) = A_\mu(x)$$

### Schrödinger functional (Lüscher et. al. '92)

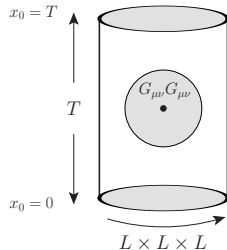
$$A_k(x)|_{x_0=0} = A_k(x)|_{x_0=T} = 0$$

$$A_\mu(x + \hat{k}L) = A_\mu(x)$$

### Basic quantity (Lüscher '10; Fodor et. al. 12'; Fritzsche, Ramos '13)

$$t^2 \langle E(t, x) \rangle, \quad E(t, x) = \frac{1}{4} G_{\mu\nu}^a(t, x) G_{\mu\nu}^a(t, x)$$

$$T = L, \quad x_0 = T/2, \quad \sqrt{8t} = 0.3 \times L$$



### NSPT observables

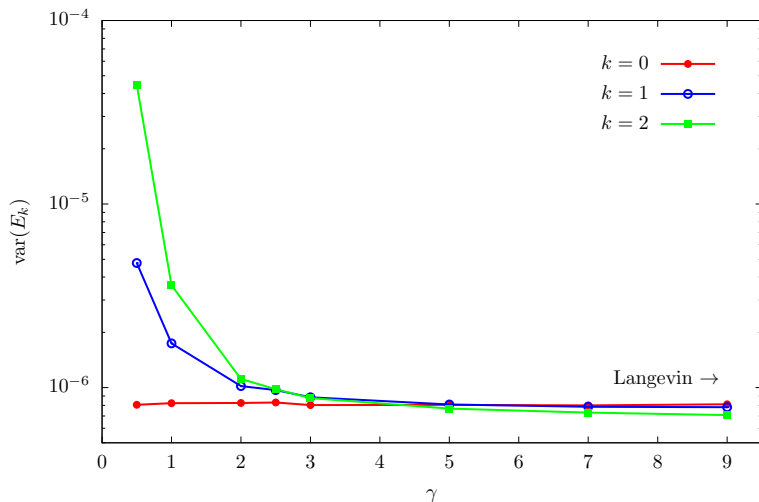
$$[ \alpha_{\overline{\text{MS}}} \leftrightarrow g_0 \text{ (Lüscher, Weisz '95)} ]$$

$$t^2 \langle E(t, x) \rangle = g_0^2 E_0(L/a) + g_0^4 E_1(L/a) + g_0^6 E_2(L/a) + \dots$$

$$\stackrel{a/L \rightarrow 0}{=} \textcolor{red}{k}_0 \{ \alpha_{\overline{\text{MS}}}(q) + \textcolor{red}{k}_1 \alpha_{\overline{\text{MS}}}(q)^2 + \textcolor{red}{k}_2 \alpha_{\overline{\text{MS}}}(q)^3 + \dots \}, \quad q = 1/\sqrt{8t}$$

# Algorithm-dependence of variances

Variances  $\text{var}(E_k)$  as a function of  $\gamma$  for  $L/a = 16$

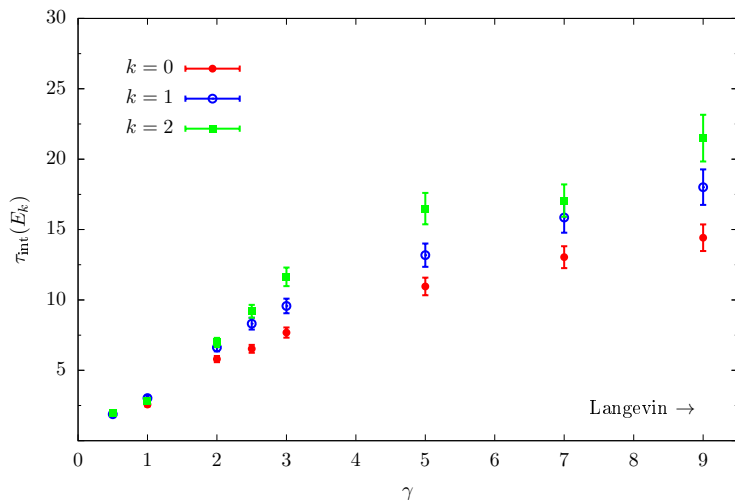


NOTE:

$\text{var}(E_{k>0}) \neq t^4 [\langle E^2 \rangle - \langle E \rangle^2] \big|_{g_0^{4(k+1)}} \Rightarrow \text{var}(E_{1,2})$  are **algorithm-dependent**!

# Autocorrelations

Integrated autocorrelations  $\tau_{\text{int}}(E_k)$  (in MDUs) as a function of  $\gamma$  for  $L/a = 16$



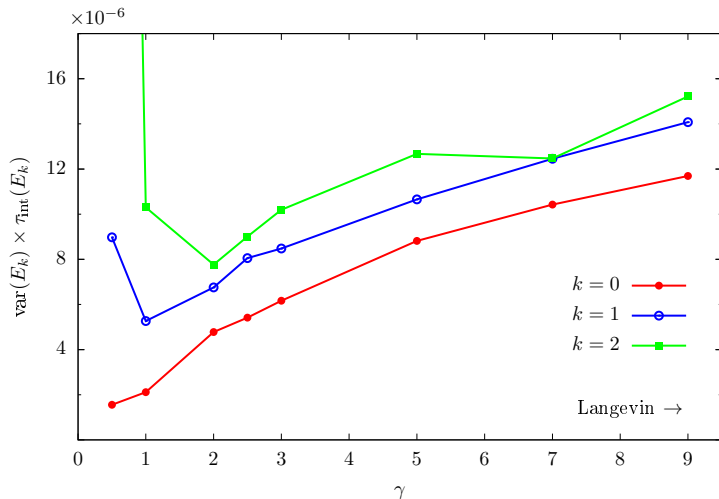
## NOTE:

The autocorrelations of the different orders appear to have similar  $\gamma$ -dependence



# Statistical errors

Products  $\text{var}(E_k) \times \tau_{\text{int}}(E_k)$  as a function of  $\gamma$  for  $L/a = 16$

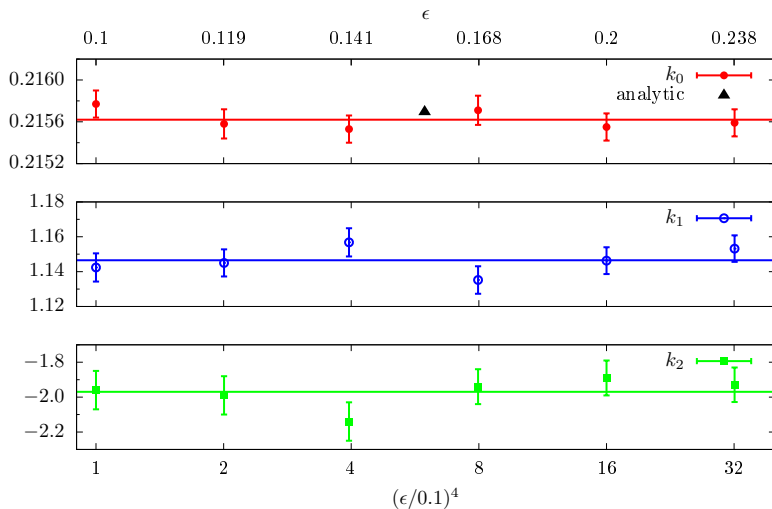


## NOTE:

- ▶ Algorithms tuned for **small autocorrelations** tend to have **large variances** and vice-versa.
- ▶ Same qualitative behavior observed in a detailed study in  $\phi^4$ -theory (MDB, Garofalo, Kennedy '17)

# Systematic errors

Coefficients  $k_0, k_1, k_2$  for  $L/a = 24$ , OMF4 integrator, 10k meas. per  $\epsilon$



NOTE:

The measured energy violations per MD step are  $\Delta H_i = O(\epsilon^5)$  w/  $H = H_0 + g_0 H_1 + \dots$

# Simulation parameters

...and other info

## Lattice sizes

$$10 \leq L/a \leq 40$$

## Step sizes

- ▶  $L/a \leq 20$ :  $\epsilon = 0.168$
- ▶  $L/a \geq 24$ :  $\epsilon = 0.168 \times 24 \times (a/L)$   
 $\Rightarrow$  Step size errors  $\propto (a/L)^4$  w/ OMF4

## Gamma

- ▶  $L/a \leq 20$ :  $\gamma = 4 - 5$
- ▶  $L/a \geq 24$ :  $\gamma = 3$   
 $\Rightarrow$  Langevin scaling (eventually)

## Autocorrelations

$$L/a = 24 \rightarrow 40: \tau_{\text{int}}(E_k) \approx 25 \rightarrow 50 \text{ MDUs} \quad [ 30\% \text{ less than } 1/a^2 ]$$

## Variances

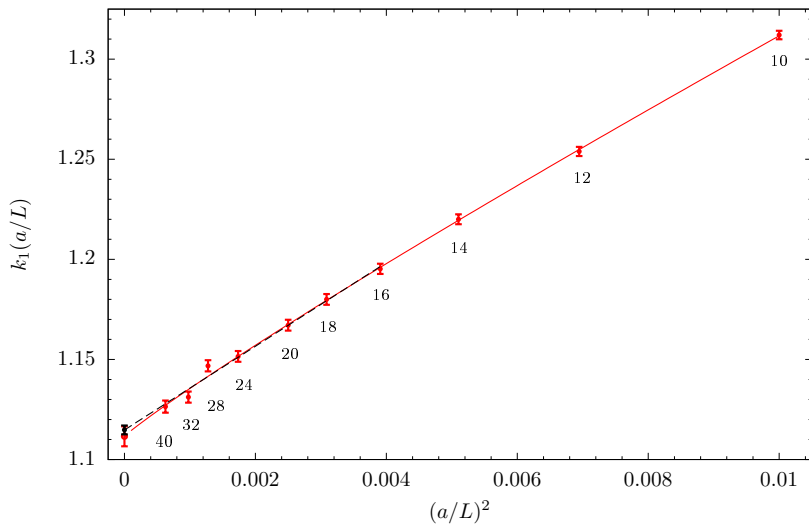
$$L/a = 24 \rightarrow 40: \text{var}(E_1) : +19\%, \quad \text{var}(E_2) : +30\% \quad [ \propto [\ln(a)]^r, r = 1, 2 ]$$

## Measurements

60k – 80k

# Continuum limit of $k_1$

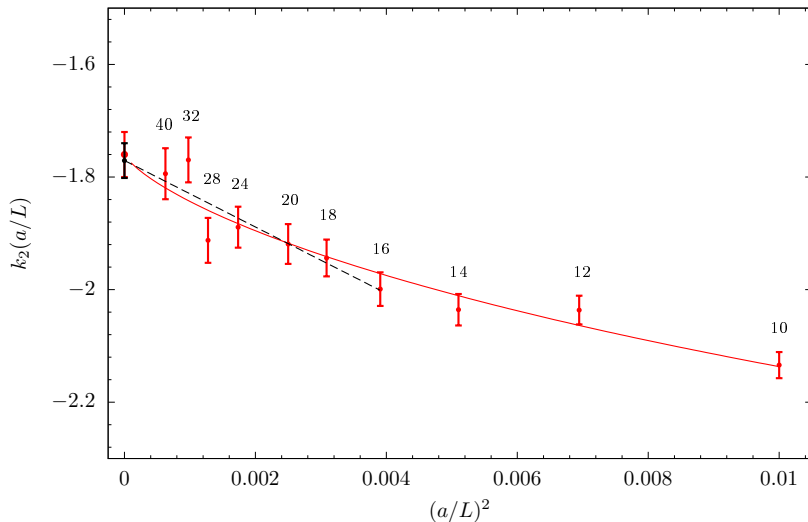
$O(a)$ -improved data, Wilson action, Wilson flow,  $E_{\text{plaq}}$



$$k_1 \stackrel{a/L \rightarrow 0}{=} a_0 + \{a_1 + b_1 \ln(L/a)\}(a/L)^2 + \dots$$

# Continuum limit of $k_2$

O( $a$ )-improved data, Wilson action, Wilson flow,  $E_{\text{plaq}}$



$$k_2 \stackrel{a/L \rightarrow 0}{=} a_0 + \{a_1 + b_1 \ln(L/a) + c_1 (\ln(L/a))^2\} (a/L)^2 + \dots$$

# The gradient flow coupling and its family

...are they all nice?

More schemes

$$\alpha(\mu) \propto \begin{cases} t^2 \langle G_{\mu\nu} G_{\mu\nu} \rangle \\ t^2 \langle G_{kl} G_{kl} \rangle & s \equiv \text{spatial} \\ t^2 \langle G_{0k} G_{0k} \rangle & t \equiv \text{temporal} \end{cases} \quad \mu^{-1} = \sqrt{8t} = cL$$

Parametric uncertainty

$$\begin{aligned} \delta k_1 &\approx 5 \times 10^{-3} \\ \delta k_2 &\approx 5 \times 10^{-2} \end{aligned} \Rightarrow \frac{\delta \alpha_{\overline{\text{MS}}}(M_Z)}{\alpha_{\overline{\text{MS}}}(M_Z)} \approx 0.1\% < 0.5\% \text{ i.e. negligible in practice!}$$

Who runs faster?

$$L \frac{\partial \alpha}{\partial L} = \beta_0 \alpha^2 + \beta_1 \alpha^3 + \beta_2 \alpha^4 + \dots$$

$$\beta_0 = \frac{11}{2\pi}, \quad \beta_1 = \frac{51}{(2\pi)^2}$$

$c$	$\beta_2/\beta_0$	$\beta_{2,s}/\beta_0$	$\beta_{2,t}/\beta_0$
0.4	-4.88(6)	-8.04(7)	-2.21(8)
0.3	-2.99(4)	-3.74(5)	-2.29(6)
0.2	-2.38(6)	-2.51(6)	-2.22(7)
0.0	-2.1751(3)	-2.1751(3)	-2.1751(3)

# Conclusions & outlook

## Conclusions

- ▶ NSPT is a **powerful** tool for automatizing LPT calculations  
⇒ Given the configurations any observable is computable
- ▶ Complicated lattice set-ups and observables can **easily** be considered
- ▶ The recent algorithmic advances opened the way for **precise** and **accurate** results  
⇒ First NSPT calculation extracting **continuum** results!
- ▶ A full implementation for SU(3) gauge theory can be downloaded at:  
[luscher.web.cern.ch/luscher/NSPT](http://luscher.web.cern.ch/luscher/NSPT)

## Outlook

- ▶ The inclusion of fermions is in principle straightforward and does not pose any technical difficulty
- ▶ Fermions are not expected to slow down the simulations by a big factor
- ▶ All sort of algorithmic tricks can be applied here too.  
Do they help? If so, why? Variances, step-size errors, ...?

(Di Renzo, Scorzato '04)





# BACKUP

# The gradient flow coupling in SU(3) Yang-Mills

## Lattice formulation

### Wilson flow

(Lüscher '10)

$$\partial_t V_t(x, \mu) V_t(x, \mu)^{-1} = -g_0^2 (\partial_{x,\mu}^a S_G)(V_t) T^a, \quad V_{t=0}(x, \mu) = U(x, \mu)$$

### Perturbative solution

(MDB, Hesse '13)

$$V_t = e^{g_0 B_\mu(t)} = 1 + g_0 V_{t,0} + g_0^2 V_{t,1} + \dots, \quad V_{t,r} = U_r$$

### Schrödinger functional

$$U(x, k)|_{x_0=0} = 1 = U(x, k)|_{x_0=T} \Rightarrow U_r(x, k)|_{x_0=0,T} = 0$$

### O(a) action counterterm

(Lüscher et. al. '92; Bode, Wolff, Weisz '98)

$$\propto c_t \sum_{\mathbf{x}} F_{0k}^a(x) F_{0k}^a(x)|_{x_0=0,T}, \quad c_t = 1 - 0.08900 g_0^2 - 0.0294 g_0^2 + \dots$$

### Basic observable

$$t^2 \langle E(t, x) \rangle = g_0^2 E_0(L/a) + g_0^4 E_1(L/a) + g_0^6 E_2(L/a) + \dots$$

### Gradient flow coupling

[  $\alpha_{\overline{\text{MS}}} \leftrightarrow g_0$  (Lüscher, Weisz '95) ]

$$t^2 \langle E(t, x) \rangle = k_0(a/L) \{ \alpha_{\overline{\text{MS}}}(q) + k_1(a/L) \alpha_{\overline{\text{MS}}}(q)^2 + k_2(a/L) \alpha_{\overline{\text{MS}}}(q)^3 + \dots \}$$

$$\lim_{a/L \rightarrow 0} k_i(a/L) = k_i$$

# NSPT in lattice QCD

Issues of convergence to an equilibrium distribution

Leading order dynamics  $[A = U_0]$

$$I_{\pi_0, h} : \pi_0 \rightarrow \pi_0 - h(\Delta A) \quad S_G = S_0 + g_0 S_1 + g_0^2 S_2 + \dots$$

$$I_{U_0, h} : A \rightarrow A + h \pi_0 \quad S_0 = \frac{1}{2} \sum_{x, y} A_\mu(x) \Delta_{\mu\nu}(x, y) A_\nu(y),$$

**PROBLEM:**  $\Delta \geq 0$

1. Gauge modes  $A_\mu(x) \sim 0$
2. In a finite volume w/ periodic bc.  $\exists A_\mu(x) \not\sim 0$  s.t.  $\Delta A = 0$

(Gonzalez-Arroyo, Jurkiewicz, Korthals-Altes '83)

**N.B.:** Issues of the perturbative expansion not (N)SPT!

**SOLUTION:**

1. Gauge damping aka stochastic gauge fixing
2. Choose proper boundary conditions for the fields  
e.g.  $A_k(x)|_{x_0=0} = A_k(x)|_{x_0=T} = 0$

(Zwanziger '81)

**RESULT:** Separate convergence criteria for the gauge modes

(MDB, Lüscher '87)

# Gauge damped SMD equations

The Zwanziger way

Time-dependent gauge transf.

$$\pi_t(x, \mu) \rightarrow \Lambda_t(x) \pi_t(x, \mu) \Lambda_t(x)^{-1}$$

$$U_t(x, \mu) \rightarrow \Lambda_t(x) U_t(x, \mu) \Lambda_t(x + \hat{\mu})^{-1}, \quad \Lambda_t(x) \in \text{SU}(3)$$

Modified SMD equations

$$\partial_t U_t(x, \mu) = g_0 \{ \pi_t(x, \mu) - \nabla_\mu \omega_t(x) \} U_t(x, \mu)$$

$$\partial_t \pi_t(x, \mu) = -g_0 (\partial_{x,\mu}^a S_G)(U_t) T^a - \gamma \pi_t(x, \mu) + \eta_t(x, \mu) + g_0 [\omega_t(x), \pi_t(x, \mu)]$$

$$\langle \eta_t^a(x, \mu) \eta_s^b(y, \nu) \rangle = 2\gamma \delta^{ab} \delta_{\mu\nu} \delta_{xy} \delta(t-s)$$

with

$$\omega_t(x) = g_0^{-1} \partial_t \Lambda_t(x) \Lambda_t(x)^{-1} \in \mathfrak{su}(3)$$

$$\nabla_\mu \omega_t(x) = U_t(x, \mu) \omega_t(x + \hat{\mu}) U_t(x, \mu)^{-1} - \omega_t(x)$$

Gauge damping [Ex.:  $L = T = \infty$ ]

$$(\partial_t + \gamma) \omega_t(x) = \lambda (d^* C)(t, x), \quad (d^* C)(t, x) = -\partial_\nu^* C_\nu(t, x), \quad \lambda > 0$$

$$C_\mu(t, x) = \frac{1}{2g_0} \left\{ U_t(x, \mu) - U_t(x, \mu)^{-1} - \frac{1}{3} \text{tr} \left[ U_t(x, \mu) - U_t(x, \mu)^{-1} \right] \right\} \xrightarrow{g_0 \rightarrow 0} A_\mu(t, x)$$

# NSPT in lattice QCD

## Gauge damping

### Gauge transformation

$$\pi(x, \mu) \rightarrow \Lambda(x) \pi(x, \mu) \Lambda(x)^{-1}, \quad U(x, \mu) \rightarrow \Lambda(x) U(x, \mu) \Lambda(x + \hat{\mu})^{-1}$$

### Gauge damping field

$$\Lambda(x) = e^{\epsilon g_0 \omega(x)} \in \text{SU}(3), \quad \omega(x) \in \mathfrak{su}(3), \quad \omega(x) = \omega_0 + g_0 \omega_1(x) + \dots$$

### Gauge-damping dynamics @ leading-order $[L = T = \infty]$

1.  $\omega_0(x) \rightarrow c_1 \omega_0(x)$   $c_1 = e^{-\epsilon \gamma}$
2.  $\omega_0(x) \rightarrow \omega_0(x) + \epsilon \lambda (d^* A)(x)$   $(d^* A)(x) = -\partial_\nu^* A_\nu(x)$
3.  $A_\mu(x) \rightarrow A_\mu(x) - \epsilon (d\omega_0)_\mu(x)$   $(d\omega_0)_\mu(x) = \partial_\mu \omega_0(x)$

$\Rightarrow \omega(x)$  assures a **restoring force** for the (longitudinal) **gauge modes!**

### Convergence criteria

1.  $\Delta|_{A^T} > 0$  (N.B.:  $d^* A^T = 0$ )
2.  $\epsilon^2 \|\Delta\| < \kappa$
3.  $\epsilon^2 \lambda \|dd^*\| < 2(1 + c_1)$  (N.B.:  $dd^* > 0$  and  $\|dd^*\| \leq 16$ )