# NSPT near the continuum limit

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*Based on work done in collaboration with Mattia Dalla Brida*

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## Introduction

Numerical stochastic perturbation theory (NSPT) Di Renzo et al. '94

- *Already led to some spectacular results, e.g.*

$$\langle \square \rangle = \sum_{n=0}^{N} c_n \alpha_0^n + \ldots$$

Horsley et al. '12 ($N$=20)

Bali et al. '14 ($N$=35)

- *But the coefficients of physical quantities are more difficult to obtain*

## Reference case

Pure SU(3) gauge theory

$L^4$ lattice with SF boundary conditions

"Gradient-flow coupling"

$$\alpha(q) = \text{const} \times t^2 \left\langle E(t,x) \right\rangle_{x_0=L/2} \quad \text{at} \quad \sqrt{8t} = 0.3 \times L \equiv 1/q$$

$E(t,x)$ : YM action density at gradient-flow time $t$

In perturbation theory

$$\alpha(q) = \alpha_s(q) + k_1 \alpha_s(q)^2 + k_2 \alpha_s(q)^3 + \ldots, \qquad \alpha_s = \alpha_{\overline{\mathrm{MS}}}$$

Fritzsch & Ramos '13

## Taking the continuum limit

$L/a \to \infty$, $t/a^2 \to \infty$ such that $t/L^2 =$ fixed

Potential obstacles

- *Autocorrelations* $\propto (L/a)^2$
- *Power-divergent variances*
- *Complicated dependence on* $a/L$

$\Rightarrow$ Need $\mathrm{O}(a)$-improvement and large lattices

$\Rightarrow$ Rapidly ends up being a large-scale project!

## Outline

## NSPT

For simplicity consider standard lattice $\phi^4$ theory

Generate a sequence of stochastic fields

$$\phi(t,x) = \sum_{k=0}^{N} g_0^k \phi_k(t,x), \qquad t = 0, \Delta t, 2\Delta t, \ldots,$$

such that

$$\langle \varphi(x_1) \ldots \varphi(x_n) \rangle = \frac{\Delta t}{T} \sum_{t=0}^{T} \phi(t,x_1) \ldots \phi(t,x_n) + \mathrm{O}(T^{-1/2})$$

up to order $g_0^N$

## Algorithms used for the generation of $\phi_0, \phi_1, \ldots$

Langevin equation Di Renzo et al. '94

$$\partial_t \phi = -\frac{\delta S}{\delta \phi} + \eta$$

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

In perturbation theory

$$\partial_t \phi_0 = (\Delta - m^2)\phi_0 + \eta$$

$$\partial_t \phi_1 = (\Delta - m^2)\phi_1 - (\delta m^2)^{(1)}\phi_0 - \tfrac{1}{3!}\phi_0^3$$

etc.

Integrated with 2nd order Runge-Kutta integrator

## Algorithms ... (cont.)

Stochastic molecular dynamics (SMD) Horowitz '85, ...

$$\partial_t \phi = \pi$$

$$\partial_t \pi = -\frac{\delta S}{\delta \phi} - 2\mu_0 \pi + \eta$$

$$\langle \eta(t,x)\eta(s,y)\rangle = 4\mu_0 \delta(t-s)\delta_{xy}$$

- May use standard symplectic integrators
- Langevin limit: $t \to 2\mu_0 t$, $\mu_0 \to \infty$
- HMC limit: $\mu_0 \to 0$ plus periodic regeneration of $\pi$

On the lattice, the adjustable parameter is $\gamma = 2\mu_0 a$

## Algorithms ... (cont.)

Instantaneous stochastic perturbation theory (ISPT) ML '14

Fourier-accelerated Langevin equation Davies et al. '86

Expected scaling of the autocorrelation times

| Langevin | SMD | ISPT | F.-a. Langevin |
|---|---|---|---|
| $a^{-2}$ | $a^{-2} \dots a^{-?}$ | n/a | $a^{-0}$ |

## Statistical errors

*In NSPT the statistical variances depend on the algorithm used!*

In general

$$\langle \mathcal{O} \rangle = c_0 + c_1 g_0 + c_2 g_0^2 + \ldots, \qquad c_k = \langle \mathcal{O}_k \rangle$$

where

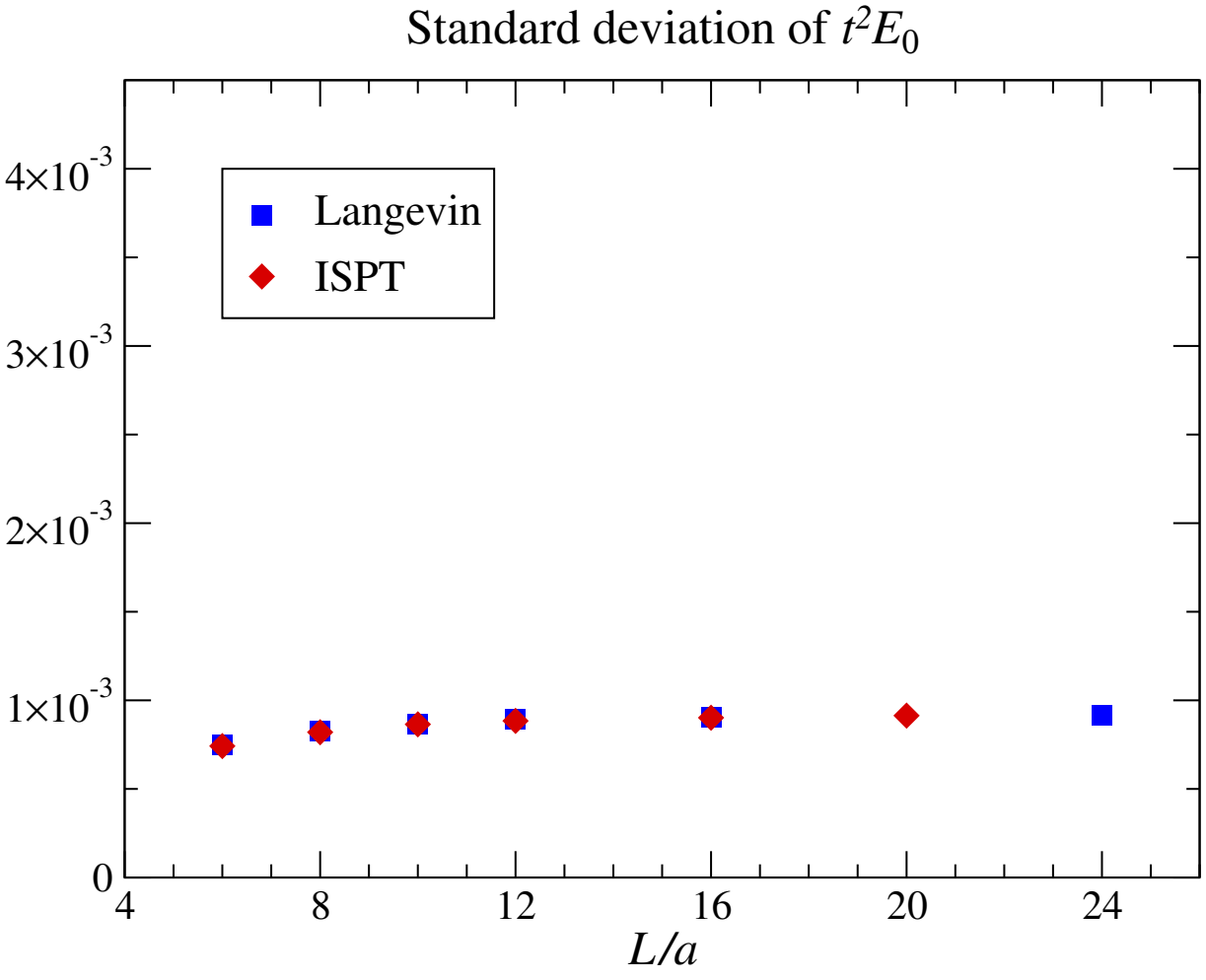
$$\mathcal{O}[\phi] = \mathcal{O}_0[\phi_0] + g_0 \mathcal{O}_1[\phi_0, \phi_1] + \ldots$$

But the variances

$$\langle \mathcal{O}_k \mathcal{O}_k \rangle - \langle \mathcal{O}_k \rangle^2$$

are <u>not</u> the order-$2k$ coefficients of any observables!

# Example: Langevin NSPT vs ISPT



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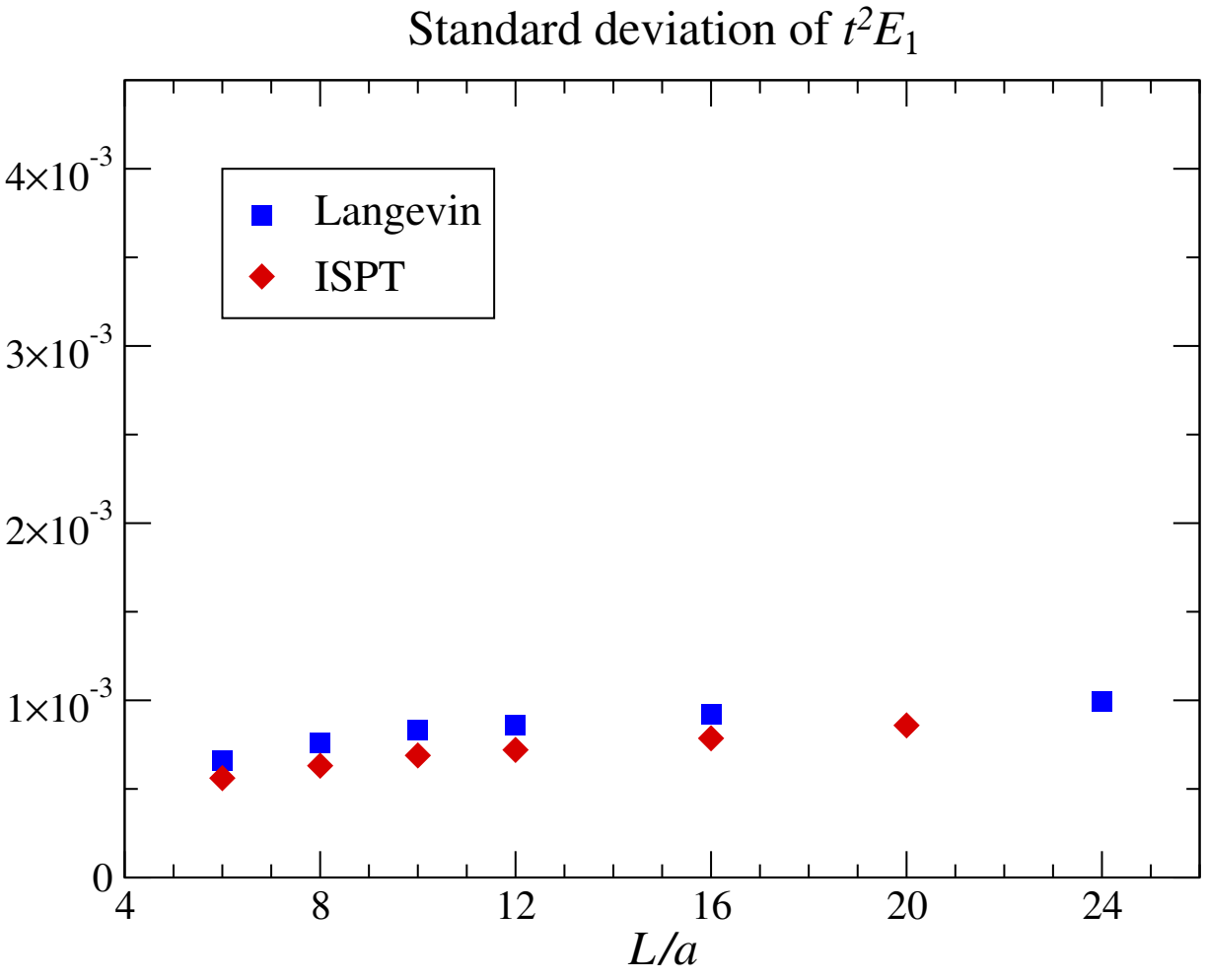

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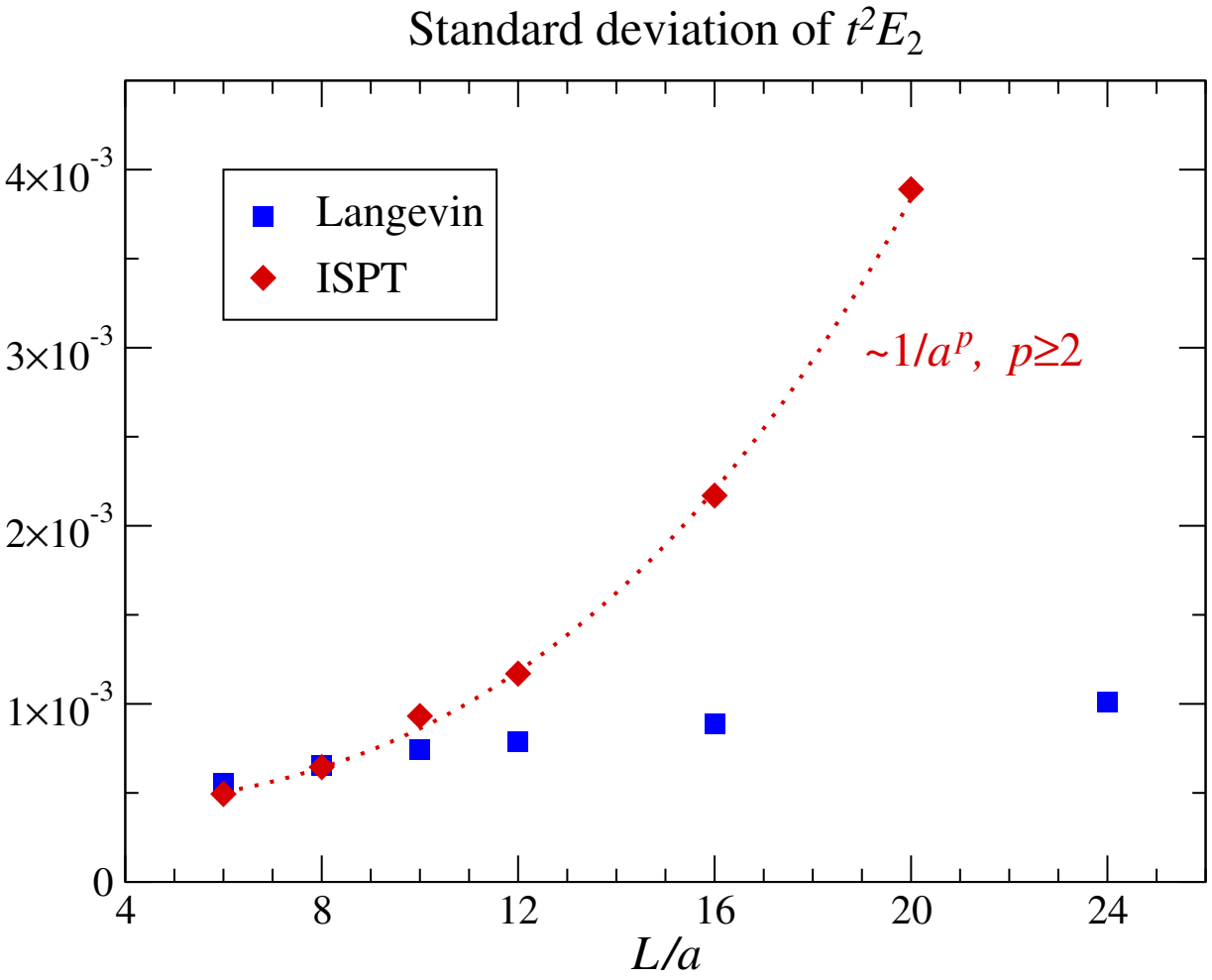


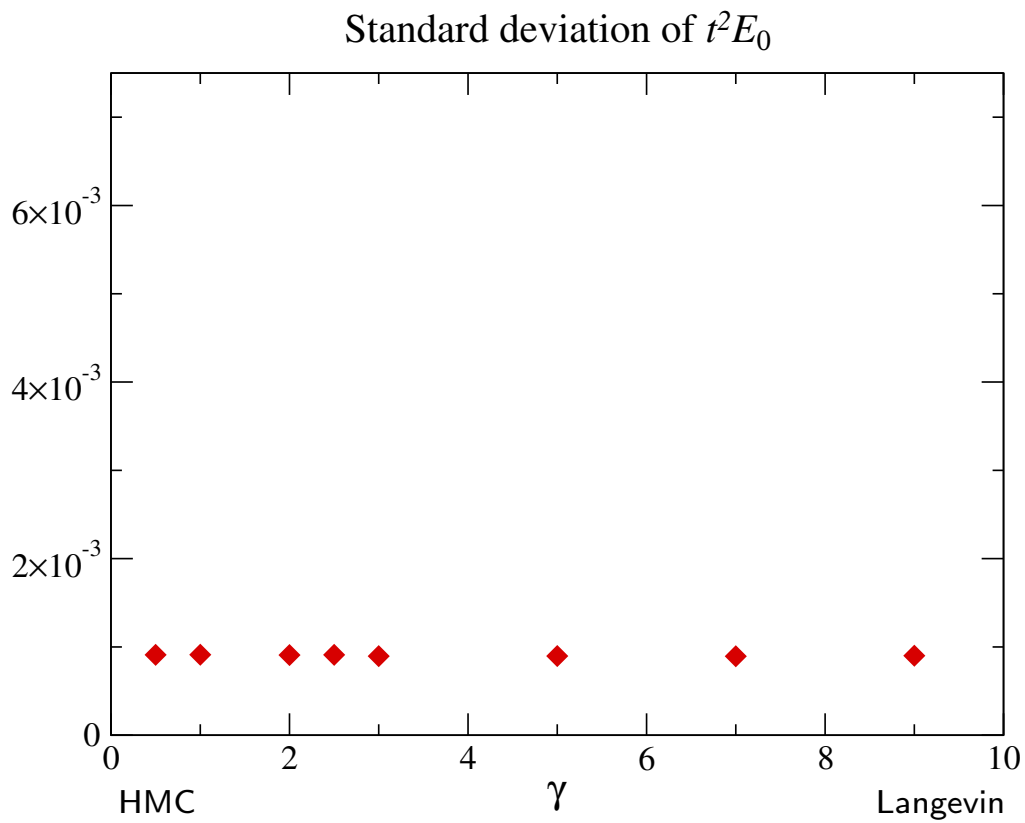

Similar behaviour observed in the $\phi^4$ theory  Dalla Brida, Kennedy & Garofalo '15

**Theorem:**

*To all orders of Langevin NSPT, the standard deviations of physical quantities grow at most logarithmically as* $a \to 0$

However, Fourier-accelerated Langevin NSPT is as bad as ISPT!

SMD at fixed L/a=16



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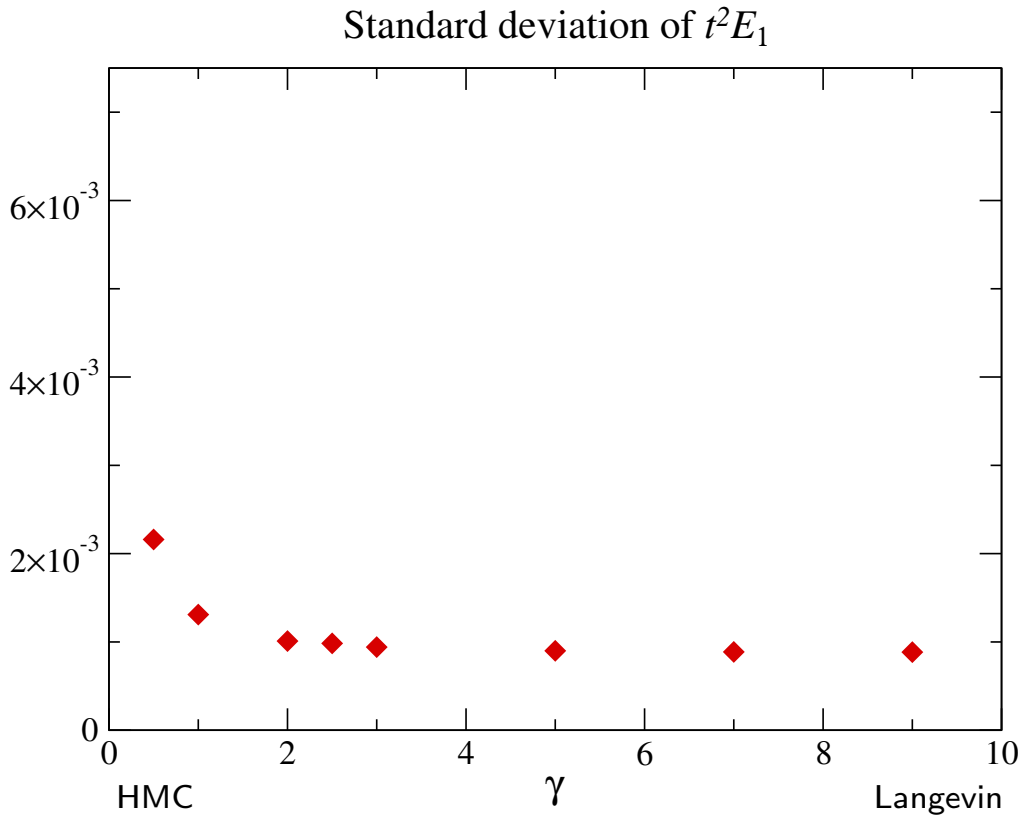

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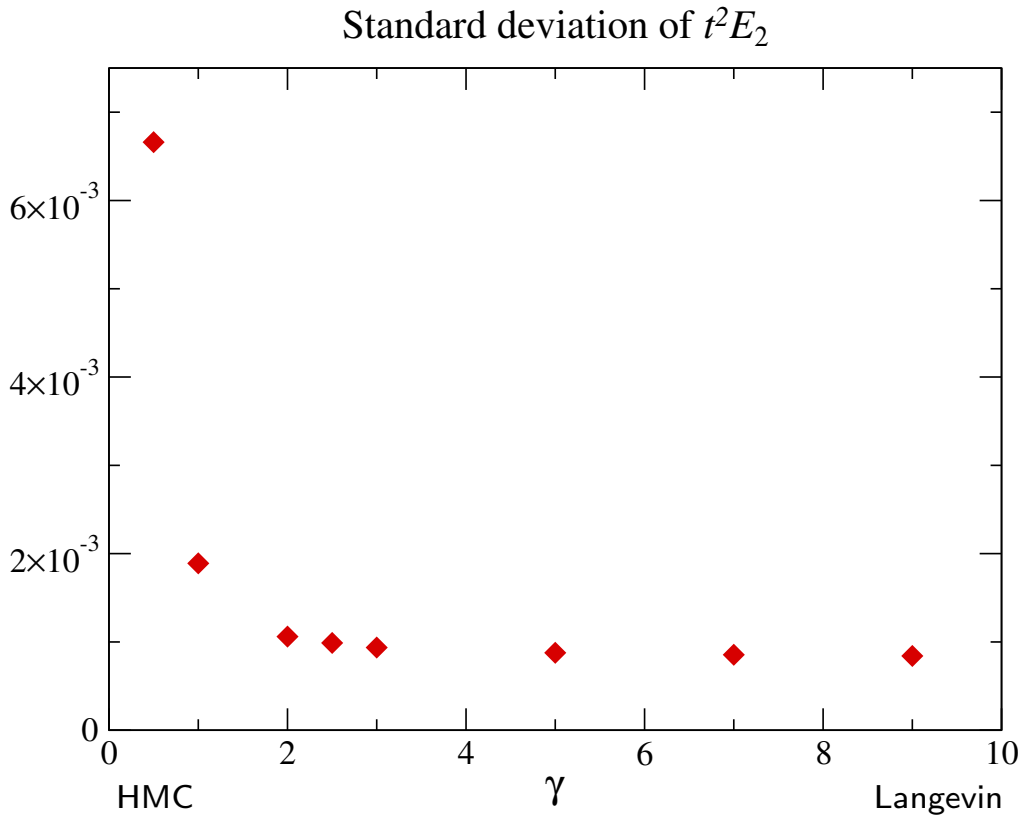


The studies conducted so far show that

- Autocorrelations $\searrow$ $\Rightarrow$ standard deviations $\nearrow$
- The SMD algorithm with $\gamma = 2 \ldots 5$ currently yields the smallest $\tau_{\mathrm{int}}(E_k) \times \mathrm{var}(E_k)$
- The molecular dynamics evolution becomes unstable when expanded in PT!

## Integration errors?

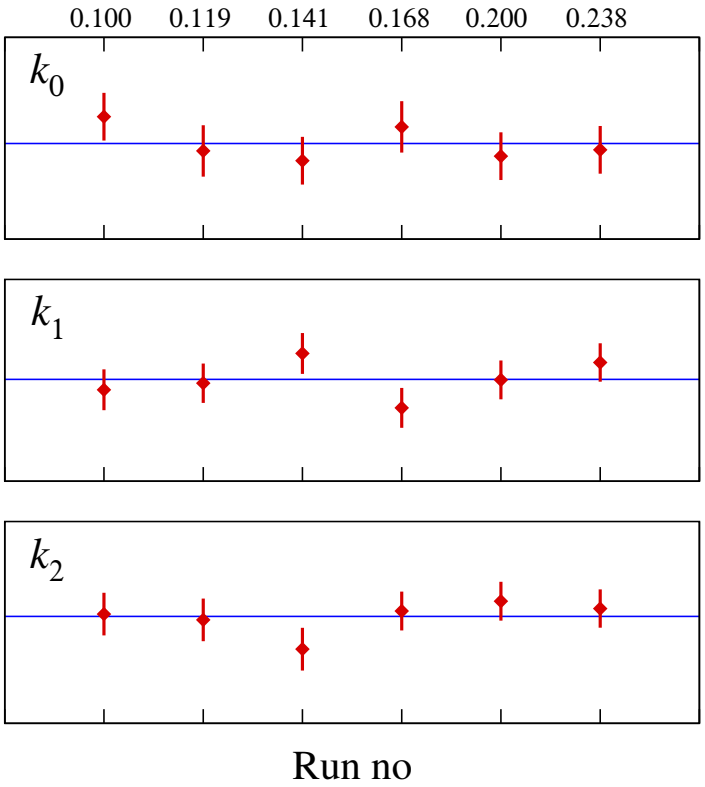
Use 4th order OMF integrator for the SMD algorithm Omelyan et al. '03

$$t^2\langle E\rangle = k_0\alpha_s\left\{1 + k_1\alpha_s + k_2\alpha_s^2 + \ldots\right\}$$

$L/a = 24$, $\gamma = 3.3$

Step size $0.10\ldots0.24$

$10^4$ measurements/run




2nd order integrator for the Langevin equation does equally well Bali et al. '13

## Extrapolation to the continuum limit

$\mathrm{O}(a)$ effects can be canceled by adding a counterterm

$$\propto c_{\mathrm{G}} \int \mathrm{d}^3x \, \mathrm{tr}\{F_{0k}(x)^2\} \quad \text{at} \quad x_0 = 0, T$$

ML et al. '92

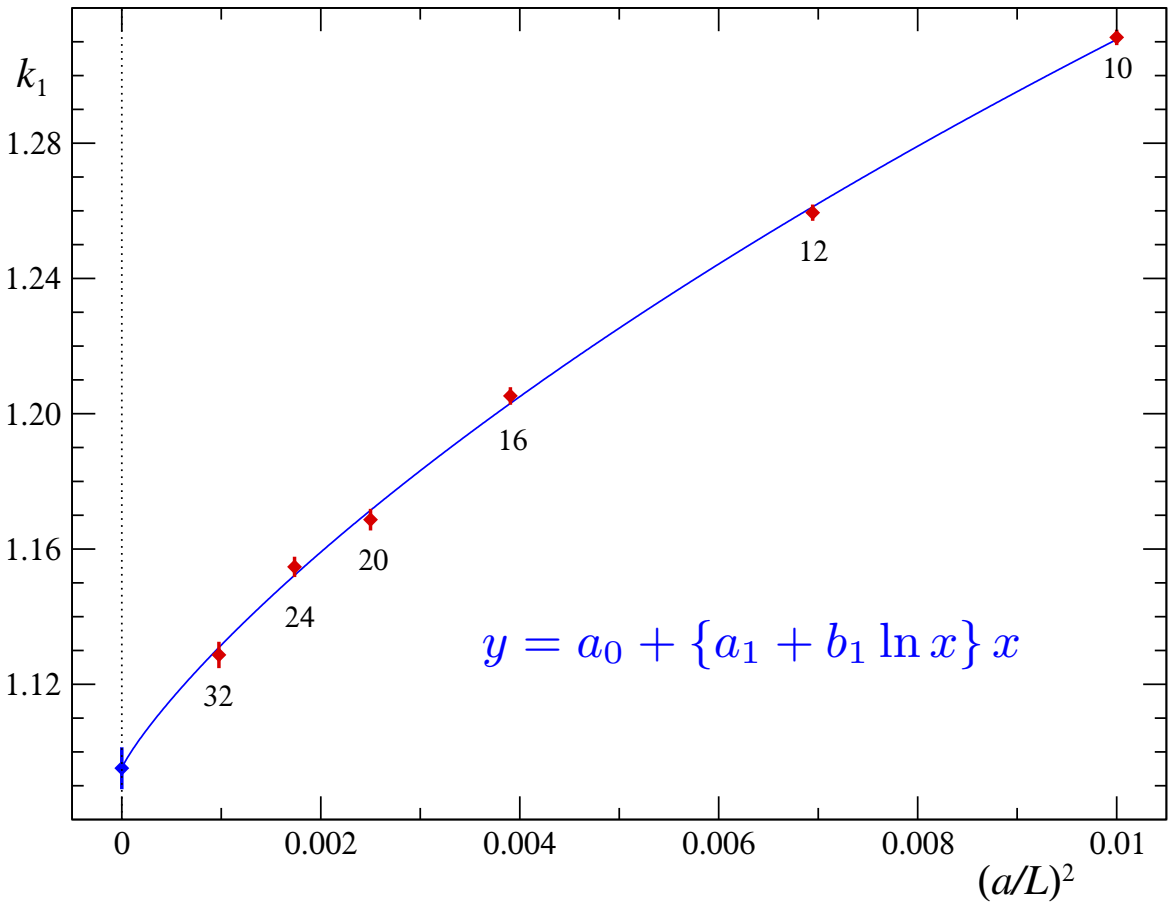
$$c_{\mathrm{G}} = 1 - 0.08900 \times g_0^2 - 0.0294 \times g_0^4 + \ldots$$

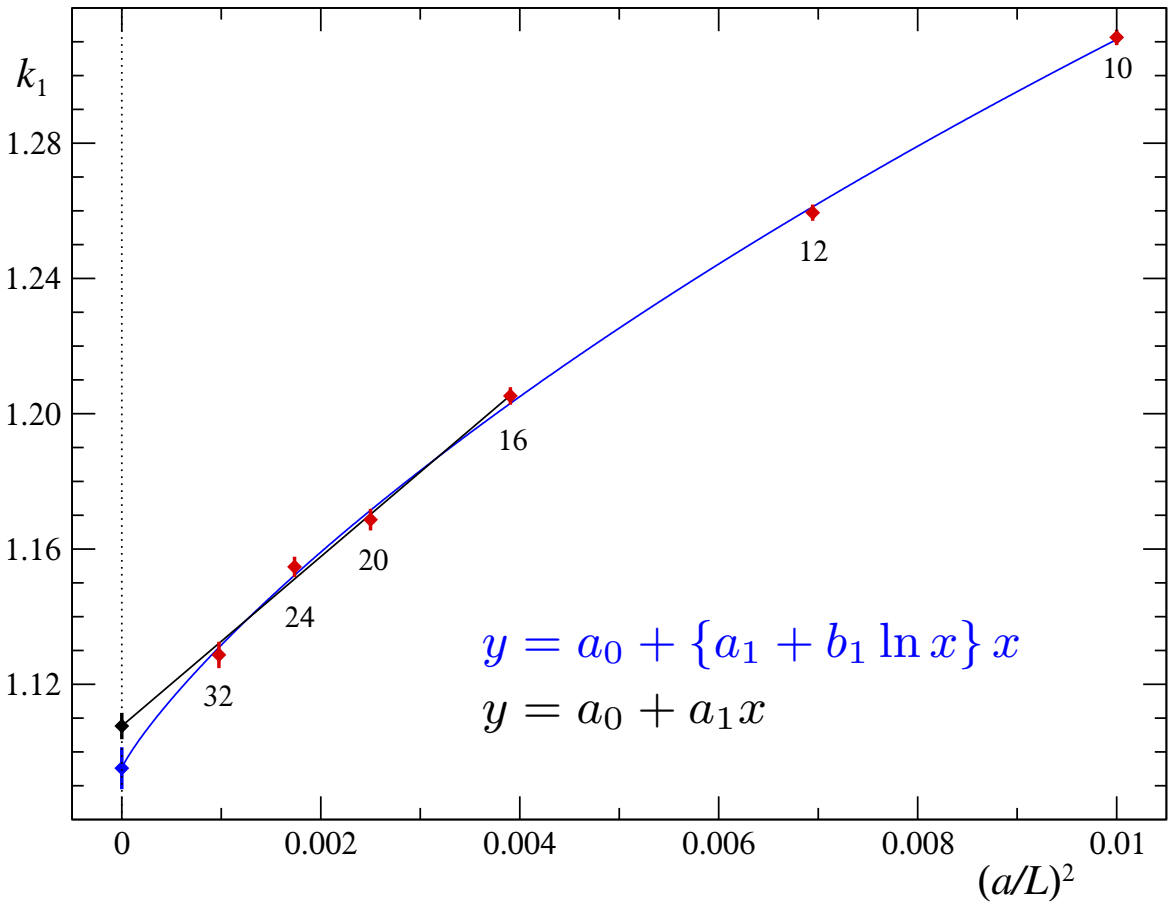
Bode, Weisz & Wolff '99f

to the action

With $\mathrm{O}(a)$-improvement in place, we have

$$k_1 \underset{a \to 0}{=} a_0 + \{a_1 + b_1 \ln(a/L)\} (a/L)^2 + \ldots$$


$k_1$
1.28
1.24
1.20
1.16
1.12
0
0.002
0.004
0.006
0.008
0.01
$(a/L)^2$
10
12
16
20
24
32
$y = a_0 + \{a_1 + b_1 \ln x\}\, x$

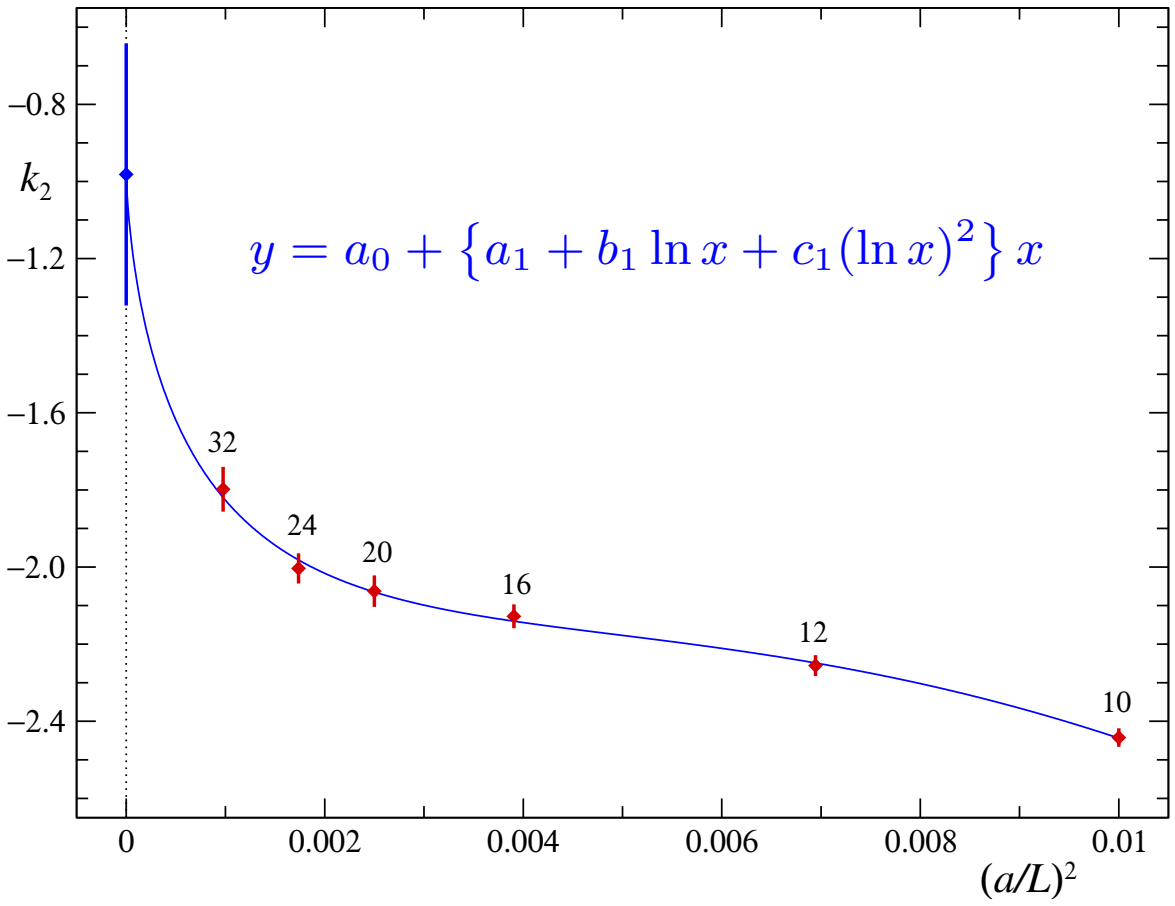



$\Rightarrow k_1 = 1.101(6)(6)$ [preliminary]

The two-loop coefficient $k_2$ is more difficult ...

- Statistical errors $10\times$ larger
- Must include $\mathrm{O}(a)$-counterterms in simulation
- More complicated $a$-dependence

$$k_2 \underset{a\to 0}{=} a_0 + \left\{a_1 + b_1 \ln(a/L) + c_1 [\ln(a/L)]^2\right\} (a/L)^2 + \ldots$$




$\Rightarrow$ need further points at $L/a > 32$ !

## Conclusions

*In NSPT we are <u>not</u> simulating a functional integral*

$\Rightarrow$ Variances are algorithm-dependent!

$\Rightarrow$ Must optimize for minimal $\tau_{\rm int} \times {\rm var}$ rather than $\tau_{\rm int}$

*Currently the best choice is the SMD algorithm with $\gamma = 2 \ldots 5$ and 4th order OMF integrator*

*Taking the continuum limit is challenging!*

$\Rightarrow$ In practice may be impossible to go beyond 2-loop order