

# Perturbative Expansions of Wilson Loops in Full QCD from MC Simulations

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# Contents

- need **higher-order** perturbation theory  
e.g.: precise determination of  $\alpha_s$  (HPQCD, PRL95, 052002, 2005)
- lattice perturbation theory → difficult
- alternative: **measure perturbative coefficients from Monte Carlo simulations at high- $\beta$  (weak coupling)**
- challenges
- results: Wilson loops in full QCD (**MILC** action)
- preliminary study for **NRQCD**
- outlook

# Need Higher-Order PT

- e.g.: precise determination of  $\alpha_s$  (HPQCD Collaboration)
- key ingredient: expansion of WL

$$-\ln W = c_1\alpha + c_2\alpha^2 + c_3\alpha^3 + \dots$$

measure this

... then solve for  $\alpha$

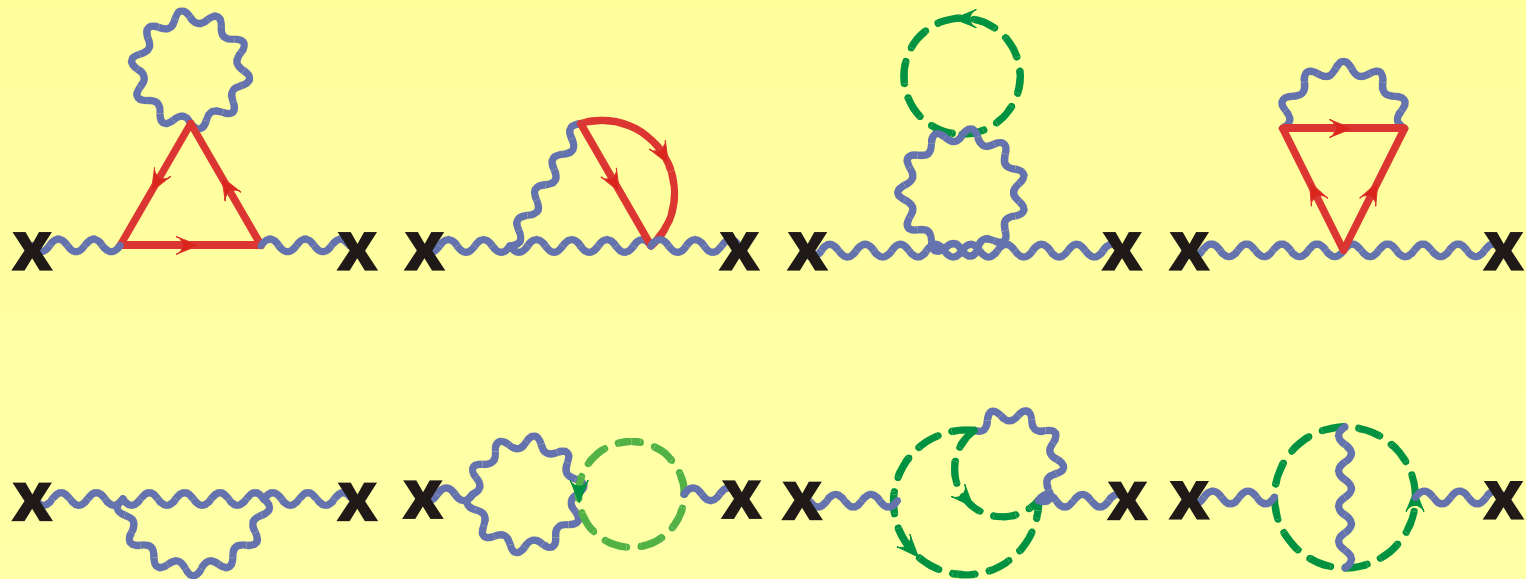
- to what order in PT → a few % error?

$$\alpha(a \approx 0.1\text{fm}) \sim 0.2 - 0.3$$

need 1-loop ( $\alpha^2$ ) or 2-loop ( $\alpha^3$ ) calculations

# Difficult! (particularly for complicated actions)

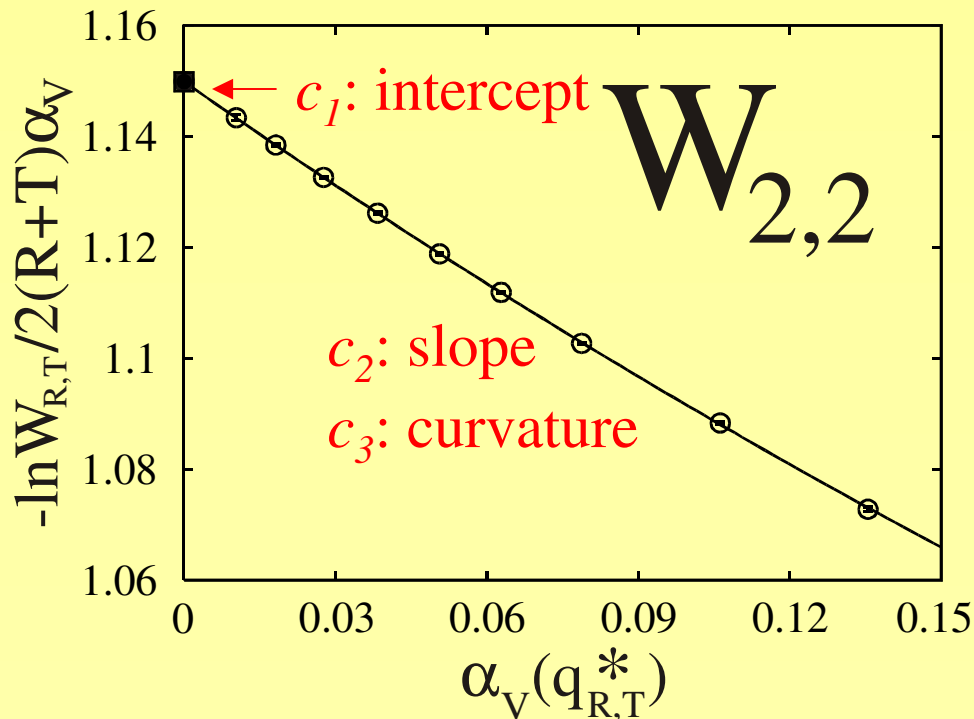
analytic calculation (**MILC** action): Q. Mason & H. Trotter



taken from Q. Mason's Ph.D Thesis (Cornell Electronic Library)

# Alternative: High- $\beta$ Simulations

- simulate the quantities of interest (Wilson loops) at **high- $\beta$**  weak coupling [ $\beta = \frac{6}{4\pi\alpha_0}$ ]
- fit results to the perturbative expansion



- 9 simulations  $\rightarrow$  9 data pts ( $\alpha_V, -\ln W_{R,T}$ )
- fit to the series

$$\frac{-\ln W_{R,T}}{2(R+T)\alpha_V} = c_1 + c_2\alpha_V + c_3\alpha_V^2 + \dots$$

# Alternative: High- $\beta$ Simulations

- high  $\beta \Rightarrow$  perturbative phase:  $(La)^{-1} \gg \Lambda_{\text{QCD}}$ , here:  $\beta \sim 9$  to  $60$   
and  $a\Lambda \sim 10^{-3}$  to  $10^{-30}$
- several studies:
  - Dimm, Lepage & Mackenzie [Nucl. Phys. B (Proc. Suppl.), **42**, 403 (1995)]  
1<sup>st</sup>-order mass renormalization for Wilson fermions
  - Trotter, Shakespeare, Lepage & Mackenzie [PRD, **65**, 094502 (2002)]  
3<sup>rd</sup>-order Wilson loops for the Wilson plaquette action
  - Hart, Horgan & Storoni [PRD, **70**, 034501 (2004)]  
tadpole factor in pure gauge theories

*this study:*

3<sup>rd</sup> –order Wilson loops **with dynamical staggered fermions**

- unimproved: Wilson action + unimproved staggered quark action
- **MILC** action: 1-loop improved gauge field action + Asqtad



important cross-check of the PT input to the determination of  $\alpha_s$  by the HPQCD Collaboration

# Challenges: Systematic Errors

- statistical errors in Wilson loops  $\sim O(10^{-5}-10^{-6})$
- probing 3<sup>rd</sup>-order coefficients

$$\alpha \sim 0.01 \Rightarrow \alpha^3 \sim O(10^{-6})$$

- account for all possible sources of errors
  - tunneling between  $Z_3$  center phases
  - fitting and truncation errors
  - zero momentum modes
  - step size errors in simulation equations
  - autocorrelation
  - inaccuracy in matrix inversions



# Tunneling and TBC

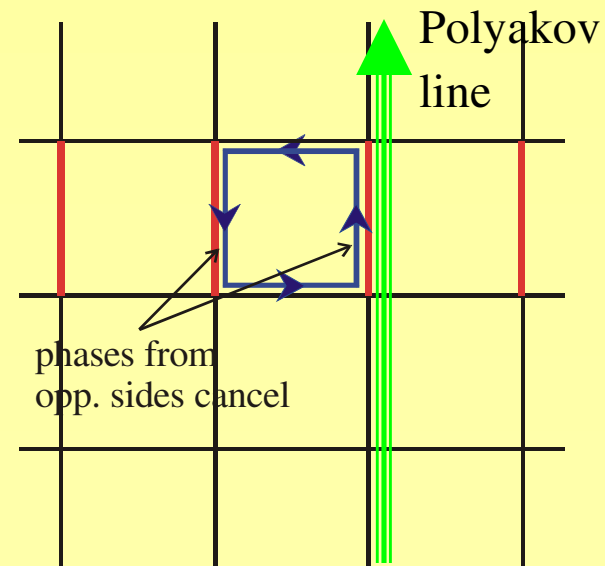
- gauge field action has a **Z<sub>3</sub> symmetry**

$$U_{x,\hat{\mu}} \rightarrow zU_{x,\hat{\mu}} \text{ where } z \in \{1, e^{i2\pi/3}, e^{i4\pi/3}\}$$

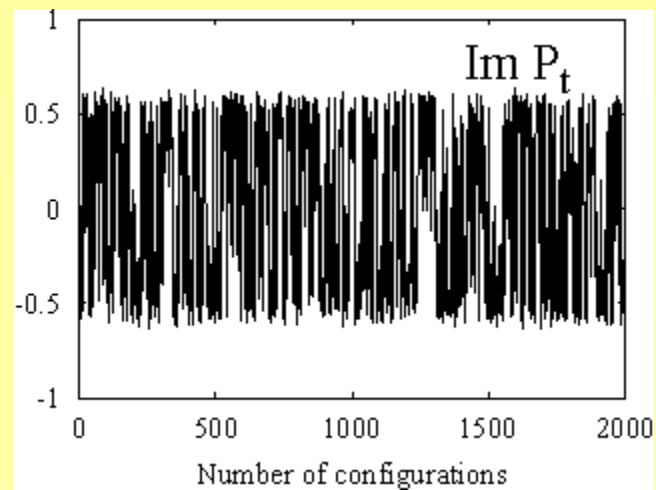
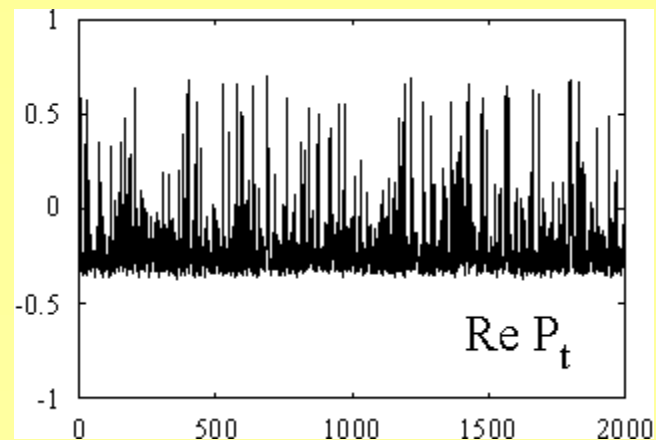
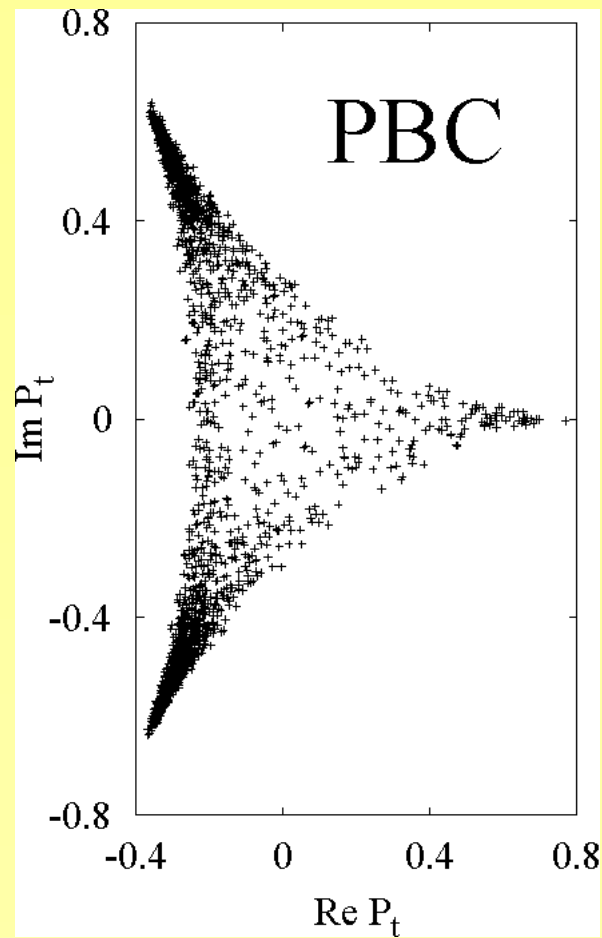
- **multiple vacuum**, analytic PT around one vacuum
- **tunneling can occur in simulations** → non-perturbative effects
- tunneling detection: Polyakov loop in one direction
- tunneling → pick up a Z<sub>3</sub> phase
- **suppressed using TBC**

$$U_{x+L\hat{\nu},\hat{\mu}} = \Omega_{\nu} U_{x,\hat{\mu}} \Omega_{\nu}^+$$

$$\psi_{x+L\hat{\nu}} = e^{i\pi/3} \Omega_{\nu} \psi_x \Omega_{\nu}^+$$

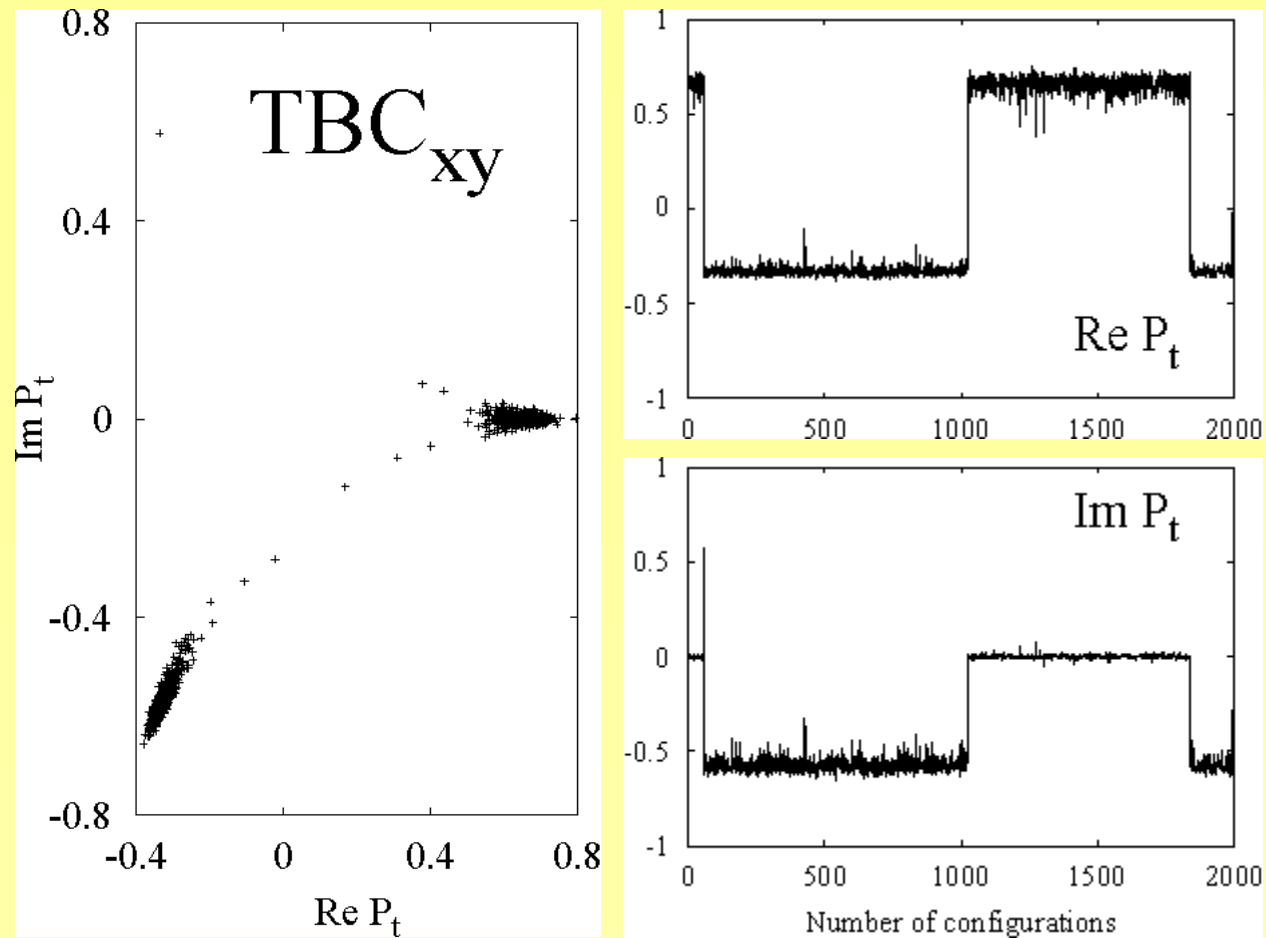


# Periodic Boundary Conditions



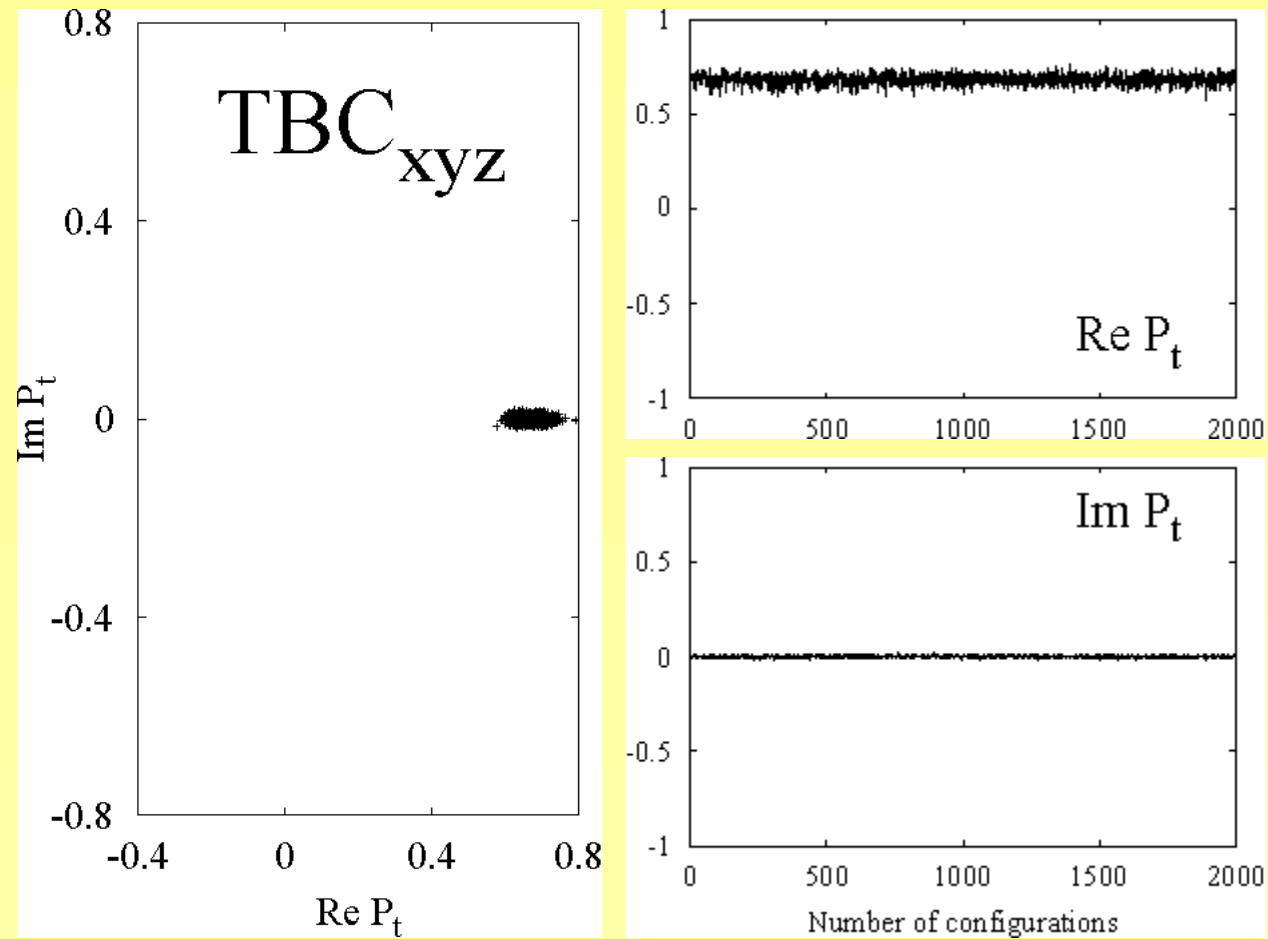
**unquenched:** the unimproved action,  $n_f = 3$ ,  $\beta = 16$ ,  $V = 4^4$

# Twisted Boundary Conditions (xy)



**unquenched:** the **unimproved** action,  $n_f = 1$ ,  $\beta = 16$ ,  $V = 4^4$

# Twisted Boundary Conditions (xyz)



**unquenched:** the **unimproved** action,  $n_f = 1$ ,  $\beta = 16$ ,  $V = 4^4$

# Simulation Parameters – MILC Action

➤ 9 values of  $\beta$ ,  $n_f = 1$ ,  $V = 8^4$ ,  $am = 0.1$

$\beta$	9.5	11.0	13.5	16.0	19.0	24.0	32.0	47.0	80.0
$\alpha_0 = \frac{6}{4\pi\beta}$	0.113	0.092	0.071	0.058	0.047	0.036	0.027	0.018	0.010
$\alpha_V(q_{1,1}^*)$	0.127	0.101	0.076	0.061	0.050	0.038	0.027	0.018	0.010
$a\Lambda$	$6 \times 10^{-2}$	$2 \times 10^{-2}$	$3 \times 10^{-3}$	$5 \times 10^{-4}$	$6 \times 10^{-5}$	$1 \times 10^{-6}$	$3 \times 10^{-9}$	$4 \times 10^{-14}$	$6 \times 10^{-25}$

➤ expansion parameter: the “V-scheme”  $V(q) = -\frac{4}{3} \frac{4\pi\alpha_V(q)}{q^2}$

➤ input from analytic PT: 3<sup>rd</sup>-order expansion of the plaquette  
→ connection between  $\alpha_0$  and  $\alpha_V$

# Fitting – MILC Action

- fit data points with  $-\frac{\ln W_{R,T}}{2(R+T)\alpha_V} = c_1 + c_2\alpha_V + c_3\alpha_V^2 + \dots$
- **constrained curve fitting**  $\chi^2 \rightarrow \chi_{\text{arg}}^2 \equiv \chi^2 + \sum_{n=1}^{n=N} \frac{(c_n - \bar{c}_n)^2}{\bar{\sigma}_n^2}$
- **data tell us how much it can determine**

vary N ( $\bar{\sigma}_n = 1.0$ )

$c_n$	$N = 4$	$N = 5$	$N = 6$
$c_1$	1.1499(4)	1.1499(4)	1.1499(4)
$c_2$	-0.641(15)	-0.641(15)	-0.641(15)
$c_3$	0.58(20)	0.58(20)	0.58(20)
$c_4$	-0.2(9)	-0.2(9)	-0.2(9)
$c_5$		-0.1(10)	-0.1(10)
$c_6$			0.0(10)
$\chi^2$	0.53	0.53	0.53

vary  $\bar{\sigma}_n$  (N = 6)

$c_n$	$\bar{\sigma}_n = 0.5$	$\bar{\sigma}_n = 1.0$	$\bar{\sigma}_n = 5.0$
$c_1$	1.1498(3)	1.1499(4)	1.1502(5)
$c_2$	-0.636(12)	-0.641(15)	-0.658(27)
$c_3$	0.51(12)	0.58(20)	0.85(43)
$c_4$	0.0(5)	-0.2(9)	-1.4(23)
$c_5$	0.0(5)	-0.1(10)	-0.8(48)
$c_6$	0.0(5)	0.0(10)	-0.2(50)
$\chi^2$	1.2	0.53	0.25

2x2 loop, analytic PT:  $c_1 = 1.1499(0)$ ,  $c_2 = -0.643(2)$ ,  $c_3 = 0.59(9)$

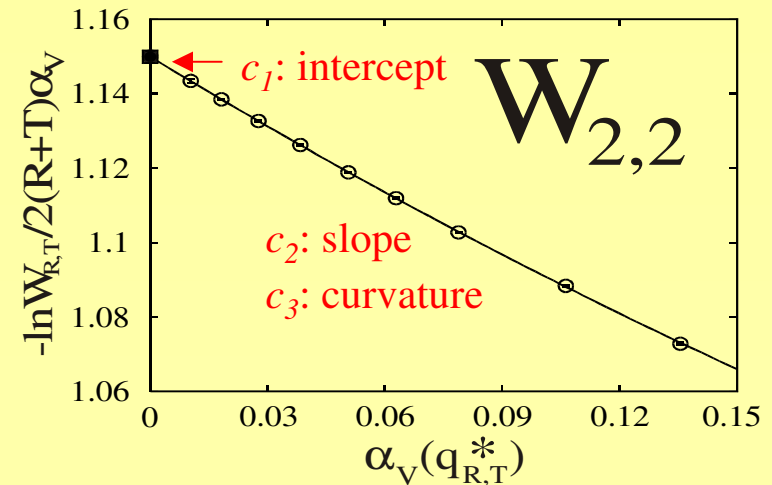
# Results – MILC Action

➤  $n_f = 1$ ,  $V = 8^4$ ,  $am = 0.1$

Perturbation Theory

Monte Carlo Simulations

Loop	$c_1$	$c_2$	$c_3$	$c_1$	$c_2$	$c_3$
1x2	0.9252(0)	-0.646(0)	0.23(5)	0.9251(3)	-0.644(13)	0.20(18)
1x3	0.9845(9)	-0.595(1)	0.38(6)	0.9845(3)	-0.599(14)	0.37(19)
2x2	1.1499(0)	-0.643(2)	0.59(9)	1.1499(4)	-0.641(15)	0.58(20)
2x3	1.2341(0)	-0.595(3)	0.85(16)	1.2342(4)	-0.599(19)	0.88(26)



## Results – MILC Action

- errors on  $c_2$  and  $c_3$  can be reduced if  $c_1$  is fixed to the analytic value in fitting

	PT		MC	
<i>Loop</i>	$c_2$	$c_3$	$c_2$	$c_3$
<i>1x2</i>	-0.646(0)	0.23(5)	-0.649(5)	0.26(12)
<i>1x3</i>	-0.595(1)	0.38(6)	-0.600(6)	0.39(13)
<i>2x2</i>	-0.643(2)	0.59(9)	-0.642(7)	0.59(14)
<i>2x3</i>	-0.595(3)	0.85(16)	-0.594(7)	0.82(15)

- fix both  $c_1$  and  $c_2$  to the analytic values

	PT	MC
<i>Loop</i>	$c_3$	$c_3$
<i>1x2</i>	0.23(5)	0.21(4)
<i>1x3</i>	0.38(6)	0.28(5)
<i>2x2</i>	0.59(9)	0.61(6)
<i>2x3</i>	0.85(16)	0.84(8)



# Energy Shift and Mass Renormalization in **NRQCD** (Preliminary)

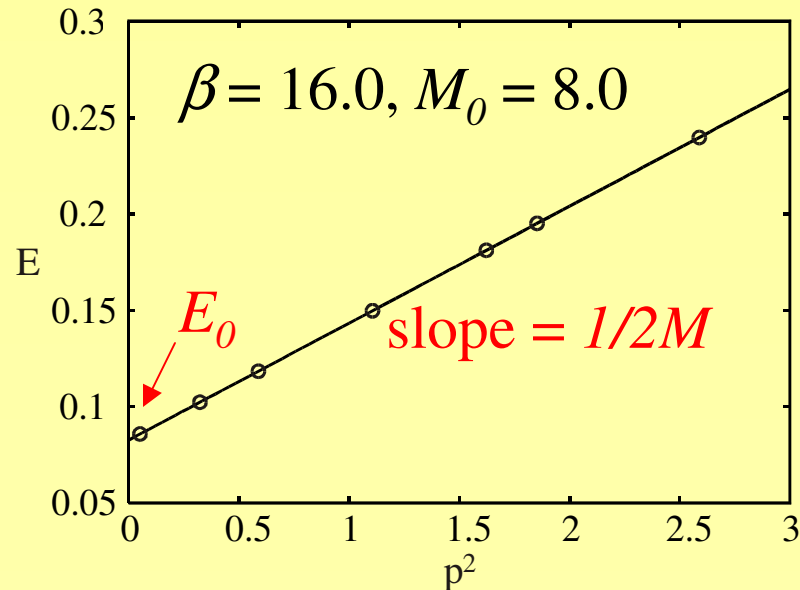
➤ quenched: Wilson plaquette action, NRQCD action  $H = -\frac{\Delta^2}{2M_0}$

➤ **observable**: dispersion relation  $E = E_0 + \frac{p^2}{2M}$

$$E_0 = c_1 \alpha_V(q_E^*) + c_2 \alpha_V^2(q_E^*) + \dots$$

$$M = M_0 \left( 1 + c_1 \alpha_V(q_M^*) + c_2 \alpha_V^2(q_M^*) + \dots \right)$$

➤ for each  $\beta$ :

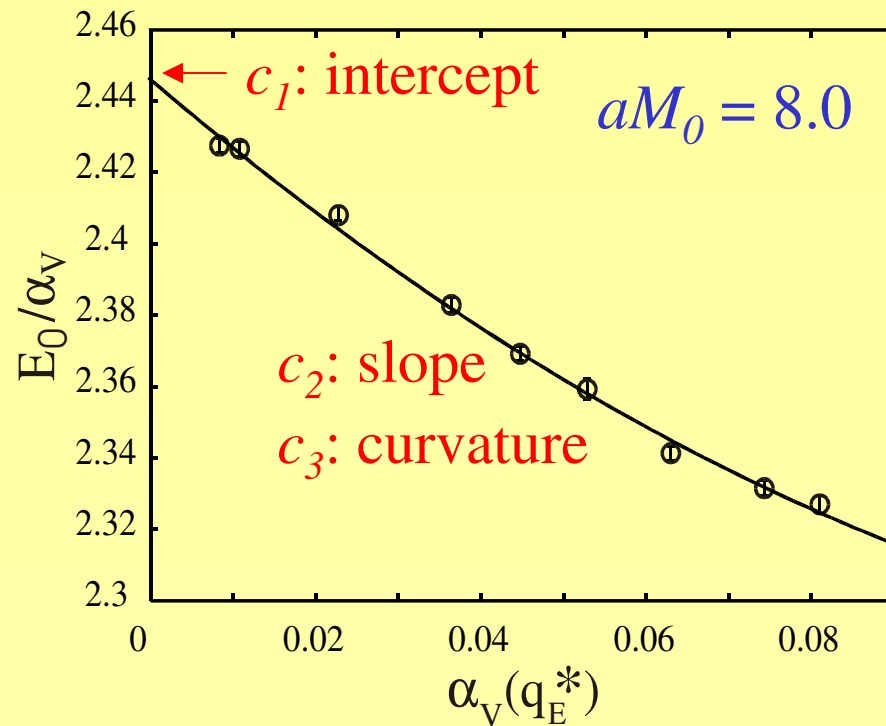


# Results (Preliminary)

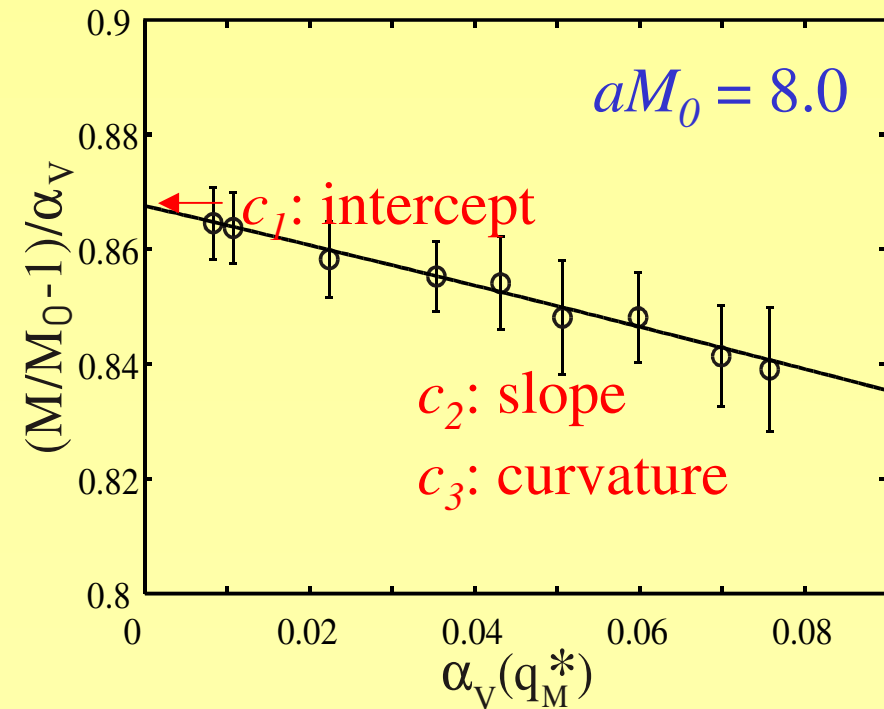
## ➤ simulations

- 9 values of  $\beta$ : 9.0 – 60.0
- 5 bare mass  $aM_0$ : 8.0, 6.0, 5.0, 4.0, 1.8

energy shift



mass renormalization



# Results for $c_1$ (Preliminary)

➤ analytic PT done by C. Morningstar [PRD, 50:5902 (1994)]

$c_1$  for  $E_0$

$c_1$  for  $M$

$M_0 a$	$PT$	$MC$	$PT$	$MC$
8.0	2.450	2.447(2)	0.850	0.867(6)
6.0	2.570	2.565(5)	0.830	0.849(7)
5.0	2.655	2.648(5)	0.820	0.842(9)
4.0	2.782	2.773(6)	0.770	0.798(10)
1.8	3.511	3.569(7)	1.100	1.245(10)

# Predictions for $c_2$ & $c_3$ (Preliminary)

*energy shift  $E_0$*       *mass renormalization  $M$*

$M_0 a$	$c_2$	$c_3$	$c_2$	$c_3$
8.0	-1.98(8)	5.9(1.4)	-0.34(37)	-0.2(4.9)
6.0	-1.91(7)	6.3(1.4)	-0.33(42)	0.5(5.3)
5.0	-2.02(7)	7.3(1.4)	-0.53(45)	0.7(6.1)
4.0	-2.13(7)	7.4(1.4)	-0.91(56)	-0.28(6.7)
1.8	-2.94(8)	7.6(1.5)	-0.87(39)	2.7(4.6)

good test run

→ future: full NRQCD & mNRQCD

# Conclusions

- perturbative coefficients of WL in full QCD (**MILC**)
- important cross-check of the PT input to the determination of  $\alpha_s$  by the HPQCD Collaboration
- can also be applied to **NRQCD**

higher-order coefficients & complicated actions

**future:** analytic PT (low order) + high- $\beta$  (high order)