Frequency-splitting estimators of single-propagator traces

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European Physical Journal C 79:586 (2019)

Short summary:

Propose efficient calculation method
for single-propagator trace and its difference

$\mathcal{O}(10)$ times efficient than usual method even in small M_π

c.f.) $g-2$ [PRD111:114509(2025)], proton radius [PRL132:211901(2024)],
$K \to \pi\ell\ell$ [PoS(LATTICE2024)258]

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- Summary

CLS configuration for test calculation: $N_{\rm cfg} = 100$, $48^3 \times 96$, $M_\pi = 268$ MeV
($m_u = 0.00207$)

Discussion is highly simplified in this report: e.g., Clover quark $\rightarrow$ naive quark

Single-propagator trace = disconnected diagram

$$\tau_\Gamma(t) = \frac{1}{L^3}\sum_{\vec{x}} \mathrm{Tr}\left[\Gamma G(x,x)\right], \quad x_0{=}t, \quad \Gamma{=}I,\ \gamma_\mu,\ \sigma_{\mu\nu}{=}\tfrac{i}{2}[\gamma_\mu,\gamma_\nu],\ \gamma_\mu\gamma_5,\ \gamma_5$$

G: fermion propagator = inverse matrix of Dirac operator $D(x,y)$

$$\sum_x D(z,x)G(x,y) = \delta_{z,y}, \quad \text{c.f.)}\ S_f = \sum_{x,y}\overline{\Psi}(x)D(x,y)\Psi(y) \text{ on lattice}$$

flavor-singlet mesons η, σ, and electromagnetic form factors for proton, neutron

In lattice QCD, difficult to calculate D^{-1} due to huge size of matrix D

One can calculate $\sum_z G(x,z)b(z)$, e.g, $\sum_z G(x,z)\delta_{z,x} = G(x,x)$

one x per one calculation

Each G calculation is not cheap.

Roughly $\mathcal{O}(L^3T) \sim 10^9$ calculations of G necessary for $\tau_\Gamma(t)$

$\times\ \mathcal{O}(10^2 \sim 10^3)$ configurations

not discuss this reduction

Large calculation cost is demanded for $\tau_\Gamma(t)$.

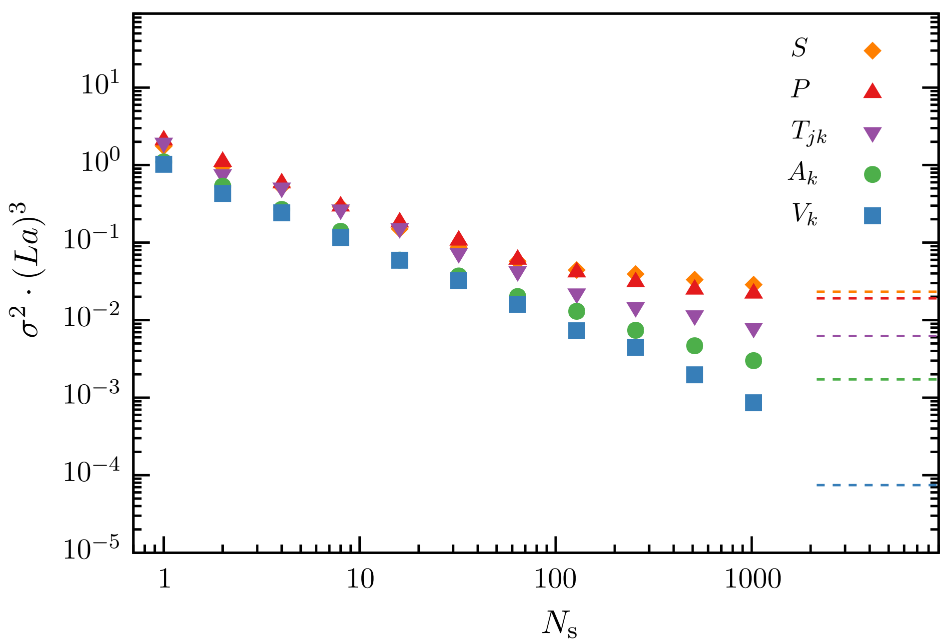
Random-noise estimator [traditional method]

[Bitar et al., NPB313:348(1989)], [UKQCD,PHD58:034506(1998)]

$\eta_i(x)$: Random noise $\lim_{N_s\to\infty} \frac{1}{N_s}\sum_{i=1}^{N_s} \eta_i^*(x)\eta_i(y) = \delta_{x,y}$

$$\tau_\Gamma^r(t) = \frac{1}{L^3}\frac{1}{N_s}\sum_i \sum_{\vec{x}} \mathrm{Tr}\left[\eta_i^*(x)\Gamma\left\{\sum_z G(x,z)\eta_i(z)\right\}\right] \sim \tau_\Gamma(t) + \mathcal{O}\left(\frac{1}{\sqrt{N_s}}\right)$$

(Error)^2 of τ_Γ^r



$\Gamma = I(S), \gamma_5(P), \sigma_{jk}(T_{jk}), \gamma_k\gamma_5(A_k), \gamma_k(V_k)$

Dashed line $\sim$ (error)^2 in $N_s \to \infty$

gauge configuration noise (estimate)

$\mathcal{O}(10^3)$ or more N_s necessary

G calculation per each N_s

further cost reduction desired

[Thron et al.,PRD57:1642(1998),$\cdots$]

Other traditional method: Hopping parameter expansion

efficient only in large quark mass

Split-even method: difference of single-propagator trace

$$D_u - D_s = (m_u - m_s)I, \quad D_q = m_q I + H, \quad G_q D_q = D_q G_q = I$$

$H \sim \sum_\mu \left[\gamma_\mu \left(U_\mu(x)\delta_{x,x+\mu} - U_\mu^\dagger(x-\mu)\delta_{x,x-\mu}\right)\right]$: hopping term independent of m_q

$$G_s - G_u = G_u D_u G_s - G_u D_s G_s = G_u(D_u - D_s)G_s = (m_u - m_s)G_u G_s$$

standard method

$$\tau_\Gamma^r(t) = \frac{1}{L^3}\frac{1}{N_s}\sum_i \sum_{\vec{x}} \mathrm{Tr}\left[\eta_i^*(x)\Gamma\left\{\sum_z G(x,z)\eta_i(z)\right\}\right]$$

$$\tau_{\Gamma,\mathrm{std}}^{r,m_2m_1}(t) = \tau_\Gamma^{r,m_2}(t) - \tau_\Gamma^{r,m_1}(t)$$

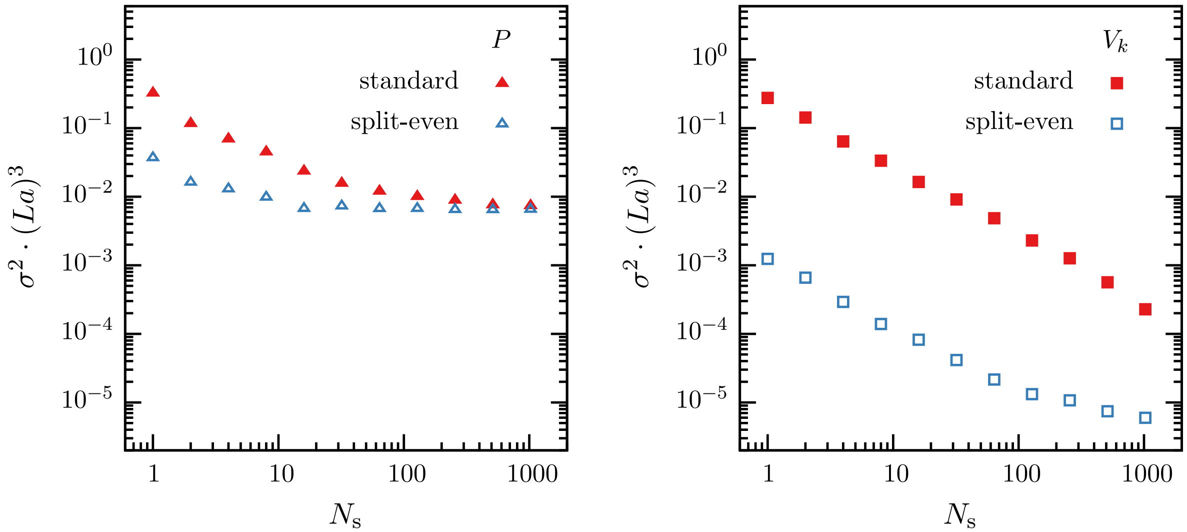
$$= \frac{m_1 - m_2}{L^3}\frac{1}{N_s}\sum_i \sum_{\vec{x}} \mathrm{Tr}\left[\eta_i^*(x)\Gamma\left\{\sum_{y,z} G_1(x,y)G_2(y,z)\eta_i(z)\right\}\right]$$

split-even method

$$\tau_{\Gamma,\mathrm{split}}^{r,m_2m_1}(t) = \frac{m_1 - m_2}{L^3}\frac{1}{N_s}\sum_i \sum_{\vec{x}} \mathrm{Tr}\left[\left\{\sum_w \eta_i^*(w)G_2(w,x)\right\}\Gamma\left\{\sum_z G_1(x,z)\eta_i(z)\right\}\right]$$

Split-even method: difference of single-propagator trace (cont'd)

(error)^2 of $\tau^{r,m_1 m_2}_{\gamma_5}$ and $\tau^{r,m_1 m_2}_{\gamma_k}$, $m_1 = 0.00207$, $m_2 = 0.0189$



split-even: 10-10^2 times more efficient than standard in small N_s
even in small m_1

Frequency-splitting estimator

$$\tau_\Gamma^{m_u}(t) = \tau_\Gamma^{m_c}(t) + \tau_\Gamma^{m_u}(t) - \tau_\Gamma^{m_c}(t) \left(= \tau_\Gamma^{m_c}(t) + \tau_\Gamma^{m_s}(t) - \tau_\Gamma^{m_c}(t) + \tau_\Gamma^{m_u}(t) - \tau_\Gamma^{m_s}(t)\right)$$

hopping parameter expansion: effective in large m_c [Thron et al.,PRD57:1642(1998)]

$$\tau_\Gamma^{r,m_u}(t) = \tau_\Gamma^{h,m_c}(t) + \tau_{\Gamma,\text{split}}^{r,m_u m_c}(t) \qquad (m_u \ll m_c)$$

difference w/ split-even method: effective even in small m_u

$$\tau_\Gamma^{r,m_u}(t) = \tau_\Gamma^{h,m_c}(t) + \tau_{\Gamma,\text{split}}^{r,m_s m_c}(t) + \tau_{\Gamma,\text{split}}^{r,m_u m_s}(t) \qquad (m_u < m_s \ll m_c)$$

$$\tau_\Gamma^{r,m_u}(t) = \tau_\Gamma^{h,m_c}(t) + \sum_{j=1}^{N_q} \tau_{\Gamma,\text{split}}^{r,m_j m_{j-1}}(t) \qquad (m_j < m_{j-1},\ m_0 = m_c,\ m_{N_q} = m_u)$$

Test calculation

FS1: $m_c = 0.1$, $m_u = 0.00207$, and $N_s = 4, 1$ for $\tau_\Gamma^{h,m_c}(t), \tau_{\Gamma,\text{split}}^{r,m_u m_c}(t)$

2.5 times more expensive than $N_s = 1$ standard

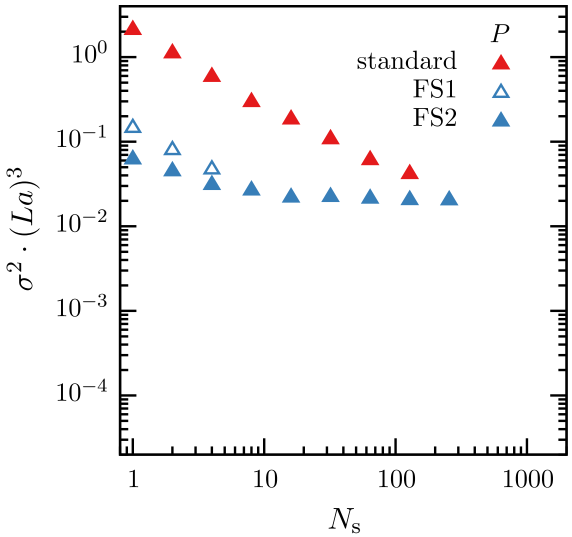
FS2: $m_j = 0.3, 0.15, 0.06, 0.02, 0.00207$,

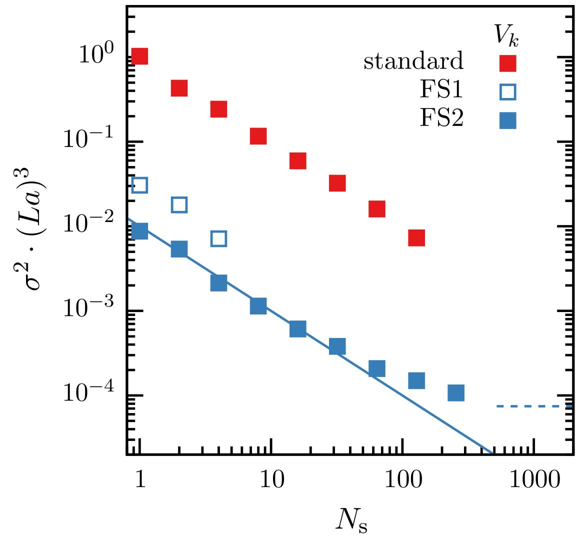
and $N_s = 10, 3, 2, 1, 1$ for $\tau_\Gamma^{h,m_c}(t), \tau_{\Gamma,\text{split}}^{r,m_j m_{j-1}}(t)$

6 times more expensive than $N_s = 1$ standard

Frequency-splitting estimator (cont'd)

(error)^2 of τ_{γ_5} and τ_{γ_k} at $m_u = 0.00207$ ($M_\pi = 268$ MeV)





FS1: $m_c = 0.1$, $m_u = 0.00207$, and $N_s = 4, 1$ for $\tau_\Gamma^{h,m_c}(t), \tau_{\Gamma,\text{split}}^{r,m_u m_c}(t)$

2.5 times more expensive than $N_s = 1$ standard

FS2: $m_j = 0.3, 0.15, 0.06, 0.02, 0.00207$ and $N_s = 10, 3, 2, 1, 1$ for $\tau_\Gamma^{h,m_c}(t), \tau_{\Gamma,\text{split}}^{r,m_j m_{j-1}}(t)$

6 times more expensive than $N_s = 1$ standard

FS1 τ_{γ_5}: 15 times smaller (error)^2 / 2.5 times cost

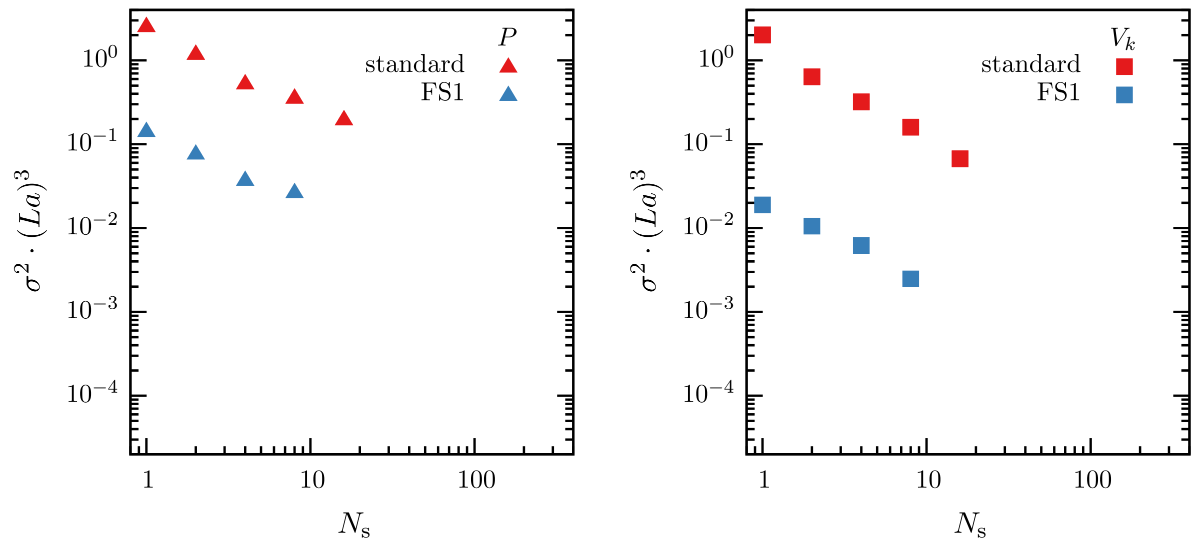
$\sim$ 6 times more efficient than standard

FS2 τ_{γ_k}: 10^2 times smaller (error)^2 / 6 times cost

$\sim$ 15 times more efficient than standard

Frequency-splitting estimator (cont'd)

(error)^2 of τ_{γ_5} and τ_{γ_k} at $M_\pi = 193$ MeV w/ $N_{\text{cfg}} = 25$ on different ensemble



FS1: $m_j = 0.1, 0.01935, 0.00108$, and $N_s = 8, 1, 1$ for $\tau_\Gamma^{h,m_c}(t), \tau_{\Gamma,\text{split}}^{r,m_j m_{j-1}}(t)$

3.3 times more expensive than $N_s = 1$ standard

τ_{γ_k}: 10^2 times smaller (error)^2 / 3.3 times cost

$\sim$ 30 times more efficient than standard

Summary

Calculation cost reduction of single-propgator trace

- split-even method : effective in difference of single-propagator trace

- Frequency-splitting estimator
  Hopping parameter expansion +
  difference(s) of single-propagator trace w/ split-even

- $\mathcal{O}(10)$ reduction of computational cost of single-propagator trace
  even in small M_π

Back up

Hopping parameter expansion

[Thron et al.,PRD57:1642(1998)], $\cdots$

$$D = mI + H = m\left(I - H_m\right), \quad H_m = -\frac{H}{m}, \quad H \propto \sum_\mu \left[\gamma_\mu \left(U_\mu(x)\delta_{x,x+\mu} - U_\mu^\dagger(x-\mu)\delta_{x,x-\mu}\right)\right]$$

H_m: hopping term, $1/m \sim$ hopping parameter

$$mD^{-1} = mG = \sum_{k=0}^{\infty} H_m^k = \sum_{k=0}^{2n-1} H_m^k + \sum_{k=2n}^{\infty} H_m^k = M_{2n} + mGH_m^{2n}$$

$$\tau_\Gamma^h(t) = \tau_\Gamma^M(t) + \tau_\Gamma^R(t), \qquad \tau_\Gamma^M(t) = \frac{1}{L^3}\sum_{\vec{x}} \mathrm{Tr}\left[\Gamma \frac{M_{2n}(x,x)}{m}\right]$$

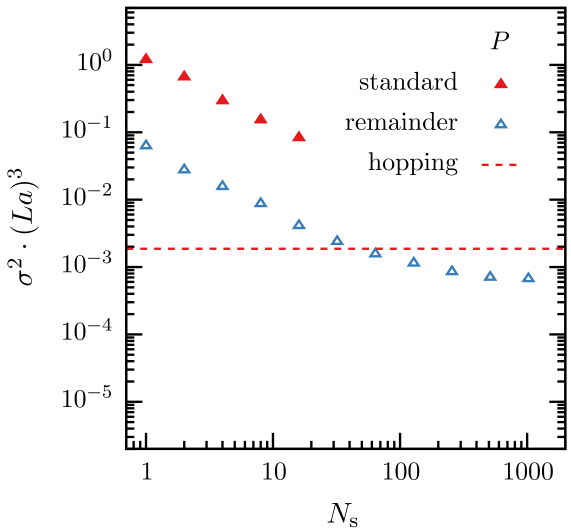
$$\tau_\Gamma^R(t) = \frac{1}{L^3}\frac{1}{N_s}\sum_i \sum_{\vec{x}} \mathrm{Tr}\left[\left\{\sum_w \eta_i^*(w) H_m^n(w,x)\right\}\Gamma\left\{\sum_{y,z} G(x,y)H_m^n(y,z)\eta_i(z)\right\}\right]$$

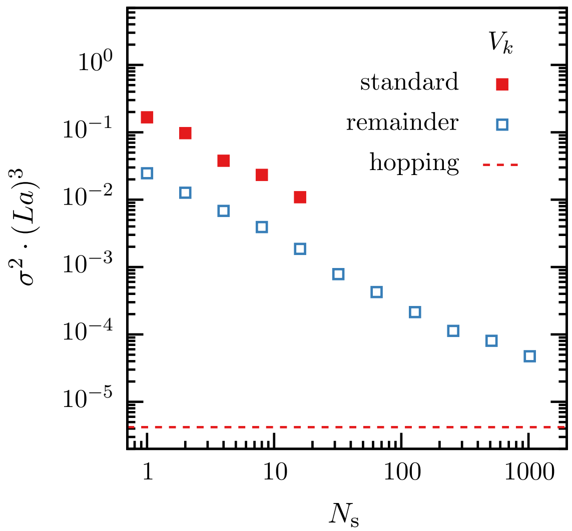
M_{2n}, H_m^n calculation is much cheaper than G calculation.

Hopping parameter expansion (cont'd) [Thron et al.,PRD57:1642(1998)], $\cdots$

(error)^2 of $\tau^h_{\gamma_5}$ and $\tau^h_{\gamma_k}$ (large $m_q = 0.3$, $n = 2$ for M_{2n}, H^{2n}_m)

$\tau^h_\Gamma = \tau^M_\Gamma + \tau^R_\Gamma$





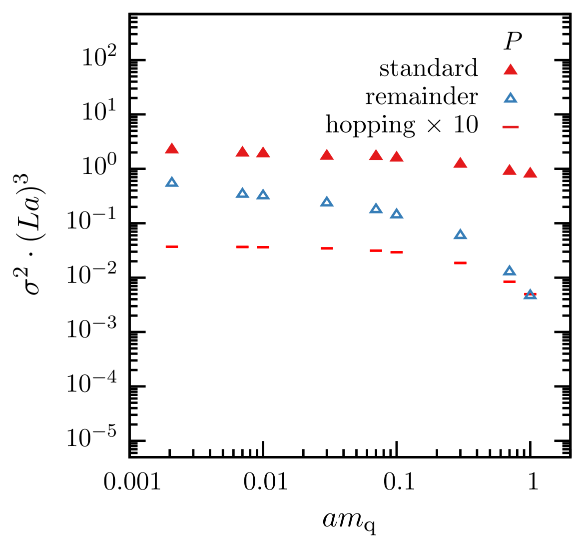
standard : random noise method previous page

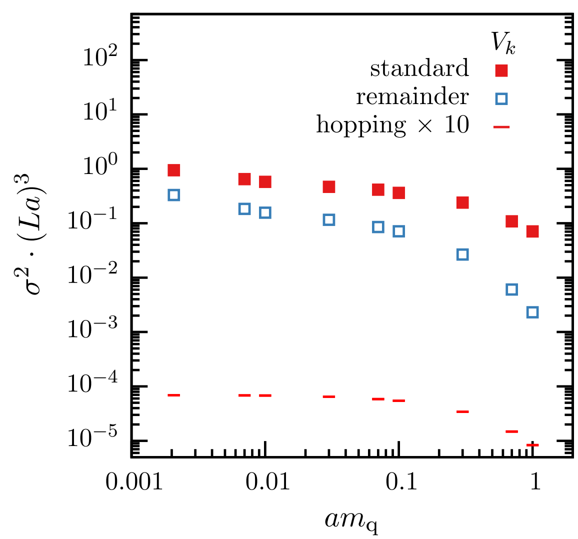
remainder : only τ^R

hopping : only τ^M w/o η

Hopping parameter expansion is better than standard

Hopping parameter expansion not effective in small m_q





Variance estimate of difference of single-progator traces

$(\text{error})^2 \sim \langle (\tau_\Gamma^r)^2 \rangle - \langle \tau_\Gamma^r \rangle^2$

Standard method $\tau_{\Gamma,\text{std}}^{r,m_2 m_1}$

$$(\text{error})^2 \sim \sigma^2 + \frac{(m_2 - m_1)^2}{L^3 N_s} \sum_{y_1, y_2, y_3} \langle S(y_1) P(y_2) S(y_3) P(0) \rangle$$

Split-evne method $\tau_{\Gamma,\text{split}}^{r,m_2 m_1}$

$$(\text{error})^2 \sim \sigma^2 + \frac{(m_2 - m_1)^2}{L^3 N_s} \sum_{y_1, \vec{y}_2, y_3} \langle P(y_1) O_\Gamma(0, \vec{y}_2) P(y_3) O_\Gamma(0) \rangle$$

$O_\Gamma = \overline{\Psi}\Gamma\Psi, \; S = O_I, \; P = O_{\gamma_5}$

standard: $L^3 \cdot T$ summation vs spilt-even: L^3 summation