

Noise Estimator and Disconnected Diagrams in Lattice QCD

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OUTLINE

1. Disconnected Diagrams

- What are these diagrams? How important are they?

2. How to calculate Disconnected Diagrams?

- Difficulties : Trace of very large matrix
- Solutions : Stochastic Noise Estimator

3. Stochastic Noise Method

4. Stochastic Noise Method and Unbiased Trace Estimator

5. What is more important? Number of noises or number of configurations?

- A Toy Model Calculation.

6. Preliminary results

- Scalar current
- $\langle x \rangle$ and $\langle x^2 \rangle$

7. Improvement

How Important are Disconnected Diagrams?

- Since nucleon do not have any valence strange quark, the only way the strangeness of the nucleon can be explained via generation of $s\bar{s}$ pair from vacuum polarization. Therefore, to obtain strangeness content of the nucleon one must calculate disconnected diagrams.
- In order to calculate complete matrix element of a current, one should always consider disconnected diagrams along with the connected ones.

Various observables

- Strangeness content term $\langle N | s\bar{s} | N \rangle$
- Disconnected diagrams for :
 - electromagnetic form factors (G_M^s and G_E^s).
 - flavor singlet axial current
 - $\pi N\sigma$ term
 - total angular momentum
 - $\langle x \rangle$ and $\langle x^2 \rangle$
- Flavor singlet mesons
- Hyperfine splitting in charmonium

Electromagnetic Form Factors and Moments

Electromagnetic vector current :

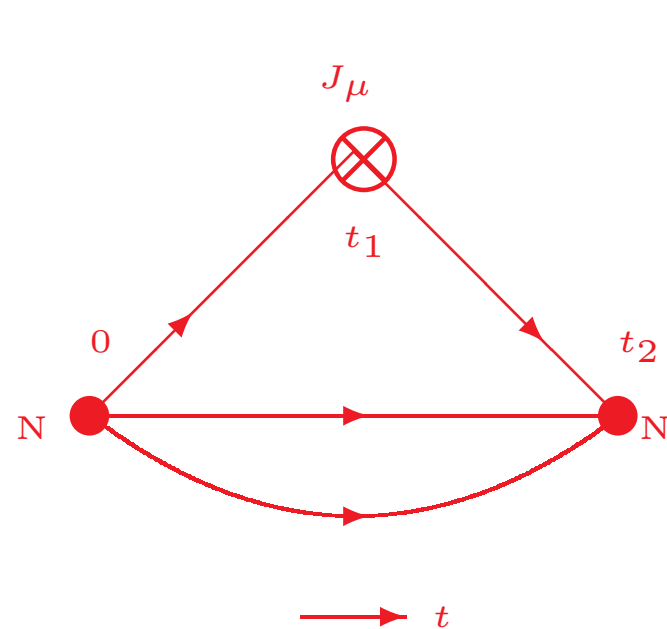
$$\langle \vec{p}s | j_\mu(0) | \vec{p}'s' \rangle = \bar{u}(\vec{p}, s) \left[\gamma_\mu F_1(q^2) - i\sigma^{\mu\nu} q_\nu \frac{F_2(q^2)}{2m} \right] u(\vec{p}', s').$$

From these one can define following form factors

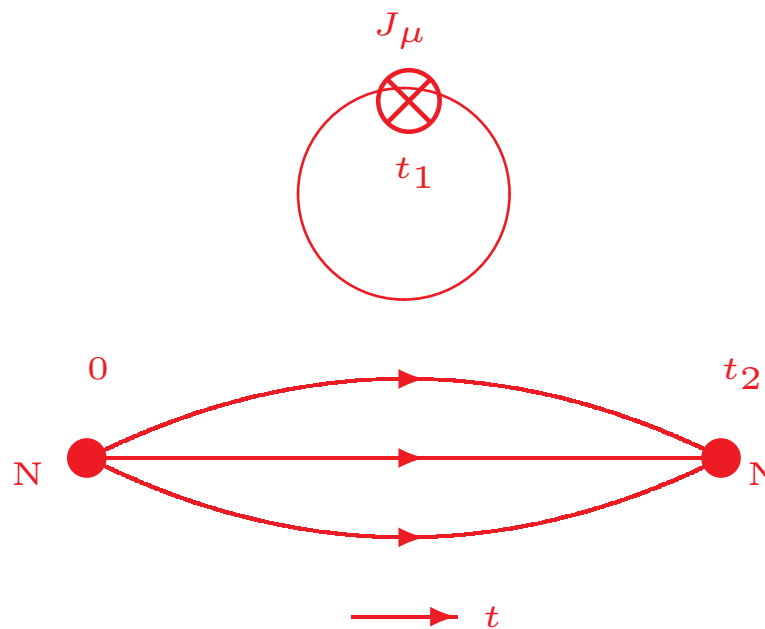
$$G_E(q^2) = F_1(q^2) - \left(\frac{q}{2m} \right)^2 F_2(q^2),$$
$$G_M(q^2) = F_1(q^2) + F_2(q^2),$$

Connected and Disconnected Insertion

$$G_{PO_\mu P}^{\alpha\beta}(t_f, t, \vec{p}, \vec{p}') = \sum_{\vec{x}_f, \vec{x}} e^{-i\vec{p}\cdot\vec{x}_f + i\vec{q}\cdot\vec{x}} \langle 0 | T \left(\chi^\alpha(x_f) O_\mu(x) \bar{\chi}^\beta(0) \right) | 0 \rangle .$$



Connected



Disconnected

Disconnected Diagrams and Noise Method

Disconnected diagrams incorporates quark loops, and to simulate those we need to calculate traces of very big matrices :

$$\sum_x \text{Tr} \left[M^{-1}(x + \mu, x) U_\mu \gamma_\mu \gamma_5 \right],$$

which involve both diagonal and off-diagonal elements of M^{-1} .

For a moderate size lattice $16^3 \times 24$, dimension of quark matrix

$$M_{\alpha\beta}^{-1ab}(x, y) \Rightarrow 16^3 \times 24 \times 2 \times 3 \times 4 \sim 10^6 \times 10^6!!$$

Therefore, it will be extremely costly to invert the whole matrix M and then take all traces.

Instead, we use stochastic noise method to calculate these traces.

Noise Method

Noise method : projection of the signal using random noise vectors as input.

- ★ To account for the Brownian motion with the Langevin and Fokker-Planck equations and to compute time dependent correlation functions in statistical mechanics.... P.C. Hohenberg and B. Halperin, *Rev. Mod. Phys.* **49**, 435 (1977).
- ★ Stochastic formulation of quantum mechanics.... E. Nelson, *Phys. Rev.* **150**, 1079 (1966).
- ★ Stochastic formulation of quantum field theory.... G. Parisi and Wu Yongshi, *Scientia Sinica* **24**, 483 (1981).

Noise Method and Matrix Inversion

Need to calculate any inverse fermion matrix element M_{ij}^{-1} stochastically.

Introduce an ensemble of L column vectors $\eta \equiv \eta^1, \dots, \eta^L$ (each of dimension $N \times 1$) with the properties of a **white noise**, i.e.,

$$\begin{aligned}\langle \eta_i \rangle &= 0, \\ \langle \eta_i \eta_j \rangle &= \frac{1}{L} \sum_{n=1}^L \eta_i^n \eta_j^n = \delta_{ij},\end{aligned}$$

where η_i^n is the i -th entry in the noise vector n .

Noise Method and Matrix Inversion

Using these noise vectors (η) as source, we solve for the solution vector x

$$\sum_i M_{ki} x_i = \eta_k,$$
$$\implies x_i = \sum_k M_{ik}^{-1} \eta_k,$$

With this solution one can obtain any inverse matrix element as

$$\langle \eta_j x_i \rangle = \sum_k M_{ik}^{-1} \langle \eta_j \eta_k \rangle = M_{ij}^{-1}.$$

Noise Method and Trace Estimation

Let us consider a general complex matrix S .

Time requires to evaluate $S\eta \sim$ time needs to evaluate λ_i .

$$\text{Trace} \equiv \sum_{i=1}^N \lambda_i$$

If we can construct a trace estimator from the matrix-vector multiplication $S\eta$, we will save a time factor $\mathcal{O}(N)$.

$$S\eta \implies \text{vector},$$

$$\text{Trace} \implies \text{number},$$

$$\text{Trace} \iff \xi S\eta, \quad \xi \text{ is a row vector.}$$

$$\xi S\eta = \text{Tr}(S)$$

Noise Method and Trace Estimation

$$\begin{aligned}\xi S \eta &= \text{Tr}(S) \\ \Rightarrow \sum_{m,n}^N S_{mn} \xi_m^* \eta_n &= \sum_n^N S_{nn} \\ \Rightarrow \xi_m^* \eta_n &= \delta_{mn} \quad \forall m, n.\end{aligned}$$

It is impossible to choose the vectors ξ and η which satisfy previous $N \times N$ conditions simultaneously. However, if ξ and η vary randomly, it is possible that the condition may be satisfied in an expectation

$$E[\xi_m^* \eta_n] = \delta_{mn} \quad \forall m, n.$$

This equality holds if η_n : an arbitrary random variables with mean zero and unit variance, and $\xi_m \equiv \eta_m$. With such a choice, it follows :

$$E[\eta^\dagger S \eta] = \text{Tr}(S).$$

Noise Method and Trace Estimation

$$\begin{aligned}
 E \left[\langle \eta^\dagger M^{-1} \eta \rangle \right] &\equiv E \left[\frac{1}{L} \sum_{j=1}^L \sum_{m,n=1}^N \langle \eta_m^{*j} M_{mn}^{-1} \eta_n^j \rangle \right] \\
 &= \frac{1}{L} \sum_{j=1}^L \left(\sum_{n=1}^N M_{nn}^{-1} \right) E \left[\langle \eta_n^{*j} \eta_n^j \rangle \right] \\
 &\quad + \frac{1}{L} \sum_{j=1}^L \left(\sum_{m \neq n}^N M_{mn}^{-1} \right) E \left[\langle \eta_m^{*j} \eta_n^j \rangle \right] \\
 &= \sum_n M_{nn}^{-1} + \left(\sum_{m \neq n}^N M_{mn}^{-1} \right) E \left[\frac{1}{L} \sum_{j=1}^L \langle \eta_m^{*j} \eta_n^j \rangle \right] \\
 &= \text{Tr} \left(M^{-1} \right).
 \end{aligned}$$

Therefore, instead of calculating the trace for M^{-1} directly, we use the estimator $E \left[\langle \eta^\dagger M^{-1} \eta \rangle \right]$. In the infinite noise limit, this trace estimation will be exact.

Noise and Variance

CHOICE OF RANDOM NOISES :

Z_2 noise :

A set of noise vectors $\eta_N^1, \eta_N^2, \dots, \eta_N^L$, where each vector has N components, and each component has one of the four values $\{\pm 1, \pm i\}$ chosen independently with equal probability.

Better than Gaussian noise:

S.J. Dong and Keh-Fei Liu, Phys. Lett. **B328**, 130 (1994).

VARIANCE : For a given L number of noises,

$$\begin{aligned}\sigma_M^2 &\equiv \text{Var} \left[\langle \eta^\dagger M^{-1} \eta \rangle \right] \\ &= E \left[\left| \langle \eta^\dagger M^{-1} \eta \rangle - \text{Tr}(M^{-1}) \right|^2 \right] \\ &= \frac{1}{L} \sum_{m \neq n}^N \left| M_{mn}^{-1} \right|^2.\end{aligned}$$

Unbiased Subtraction

$$\text{Tr}A^{-1} = E \left[\left\langle \eta^\dagger \left(A^{-1} - \sum_{p=1}^P \lambda_p Q^{(P)} \right) \eta \right\rangle \right]$$

$\eta : Z_2$ noise vectors,

Q^P : set of traceless matrices,

λ_p : variational coefficients needed to be tuned to get the minimum variance.

$$\begin{aligned} \sigma_A^2(\lambda) &= \text{Var} \left[\left\langle \eta^\dagger \left(A^{-1} - \sum_{p=1}^P \lambda_p Q^{(P)} \right) \eta \right\rangle \right] \\ &= \frac{1}{L} \sum_{m \neq n} \left| A_{m,n}^{-1} - \sum_{p=1}^P \lambda_p Q_{m,n}^{(P)} \right|^2. \end{aligned}$$

....C. Thron et al., Phys. Rev. **D57**, 1642 (1998).

Unbiased Subtraction

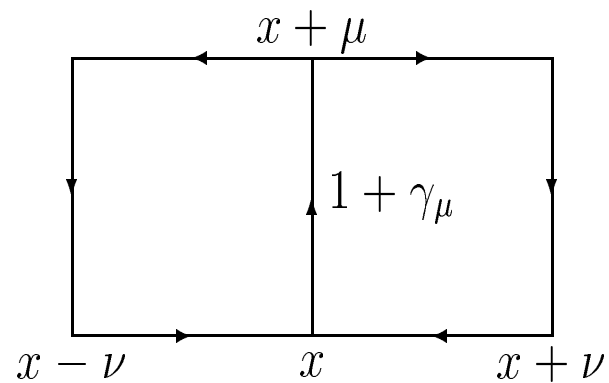
CHOICE OF Q^P

Any traceless matrix. However, it should match the off-diagonal behavior of the matrix A . We used a set of traceless matrices obtained from the hopping parameter expansion of the Wilson fermion matrix M .

$$M^{-1} = I + \kappa D + \kappa^2 D^2 + \kappa^3 D^3 + \dots$$

Unbiased Subtraction

Need to subtract trace-full part like (for vector current) :



CH-Symmetry

By CH-symmetry we mean the charge conjugation (C) and Euclidean hermiticity (H).

$$M^{-1}(x, y, U) = C^{-1} \tilde{M}^{-1}(y, x, U^*) C.$$

Euclidean hermiticity :

$$\gamma_5 M^{-1}(x, x + a_\mu) \gamma_5 = M^{-1\dagger}(x + a_\mu, x),$$

Under CH-transformation,

$$M^{-1}(x, y, U) = C^{-1} \gamma_5 M^{-1*}(x, y, U^*) \gamma_5 C.$$

Using CH-symmetry one can prove that

$$O_{vc}(U, M^{-1}[U]) = O_{vc}^*(U^*, M^{-1}[U^*]),$$

i.e., the three-point function of the vector current is REAL.

Loop Reduction

Loop Part :

$$\begin{aligned} & \text{Tr} \left[M^{-1}(x, x + a_\mu) (1 + \gamma_\mu) U_\mu^\dagger(x_1) \right] \\ & \quad - \text{Tr} \left[M^{-1}(x + a_\mu, x) (1 - \gamma_\mu) U_\mu(x) \right]. \end{aligned}$$

Now, using the identity, $\gamma_5 M^{-1}(x, y) \gamma_5 = M^{-1\dagger}(y, x)$,

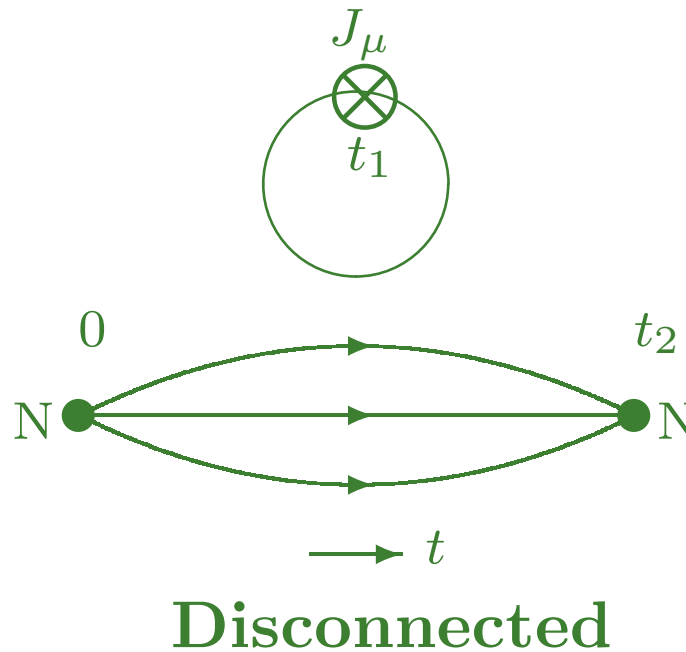
$$\begin{aligned} & \text{Tr} \left[M^{-1}(x + a_\mu, x) (1 - \gamma_\mu) U_\mu(x) \right] \\ & = \text{Tr} \left[\gamma_5 M^{-1}(x + a_\mu, x) (1 - \gamma_\mu) U_\mu(x) \gamma_5 \right] \\ & = \text{Tr} \left[M^{-1\dagger}(x, x + a_\mu) (1 + \gamma_\mu) U_\mu(x) \right] \\ & = \text{Tr} \left[M^{-1}(x, x + a_\mu) (1 + \gamma_\mu) U_\mu^\dagger(x) \right]^\dagger \end{aligned}$$

Therefore,

$$\begin{aligned} & \text{Tr} \left[M^{-1}(x, x + a_\mu) (1 + \gamma_\mu) U_\mu^\dagger(x_1) \right] \\ & \quad - \text{Tr} \left[M^{-1}(x + a_\mu, x) (1 - \gamma_\mu) U_\mu(x) \right] \\ & = 2\text{Im} \text{Tr} \left[M^{-1}(x, x + a_\mu) (1 + \gamma_\mu) U_\mu^\dagger(x_1) \right] \end{aligned}$$

Thus, after Fourier transformation only **REAL** part of the loop exists.

Loop Reduction



$$\begin{aligned}
 & \{ \cos(qx) + i \sin(qx) \} \{ (Loop)_R + (Loop)_I \} \times \{ (2Pt)_R + (2Pt)_I \} \\
 & = -\sin(qx)(Loop)_I \times \{ (2Pt)_R + (2Pt)_I \} \\
 & = -\sin(qx)(Loop)_I \times \{ (2Pt)_R \}
 \end{aligned}$$

Error Calculation over Configurations and Noises

$\{x_1, x_2, \dots, x_N\}$: a set of configurations.

$$\text{Average, } a = \frac{1}{N} \sum_{i=1}^N x_i,$$

$$\text{Error, } \epsilon_1 = \frac{\sigma_1}{\sqrt{N}}.$$

Next, each x_i is stochastically estimated with n noises with mean x_i and variance σ_2 :

$$x_i = \frac{1}{n} \sum_{j=1}^n x_{ij},$$

$$\text{Error, } \epsilon_2 = \frac{\sigma_2}{\sqrt{n}}.$$

The characteristic function (fourier transform of the probability distribution for the deviation of the compound noise and configuration average) is given by,

$$\begin{aligned}
 \Phi(k) &= \int e^{ik(a-\bar{x})} Q(a-\bar{x}) da \\
 &= \prod_{ij} \int \int \exp \frac{ik}{N} \left[\frac{1}{n} (x_{ij} - \bar{x}) + (x_i - \bar{x}) \right] \\
 &\quad \times q(x_{ij}) p(x_i) dx_{ij} dx_i \\
 &\sim e^{-k^2 (\sigma_1 + \sigma_2^2/n)/2N},
 \end{aligned}$$

where p and q are the distribution functions for the Monte Carlo and noise estimator, respectively.

$$\sigma_2^2 = \left\langle \sum_{i,k \neq i} [M_{ik}^{-1}]^2 \right\rangle$$

is the configuration average of individual $\sigma_2^2(m)$. σ_1 is the standard deviation for $\text{Tr}(M^{-1})$ in configuration averaging. Combined standard error squared is

$$\epsilon^2 = \frac{\sigma_1^2}{N} + \frac{\sigma_2^2}{Nn}.$$

For $\text{Tr}(M^{-1})$,

$$\epsilon^2 = \frac{\sigma_1^2}{N} + \frac{\langle \sum_{i,k \neq i} [M_{ik}^{-1}]^2 \rangle}{Nn}$$

Consider an extreme case of $n = 1$, for which,

$$\begin{aligned} E[\text{Tr}(M^{-1})] &= \sum_i \eta_i X_i = \sum_{i,k} M_{ik}^{-1} \eta_i \eta_k \\ &= \sum_i M_{ii}^{-1} + \sum_{i,k \neq i} M_{ik}^{-1} \eta_i \eta_k \\ &= \sum_i M_{ii}^{-1} \pm \sum_{i,k \neq i} M_{ik}^{-1}. \end{aligned}$$

However, one can change this $n = 1$ noise as one moves through the Markov chain for the gauge configurations.

Variance in this case involves the combined distribution of M_{ik}^{-1} and $\eta_i \eta_k$ which can be written as

$$P(x) \sim \exp\left[-\frac{(x - \bar{x})^2}{2\sigma^2}\right] + \exp\left[-\frac{(x + \bar{x})^2}{2\sigma^2}\right].$$

where $\bar{x} = M_{ik}^{-1}$ and $\sigma = \sigma_{ik}$ for the matrix element M_{ik}^{-1} over the configuration space. Standard error squared is

$$\epsilon^2 = \frac{\sigma_1}{N} + \frac{\langle \sum_{i,k \neq i} [M_{ik}^{-1}]^2 \rangle + \sum_{i,k \neq i} \sigma_{ik}^2}{Nn}.$$

Extra term σ_{ik}^2 will increase error.

Which one is more important?

More Configurations

with

Less Noises

Less Configurations

with

More Noises

A Toy Model Calculation

$\{X_1, X_2, \dots, X_N\}$: Gaussian Distribution with mean 0 and variance σ_G .

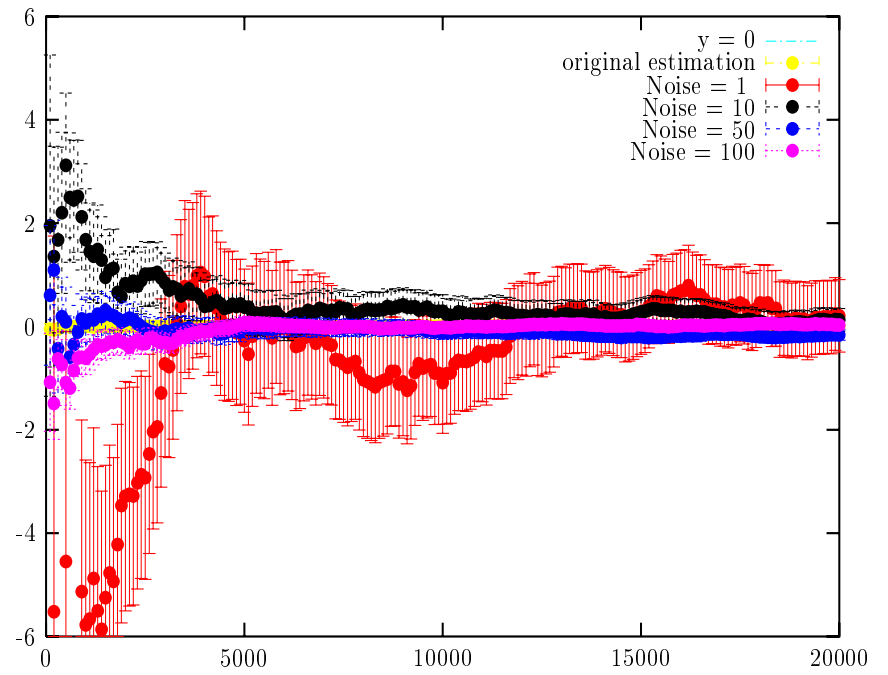
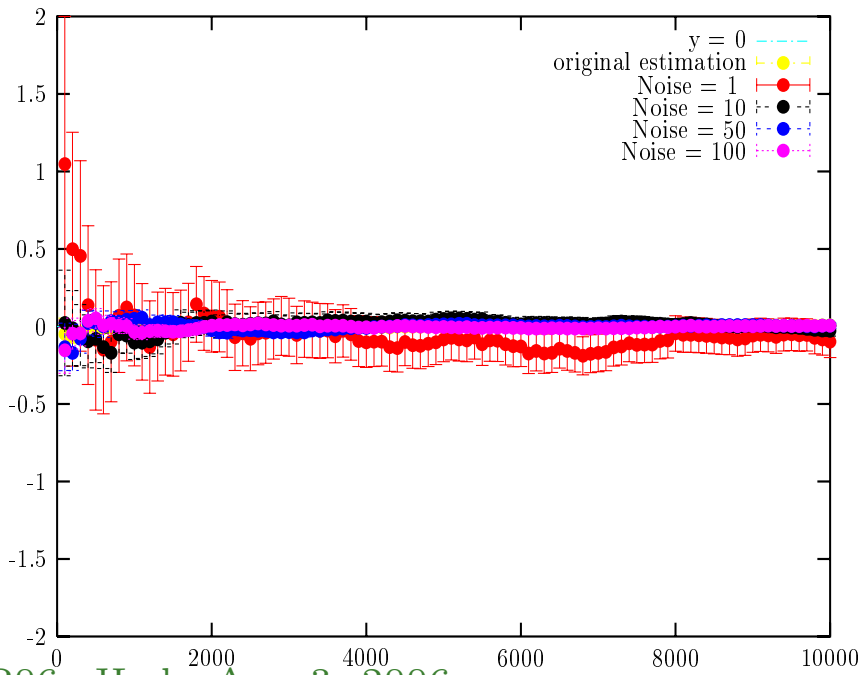
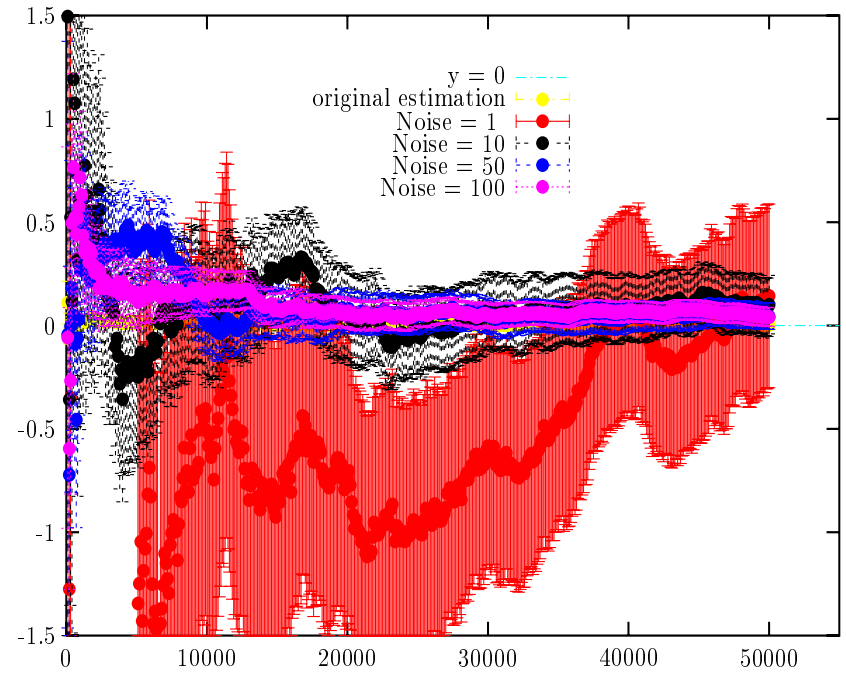
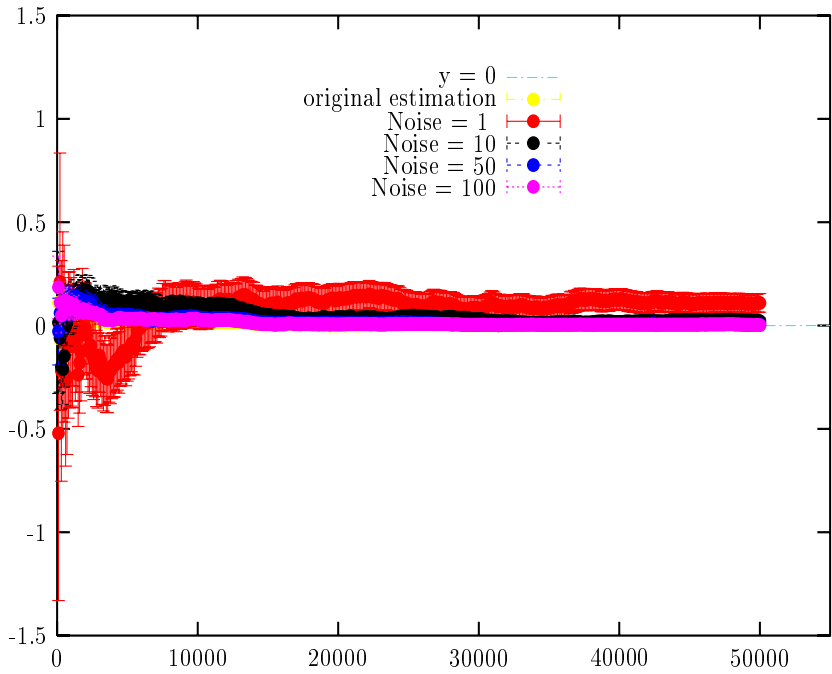
$$\text{Mean, } M_N = \frac{1}{N} \sum_{i=1}^N X_i,$$

$$\text{Error, } \epsilon = \frac{\sigma_N}{\sqrt{N}}.$$

Next, stochastically estimate each X_i :

For each X_i , generate n samples ($x_{ij}, j = 1..n$) from a Gaussian distribution with mean X_i and variance σ_n ($\sigma_n/\sigma_G = \lambda$). Corresponding to each X_i , we get a noise average

$$\tilde{X}_i = \frac{1}{n} \sum_{j=1}^n x_{ij}.$$



A Toy Model Calculation

What is the fraction (f) of configurations whose means and errors touch $M_N \pm \sigma_N/\sqrt{N}$?

- Calculate cumulative mean and error

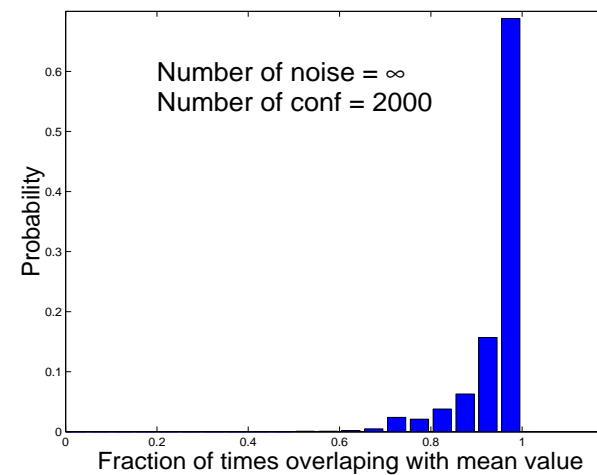
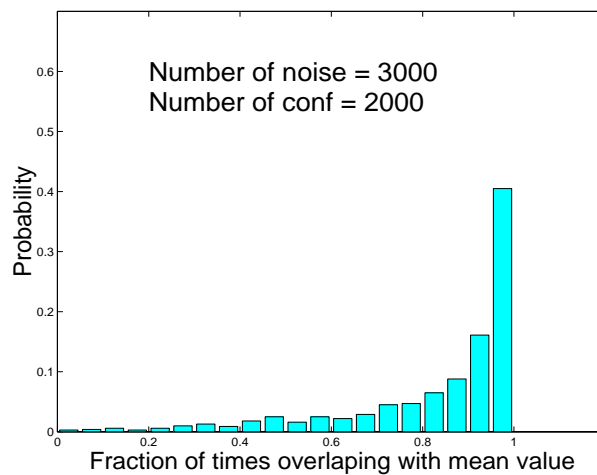
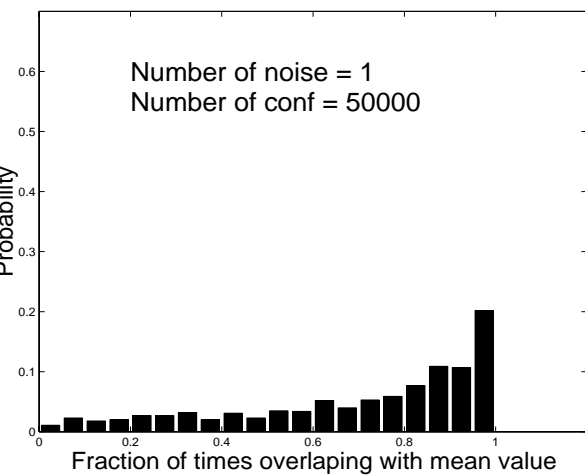
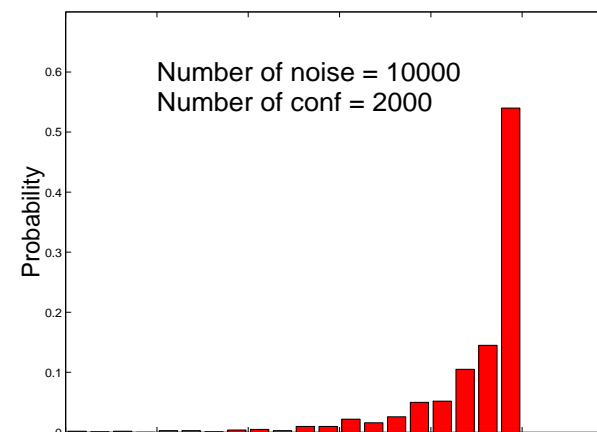
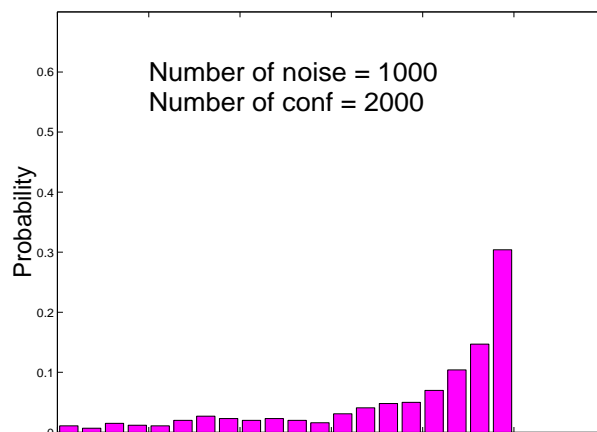
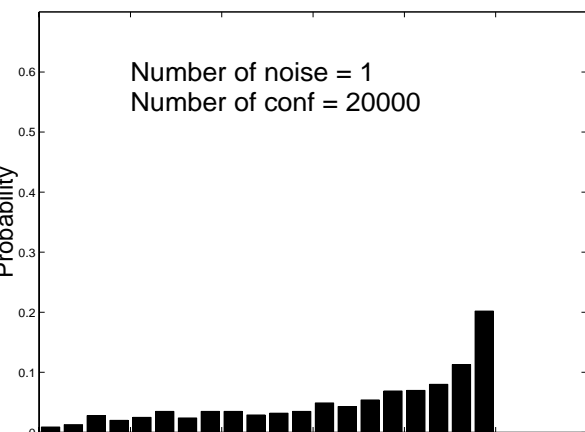
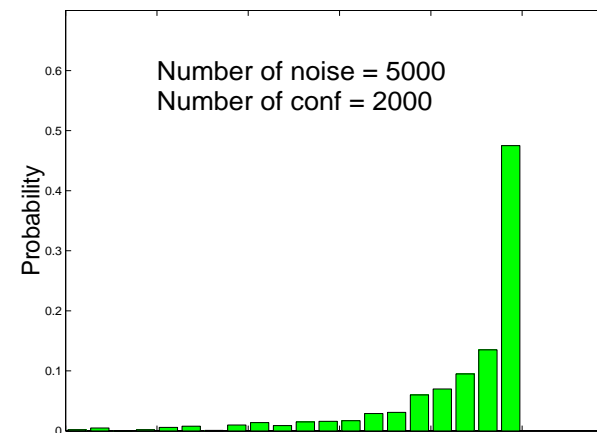
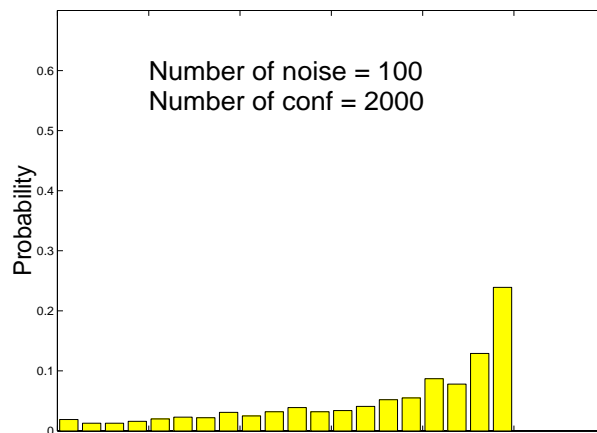
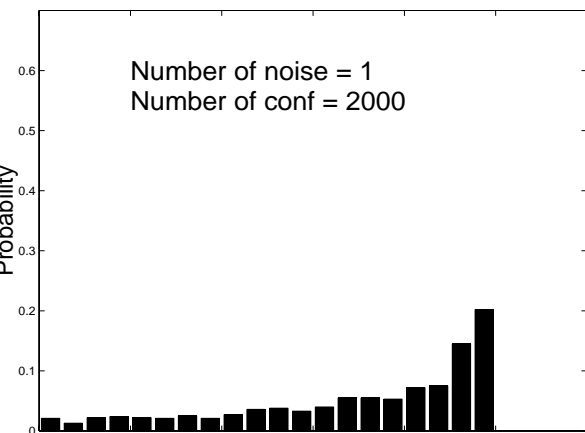
$$m_k = \frac{1}{k} \sum_{i=1}^k \tilde{X}_i,$$

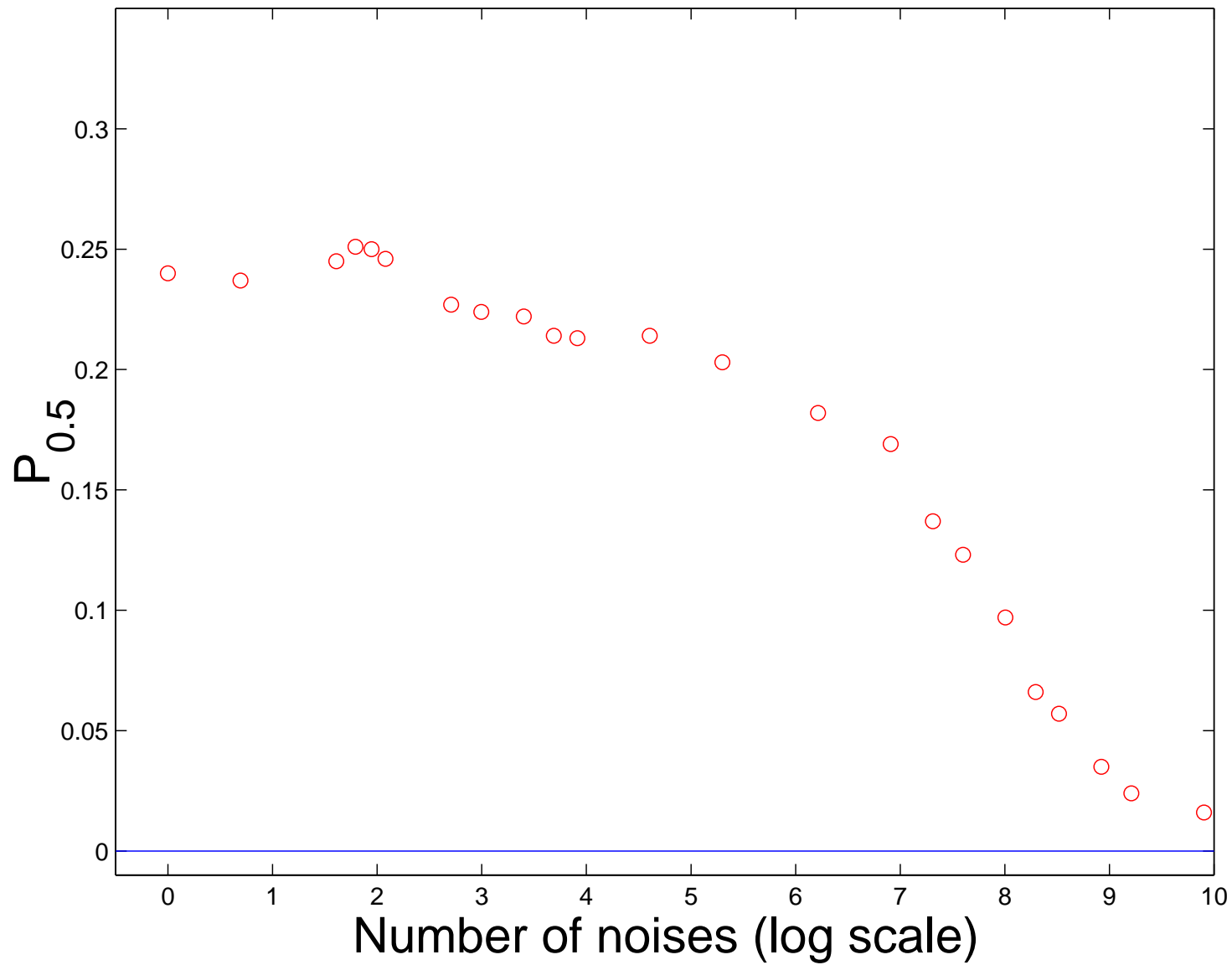
$$\epsilon_k = \sigma_k/\sqrt{k},$$

where k is the cumulative # of configurations starting from 2 to N .

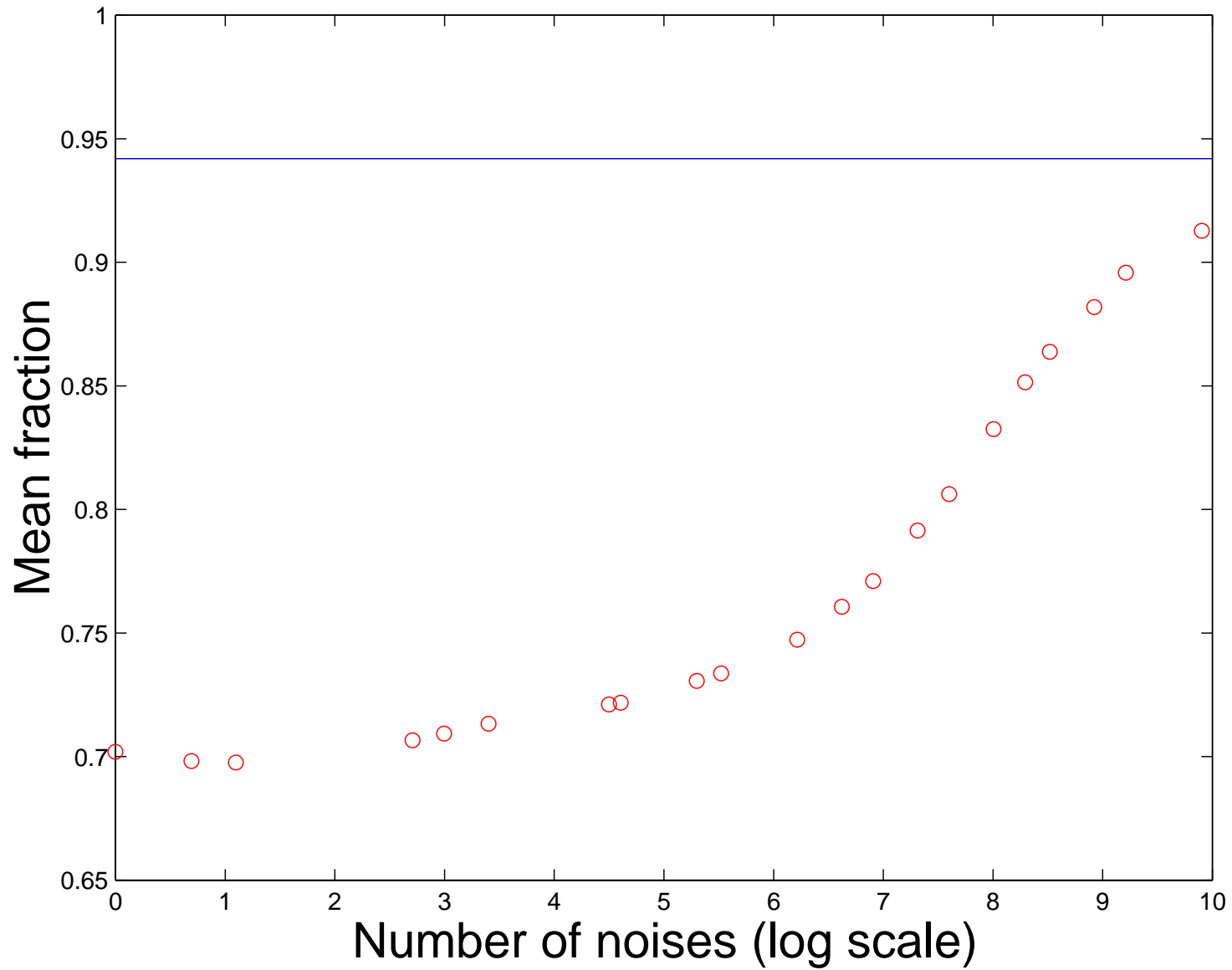
- Check for each k whether $m_k \pm \sigma_k/\sqrt{k}$ is consistent with $M_N \pm \sigma_N/\sqrt{N}$.
- If out of k ($k = 2$ to N) cumulative estimates, I estimates are consistent with $M_N \pm \sigma_N/\sqrt{N}$, then the corresponding fraction

$$f = I/(N - 1).$$





Probability (p) to be below fraction (f) 0.5 for different noise cases



Mean fraction ($p_i f_i$) for different noise cases.

A detail study for noise versus configuration

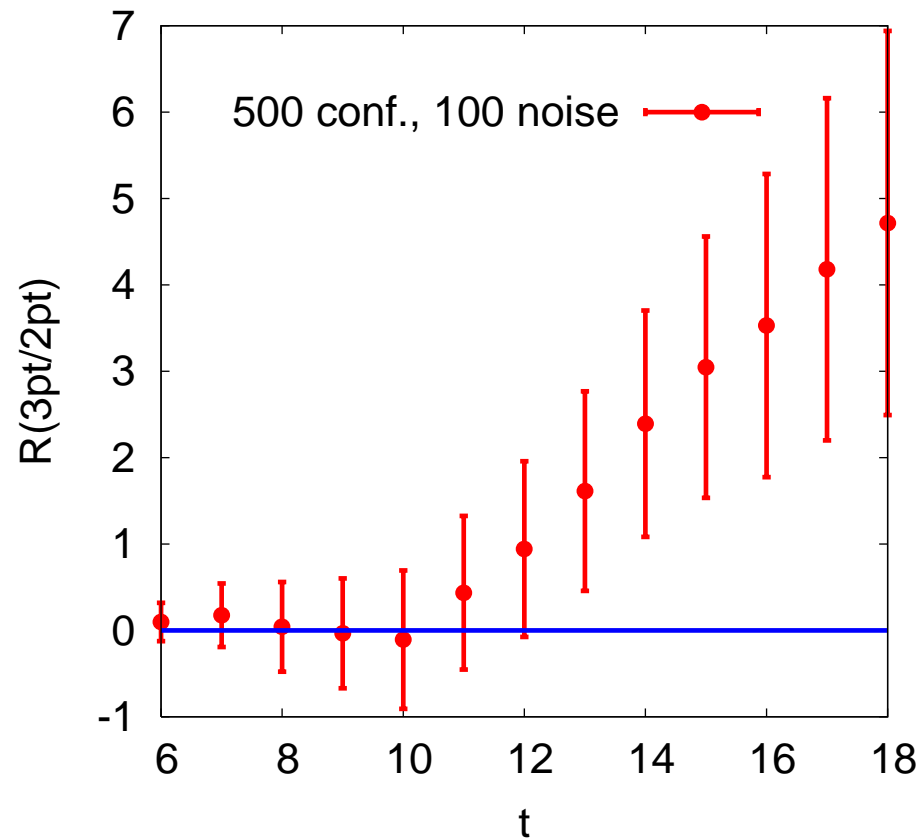
- Simulation details
 - Wilson action, $16^3 \times 24$, $a = 0.1$ fm
 - 500 configurations and 500 noises/configs, (in future 1000 configs and 500 noises/configs).
 - four loop masses
 - unbiased subtraction up to order 8 in D

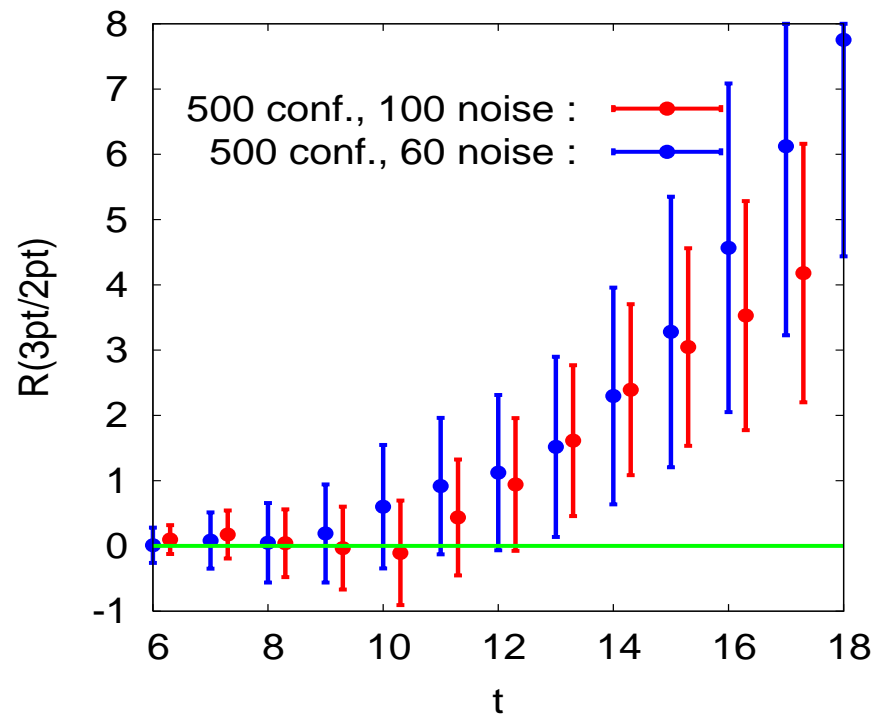
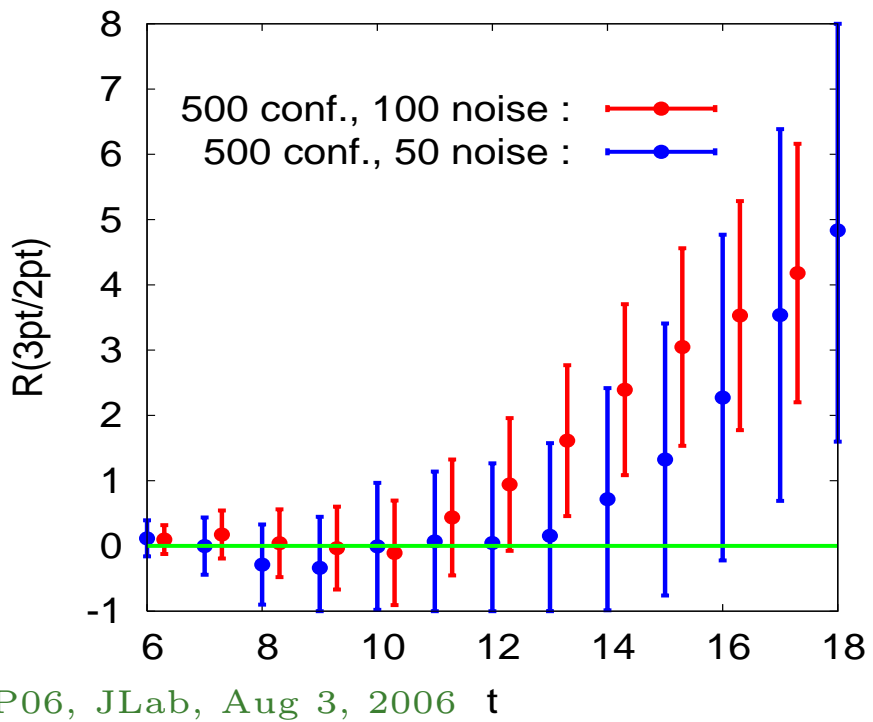
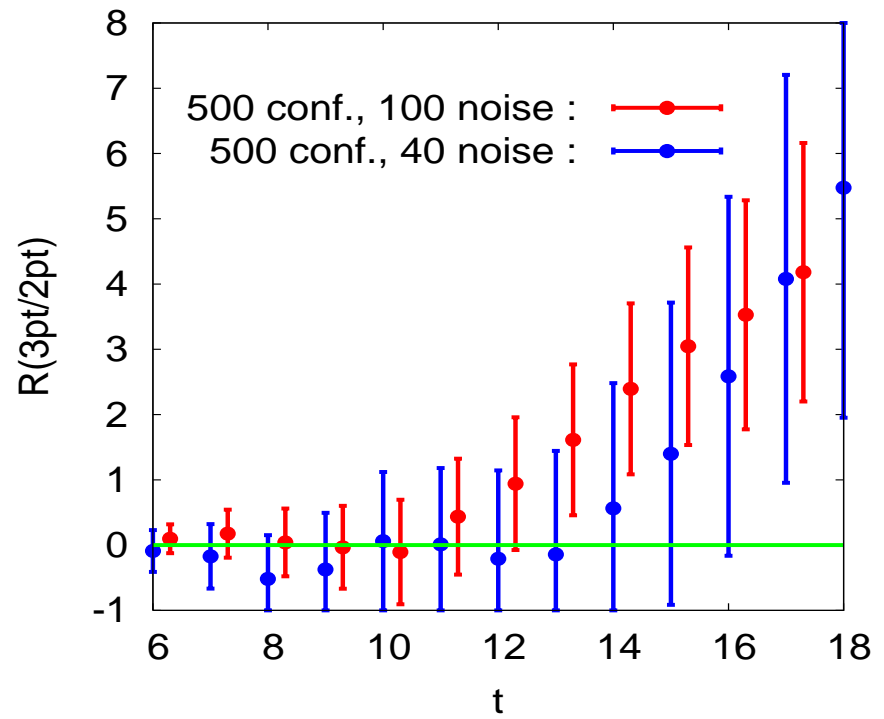
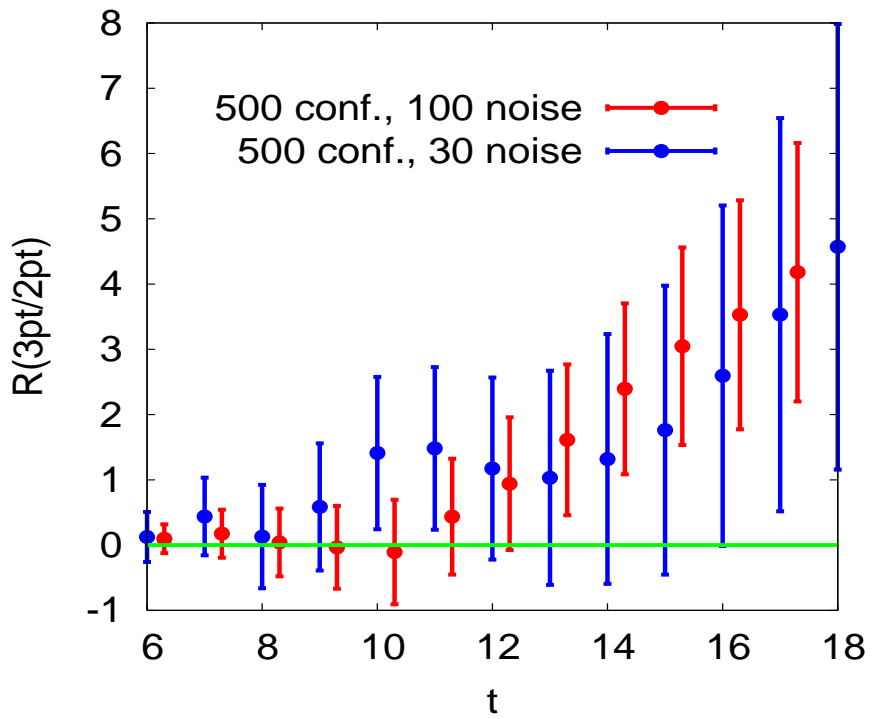
$$R(3pt/2pt) = \sum_t \frac{\Gamma_1^{\alpha\beta} G_{NSN}^{\beta\alpha}(t_f, \vec{p}, t, \vec{q}) \Gamma_2^{\alpha\beta} G_{NN}^{\beta\alpha}(t, \vec{p})}{\Gamma_2^{\alpha\beta} G_{NN}^{\beta\alpha}(t_f, \vec{p}) \Gamma_2^{\alpha\beta} G_{NN}^{\beta\alpha}(t, \vec{q})} \implies const. + t_f g_{dis}(q^2)$$

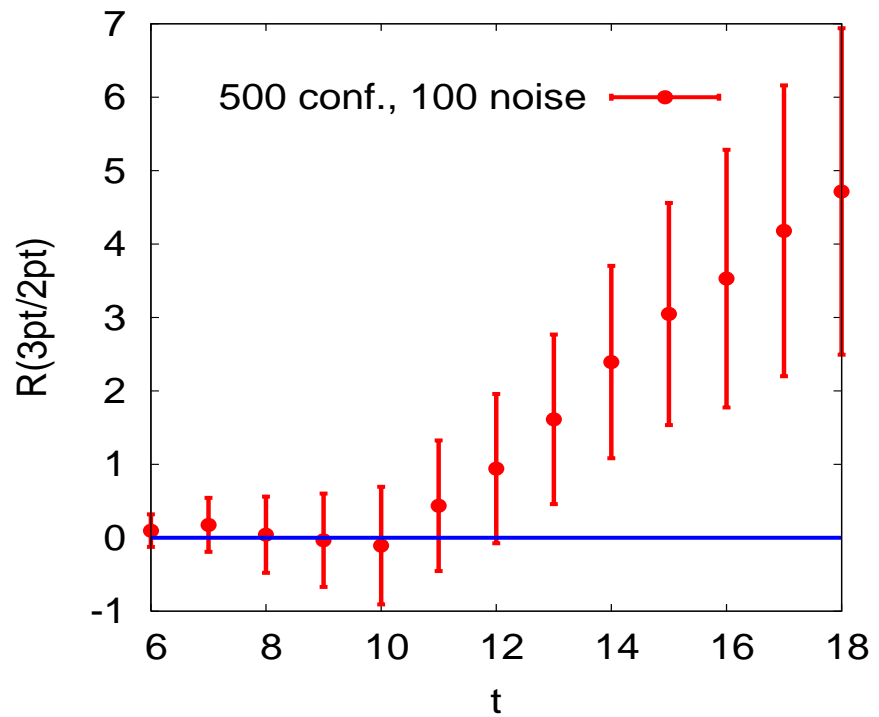
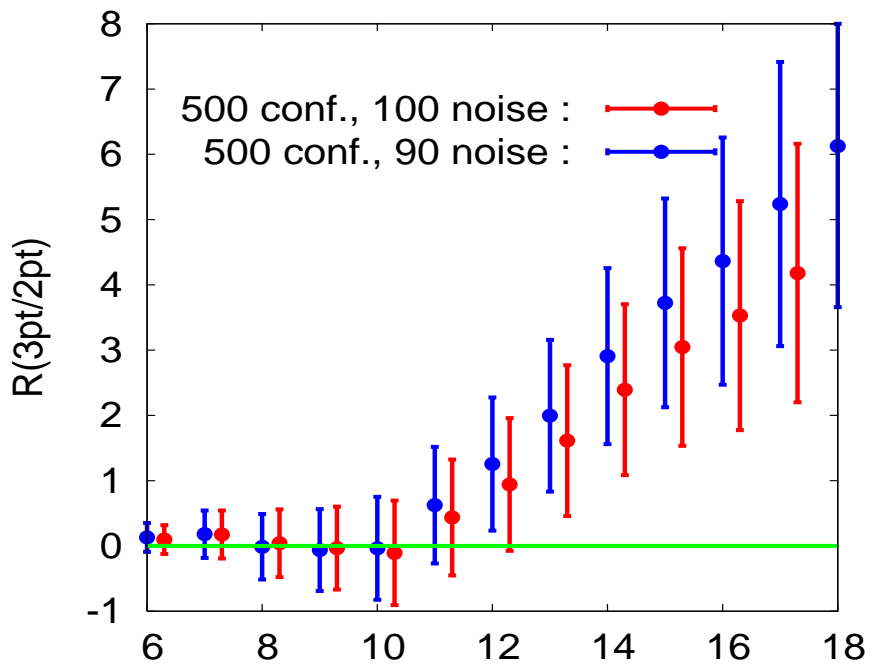
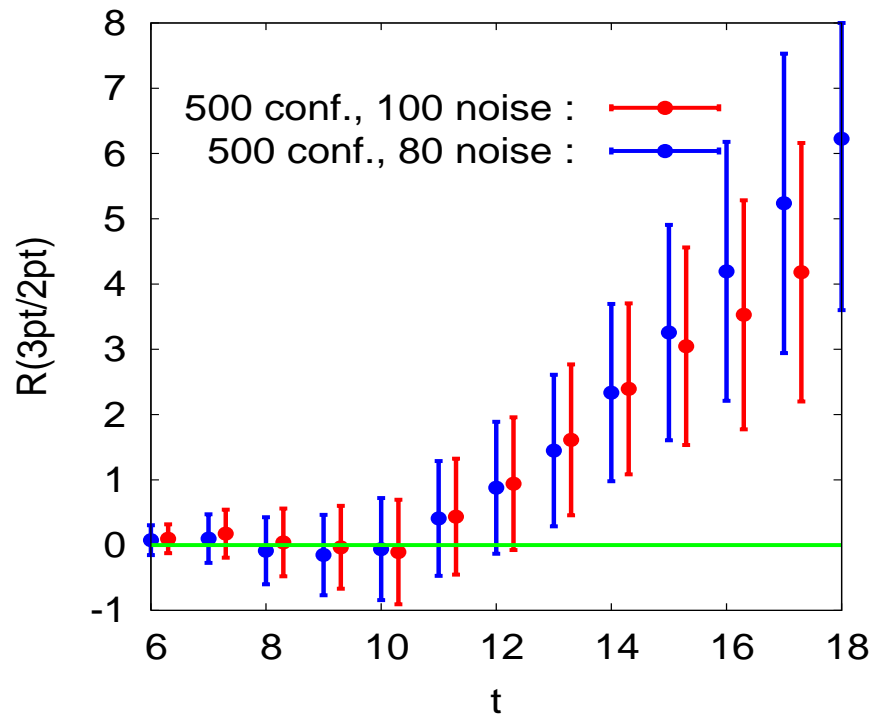
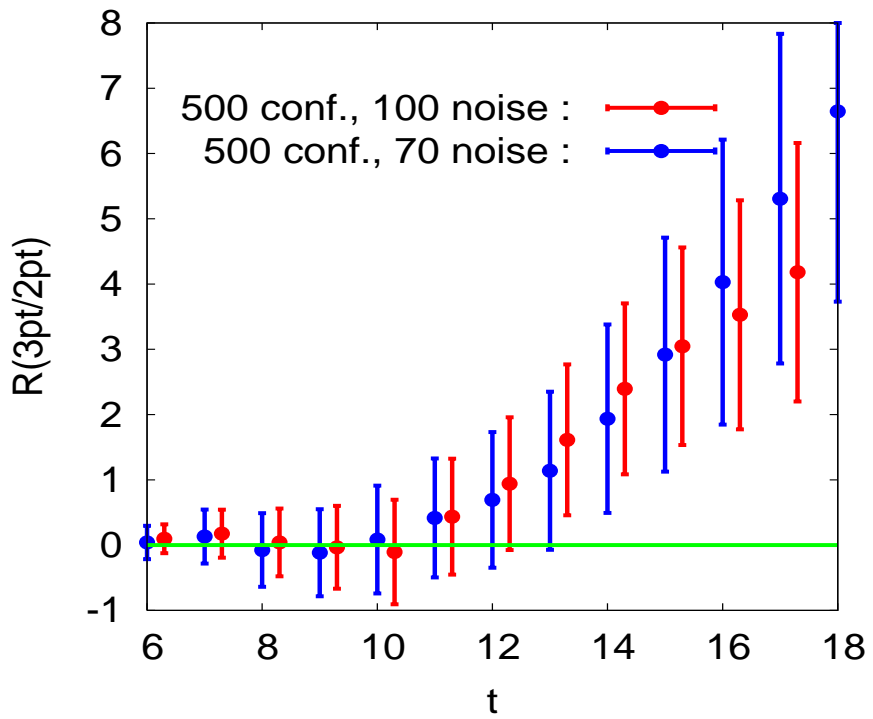
Slope will give disconnected contribution

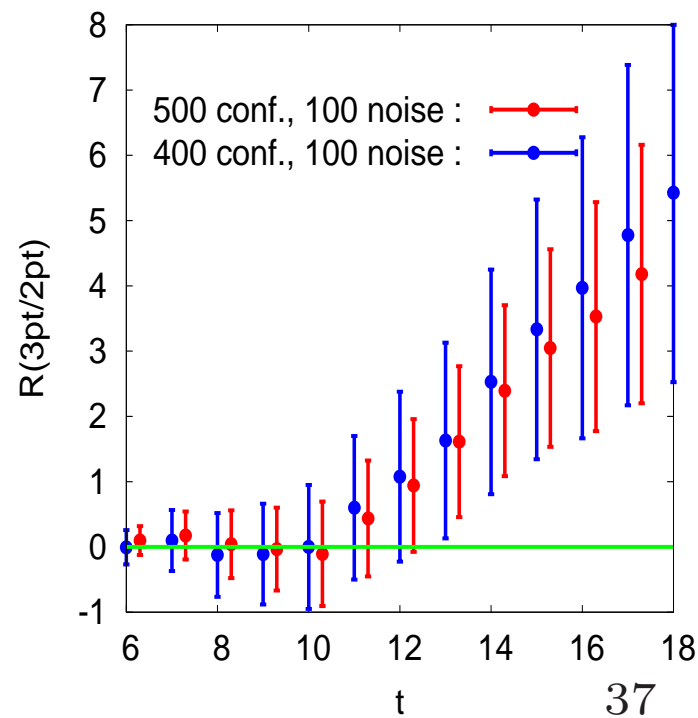
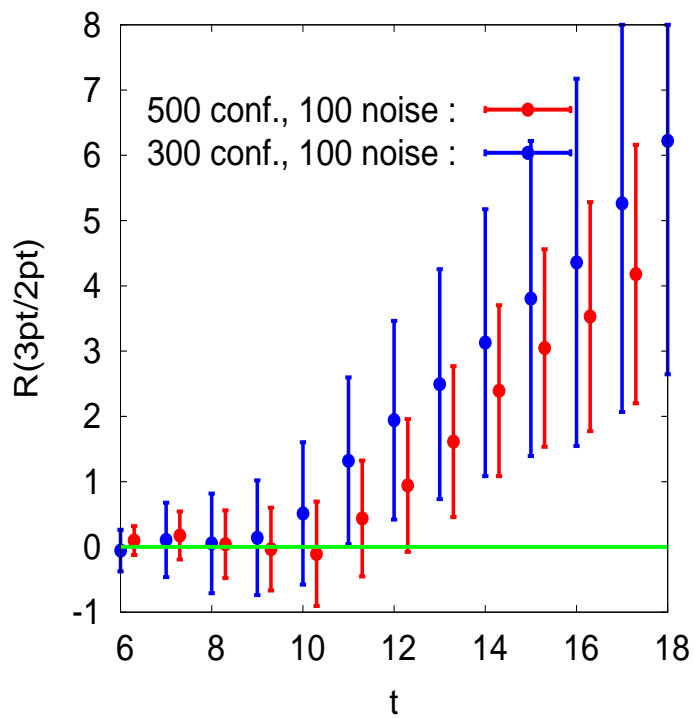
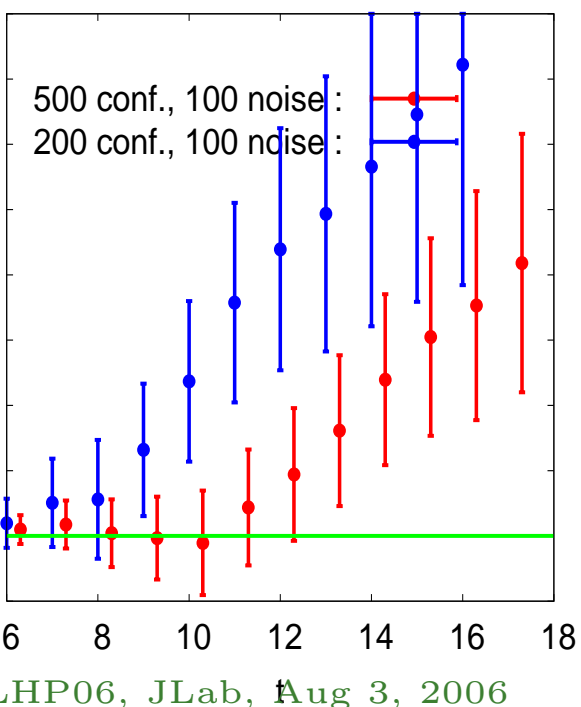
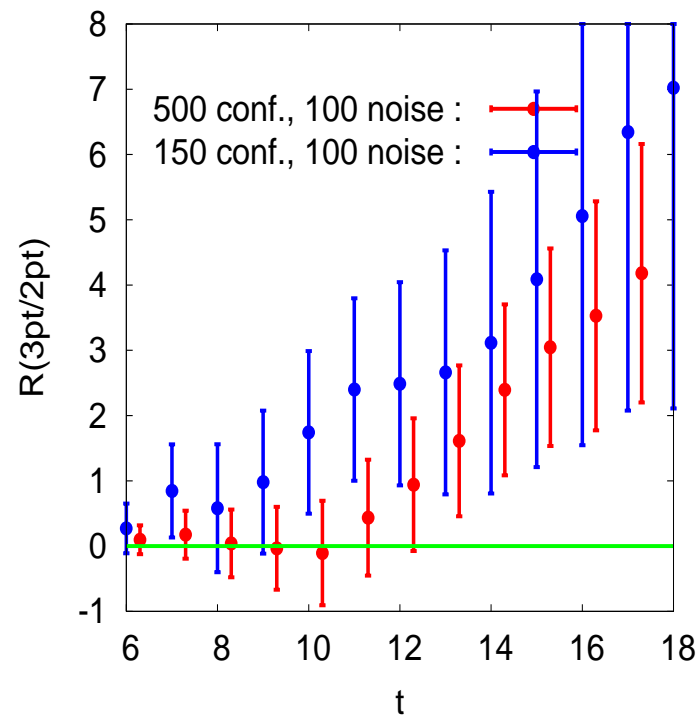
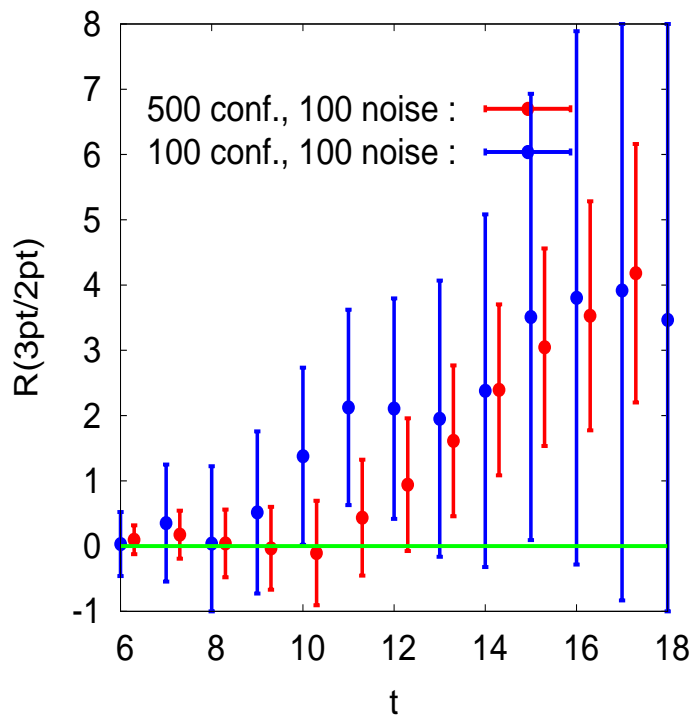
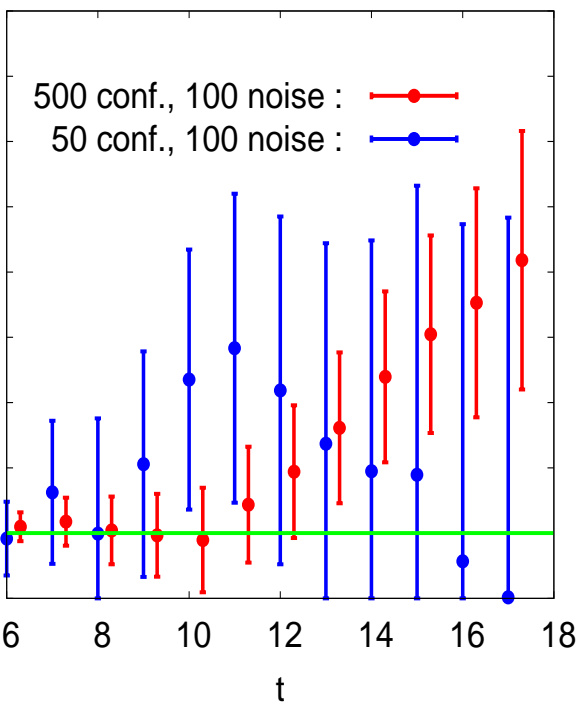
One can also take difference of ratios to avoid fitting in slope ...Wilcox

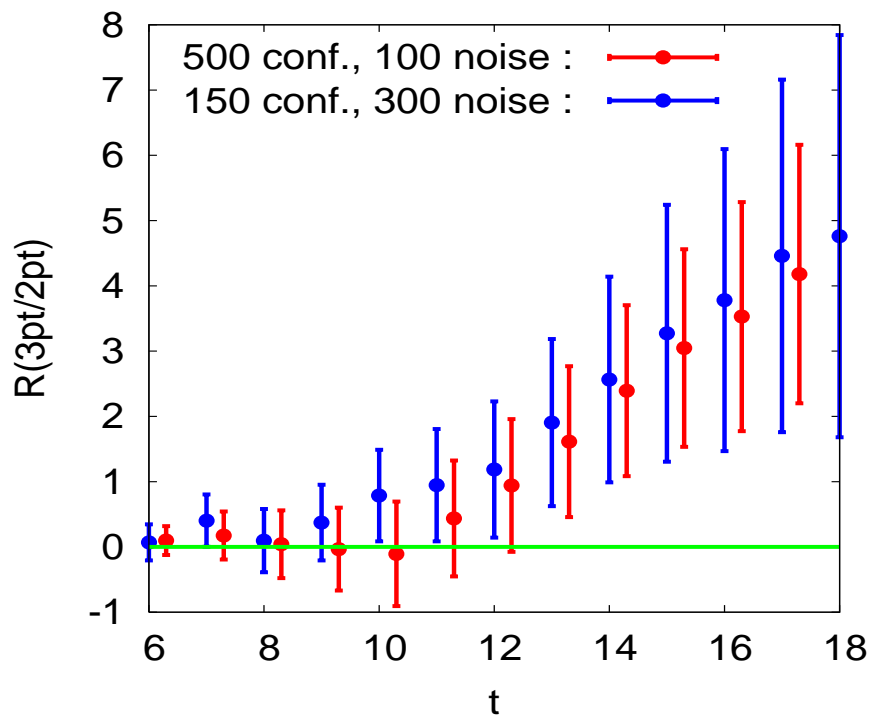
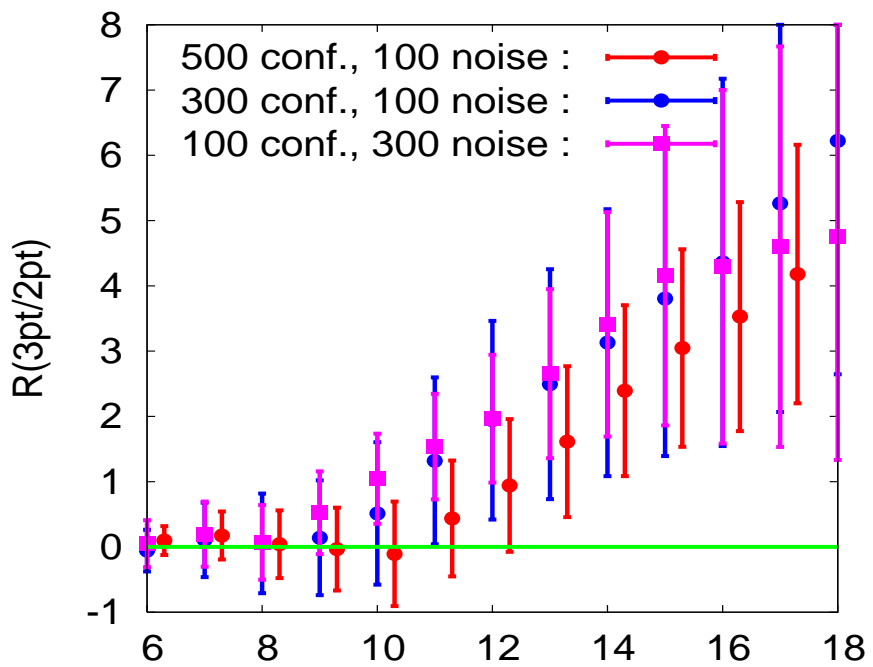
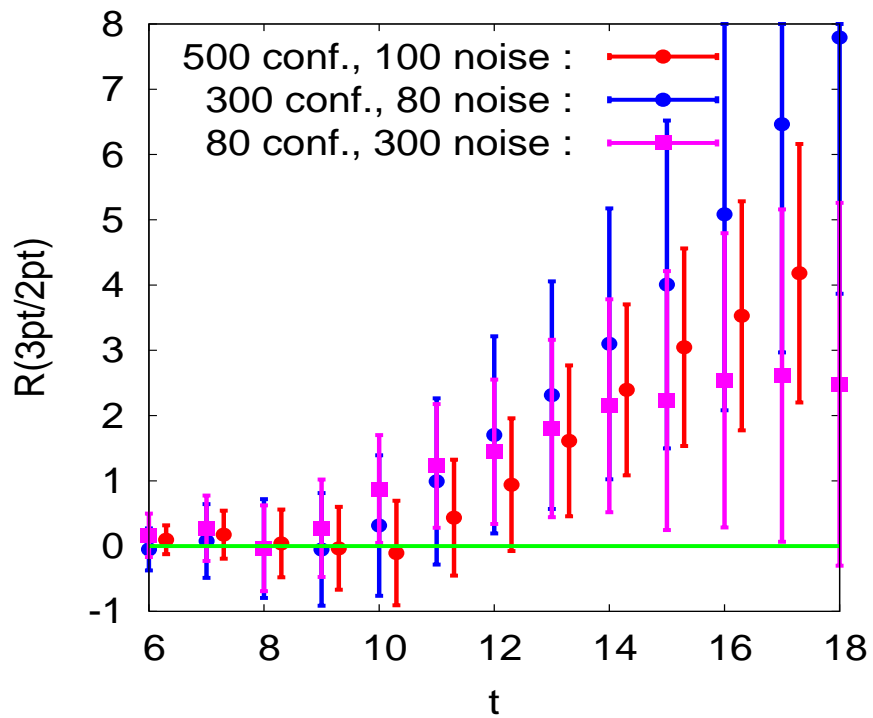
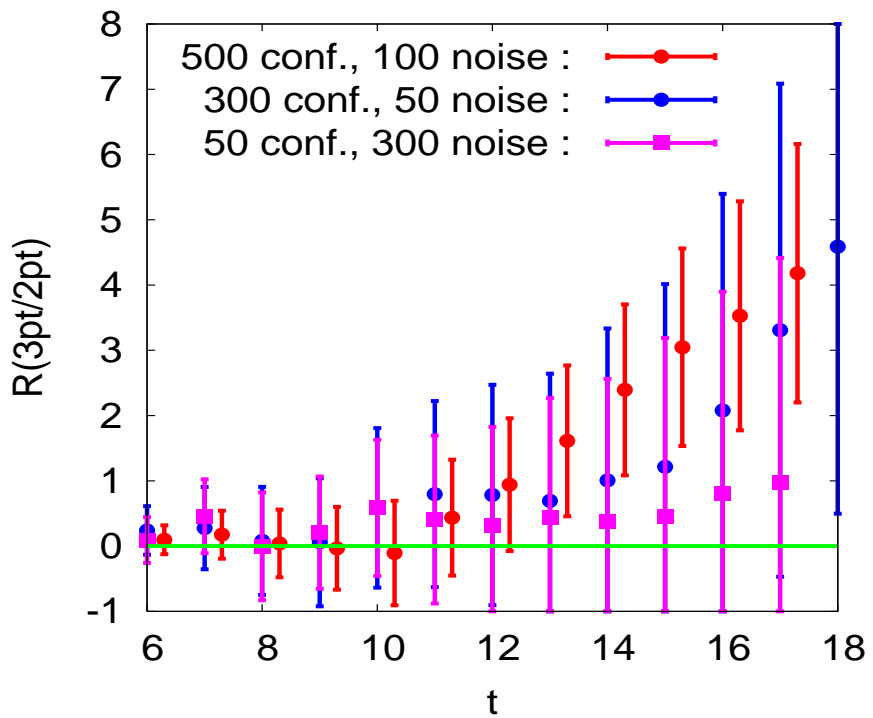
Preliminary results for scalar current











Strangeness content in parton distribution function

$$\langle P | \mathcal{O}_f^{(n)\{\mu_1 \dots \mu_n\}} | P \rangle = 2A_f^n P^{\mu_1} \dots P^{\mu_n} \quad - \text{traces}$$

where,

$$A_f^n = \int_0^1 dx x^{n-1} [\zeta_f(x) + (-1)^n \zeta_{\bar{f}}(x)]$$

$\zeta_f(x)$ is the parton distribution function.

- For s quark

$$A_s^2 = \langle x \rangle = \int_0^1 dx x [s(x) + \bar{s}(x)], \quad \text{is the first moment}$$

$$A_s^3 = \langle x^2 \rangle = \int_0^1 dx x^2 [s(x) - \bar{s}(x)], \quad \text{is the second moment}$$

- Analytical expressions for $\langle x \rangle$

for $\mathcal{O}_{\{4i\}}$ operator ($i = 1, 2, 3$)

$$R_{\{4i\}}^{\text{dis}} = \sum_{t_1} \frac{\text{Tr} [\Gamma G_{N\mathcal{O}_{\{4i\}}N}(t_2, t_1, p_i)]}{\text{Tr} [\Gamma G_{NN}(t_2, \vec{p})]} \frac{2}{-ip_i} \rightarrow \text{const.} + t_2 \langle x \rangle_{\text{dis}}$$

$$R_{\{4i\}}^{\text{con}} = \frac{\text{Tr} [\Gamma G_{N\mathcal{O}_{\{4i\}}N}(t_2, t_1, p_i)]}{\text{Tr} [\Gamma G_{NN}(t_2, \vec{p})]} \frac{2}{-ip_i} \rightarrow \langle x \rangle_{\text{con.}}$$

for $\mathcal{O}_{\{44\}} - \frac{1}{3}(\mathcal{O}_{\{11\}} + \mathcal{O}_{\{22\}} + \mathcal{O}_{\{33\}})$ operator

$$R_{\{44\}}^{\text{con}} = - \frac{\text{Tr} [\Gamma G_{N\mathcal{O}_{\{44\}}N}(t_2, t_1, \vec{p})]}{\text{Tr} [\Gamma G_{NN}(t_2, \vec{p})]} \frac{2E_p}{E_p^2 + \frac{p^2}{3}} \rightarrow \langle x \rangle_{\text{con.}}$$

- Analytical expressions for $\langle x^2 \rangle$

For $\mathcal{O}_{\{4ii\}} = \frac{1}{2}(\mathcal{O}_{\{4jj\}} + \mathcal{O}_{\{4kk\}})$ ($i, j, k = 1, 2, 3$ and $i \neq j \neq k$)

$$R_{\{4ii\}}^{\text{dis}} = \sum_{t_1} - \frac{\text{Tr} [\Gamma G_{N\mathcal{O}_{\{4ii\}}N}(t_2, t_1, p_i)]}{\text{Tr} [\Gamma G_{NN}(t_2, \vec{p})]} \frac{2}{p_i^2}$$

$$\rightarrow \text{const.} + t_2 \langle x^2 \rangle_{\text{dis}}$$

$$R_{\{4ii\}}^{\text{con}} = - \frac{\text{Tr} [\Gamma G_{N\mathcal{O}_{\{4ii\}}N}(t_2, t_1, p_i)]}{\text{Tr} [\Gamma G_{NN}(t_2, \vec{p})]} \frac{2}{p_i^2} \rightarrow \langle x^2 \rangle_{\text{con}}$$

The $\mathcal{O}_{\{4i\}}$ operator is defined as,

$$\mathcal{O}_{\{4i\}}(x) = \bar{\psi}(x)(\gamma)_{\{4(-\frac{i}{2} \overleftrightarrow{\mathcal{D}})_i\}} \psi(x)$$

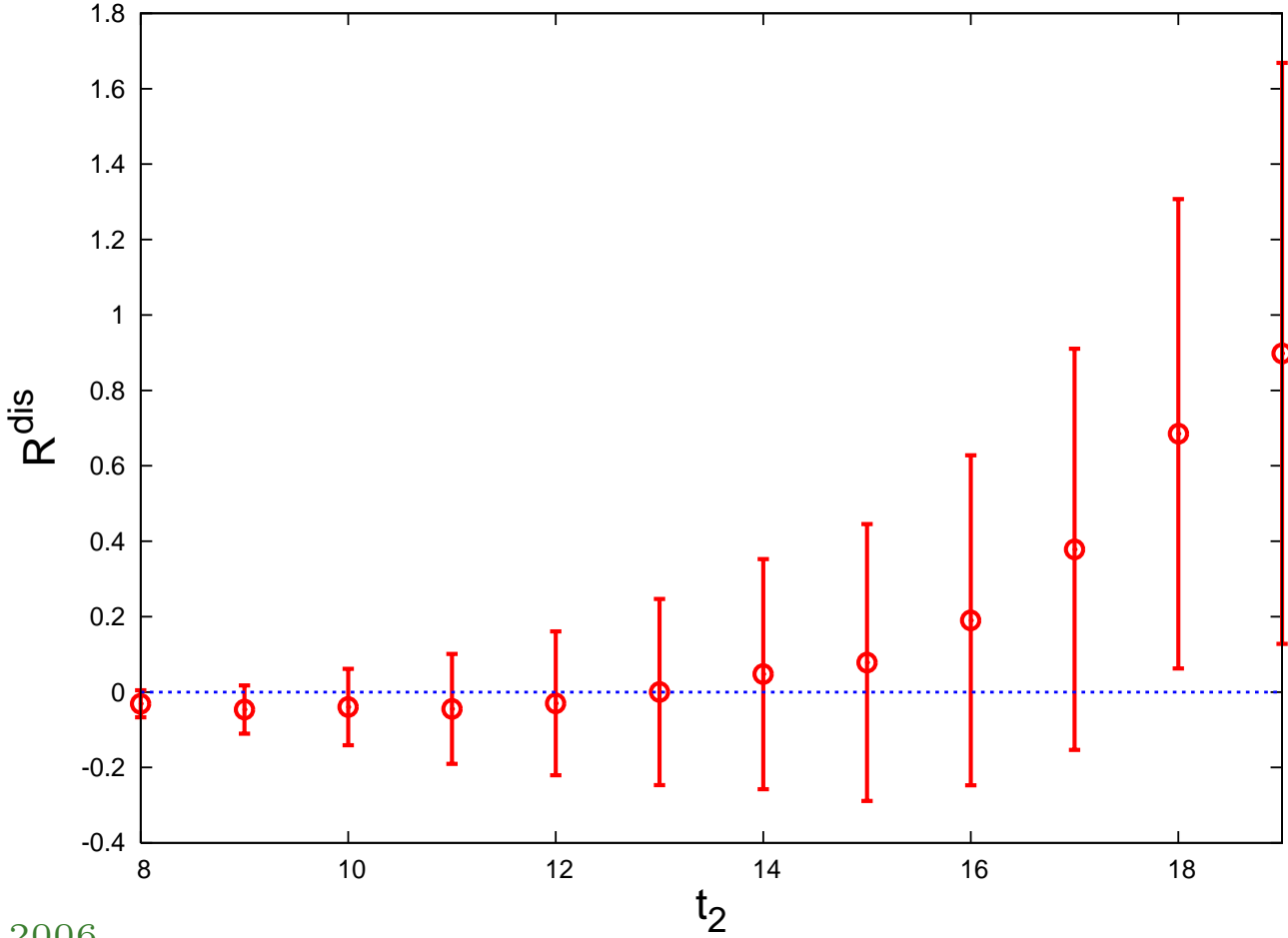
The $\mathcal{O}_{\{4ii\}}$ operator is defined as,

$$\mathcal{O}_{\{4ii\}}(x) = \bar{\psi}(x)(\gamma)_{\{4(-\frac{i}{2} \overleftrightarrow{\mathcal{D}})_i(-\frac{i}{2} \overleftrightarrow{\mathcal{D}})_i\}} \psi(x)$$

PRELIMINARY RESULTS

First Moment

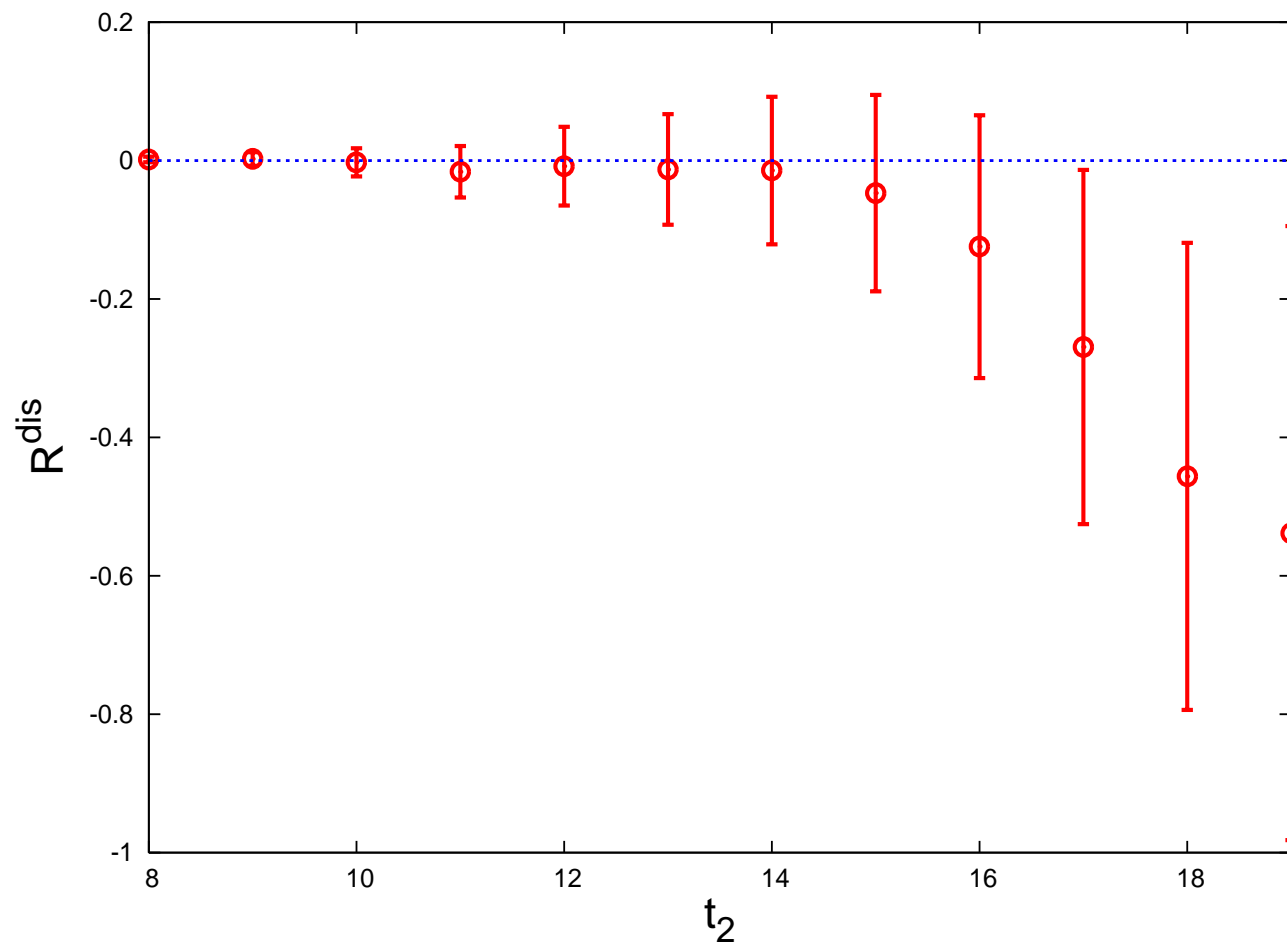
$\kappa = 0.154$,
of noise=100, # of conf = 500



Second Moment

$$\kappa = 0.154 ,$$

of noise=100, # of conf = 500



Comments

- Preliminary results from scalar current indicate that
 - only a handful of noise vector and large number of configurations is not good
 - only a handful of configuration and large number of noise vectors is also not good
 - One needs a optimal set
- Our calculation with larger set of configurations and noise vectors with unbiased subtraction is ongoing.

Improvements

Use all-to-all propagators

..... M. Peardon's talk

- Use Dilution : **spin and color**
- Projection of a few eigenvalues
- Unbiased subtraction