Lattice QCD
Beyond Ground States

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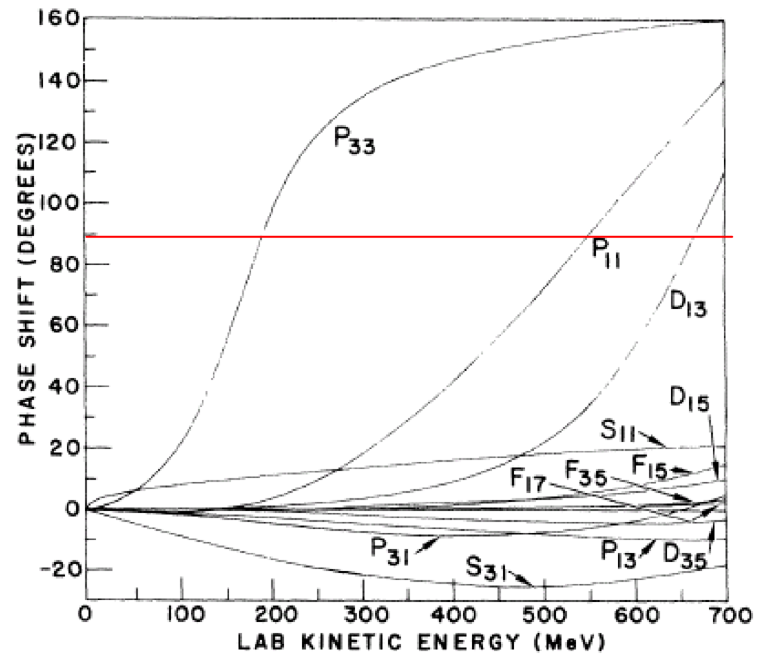
Outline

- Motivation and background
- Two-point Green function
  - Black box methods
  - Variational method
- Three-point Green function

Example: Roper (P_{11}) Spectrum

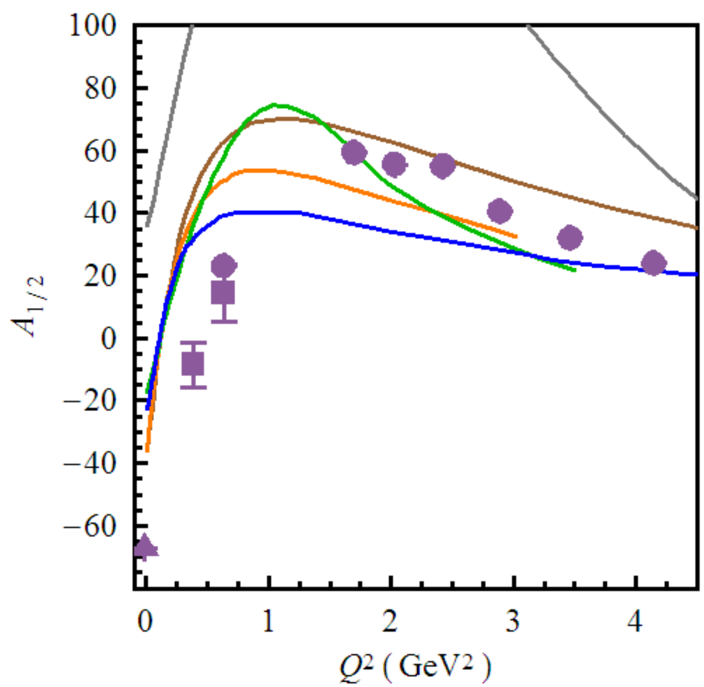
- First positive-parity excited state of nucleon (discovered in 1964)
- Unusual feature: 1st excited state is lower than its negative-parity partner!

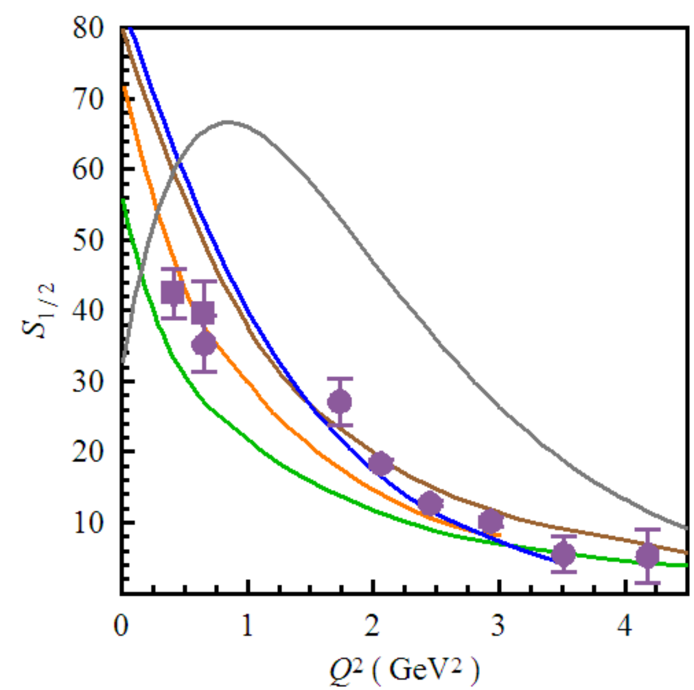


- Long-standing puzzle
  - Quark-gluon (hybrid) state [C. Carlson et al. (1991)]
  - Five-quark (meson-baryon) state [O. Krehl et al. (1999)]
  - Constituent quark models (many different specific approaches)
  - and many other models…
- Shopping list: full dynamical lattice QCD with proper extrapolation to (or calculation nearby) the physical pion mass

Example: Roper Form Factor

- Experiments at Jefferson Laboratory (**CLAS**), MIT-Bates, LEGS, Mainz, Bonn, GRAAL, and Spring-8
- Great effort has been put in by phenomenologists; Many models disagree (a selection are shown below)



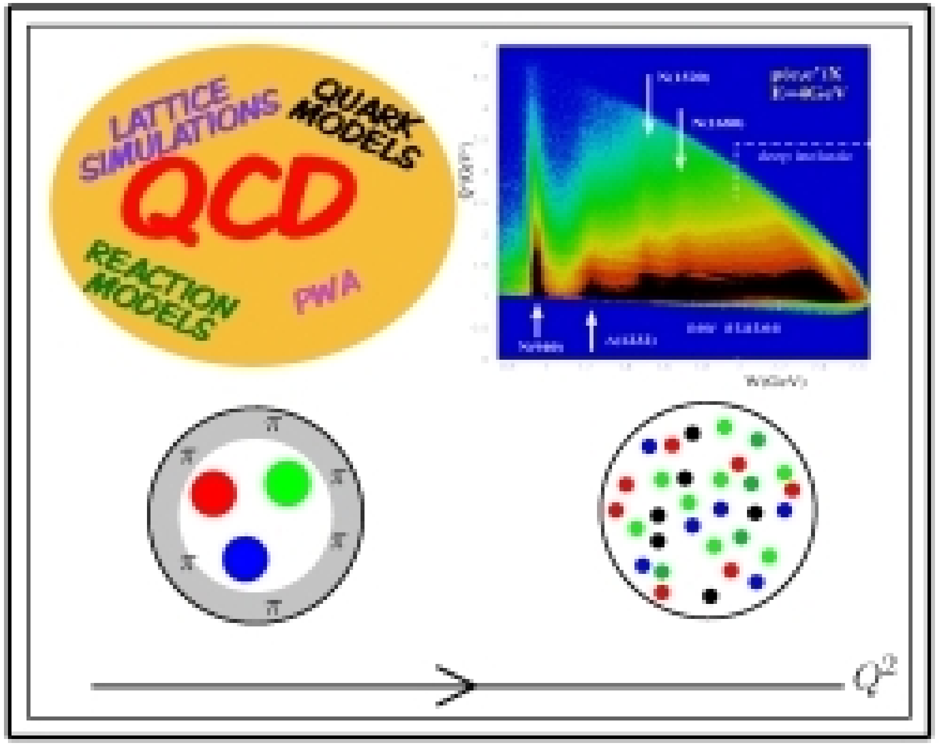


Helicity amplitudes are measured (in 10^{-3} GeV$^{-1/2}$ units)

EBAC

- Excited Baryon Analysis Center (EBAC)

"an international effort which incorporates researchers from institutes around the world"

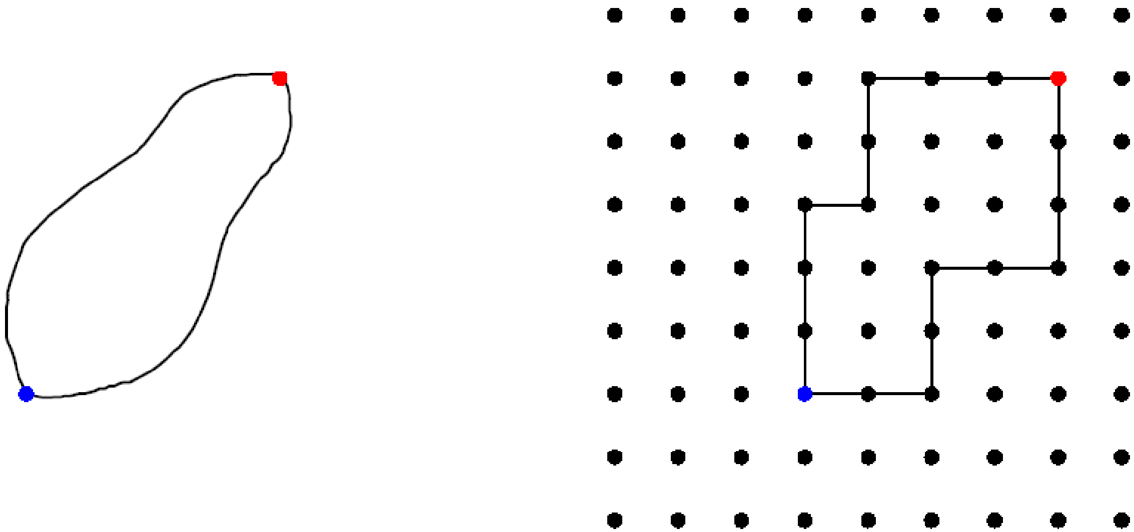


Lattice QCD

- Physical observables are calculated from the path integral

$$\langle 0|O(\overline{\psi},\psi,A)|0\rangle = \frac{1}{Z}\int [dA][d\overline{\psi}][d\psi]\, O(\overline{\psi},\psi,A)\, e^{i\int d^4x\, \mathcal{L}^{\mathrm{QCD}}(\overline{\psi},\psi,A)}$$

- Lattice QCD is a discrete version of continuum QCD theory



- Use Monte Carlo integration combined with the "importance sampling" technique to calculate the path integral.
- Take $a \rightarrow 0$ and $V \rightarrow \infty$ in the continuum limit

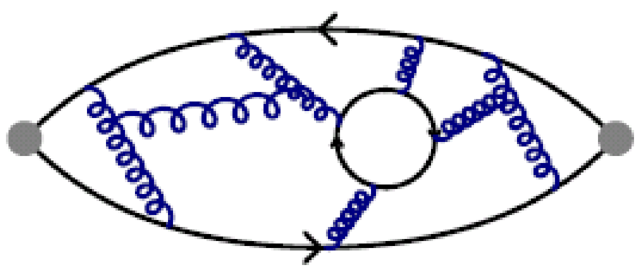
Lattice QCD: Observables

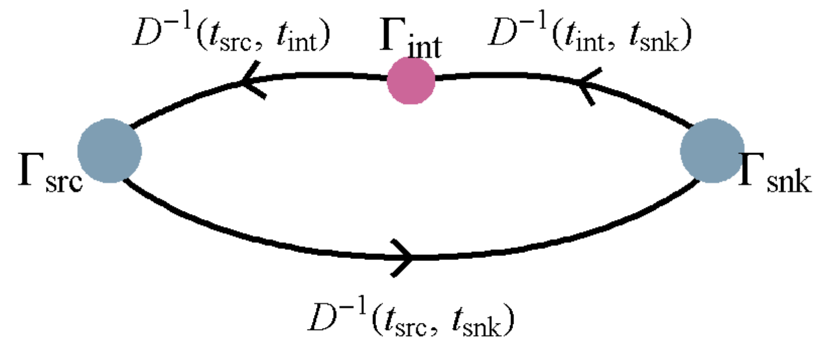
- Two-point Green function

  e.g. Spectroscopy

- Three-point Green function

  e.g. Form factors, Structure functions, …





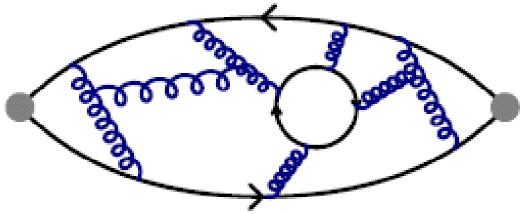
$$\sum_{\alpha,\beta} \Gamma^{\alpha,\beta} \langle J(X_{\rm snk}) J(X_{\rm src}) \rangle_{\alpha,\beta}$$

$$\sum_{\alpha,\beta} \Gamma^{\alpha,\beta} \langle J(X_{\rm snk}) O(X_{\rm int}) J(X_{\rm src}) \rangle_{\alpha,\beta}$$

Lattice QCD: Observables

- Two-point Green function

  e.g. Spectroscopy



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- Three-point Green function

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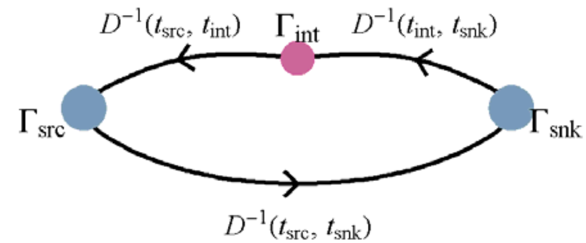


$$\sum_{\alpha,\beta} \Gamma^{\alpha,\beta} \langle J(X_{\rm snk}) O(X_{\rm int}) J(X_{\rm src}) \rangle_{\alpha,\beta}$$

After taking spin and momentum projection

(ignore the variety of boundary condition choices)

Two-point correlator

$$\sum_n Z_{n,B} e^{-E_n(\vec{P})t}$$

Three-point correlator

$$\sum_n \sum_{n'} Z_{n',B}(p_f) Z_{n,A}(p_i)$$

$$\times \text{FF's} \times e^{-(t_f - t)E'_n(\vec{p}_f)} e^{-(t-t_i)E_n(\vec{p}_i)}$$

Different states are mixed and the signal decays exponentially as a function of *t*

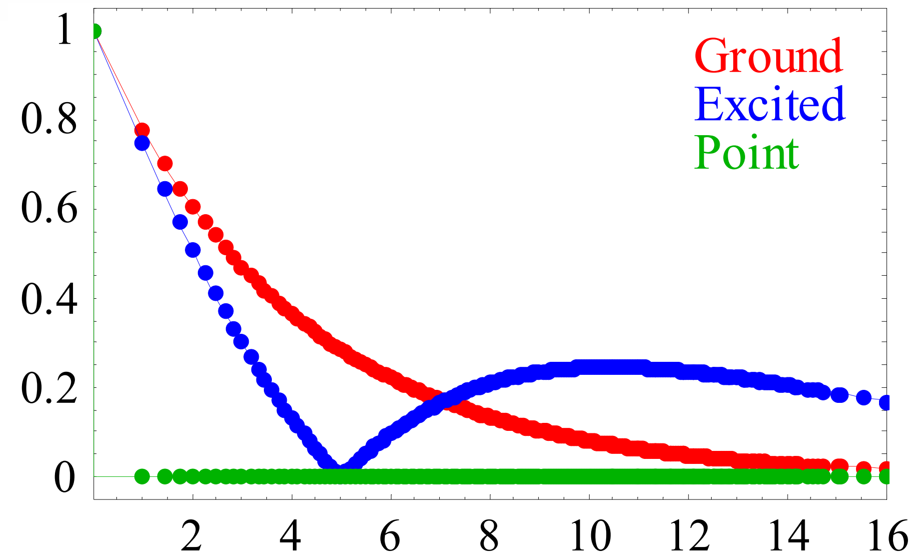
Lattice QCD: Improvements

- Obtain the ground state observables at large *t*, after the excited states die out: Need large time dimension
- The lighter the particle is, the longer the *t* required
- Smaller lattice spacing in time (anisotropic lattices)
- Multiple smearing techniques to overlap with different states

$$\psi^s(0) = \sum_{\vec{y}} F(\vec{y}, 0)\, \psi(\vec{y}, 0)$$

- Example:

Hydrogen wavefunction



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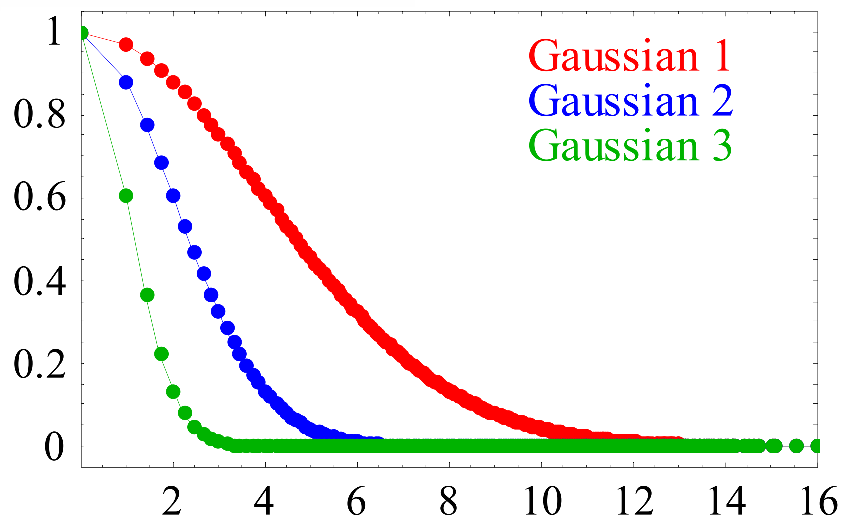
- Example:

Gaussian function



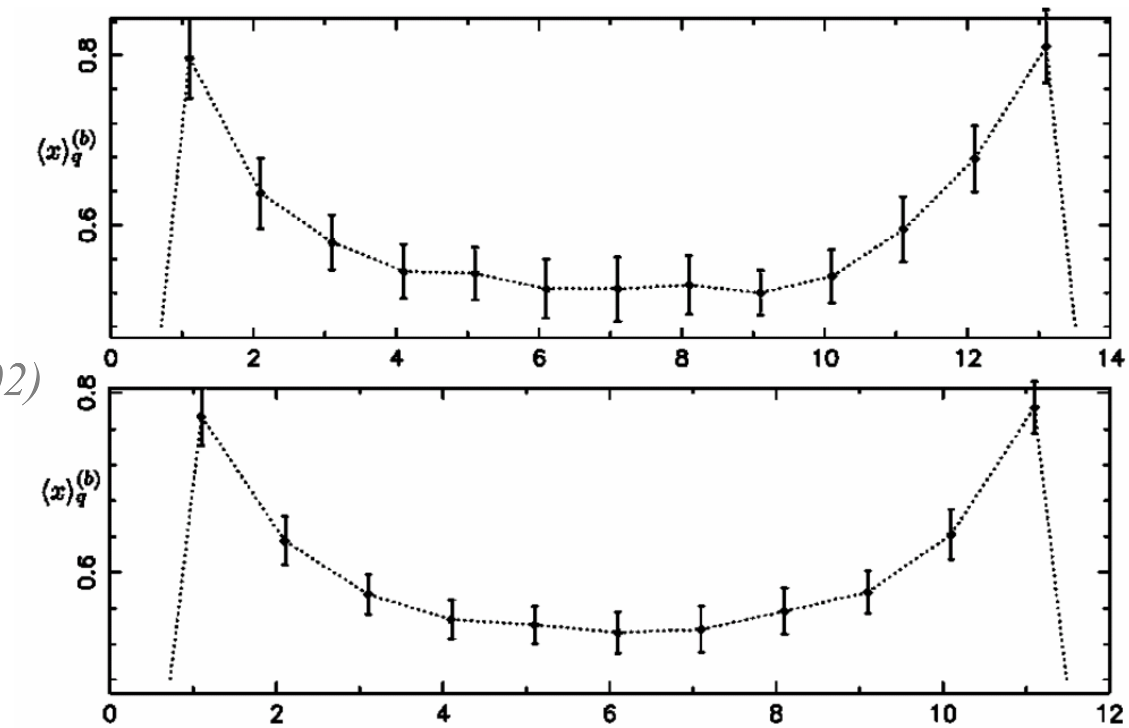
Only Interested in Ground State?

- Larger *t* solution does not always work well with three-point correlators
- Example:

  Quark helicity distribution

  LHPC & SESAM

  Phys. Rev. D ***66****, 034506 (2002)*



50% increase in error budget at $t_{sep} = 14$

- Confronting the excited states might be a better solution than avoiding them.

Probing Excited-State Signals

- Lattice spectrum (two-point Green function) case
  - *Black box method*
    (modified correlator method)
  - Multiple correlator fits
  - Variational methods
  - Bayesian Methods
    (as in G. Fleming's and P. Petreczky's talks)
- Form factor (three-point Green function) case
  - Fit the amplitude
  - Modified variational method

Black Box Methods

- In the 3rd iteration of this workshop, G. T. Fleming (*hep-lat/0403023*) talked about "black box methods" used in NMR:

$$y_n = \sum_{k=1}^{K} a_k e^{i\phi_k} e^{(-d_k + i2\pi f_k)t_n} + e_n$$

- Similar to the lattice correlators, which have the general form

$$y_n = \sum_{k=1}^{K} a_k \alpha_k^n$$

This forms a Vandermonde system

$$\mathbf{y} = \mathbf{\Phi a} \quad \text{with} \quad \mathbf{\Phi} = \begin{pmatrix} \phi_1(t_1, \boldsymbol{\alpha}) & \cdots & \phi_K(t_1, \boldsymbol{\alpha}) \\ \vdots & \ddots & \vdots \\ \phi_1(t_N, \boldsymbol{\alpha}) & \cdots & \phi_K(t_N, \boldsymbol{\alpha}) \end{pmatrix}$$

Black Box Method: *N*-State Effective Mass

- Given a single correlator (with sufficient length of *t*), one can, in principle, solve for multiple *a*'s and *α*'s

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = \begin{pmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_K \\ \alpha_1^2 & \alpha_2^2 & \cdots & \alpha_K^2 \\ \vdots & \cdots & \cdots & \vdots \\ \alpha_1^N & \alpha_2^N & \cdots & \alpha_K^N \end{pmatrix} \times \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_K \end{pmatrix}$$

- Can one solve *N*/2 states from one correlator of length *N* ?

Black Box Methods: Effective Mass

- System dominated by ground state ($K = 1$) case,

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = \begin{pmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_K \\ \alpha_1^2 & \alpha_2^2 & \cdots & \alpha_K^2 \\ \vdots & \cdots & \cdots & \vdots \\ \alpha_1^N & \alpha_2^N & \cdots & \alpha_K^N \end{pmatrix} \times \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_K \end{pmatrix}$$

easy solution: $\alpha_1 = y_{n+1}/y_n$

Thus, "effective mass" $M_{\text{eff}} = \ln(y_{n+1}/y_n)$

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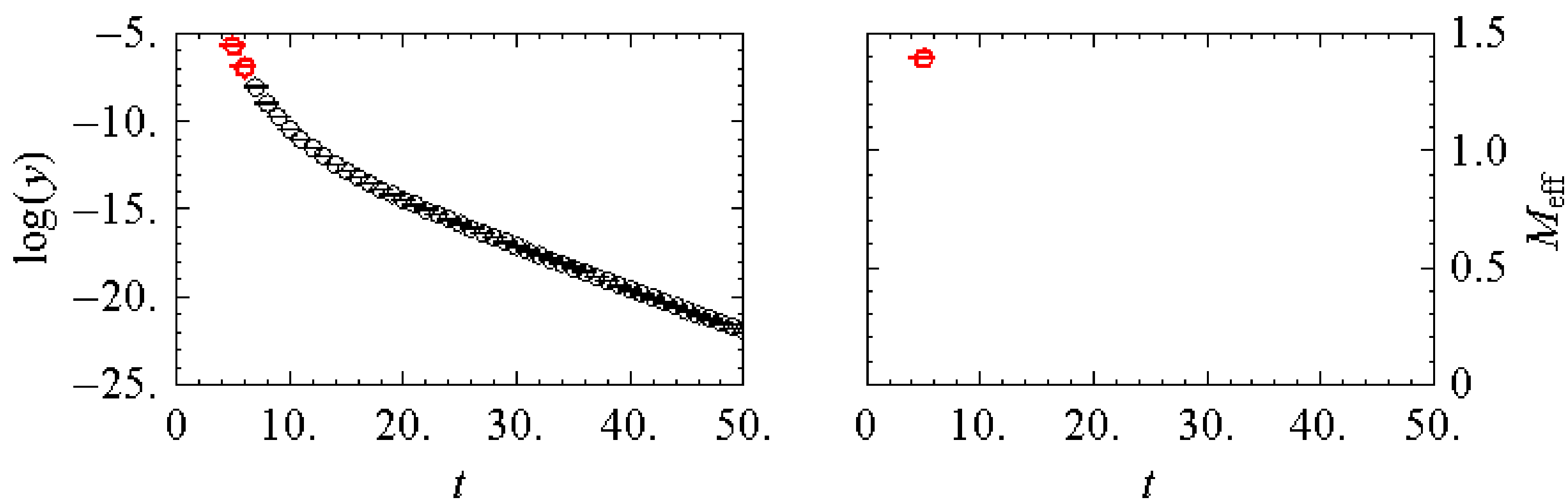


Black Box Methods: 1st Excited State

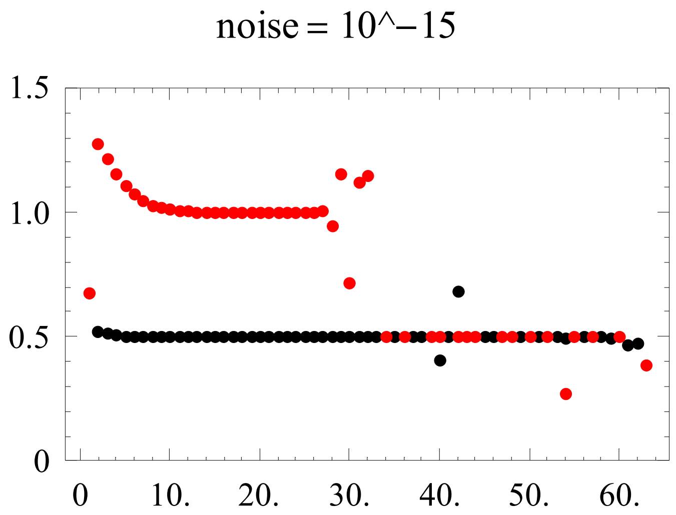
- Extracting two states ($K = 2$) case,

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} \alpha_1 & \alpha_2 \\ \alpha_1^2 & \alpha_2^2 \\ \alpha_1^3 & \alpha_2^3 \\ \alpha_1^4 & \alpha_2^4 \end{pmatrix} \times \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

which leads to a more complicated solution

$$\alpha_{1,2} = \frac{\left(y_1\, y_4 - y_2\, y_3 \pm \sqrt{(y_2\, y_3 - y_1\, y_4)^2 + 4\,(y_2^2 - y_1\, y_3)\,(y_2\, y_4 - y_3^2)}\right)}{2\,(y_1\, y_3 - y_2^2)}$$

- Toy model: consider three states with masses 0.5, 1.0, 1.5 and with the same amplitude



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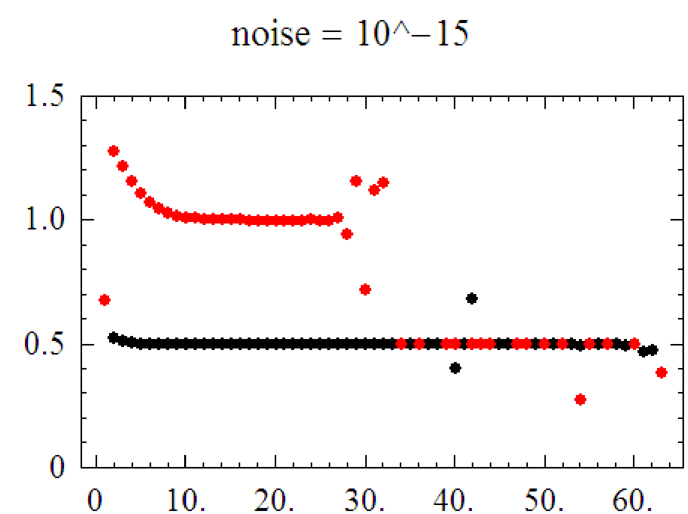
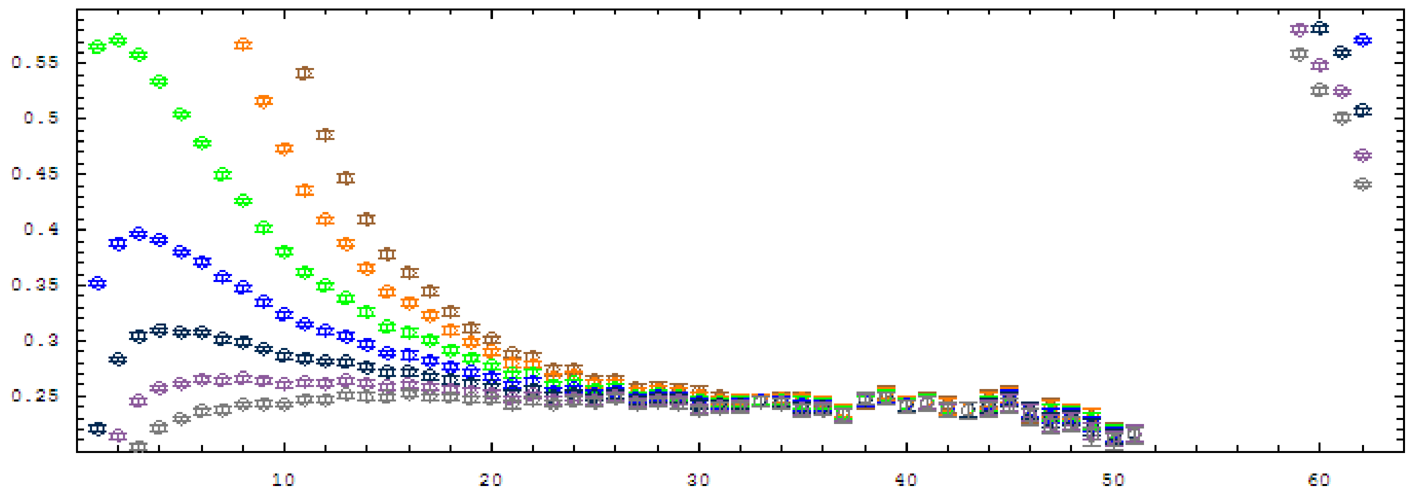
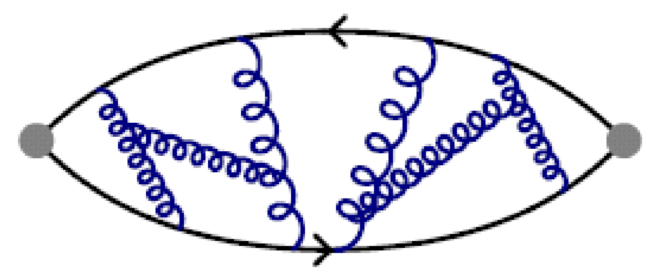


Lattice Data

- Real World: proton case

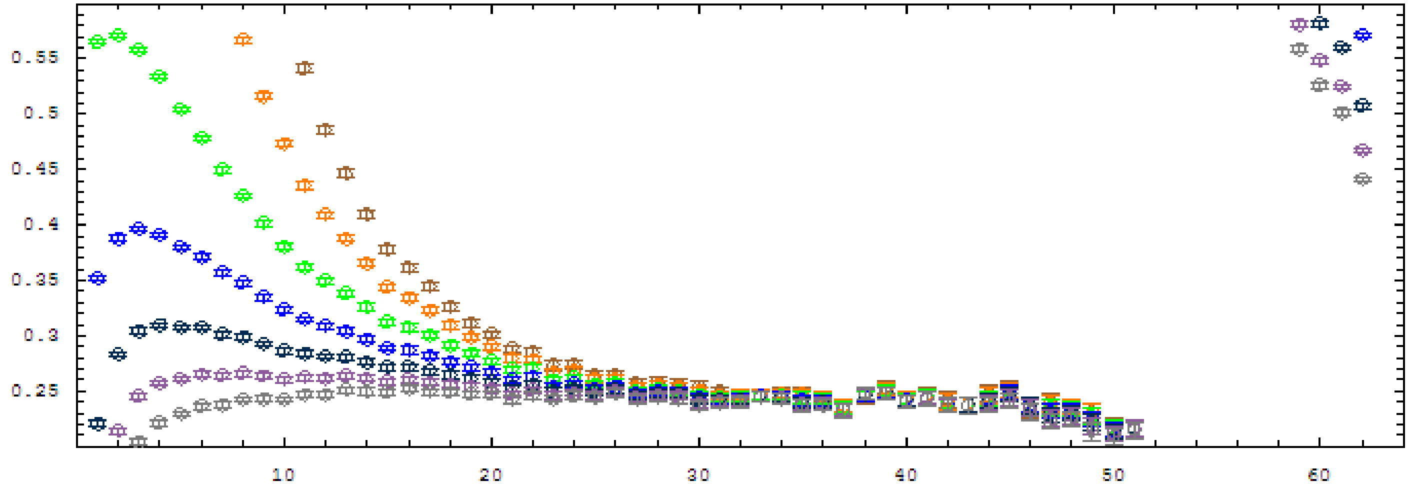


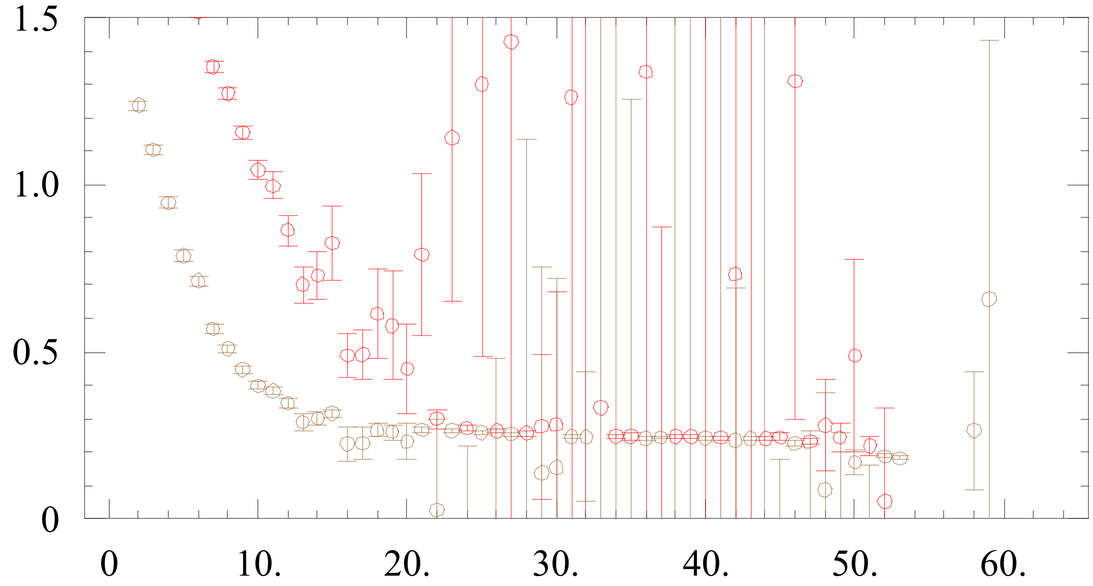
- "Quenched" study on $16^3 \times 64$ **an**isotropic lattice
- Wilson gauge action + nonperturbative clover fermion action
- $a_t^{-1} \approx 6$ GeV and $a_s \approx 0.125$ fm
- 7 effective mass plots from Gaussian smeared-point



Black Box Methods: 1st Excited State

- Real World: proton case





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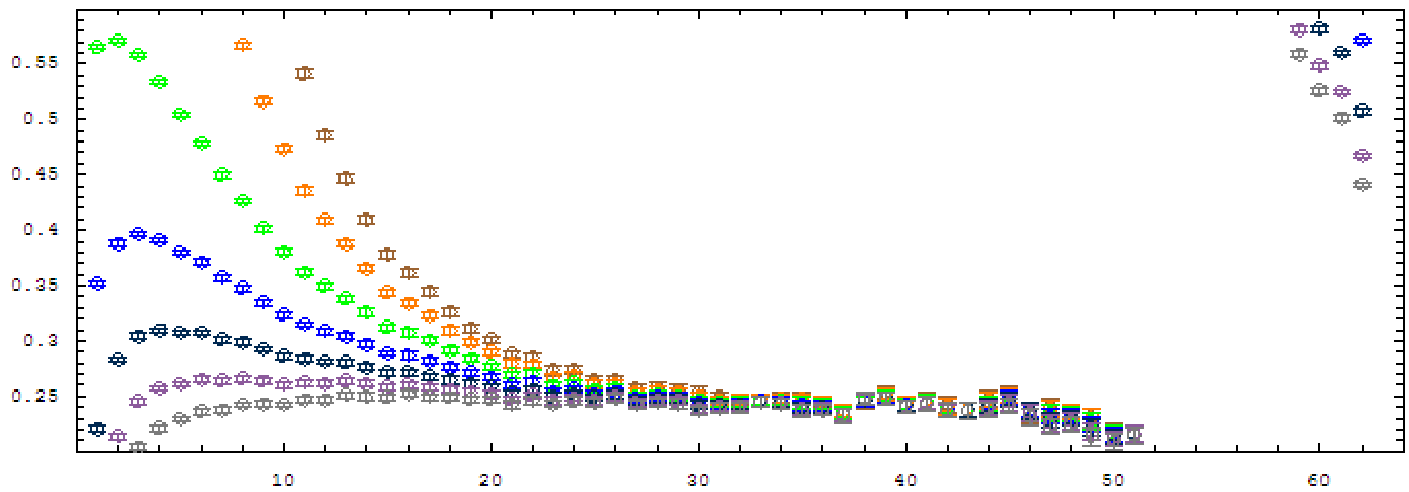
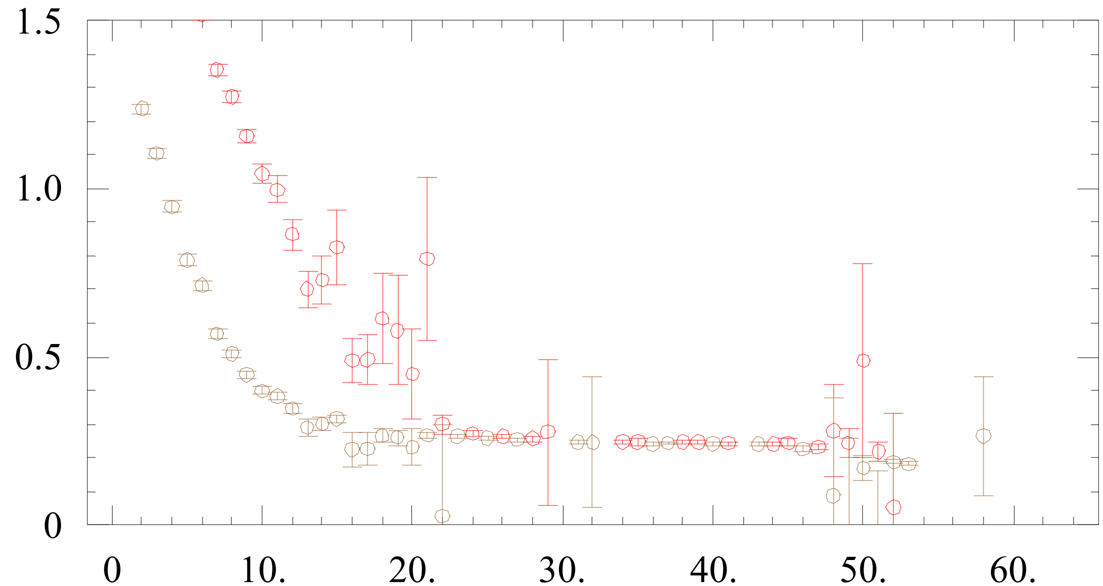
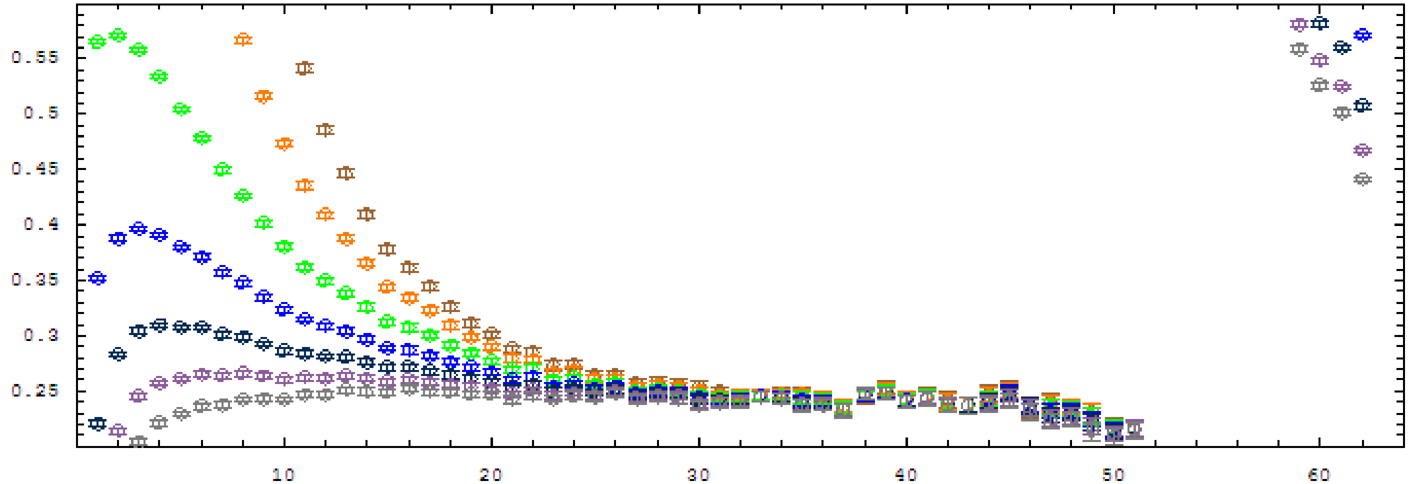


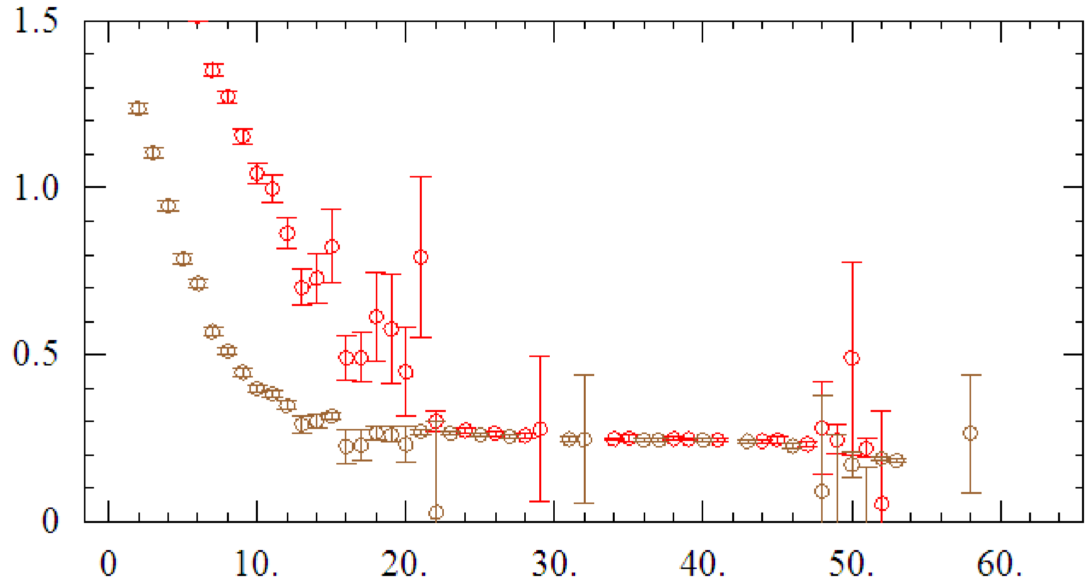
Cut



Black Box Methods: 1st Excited State

- Real World: proton case

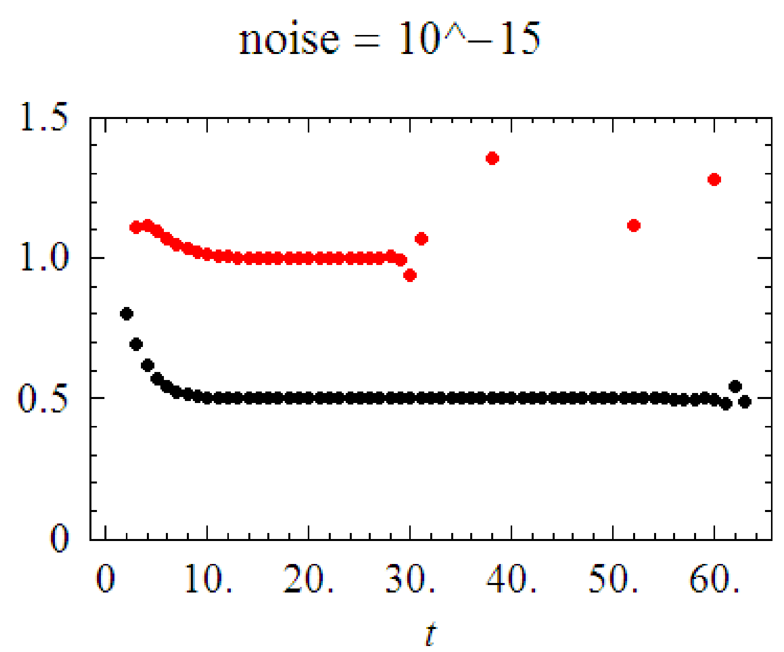




Modified Correlator

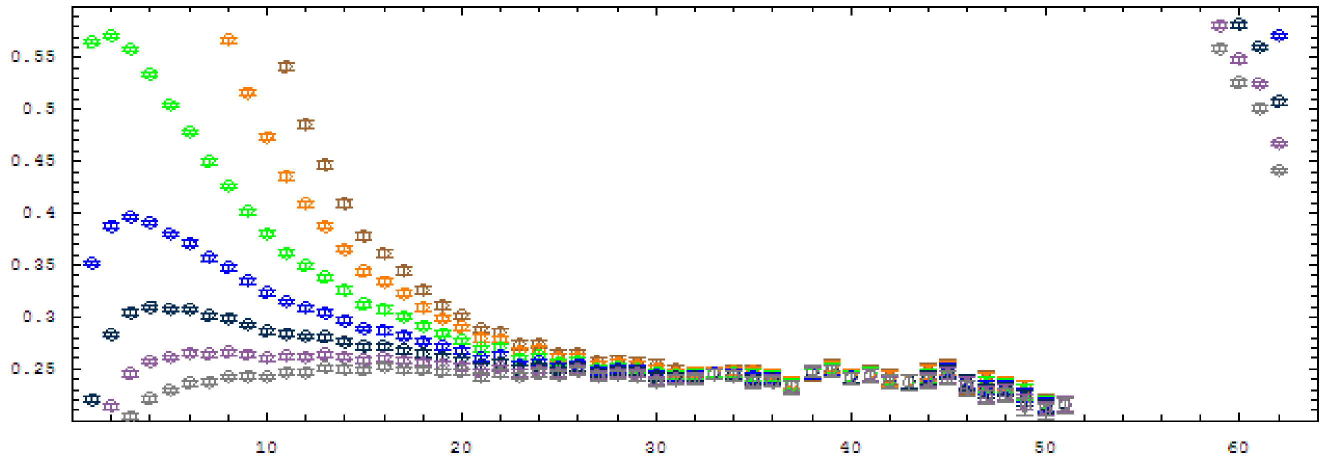
[*D. Gaudagnoli, Phys. Lett. B604, 74 (2004)*]

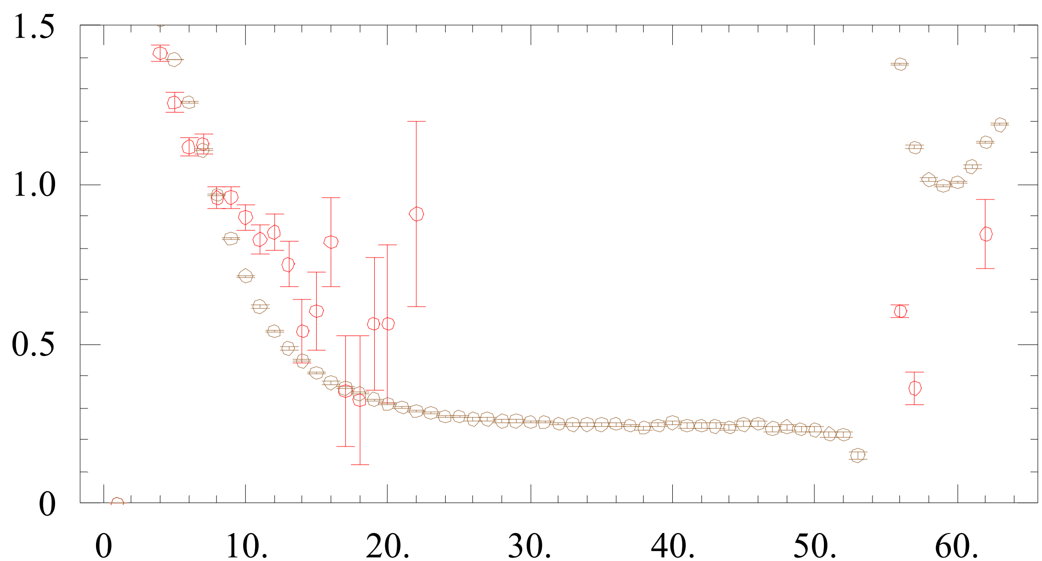
- Instead of using a direct solution, define a modified correlator as $\mathcal{Y}_t = y_{t-1}\, y_{t+1} - y_t^2\ (= \alpha_1 \times \alpha_2)$
- $-\ln(\mathcal{Y}_{t+1}/\mathcal{Y}_t) = E_1 + E_2$
- Toy model: consider three states with masses 0.5, 1.0, 1.5 and with the same amplitude



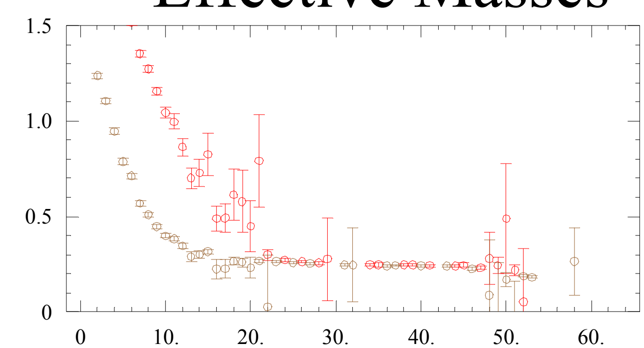
Modified Correlator

- Real World: proton case





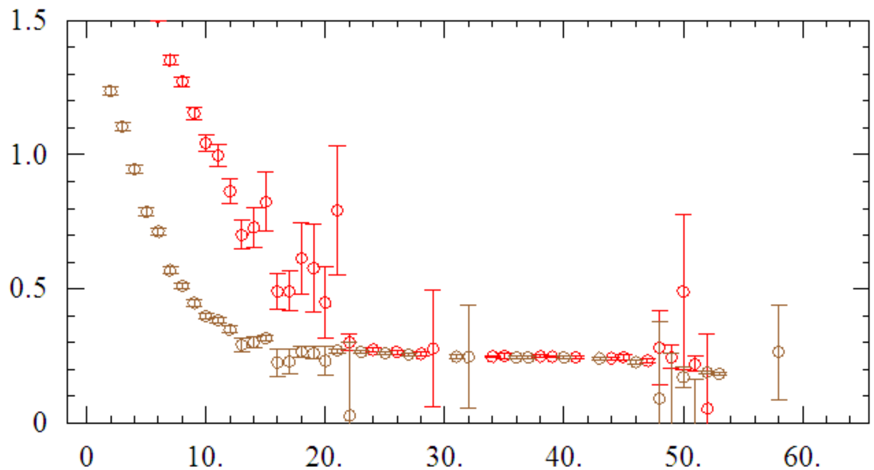
2-State
Effective Masses



N-State Masses vs Modified Correlator

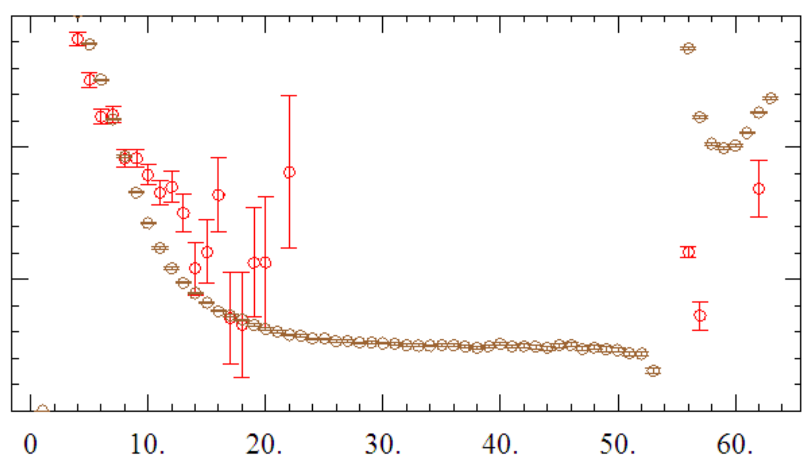
[*George T. Fleming, hep-lat/0403023*]

- *N*-state effective mass method



[*D. Gaudagnoli, Phys. Lett. B604, 74 (2004)*]

- Modified correlator method



Black Box Methods: Recap

- Different point of view from what we normally do in lattice calculations
- Neat idea. Simple algebra excise gives us multiple states from single correlator. Great difficulty to achieve with least-square fits.
- How about 2nd excited state?
- Limitation: Abel's Impossibility Theorem

  algebraic solutions are only possible for $N \leq 5$

Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

- Consider a *K*-state system:
  - Construct a polynomial with coefficients

$$\prod_{k=1}^{K}(\alpha-\alpha_k)=\sum_{i=0}^{K}p_i\alpha^{K-i}$$

  - We know that

$$y_m=-\sum_{k=1}^{K}p_k\, y_{m-k}, \quad m\geq K.$$

  - Solving the system of equations

$$\begin{bmatrix}\bar{y}_K\\ \bar{y}_{K+1}\\ \vdots\\ \bar{y}_{N-1}\end{bmatrix} = -\begin{bmatrix}\bar{y}_0 & \cdots & \bar{y}_{K-1}\\ \bar{y}_1 & \cdots & \bar{y}_K\\ \vdots & \ddots & \vdots\\ \bar{y}_{N-K-1} & \cdots & \bar{y}_{N-2}\end{bmatrix}\begin{bmatrix}p_K\\ p_{K-1}\\ \vdots\\ p_1\end{bmatrix}$$

for ideal data

Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

- Consider a K-state system:
  - Construct a polynomial with coefficients
    $$\prod_{k=1}^{K}(\alpha-\alpha_k)=\sum_{i=0}^{K}p_i\alpha^{K-i}$$
  - We can make the linear prediction
    $$y_n \approx -\sum_{k=1}^{M} p_m y_{n-k} + v_n$$
  - Solving the system now gives

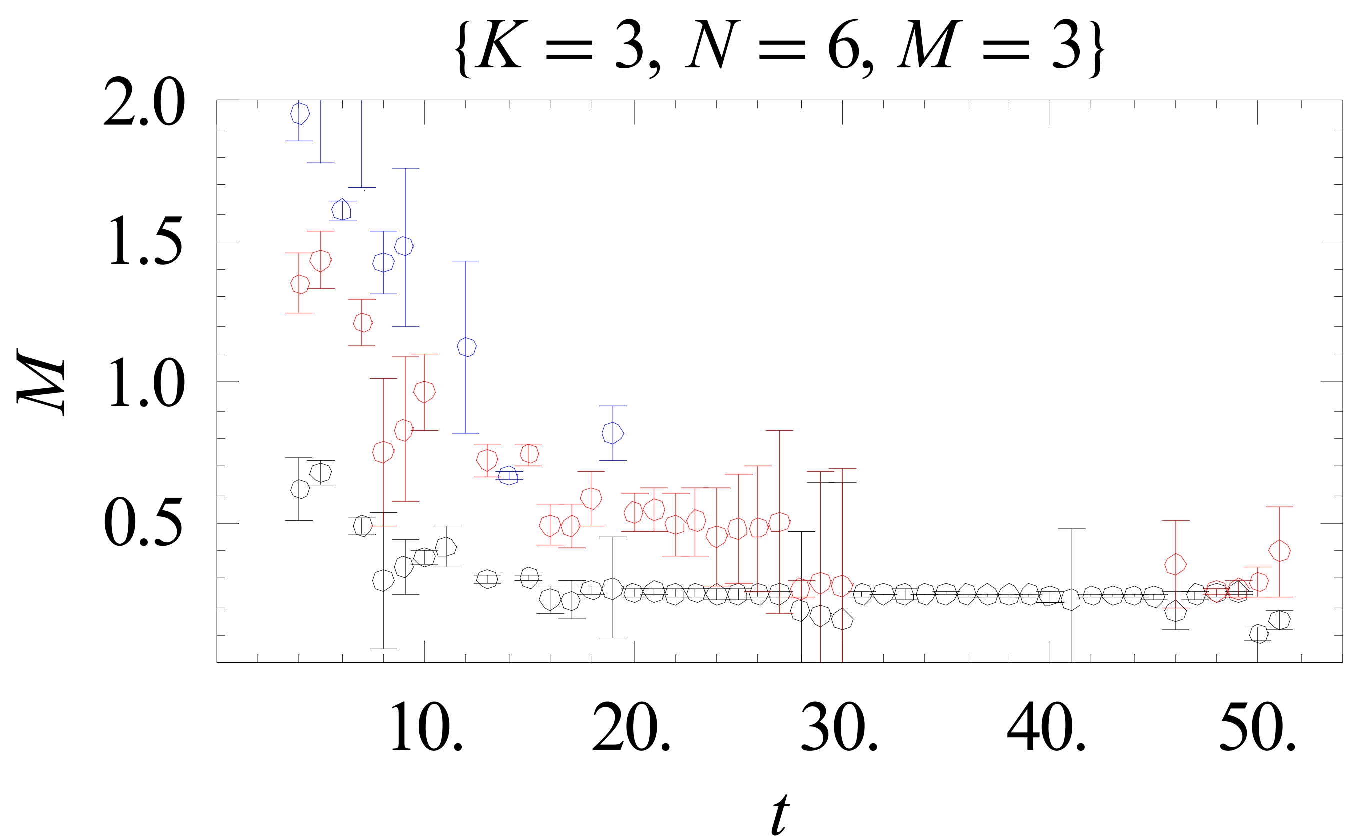
$$\begin{bmatrix} y_M \\ y_{M+1} \\ \vdots \\ y_{N-1} \end{bmatrix} \approx -\begin{bmatrix} y_0 & \cdots & y_{M-1} \\ y_1 & \cdots & y_M \\ \vdots & \ddots & \vdots \\ y_{N-M-1} & \cdots & y_{N-2} \end{bmatrix} \begin{bmatrix} p_M \\ p_{M-1} \\ \vdots \\ p_1 \end{bmatrix}$$

for real data ($N \geq 2M$)

Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

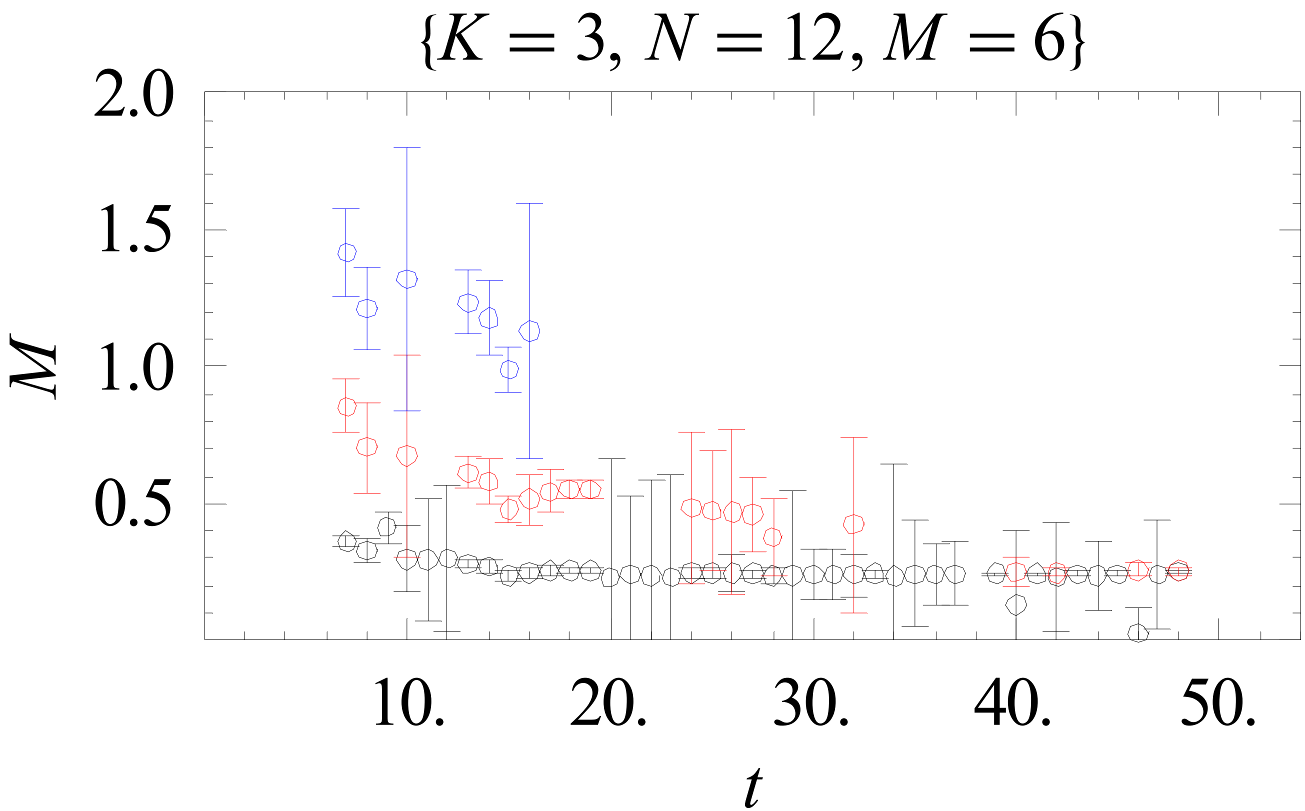
- 3-state results on the smallest Gaussian smeared-point correlator; using the minimal *M*:



Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

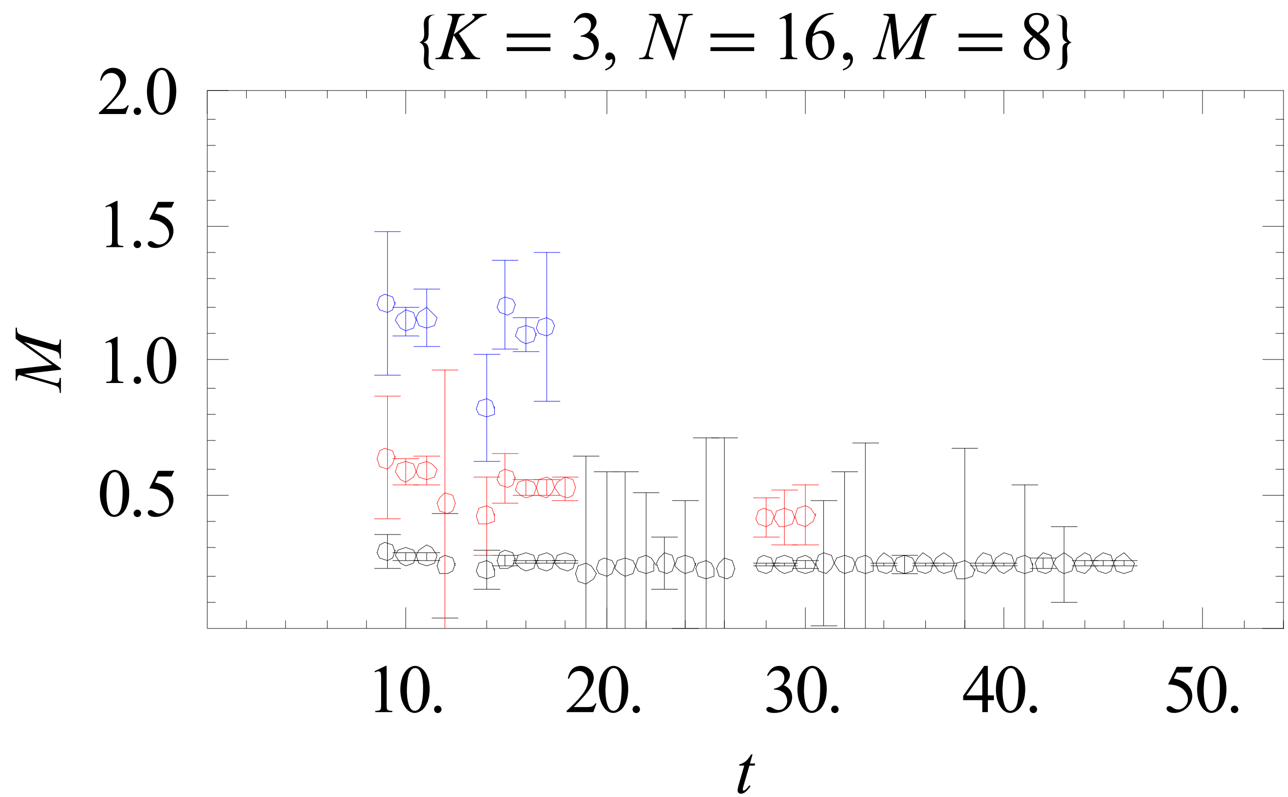
- Increase M. A higher-order polynomial means bad roots can be thrown out without affecting the K roots we want.



Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

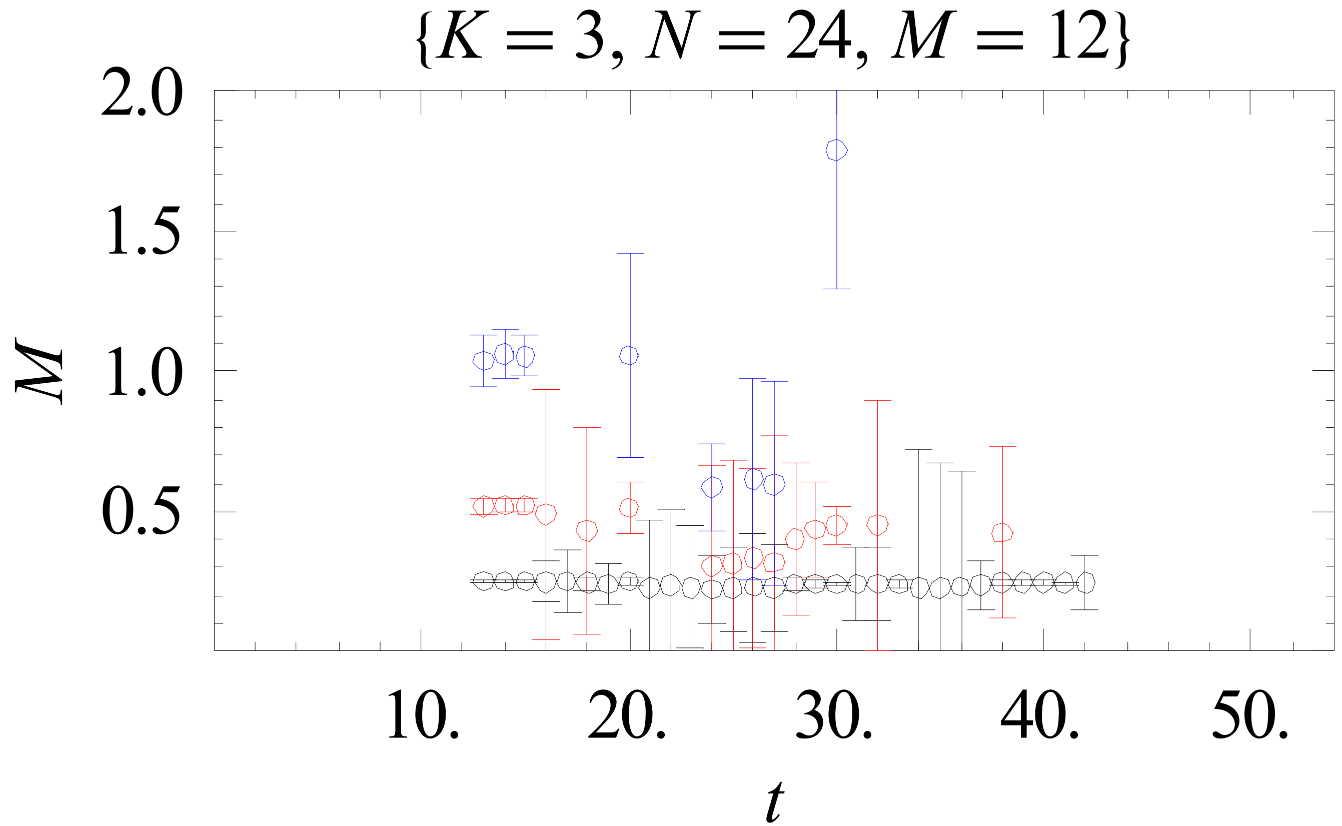
- Still higher *M*...



Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

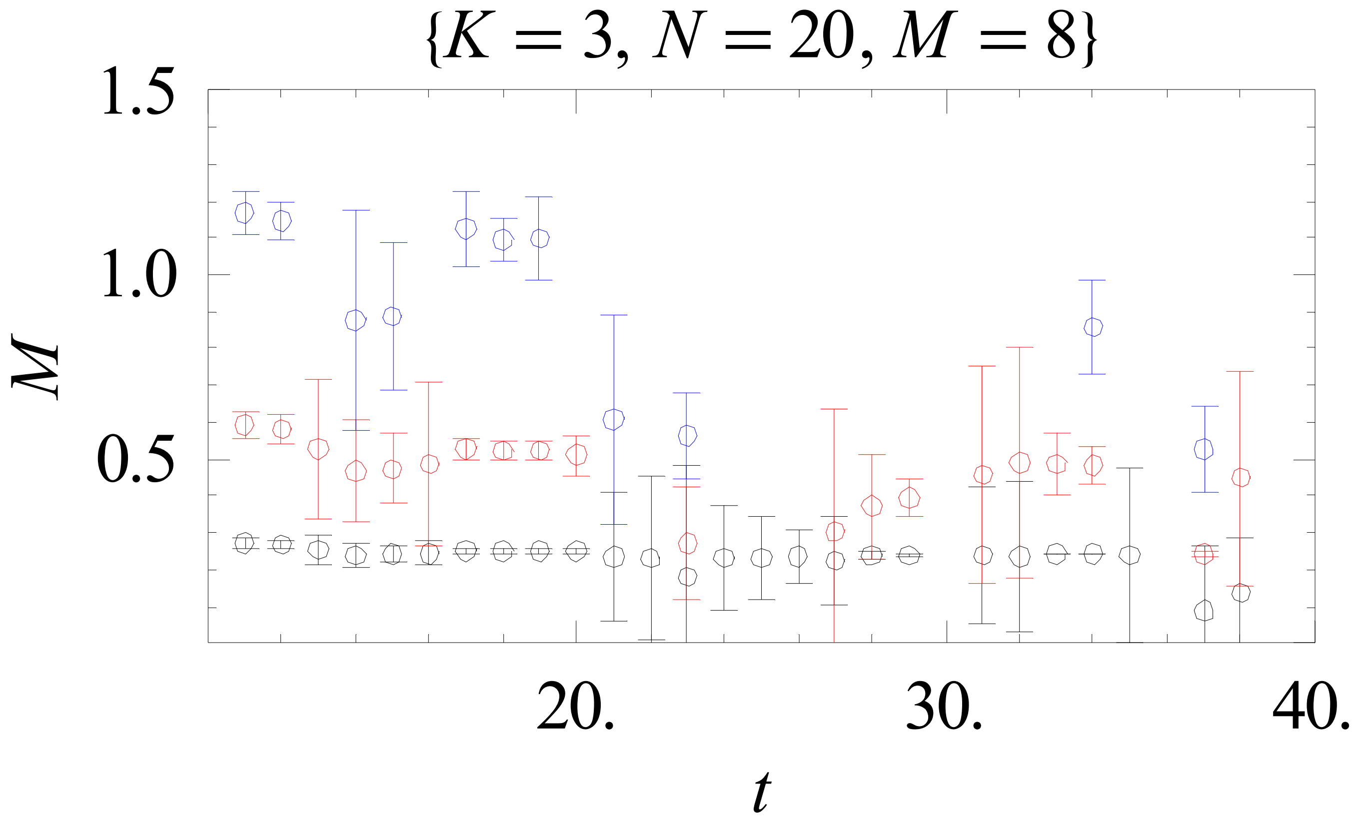
- As N becomes large compared to the total length, not many independent measurements can be made.



Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

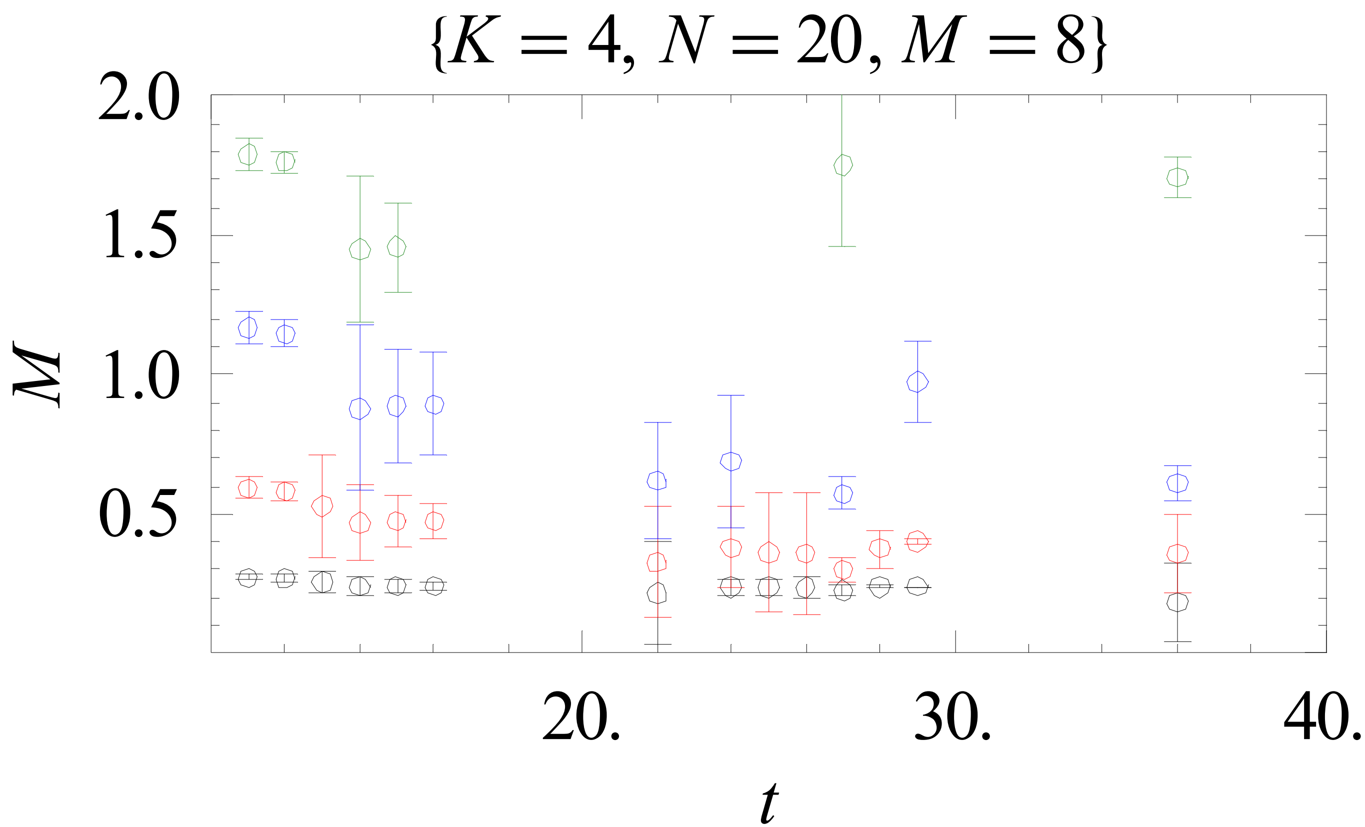
- These settings seem to be a happy medium.



Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

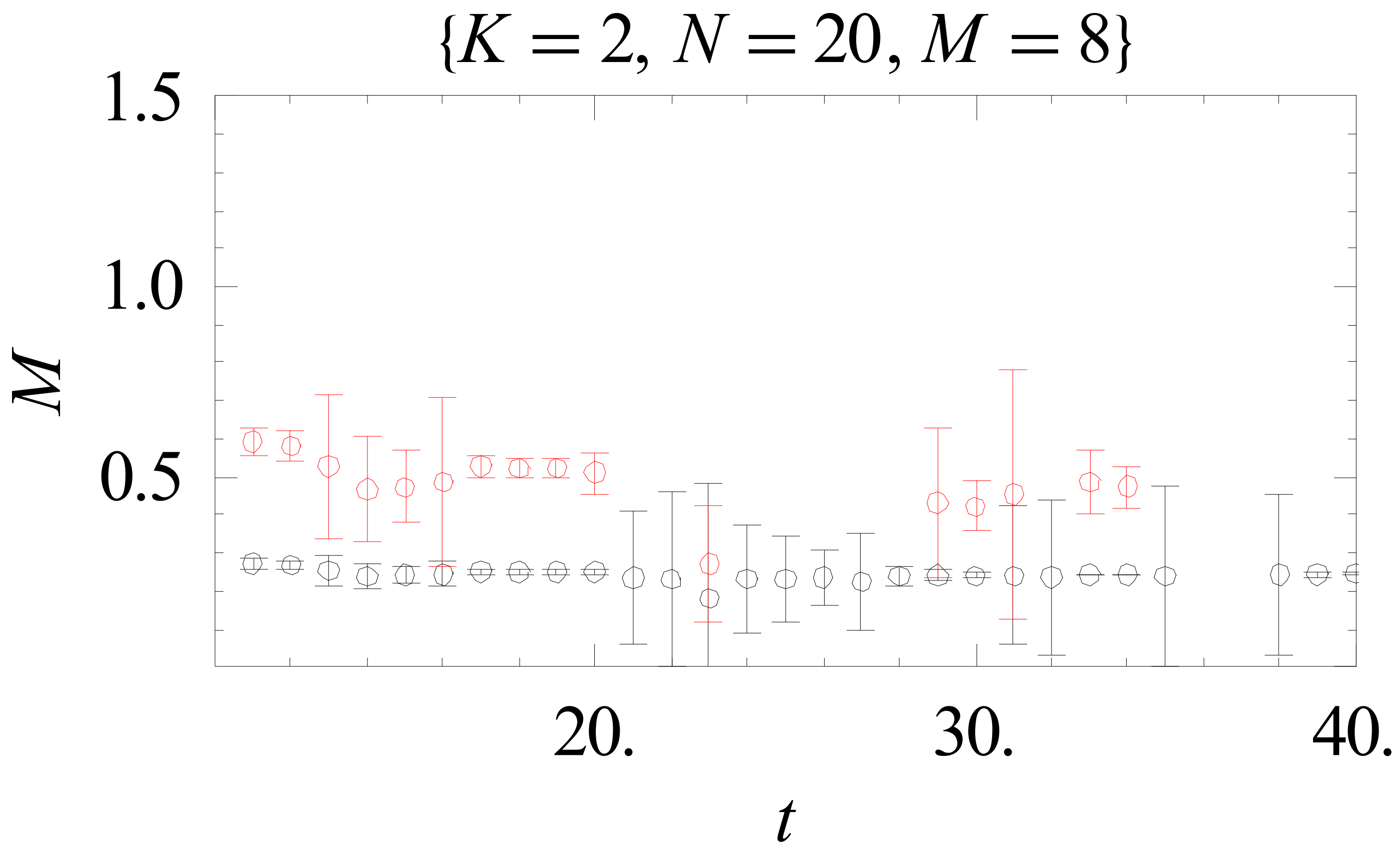
- Can we extract even higher energies?



Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

- Can we get better results if we're only interested in the lowest energies?



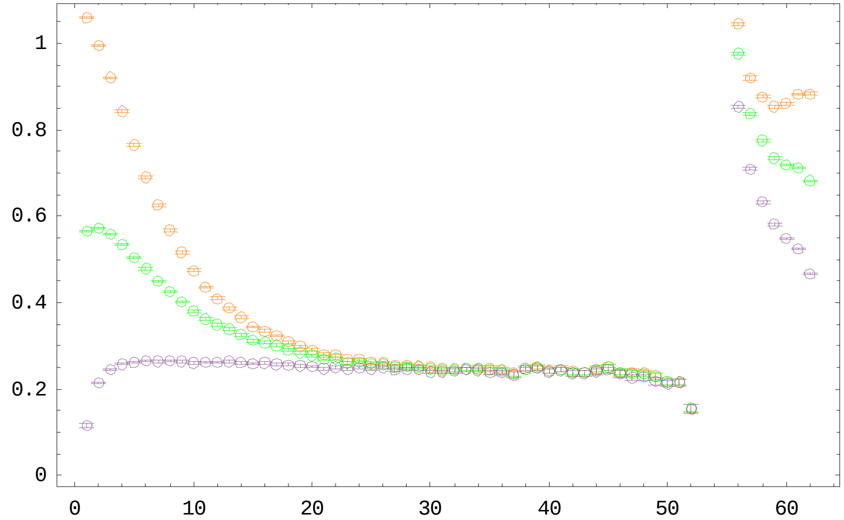
Multiple Least-Squares Fit

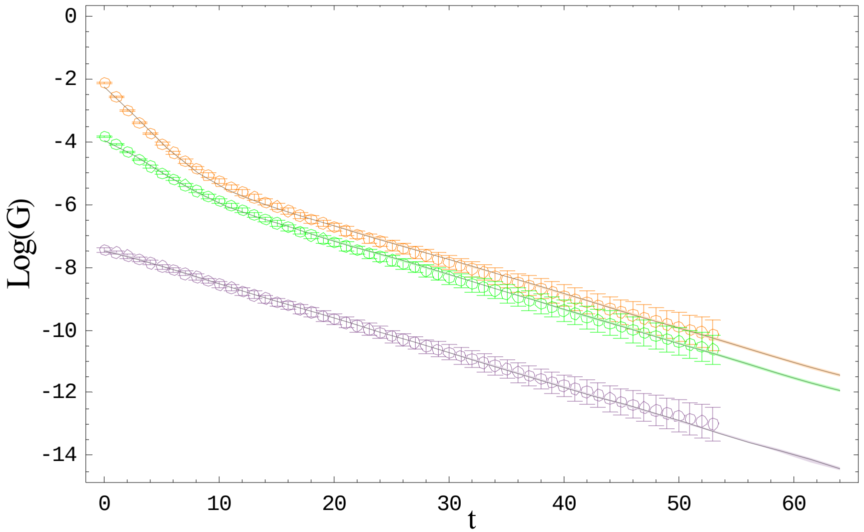
- With multiple smeared correlators, one minimizes the quantity

$$\chi^2 = \sum_s \frac{\left(G_s(t) - \sum_n a_n e^{-E_n t}\right)^2}{\sigma_s^2(t)}$$

  to extract E_n.

- Example:





- To extract n states, one at needs at least n “distinguished” input correlators

Variational Method

- Generalized eigenvalue problem:

  [*C. Michael, Nucl. Phys. B 259, 58 (1985)*]

  [*M. Lüscher and U. Wolff, Nucl. Phys. B 339, 222 (1990)*]

  - Construct the matrix

    $$C_{i\ j}(t) = \langle 0 \mid \mathcal{O}_i(t)^\dagger \mathcal{O}_j(0) \mid 0 \rangle$$

  - Solve for the generalized eigensystem of

    $$C(t_0)^{-1/2} C(t) C(t_0)^{-1/2} \psi = \lambda(t, t_0) \psi$$

  with eigenvalues

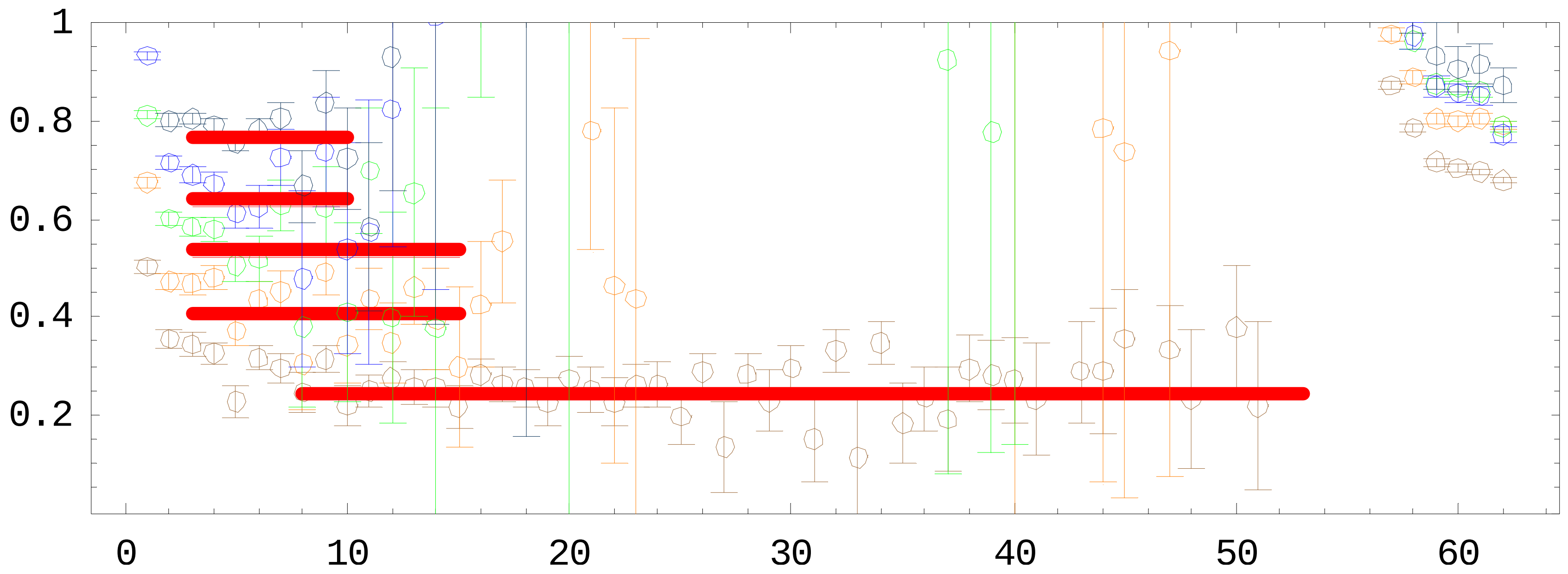
  $$\lambda_n(t, t_0) = e^{-(t-t_0)E_n}$$

  and the original correlator matrix can be approximated by

  $$C_{ij} = \sum_{n=1}^{r} v_i^{n*} v_j^n e^{-tE_n}$$

Variational Method

- Example: 5×5 smeared-smeared correlator matrices
- Solve eigensystem for individual λ_n
- Fit them individually with exponential form (red bars)
- Plotted along with effective masses



Three-Point Correlators

- The form factors are buried in the amplitudes

$$
\begin{aligned}
&\Gamma^{(3),T}_{\mu,AB}(t_i,t,t_f,\vec{p}_i,\vec{p}_f) \\
&= a^3 \sum_n \sum_{n'} \frac{1}{Z_j} \frac{Z_{n',B}(p_f) Z_{n,A}(p_i)}{4E'_n(\vec{p}_f)E_n(\vec{p}_i)} e^{-(t_f-t)E'_n(\vec{p}_f)} e^{-(t-t_i)E_n(\vec{p}_i)} \\
&\times \sum_{s,s'} T_{\alpha\beta} u_{n'}(\vec{p}_f,s')_\beta \langle N_{n'}(\vec{p}_f,s') | j_\mu(0) | N_n(\vec{p}_i,s)\rangle \overline{u}_n(\vec{p}_i,s)_\alpha
\end{aligned}
$$

- Brute force approach: multi-exponential fits to two-point correlators to extract overlap factors *Z* and energies *E*
- Modified variational method approach: use the eigensystem solved from the two-pt correlator as inputs; works for the diagonal elements.
  - Any special trick for the non-diagonal elements?

Summary

- A lot of interesting physics involves excited states, but they're difficult to handle.
- NMR-inspired methods provide an interesting alternate point of view for looking at the lattice QCD spectroscopy
- Remarkable! Multiple excited states can be extracted from a single correlator
- Extends further to multiple correlators to be compatible with other approaches, such as variational method