



Lattice QCD

Beyond Ground States

Huey-Wen Lin

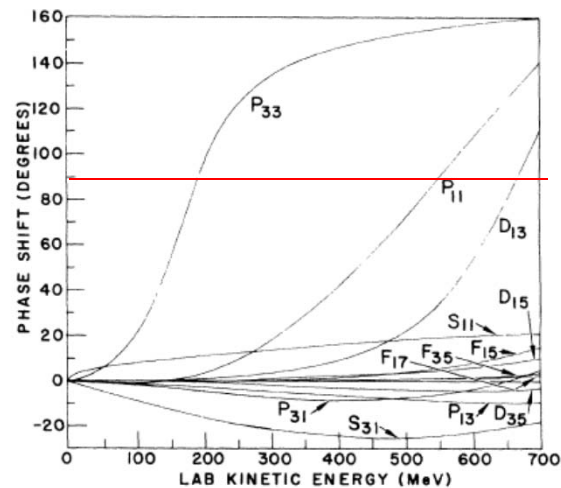


Outline

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

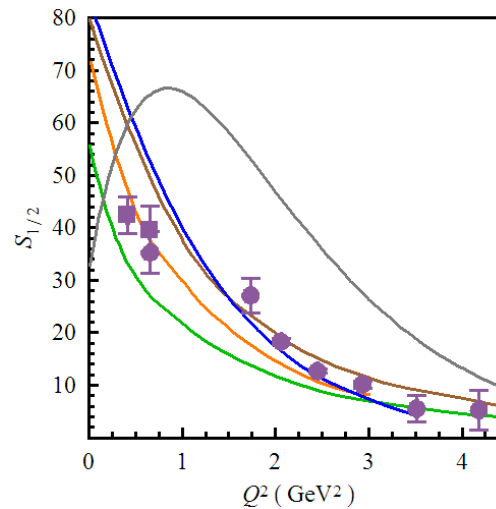
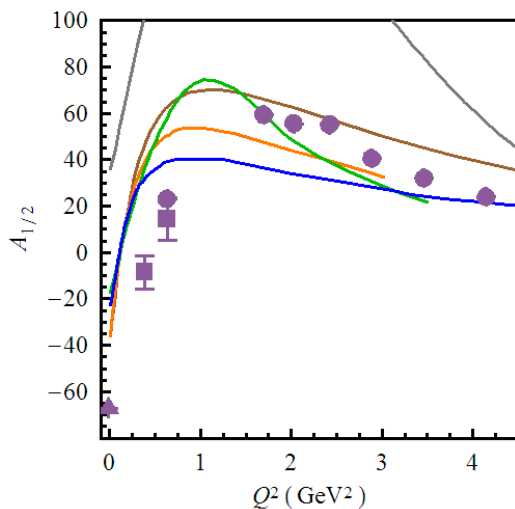
Example: Roper (P_{11}) Spectrum

- ◆ 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)

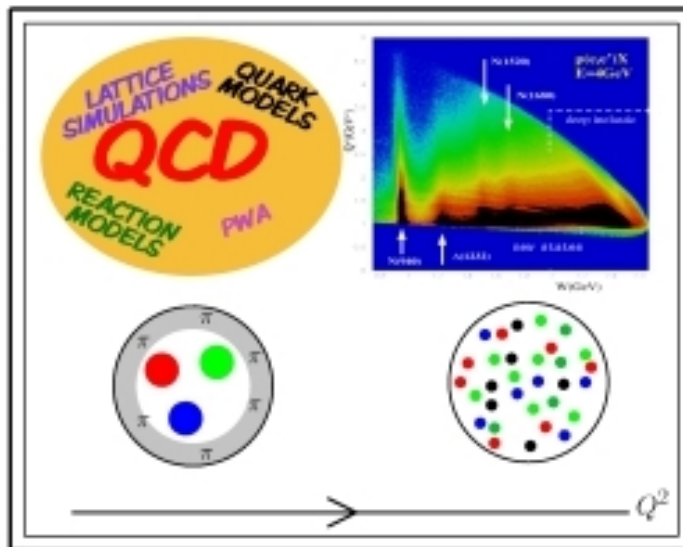


Helicity amplitudes are measured (in 10^{-3} GeV^{-1/2} units)

EBAC

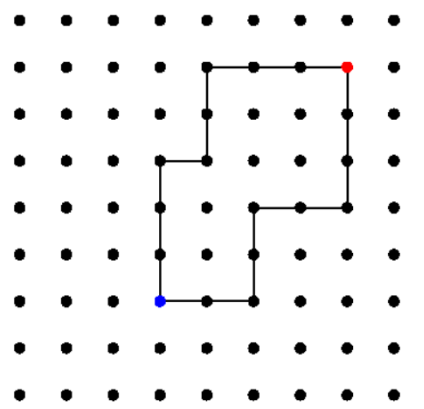
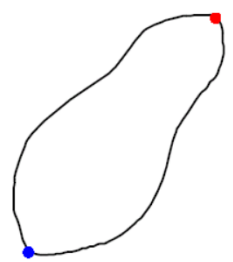
◆ Excited Baryon Analysis Center (EBAC)

“an international effort which incorporates researchers from institutes around the world”



Lattice QCD

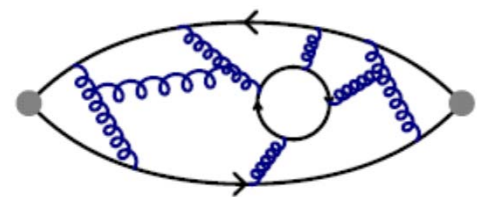
- Physical observables are calculated from the path integral
- $$\langle 0 | O(\bar{\psi}, \psi, A) | 0 \rangle = \frac{1}{Z} \int [dA][d\bar{\psi}][d\psi] O(\bar{\psi}, \psi, A) e^{i \int d^4x \mathcal{L}^{\text{QCD}}(\bar{\psi}, \psi, A)}$$
- Lattice QCD is a discrete version of continuum QCD theory



- 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

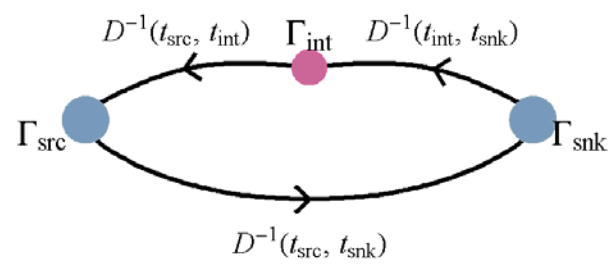
Lattice QCD: Observables

◆ Two-point Green function
 e.g. Spectroscopy



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

◆ Three-point Green function
 e.g. Form factors, Structure functions, ...

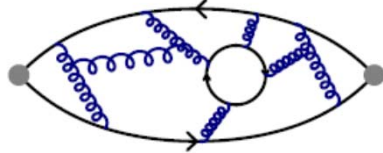


$$\sum_{\alpha, \beta} \Gamma^{\alpha, \beta} \langle J(X_{\text{snk}}) O(X_{\text{int}}) J(X_{\text{src}}) \rangle_{\alpha, \beta}$$

Lattice QCD: Observables

Two-point Green function

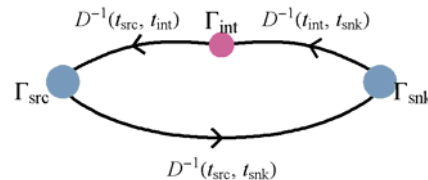
e.g. Spectroscopy



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

Three-point Green function

e.g. Form factors. Structure functions, ...



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

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

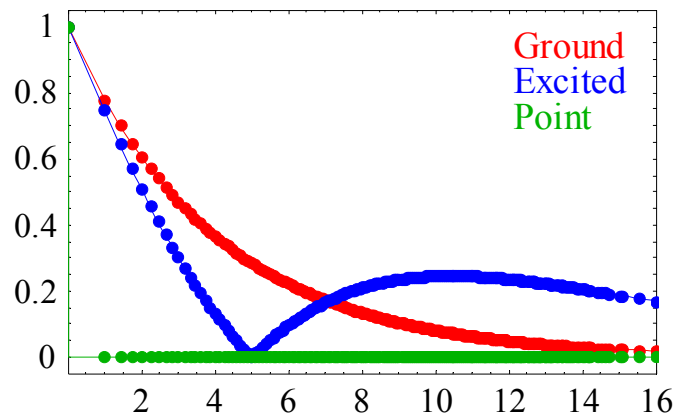
Lattice QCD: Improvements

- ◆ 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



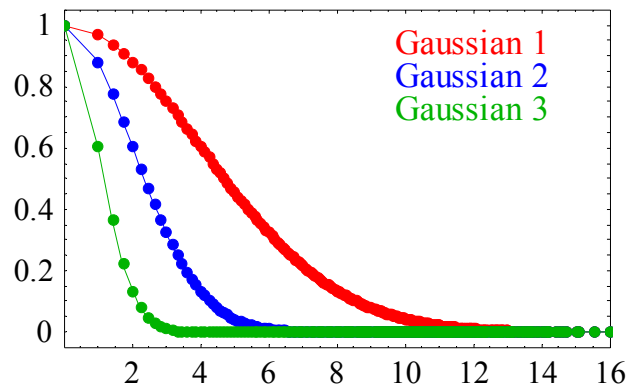
Lattice QCD: Improvements

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

- ◆ Example:

Gaussian function



Only Interested in Ground State?

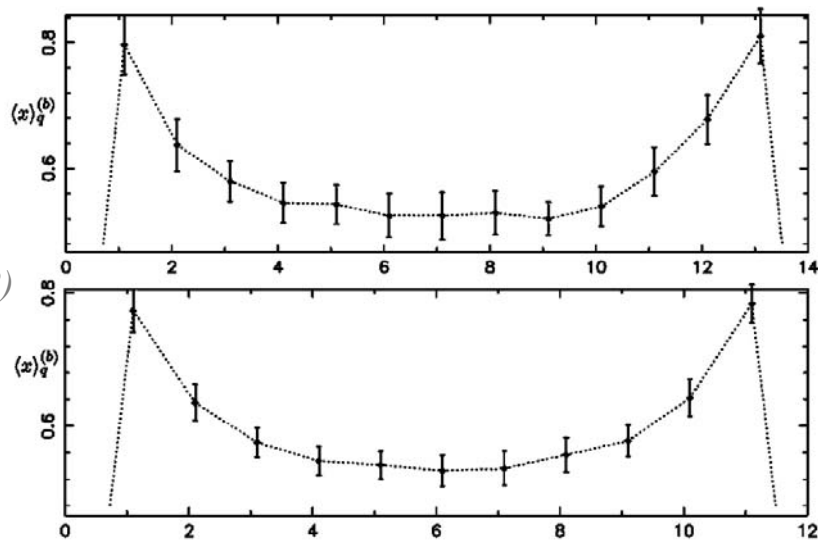
- ◆ Larger t solution does not always work well with three-point correlators

- ◆ Example:

Quark helicity distribution
LHPC & SESAM

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

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



- ◆ 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

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

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” $M_{\text{eff}} = \ln(y_{n+1}/y_n)$

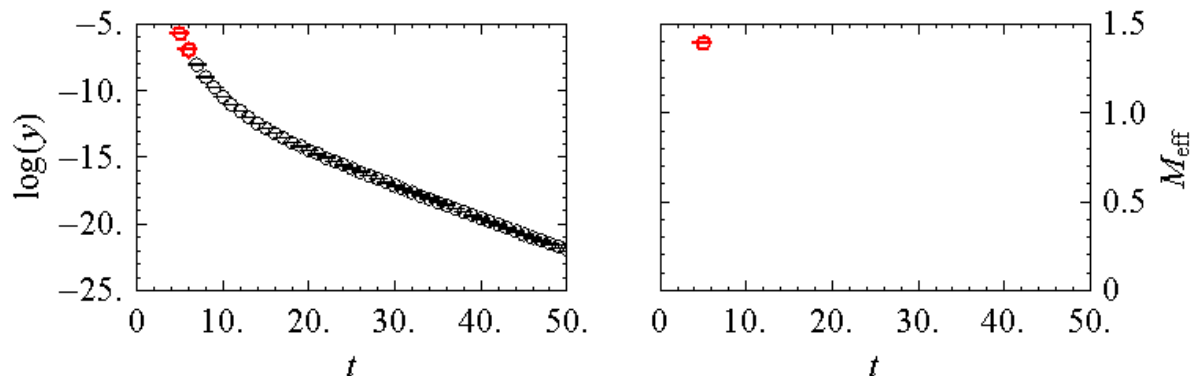
Black Box Methods: Effective Mass

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Black Box Methods: 1st Excited State

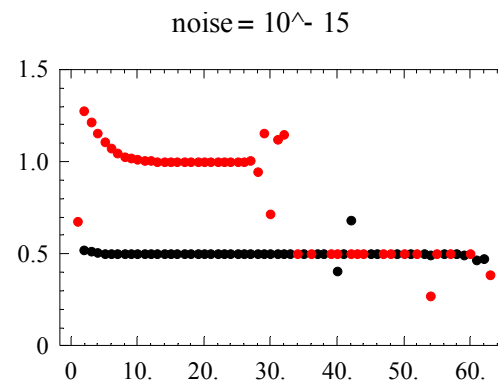
Extracting two states ($K = 2$) case,

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

which leads to a more complicated solution

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

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



Black Box Methods: 1st Excited State

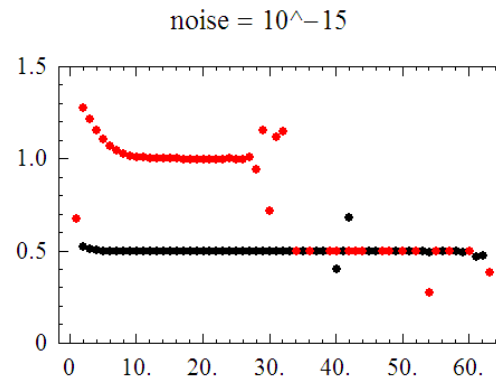
Extracting two states ($K = 2$) case,

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

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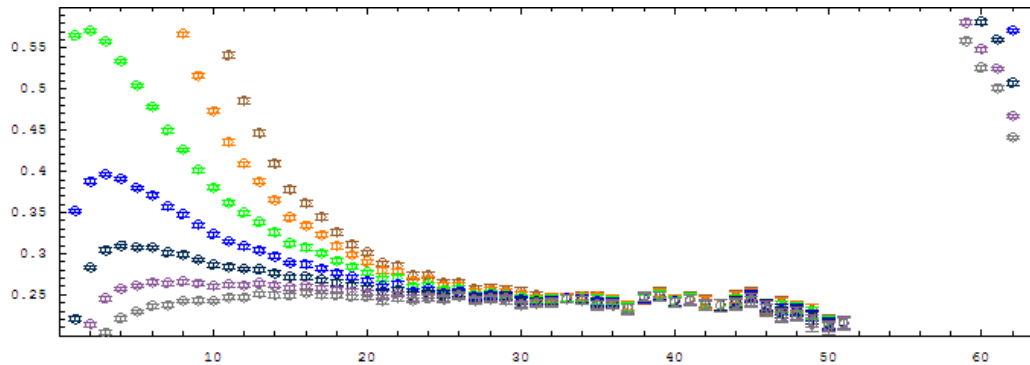
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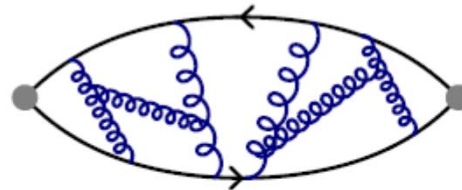


Lattice Data

◆ Real World: proton case

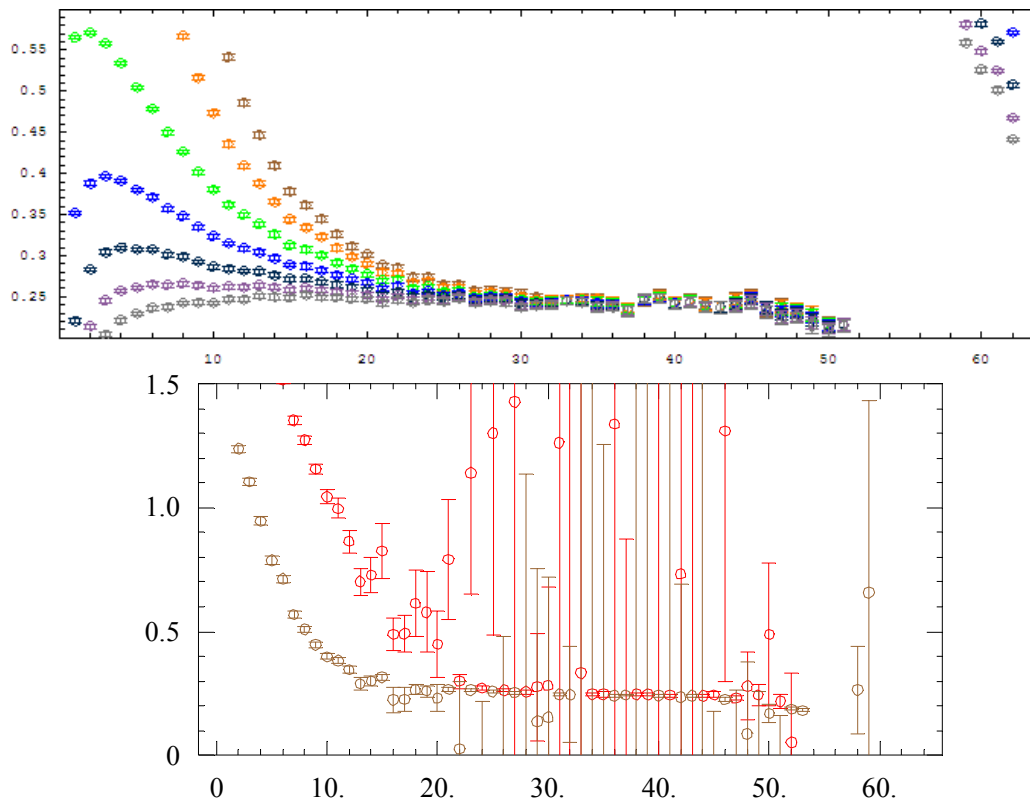


- ◆ “Quenched” study on $16^3 \times 64$ **anisotropic** lattice
- ◆ Wilson gauge action + nonperturbative clover fermion action
- ◆ $a_t^{-1} \approx 6$ GeV and $a_s \approx 0.125$ fm
- ◆ 7 effective mass plots from Gaussian smeared-point



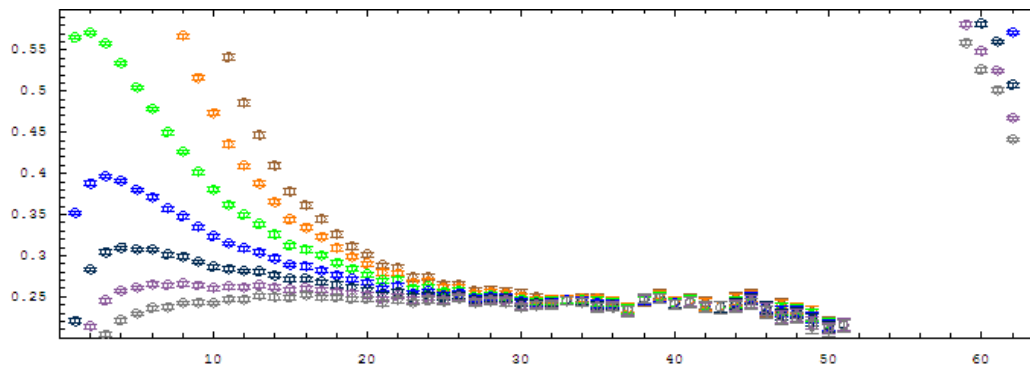
Black Box Methods: 1st Excited State

◆ Real World: proton case

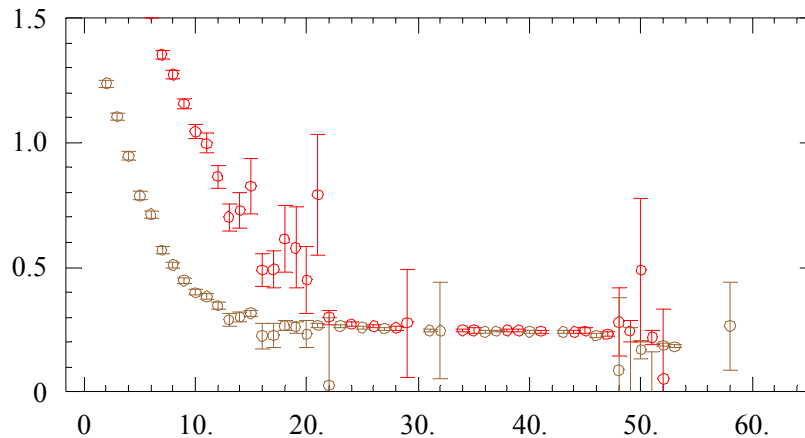


Black Box Methods: 1st Excited State

◆ Real World: proton case

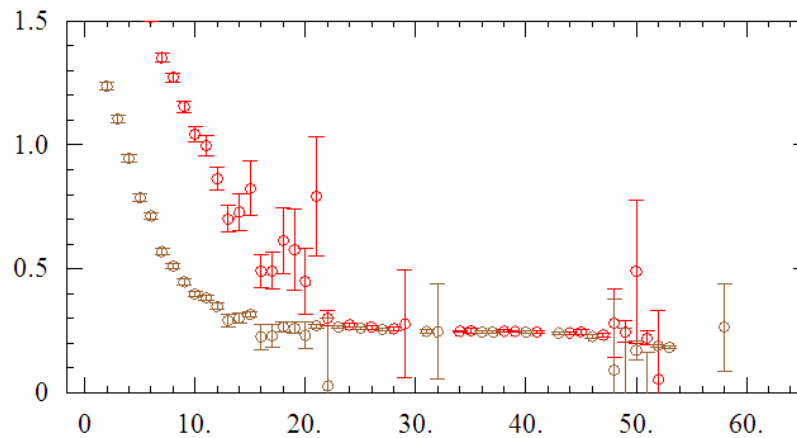
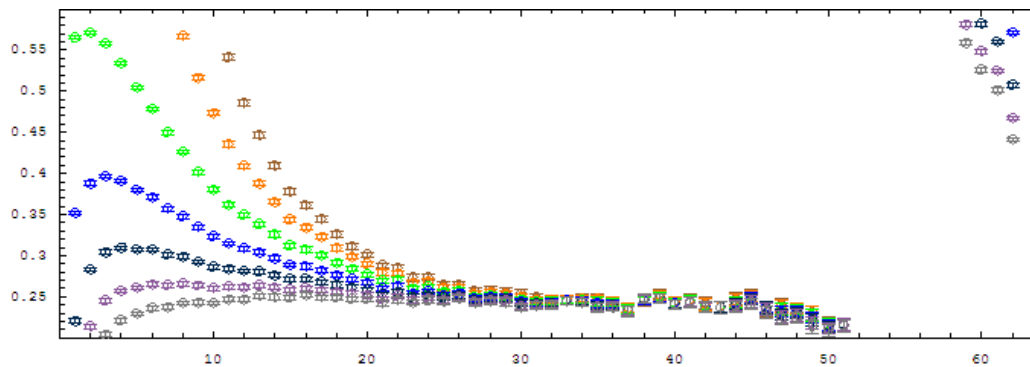


Cut



Black Box Methods: 1st Excited State

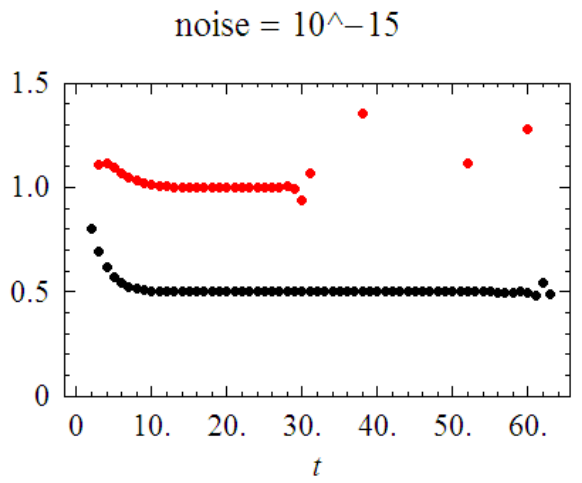
◆ Real World: proton case



Modified Correlator

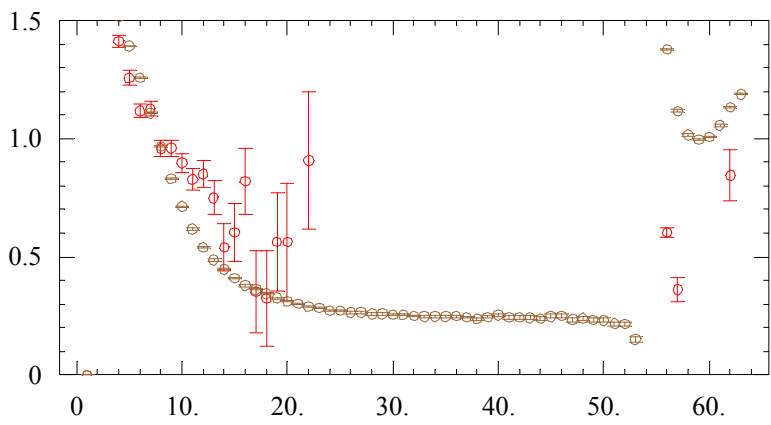
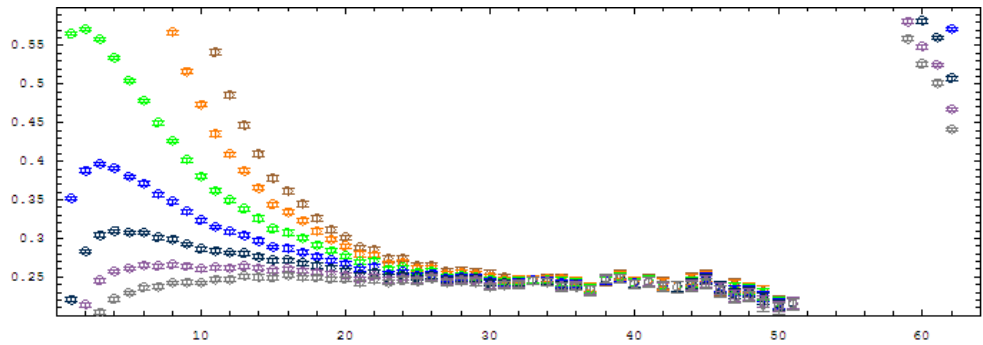
[D. Gaudagnoli, Phys. Lett. B604, 74 (2004)]

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

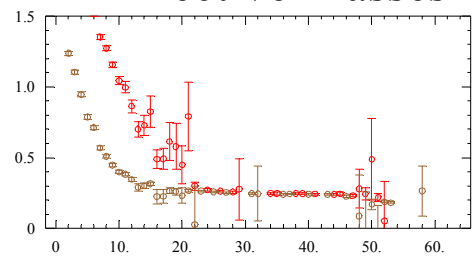


Modified Correlator

◆ Real World: proton case



2-State Effective Masses



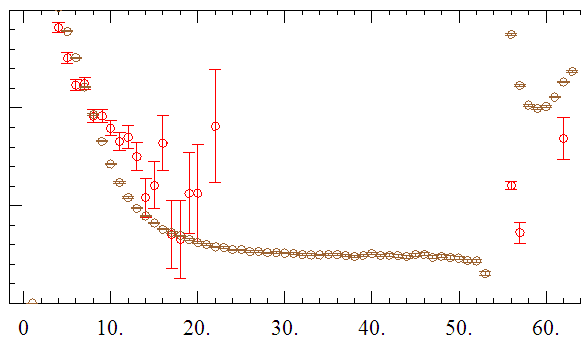
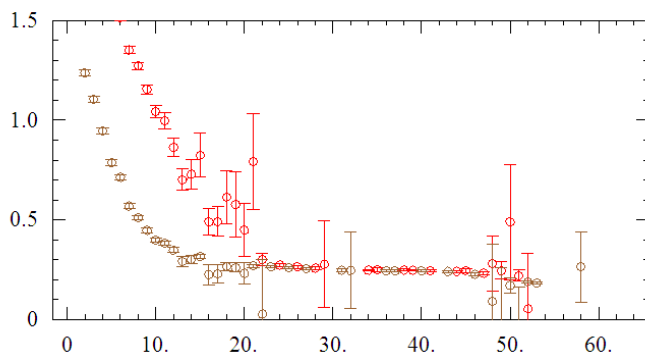
N -State Masses vs Modified Correlator

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

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

◆ N -state effective mass method

◆ 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

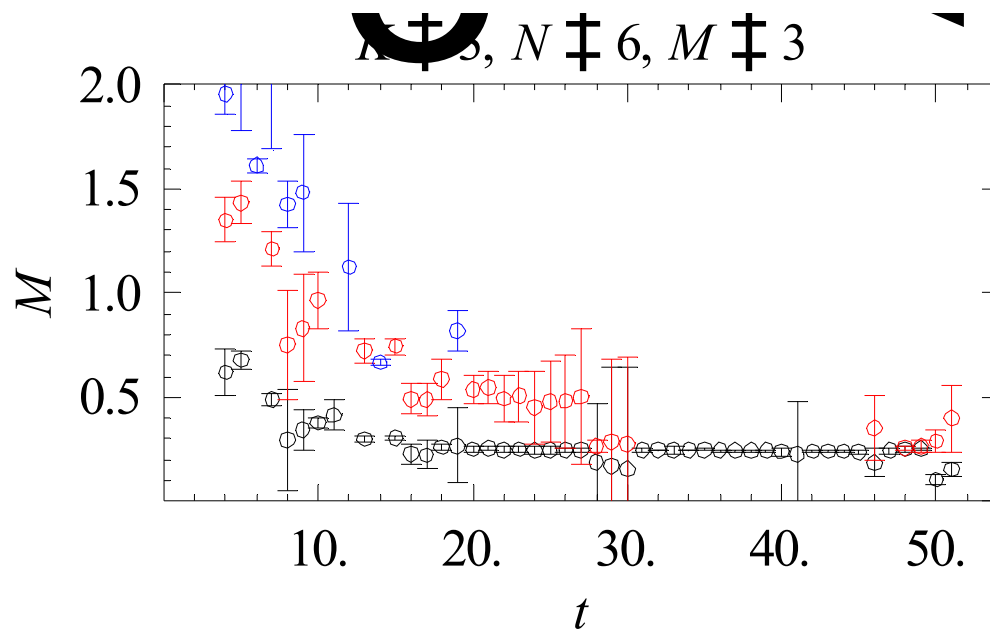
$$\begin{bmatrix} y_M \\ y_{M+1} \\ \vdots \\ y_{N-1} \end{bmatrix} \approx - \begin{bmatrix} y_0 & \dots & y_{M-1} \\ y_1 & \dots & y_M \\ \vdots & \ddots & \vdots \\ y_{N-M-1} & \dots & y_{N-2} \end{bmatrix} \begin{bmatrix} p_M \\ p_{M-1} \\ \vdots \\ p_1 \end{bmatrix}$$

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

Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

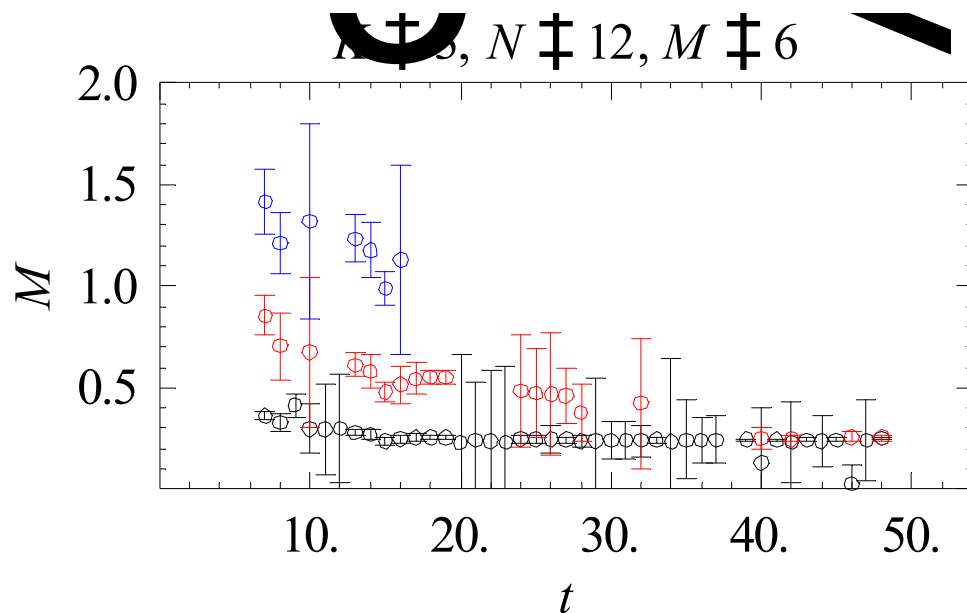
- ◆ 3-state results on the smallest Gaussian smeared-point correlator; using the minimal M :



Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

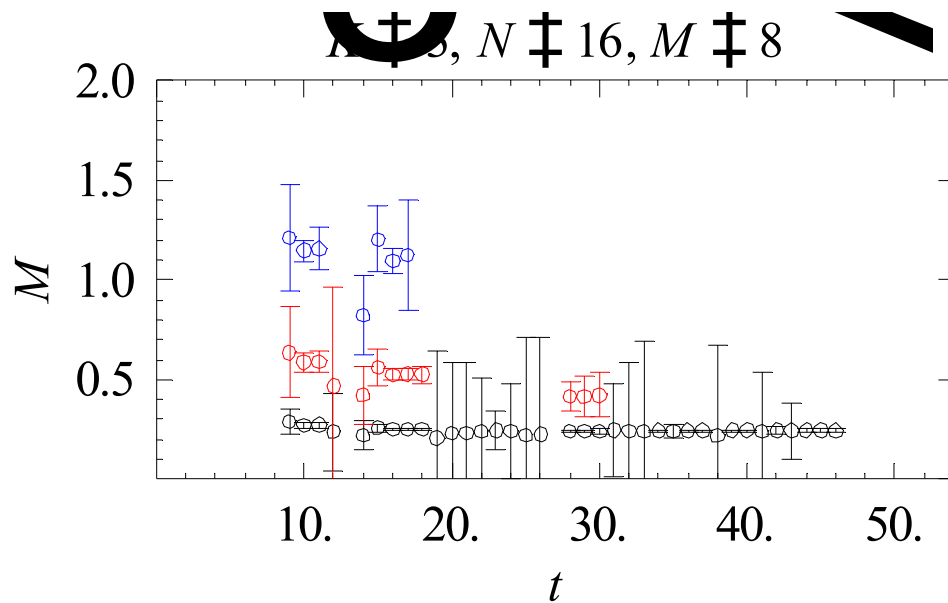
- ◆ Increase M . A higher-order polynomial means bad roots can be thrown out without affecting the K roots we want.



Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

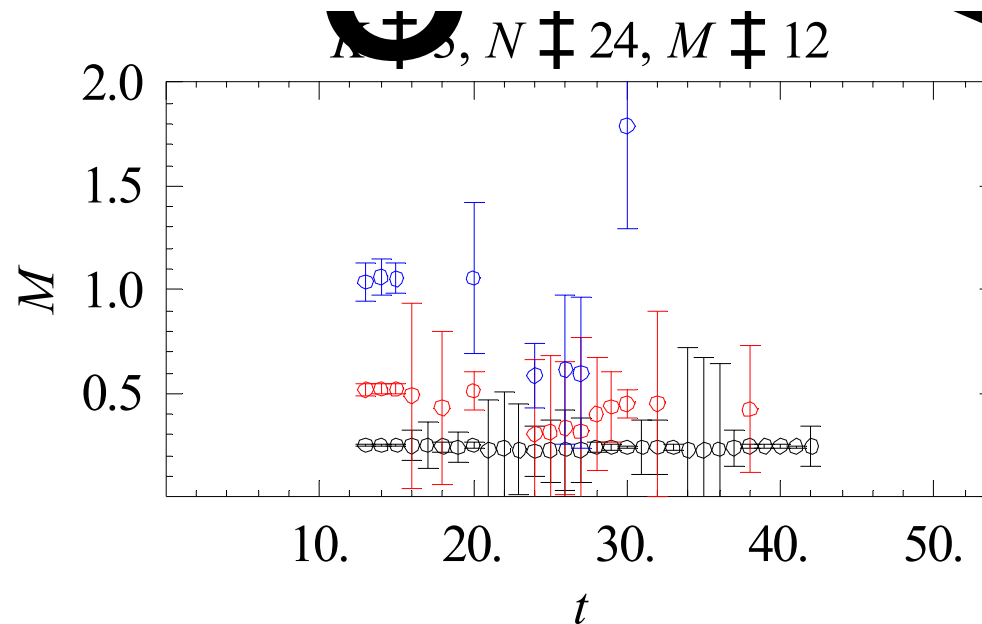
- ◆ Still higher M ...



Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

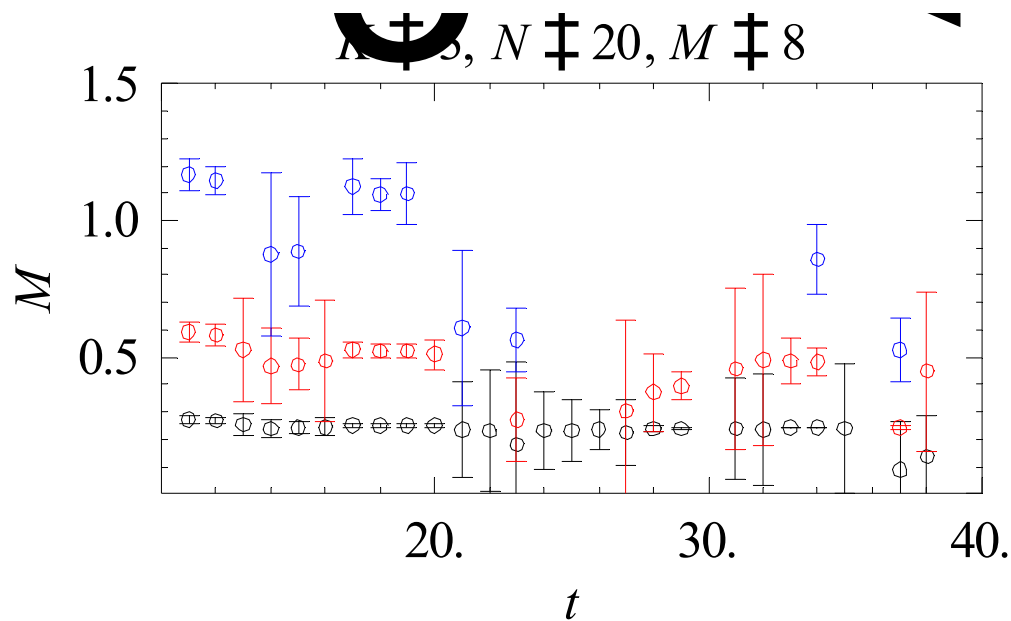
- As N becomes large compared to the total length, not many independent measurements can be made.



Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

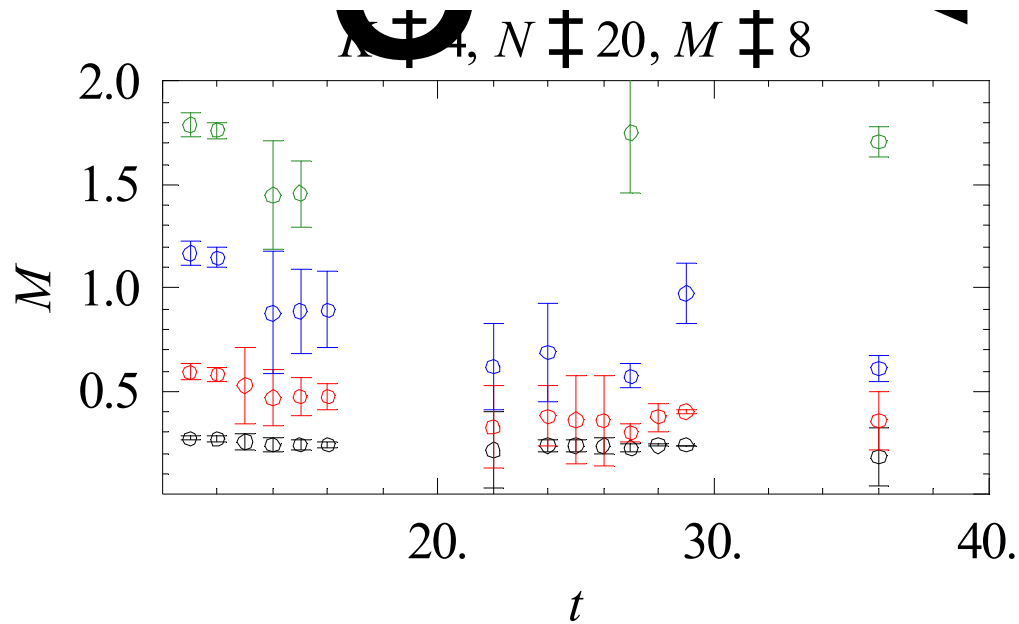
- ◆ These settings seem to be a happy medium.



Black Box Method: Linear Prediction

In collaboration with *Saul D. Cohen*

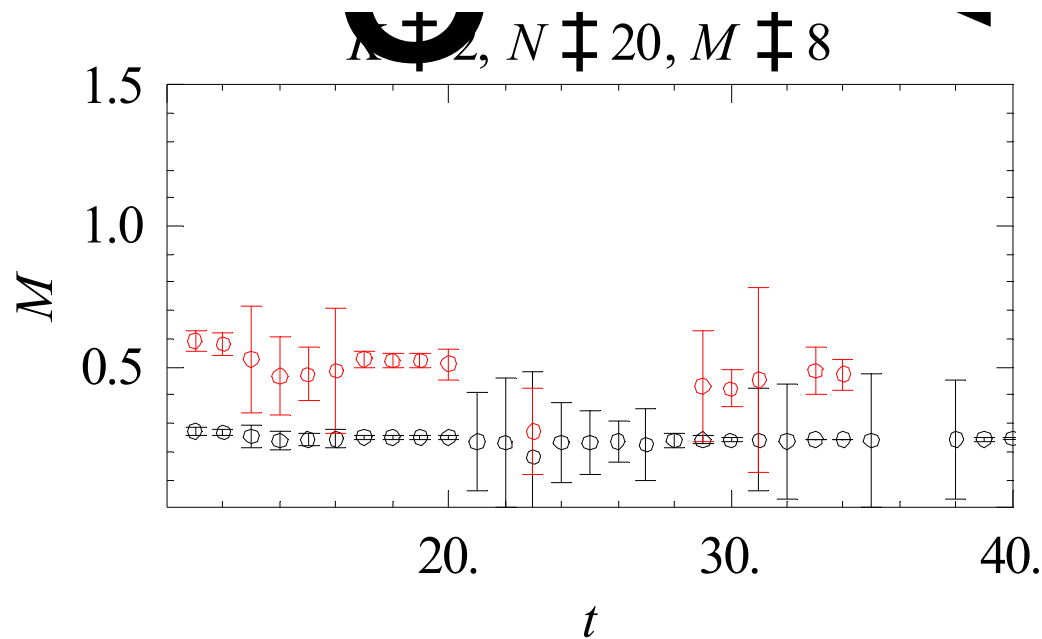
- ◆ Can we extract even higher energies?



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?



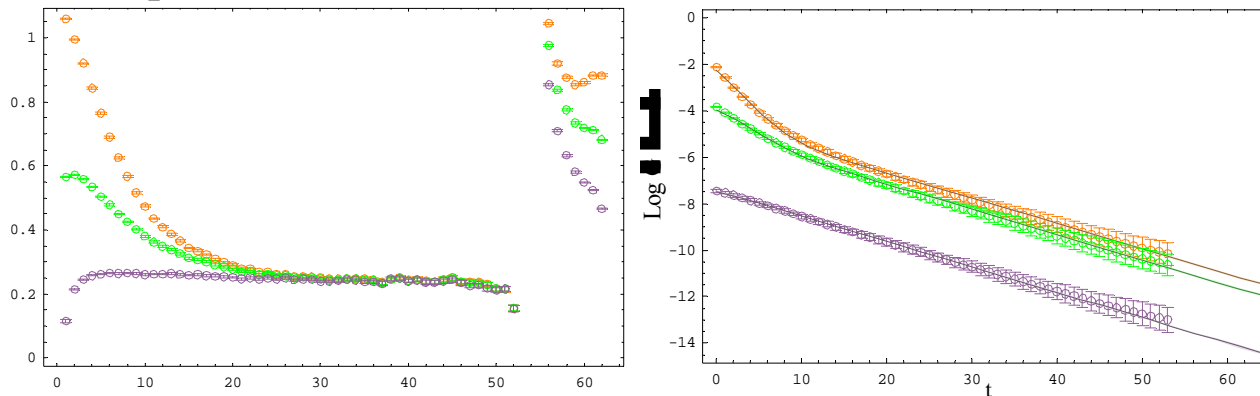
Multiple Least-Squares Fit

- With multiple smeared correlators, one minimizes the quantity

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

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

$$C_{ij}(t) = \langle 0 | \mathcal{O}_i(t)^\dagger \mathcal{O}_j(0) | 0 \rangle$$

◆ 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

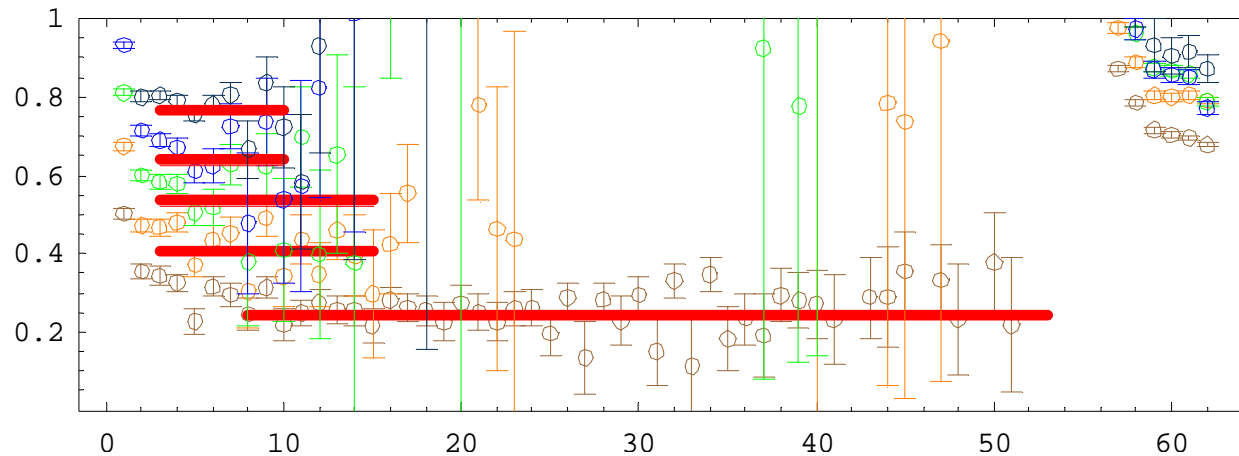
$$\lambda_n(t, t_0) = e^{-(t-t_0)E_n}$$

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

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

- ◆ 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
- ◆ Sparks for new ideas are generated in workshops like this where flinty lattice theorists meet steely numerical mathematicians
- ◆ What do I gain from this workshop?