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## Construction and Analysis of Two Baryon Correlation functions

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## Summary

The problem

Hadron-Hadron scattering phase shifts

Methods for extracting masses from correlators

The variable projection method

A new use of the generalized eigenvalue problem

Application to Baryon-Baryon spectrum

# Elastic Scattering Phases shifts

Maiani-Testa no-go theorem

- Luscher: Finite volume two particle spectrum is related to elastic scattering phase shifts
- Computational problem: Calculate in Euclidean space and finite volume the two particle spectrum
- Extract energy levels from exponentially decaying correlation functions
- Baryons: Signal to noise ratio grows exponentially with Euclidean time

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24<sup>3</sup> x 128 M<sub>π</sub>=390MeV

# Signal to Noise

NPLQCD data





## Expected Two Nucleon spectrum



# Needed Time Separation $e^{-\Delta E \delta t} \approx 10^{-2}$



## Conclusion

We need to fit for several low lying states for reliable estimation of the ground state of the two particle system in a finite box

The Variable Projection method (VarPro) Golub and Pereyra, SIAM J. Numer. Anal. Vol 10 No 2, 1973

 $t^{2}(Z, E) = \sum_{ij} \left[ \bar{G}(t_{i}) - F(t_{i}, Z, E) \right] C_{ij}^{-1} \left[ \bar{G}(t_{j}) - F(t_{j}, Z, E) \right]$  $F(t, Z, E) = \sum_{n=0}^{N} Z_{n} e^{-E_{n} t}$ 

Separable Least Squares problem:

Solve analytically for for the minimum for Z's at a given choice for E's

Minimize numerically the resulting  $t^2$  as a function of E's

The Variable Projection method (VarPro) Golub and Pereyra, SIAM J. Numer. Anal. Vol 10 No 2, 1973

$$F(t_i, Z, E) = \sum_{n=0}^{N} Z_n e^{-E_n t_i}$$

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 $F(t_i, Z, E) = \sum^N A_{in} Z_n$ n=0

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$$F(t_i, Z, E) = \sum_{n=0}^{N} A_{in} Z_n$$

 $A_{in} = e^{-E_n t_i}$ 

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$$F(t_i, Z, E) = \sum_{n=0}^{N} A_{in} Z_n$$

$$A_{in} = e^{-E_n t_i}$$

Solution for Z's:

 $Z(E) = [A^{\dagger}C^{-1}A]^{-1}A^{\dagger}C^{-1}Y$  $Y_i = \bar{G}(t_i)$ 

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$$t^{2}(E) = \sum_{ij} d_{i}(E) C_{ij}^{-1} d_{j}(E)$$

$$d_{i}(E) = \bar{G}(t_{i}) - \sum_{n=1}^{N} A_{in} Z_{n}(E)$$

## $d(E) = Y - [A(E)^{\dagger} C^{-1} A(E)]^{-1} A(E)^{\dagger} C^{-1} Y$

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VarPro can be generalized for multiple correlation functions with full covariance

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Fitting exponentials is hard....

## Alternative Methods

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Use multiple correlators and construct linear combinations that couple predominately to one state

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Use multiple correlators and construct linear combinations that couple predominately to one state

"Variational": Symmetric positive definite matrix of correlators [C. Michael, '85; Luscher&Wolf '90; ...]

Prony methods: [Fleming '04; NPLQCD '08; Fleming et.al. '09 ]

Matrix Prony [NPLQCD '08]

Similar to "Variational"

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Applicable to non-symmetric matrices

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Requires correlators less expensive to construct

Similar to "Variational"

Applicable to non-symmetric matrices

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## Generalized Pensile of Matrix

Similar to "Variational"

Applicable to non-symmetric matrices

Requires correlators less expensive to construct

## Generalized Pensile of Matrix

#### GPOF

Y. Hua and T. Sarkar IEEE Transactions of Antennas and Propagation Vol. 37 No. 2 p.229 '89

#### Consider

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

 $K_{ij}^{lm}(t) = \langle \mathcal{O}_i(t+l\tau)\mathcal{O}_j^{\dagger}(-m\tau) \rangle = G_{ij}(t+(l+m)\tau)$ 

#### Organized into a matrix

 $K(t) = \begin{pmatrix} G(t) & G(t+\tau) & G(t+2\tau) & G(t+3\tau) & \cdots \\ G(t+\tau) & G(t+2\tau) & G(t+3\tau) & G(t+4\tau) & \cdots \\ G(t+2\tau) & G(t+3\tau) & G(t+4\tau) & G(t+5\tau) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \cdots \end{pmatrix}$ 

If N operators and M shifts are used then K is an NMXNM matrix

 $G_{ij}(t) = \sum \langle 0|e^{Ht}\mathcal{O}_i e^{-Ht}|n\rangle \langle n|\tilde{\mathcal{O}}_j^{\dagger}|0\rangle$ 

Using the operators  $\mathcal{O}_i(t)$   $ilde{\mathcal{O}}_i^\dagger(t)$  and

 $\mathcal{O}(t+m\tau) = e^{m\tau H} \mathcal{O}(t) e^{-m\tau H}$  $\mathcal{O}^{\dagger}(t-m\tau) = e^{-m\tau H} \mathcal{O}^{\dagger}(t) e^{m\tau H}$ 

The K(t) is the matrix of correlators resulting from

 $ilde{\mathcal{O}}_i^\dagger(t-m au)$  Ci

creation operators

annihilation operators

 $\mathcal{O}_i(t+m\tau)$ 

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and

#### In general K(t) is:

A positive definite and symmetric if G(t) is positive definite and symmetric

A rectangular matrix if the basic creation and annihilation operators are not the same set

An (M<sub>1</sub> N<sub>1</sub>) x (M<sub>2</sub> N<sub>2</sub>) matrix if M<sub>1</sub> shifts with N<sub>1</sub> basic annihilation operators and M<sub>2</sub> shifts with N<sub>2</sub> basic creation operators are used

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From now on I consider K(t) an NxM matrix

# Estimating Energies

Assuming finite number (S) of states contributing to the correlators with S < min(N,M)

$$K_{ij}(t) = \sum_{n} Z_{i}^{n} (\tilde{Z}_{j}^{n})^{*} e^{-E_{n}t}$$
Look for vectors  $\omega^{n}$  and  $\tilde{\omega}^{n}$  that
$$\omega^{n\dagger}Z^{m} = \sum_{i=1}^{N} \omega_{i}^{n*}Z_{i}^{m} = \delta_{nm} \qquad \tilde{Z}^{n\dagger}\tilde{\omega}^{m} = \sum_{i=1}^{M} \tilde{Z}_{i}^{n*}\tilde{\omega}_{i}^{m} = \delta_{nm}$$

 $\overline{K(t)\tilde{\omega}^n} = Z^n e^{-E_n t} = e^{-E_n (t-t_0)} K(t_0) \tilde{\omega}^n$ 

# Estimating Energies

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 $K(t)\tilde{\omega}^n = \lambda K(t_0)\tilde{\omega}^n$ 

# Estimating Energies

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 $\overline{K(t)\tilde{\omega}^n} = \lambda \overline{K(t_0)}\tilde{\omega}^n$ 

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

 $K(t)\tilde{\omega}^n = \lambda K(t_0)\tilde{\omega}^n$ 

 $\omega^{n\dagger}K(t) = \lambda\omega^{n\dagger}K(t_0)$ 

#### $K(t)\tilde{\omega}^n = \lambda K(t_0)\tilde{\omega}^n$

 $\omega^{n\dagger}K(t) = \lambda\omega^{n\dagger}K(t_0)$ 

Generalized eigenvalue problem but K is not symmetric and not positive
#### $\overline{K(t)\tilde{\omega}^n} = \lambda \overline{K(t_0)}\tilde{\omega}^n$

 $\omega^{n\dagger}K(t) = \lambda\omega^{n\dagger}K(t_0)$ 

Generalized eigenvalue problem but K is not symmetric and not positive

Consider the singular value decomposition  $K(t_0) = U \Sigma V^{\dagger}$ 

#### $K(t)\tilde{\omega}^n = \lambda K(t_0)\tilde{\omega}^n$

 $\omega^{n\dagger}K(t) = \lambda\omega^{n\dagger}K(t_0)$ 

Generalized eigenvalue problem but K is not symmetric and not positive

Consider the singular value decomposition  $K(t_0) = U \Sigma V^{\dagger}$ 

Let M<N Then we have M singular values But only S (the number of states contributing to the correlator) of them are non-zero

# $K(t) = \begin{pmatrix} G(t) & G(t+\tau) & G(t+2\tau) & G(t+3\tau) & \cdots \\ G(t+\tau) & G(t+2\tau) & G(t+3\tau) & G(t+4\tau) & \cdots \\ G(t+2\tau) & G(t+3\tau) & G(t+4\tau) & G(t+5\tau) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \cdots \end{pmatrix}$

The S+1 column is a linear combination for the first S columns given that the signal is a sum of exponentials

#### Let $\sigma_i$ be the non-zero singular values of K(t<sub>0</sub>)

$$\Sigma' = \begin{pmatrix} \sigma_1 & 0 & \cdots \\ 0 & \sigma_2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$
 SxS mo

### U' = U(:, 1:S) NxS matrix V' = V(:, 1:S) MxS matrix

$$K(t_0) = U' \Sigma' V'^{\dagger}$$

$$V'^{\dagger}V' = \mathbf{1}_{S \times S}$$

 $U'^{\dagger}U' = \mathbf{1}_{S \times S}$ 

trix

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Let 
$$A = \Sigma'^{-\frac{1}{2}} U' K(t) V' \Sigma'^{-\frac{1}{2}}$$
 SxS matrix

Then  $A\tilde{q}^n = \lambda_n \tilde{q}^n$   $q^{n\dagger}A = \lambda_n q^{n\dagger}$   $q^{n\dagger}\tilde{q}^m = \delta_{nm}$ 

with  $\tilde{\omega}^n = V' \Sigma'^{-\frac{1}{2}} \tilde{q}^n$   $\omega^{n\dagger} = q^{n\dagger} \Sigma'^{-\frac{1}{2}} U'^{\dagger}$ 

#### is an eigenvalue problem of a non-symmetric matrix

Let 
$$A = \Sigma'^{-\frac{1}{2}} U' K(t) V' \Sigma'^{-\frac{1}{2}}$$
 SxS matrix

Then  $A\tilde{q}^n = \lambda_n \tilde{q}^n$   $q^{n\dagger}A = \lambda_n q^{n\dagger}$   $q^{n\dagger}\tilde{q}^m = \delta_{nm}$ 

with  $\tilde{\omega}^n = V' \Sigma'^{-\frac{1}{2}} \tilde{q}^n$   $\omega^{n\dagger} = q^{n\dagger} \Sigma'^{-\frac{1}{2}} U'^{\dagger}$ 

is an eigenvalue problem of a non-symmetric matrix

Z factor reconstruction

 $\tilde{Z}^{\dagger} = Q^{\dagger} \Sigma'^{\frac{1}{2}} V'^{\dagger} \quad Z = U' \Sigma'^{\frac{1}{2}} \tilde{Q}$ 

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Keep singular values that

 $\frac{\sigma_k}{\max(\sigma_i)} > tol$ 

The tolerance can be taken to be of the order of the signal to noise ratio

 $tol \sim \frac{\operatorname{err}[G(t_0)]}{\bar{G}(t_0)}$ 

Typical tolerance values  $10^{-2}$  to  $10^{-3}$ 

 $A(t) = \Sigma'^{-\frac{1}{2}} U' K(t) V' \Sigma'^{-\frac{1}{2}}$  $A(t)\tilde{q}^{n} = \lambda_{n}(t)\tilde{q}^{n}$ 

 $\lambda_n(t) = \left(1 - \sum_i z_i\right) e^{-E_n(t-t_0)} + \sum_i z_i e^{-E'_i(t-t_0)}$ 

 $A(t) = \Sigma'^{-\frac{1}{2}} U' K(t) V' \Sigma'^{-\frac{1}{2}}$  $A(t)\tilde{q}^n = \lambda_n(t)\tilde{q}^n$ 

 $\lambda_n(t) = \left(1 - \sum_i z_i\right) e^{-E_n(t-t_0)} + \sum_i z_i e^{-E'_i(t-t_0)}$ principal correlator

o Scan over several t<sub>0</sub> values

- Chose tolerance based on signal to noise ratio
- The principal correlators in (t<sub>0</sub>+1,t<sub>max</sub>)  $\lambda_n(t) = e^{-E_n(t-t_0)}$
- t<sub>max</sub> as large possible with λ(t) resolved
   Confidence level is checked

### Single Baryon spectrum

Use smeared-smeared correlation functions
Use a basis of all local independent interpolating fields
JLab anisotropic lattices at 390MeV pion mass

Compare GPOF with regular "variational"

### Nucleon Mass



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### Nucleon Mass

16<sup>3</sup>×128



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#### Nucleon Mass



### Delta Mass



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### Delta Mass



#### 16<sup>3</sup>x128

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#### Delta Mass



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### Two Baryon Correlation functions



- Single smeared quark source
- Multiple sink interpolating fields
  - Smeared, Point and Smeared-Point
- Resulting G is a 3x1 matrix
- No-need for all-to-all propagators
- Very high statistics (300K correlation functions on 2K lattices)

### NPLQCD data



NPLQCD data

single operator

one source smearing

smeared and point sink

two source shifts



### NPLQCD data

single operator

one source smearing

smeared and point sink

two source shifts



### NPLQCD data

single operator

one source smearing

smeared and point sink

two source shifts



NPLQCD data

single operator

one source smearing

smeared and point sink

two source shifts



NPLQCD data

single operator

one source smearing

smeared and point sink

two source shifts



NPLQCD data

single operator

one source smearing

smeared and point sink

two source shifts



NPLQCD data

single operator

one source smearing

smeared and point sink

two source shifts



NPLQCD data

single operator

one source smearing

smeared and point sink

two source shifts



NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink

three source shifts



NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink

three source shifts



NPLQCD data

single operator

one source smearing smeared, point and smeared-point sink

three source shifts



NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink

three source shifts



single operator one source smearing smeared, point and smeared-point sink

three source shifts



NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink

three source shifts



NPLQCD data

single operator one source smearing smeared, point and smeared-point sink

three source shifts



NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink

three source shifts



single operator

one source smearing

smeared, point and smeared-point sink

three source shifts



single operator

one source smearing

smeared, point and smeared-point sink

three source shifts


NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink

three source shifts



single operator

one source smearing

smeared, point and smeared-point sink

three source shifts



NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink

three source shifts



single operator

one source smearing

smeared, point and smeared-point sink

three source shifts



NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink

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NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink

three source shifts



single operator

one source smearing

NPLQCD data

smeared and point sink

### NPLQCD data



single operator

one source smearing

smeared and point sink



#### NPLQCD data

one source smearing

single operator

smeared and point sink

### NPLQCD data



single operator

one source smearing

smeared and point sink



#### NPLQCD data

single operator one source smearing smeared and point sink VarPro 3 state fits

### NPLQCD data



single operator

one source smearing

smeared and point sink

VarPro 3 state fits

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#### NPLQCD data

one source smearing

single operator

smeared and point sink

### NPLQCD data



single operator

one source smearing

smeared and point sink



### NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink

### NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink





### NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink



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smeared, point and smeared-point sink



NPLQCD data

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smeared, point and smeared-point sink

#### sigsig 0.475 0.47 0.465 0.46 E 0.455 Φ 0.45 0.445 0.44 0.435 12 8 10 16 18 6 14 20 $\mathbf{t}_0$

NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink



NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink



### NPLQCD data

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### NPLQCD data

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one source smearing

smeared, point and smeared-point sink



NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink



NPLQCD data

single operator

one source smearing

smeared, point and smeared-point sink

### Conclusions

- The Generalized Pencil of Matrix provides an alternative "diagonalization" method for correlator matrices
- Shifting" is not a substitute for a good set of interpolating fields
- Non-symmetric correlator matrices can be treated
- Symmetric positive definite correlator matrices are preferable
- Could be useful for variational approach to Form Factor calculations