New avenues for noise reduction in QCD correlation functions

Michael G. Endres
MIT

YITP, Kyoto
March 6, 2015

In collaboration with W. Detmold
Phys. Rev. D 90 (2014) 034503, [arXiv:1404.6816]
PoS LAT2014 (2014) 170, [arXiv:1409.5667]

Correlation functions on the lattice

- Two point correlators
  - spectrum, binding energies
  - scattering parameters (via Luscher's formula)
  - finite density (e.g., equation of state at T=0, etc.)
  - transport coefficients (via Kubo relations)
- Three point correlators
  - matrix elements

Correlation functions in Euclidean spacetime

$$C_{ij}(\tau) = \langle\Omega|\hat{\mathcal{O}}'_i e^{-\hat{H}\tau}\hat{\mathcal{O}}^\dagger_j|\Omega\rangle$$

N`xN matrix

$$= \sum_n Z'_{in} Z^*_{jn} e^{-E_n\tau}$$

sum over states n with quantum numbers equal to those of $\mathcal{O}_i$ $(\mathcal{O}_j)$

overlap factors

$$\hat{H}|n\rangle = E_n|n\rangle \qquad Z'_{in} = \langle\Omega|\hat{\mathcal{O}}'_i|n\rangle \qquad Z_{jn} = \langle\Omega|\hat{\mathcal{O}}_j|n\rangle$$

Correlation functions in Euclidean spacetime

$$C_{ij}(\tau) = \langle\Omega|\hat{\mathcal{O}}'_i e^{-\hat{H}\tau}\hat{\mathcal{O}}_j^\dagger|\Omega\rangle$$

N`xN matrix

$$= \langle\mathcal{C}_{ij}\rangle + \text{stat. errors}$$

ensemble average over "individual" correlators measured on background gauge field configurations

$$\hat{H}|n\rangle = E_n|n\rangle \qquad Z'_{in} = \langle\Omega|\hat{\mathcal{O}}'_i|n\rangle \qquad Z_{jn} = \langle\Omega|\hat{\mathcal{O}}_j|n\rangle$$

Extraction of energies at late times

typically one lattice spacing

N-dimensional source vector; specifies a linear combination of source operators

exponential suppression at late times

$$m_{eff}(\tau) = -\frac{1}{\Delta\tau}\log\frac{\psi'^{\dagger}C(\tau+\Delta\tau)\psi}{\psi'^{\dagger}C(\tau)\psi}$$

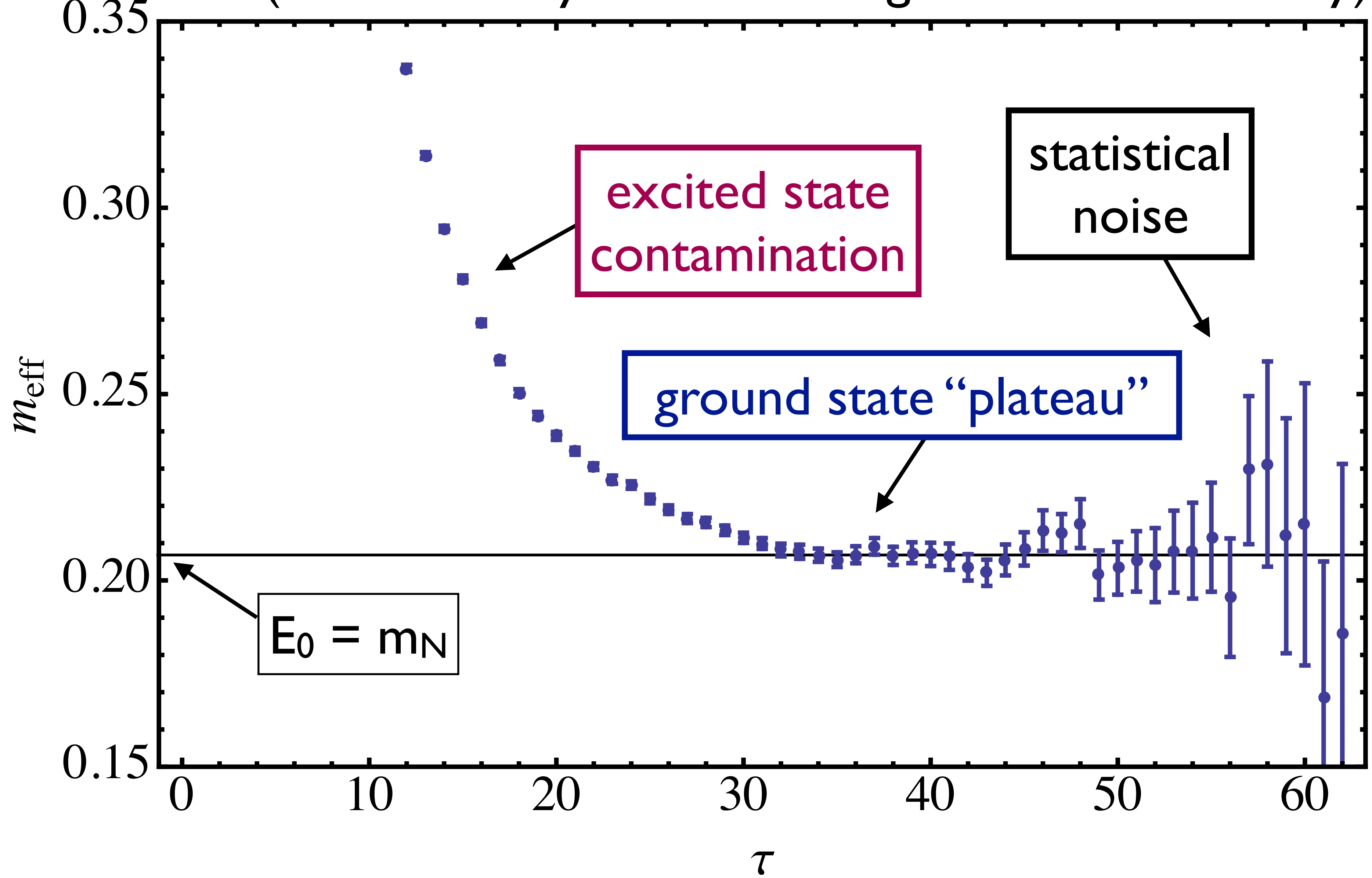
$$\approx \underline{E_0} + \underline{\frac{(\psi'^{\dagger}Z_1')(Z_1^{\dagger}\psi)}{(\psi'^{\dagger}Z_0')(Z_0^{\dagger}\psi)}\left[\frac{1-e^{-(E_1-E_0)\Delta\tau}}{\Delta\tau}\right]e^{-(E_1-E_0)\tau}}$$

ground state energy

"excited state contamination"

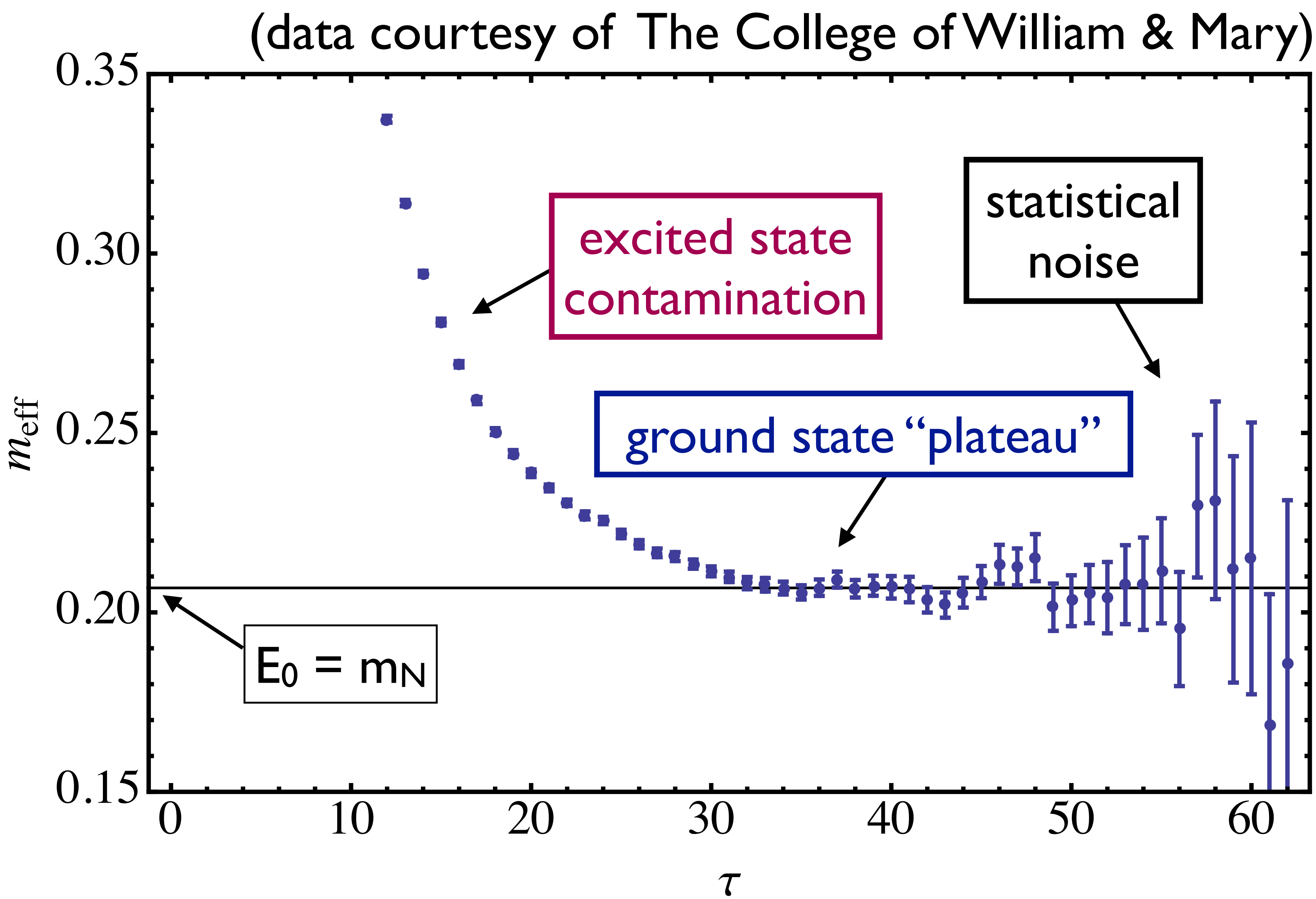
Example: nucleon correlator

(data courtesy of The College of William & Mary)



"Plateau region" can be short; or worse yet, nonexistent

Example: nucleon correlator

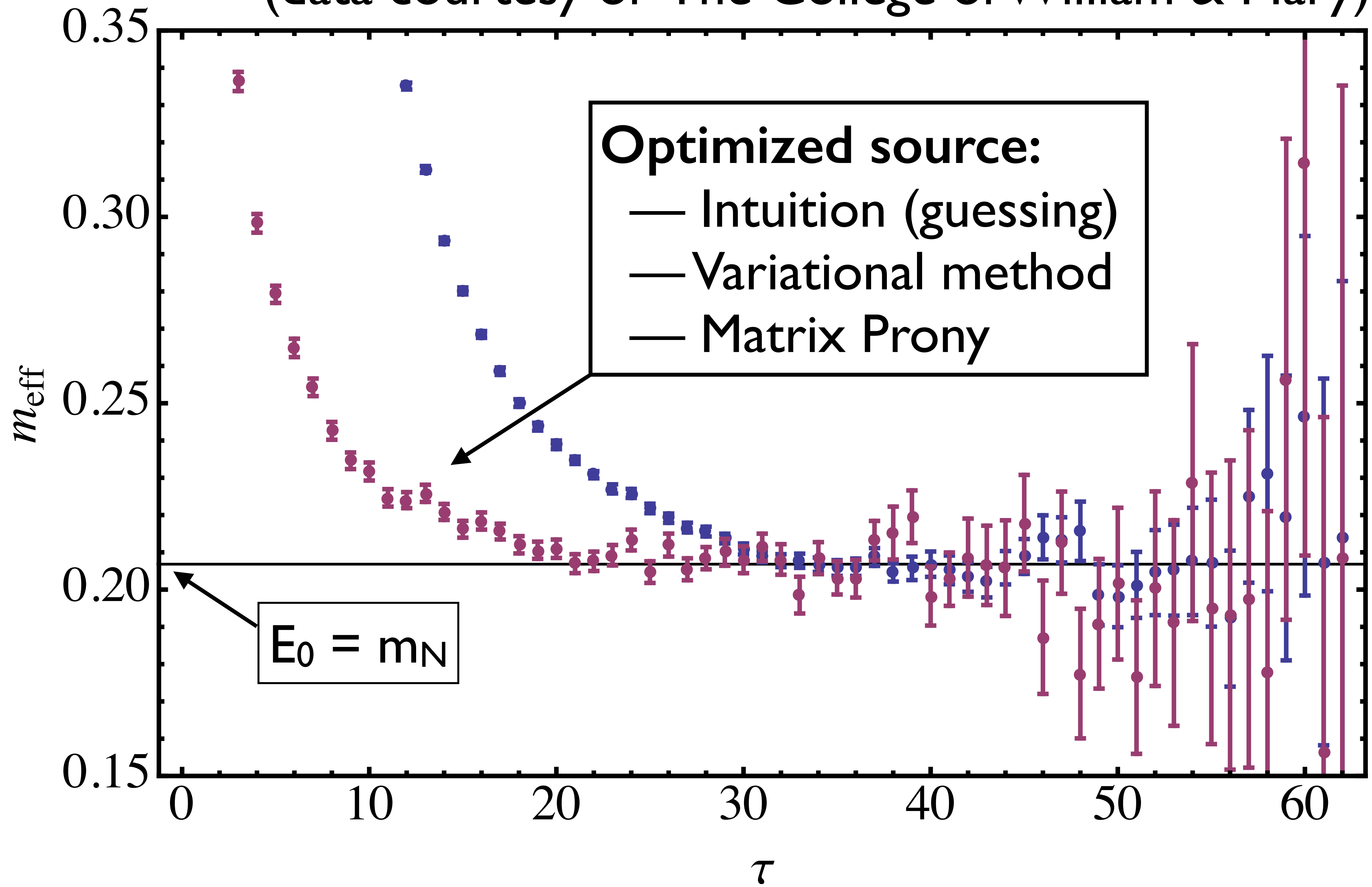


To extend plateau, one can either:

1) *reduce contamination at early times*
2) *reduce statistical noise at late times*

Example: nucleon correlator

(data courtesy of The College of William & Mary)



Optimized source yields an earlier plateau for ground state, yet the late time uncertainties are significantly larger

Can we understand the interplay between excited state contamination at early times and signal/noise degradation at late times?

— *are optimizations mutually compatible?*
— *what is the ideal balance between strategies?*
— *can this be understood theoretically?*

Behavior of the variance

The variance of a correlator is itself a correlator

$$\sigma^2(\psi', \psi) = \left(\psi' \otimes \psi'^*\right)^\dagger \Sigma^2 \left(\psi \otimes \psi^*\right)$$

N`²xN² matrix

$$\Sigma^2 = \langle \mathcal{C} \otimes \mathcal{C}^* \rangle$$

$$\Sigma^2_{ik;jl}(\tau) = \sum_n \tilde{Z}'_{ik,n} \tilde{Z}^*_{jl,n} e^{-\tilde{E}_n \tau}$$

noise state energies

sum over states with nontrivial valence quantum numbers

NxN positive semidefinite matrix

Signal/noise ratio at late times

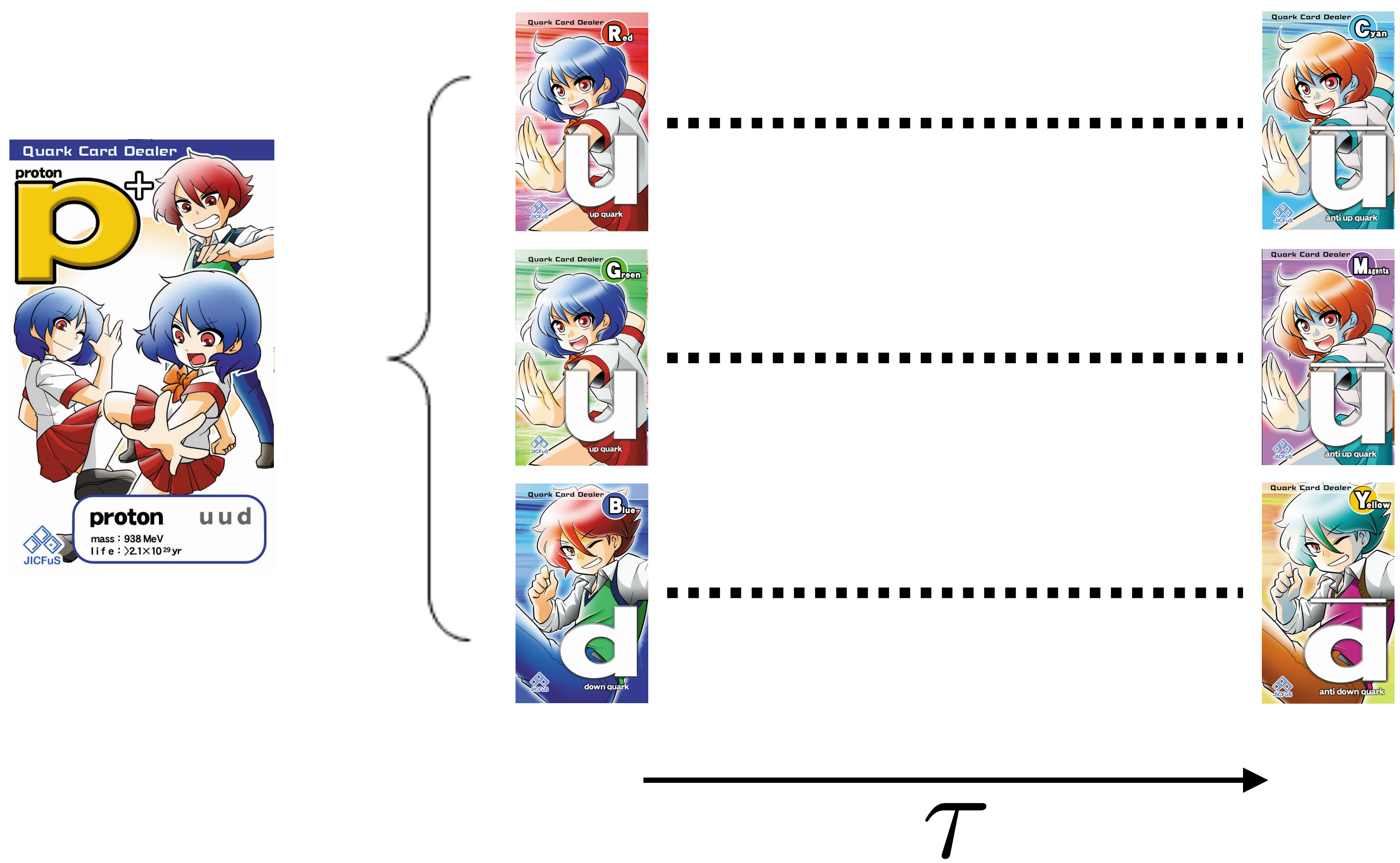
At sufficiently late times:

$$\theta(\psi', \psi) \sim \frac{|\psi'^\dagger Z_0'|}{\sqrt{\psi'^\dagger \tilde{Z}_0' \psi'}} \frac{|Z_0^\dagger \psi|}{\sqrt{\psi^\dagger \tilde{Z}_0 \psi}} e^{-\left(E_0 - \frac{1}{2}\tilde{E}_0\right)\tau}$$

$$2E_0 > \tilde{E}_0$$

“Lepage’s argument”

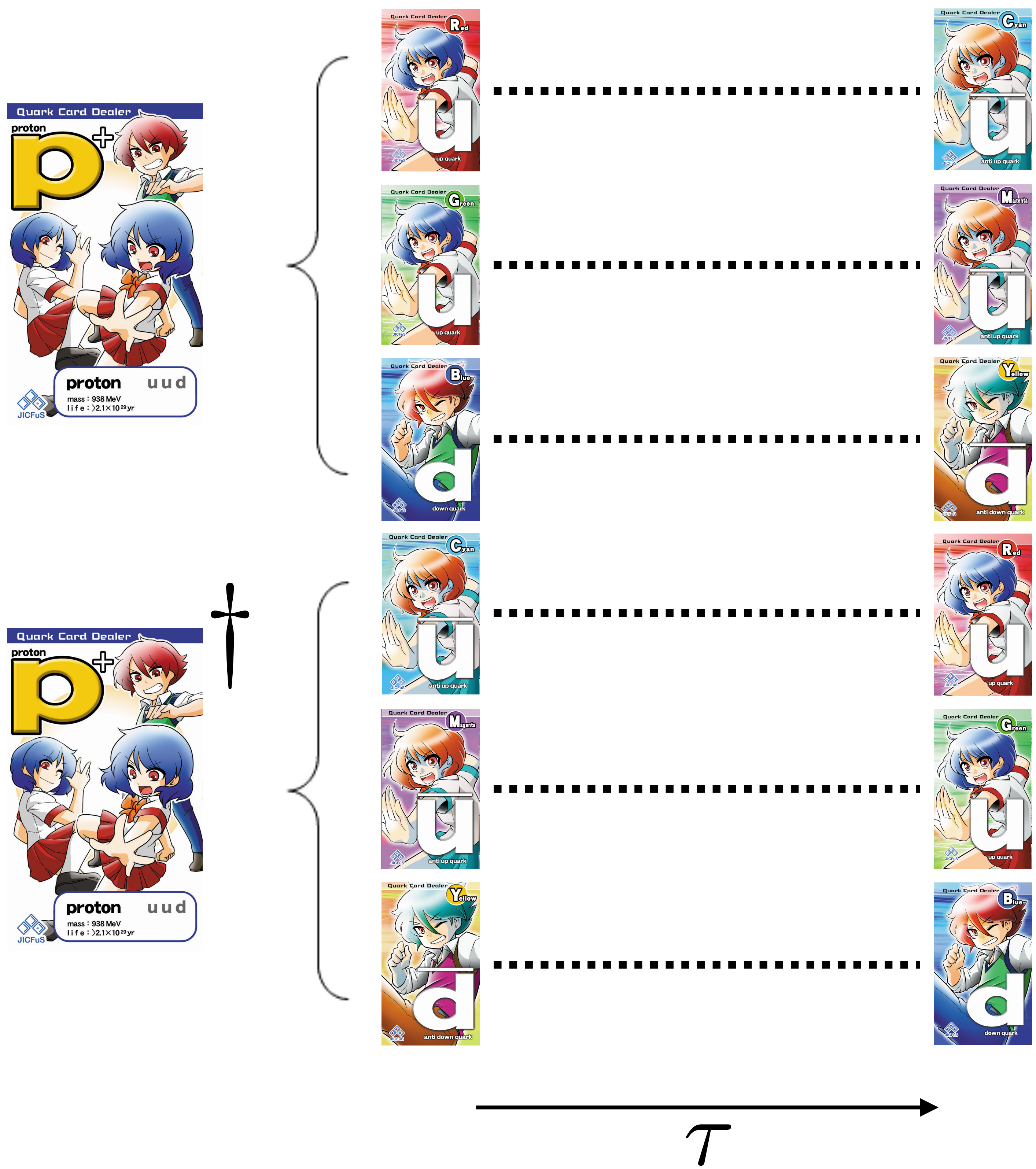
Physical origins of noise



"signal"

$$C_p(\tau) \sim e^{-m_p \tau}$$

Physical origins of noise



"noise"

$$\sigma_p^2(\tau) \overset{?}{\sim}$$

Physical origins of noise

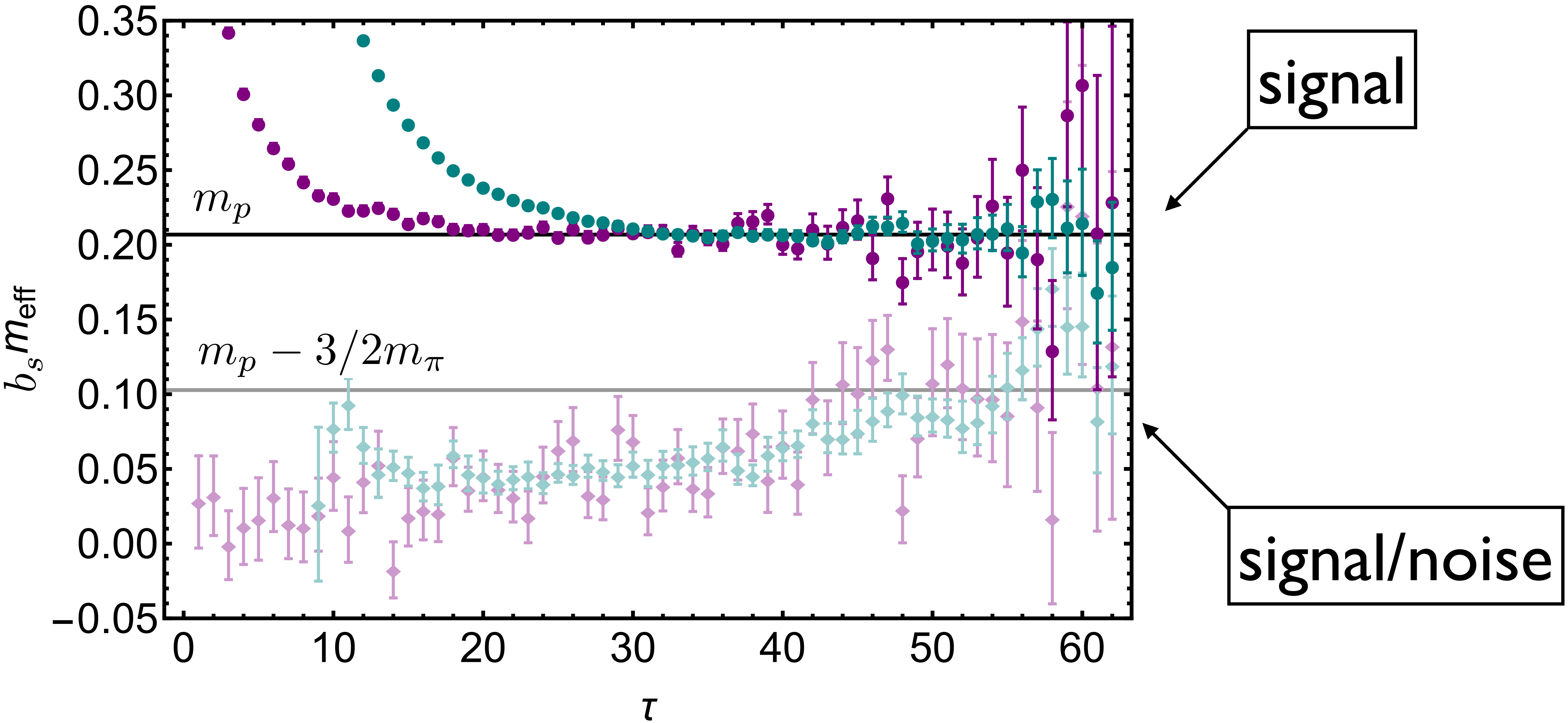
"noise"

$$\sigma_p^2(\tau) \sim e^{-3m_\pi \tau}$$

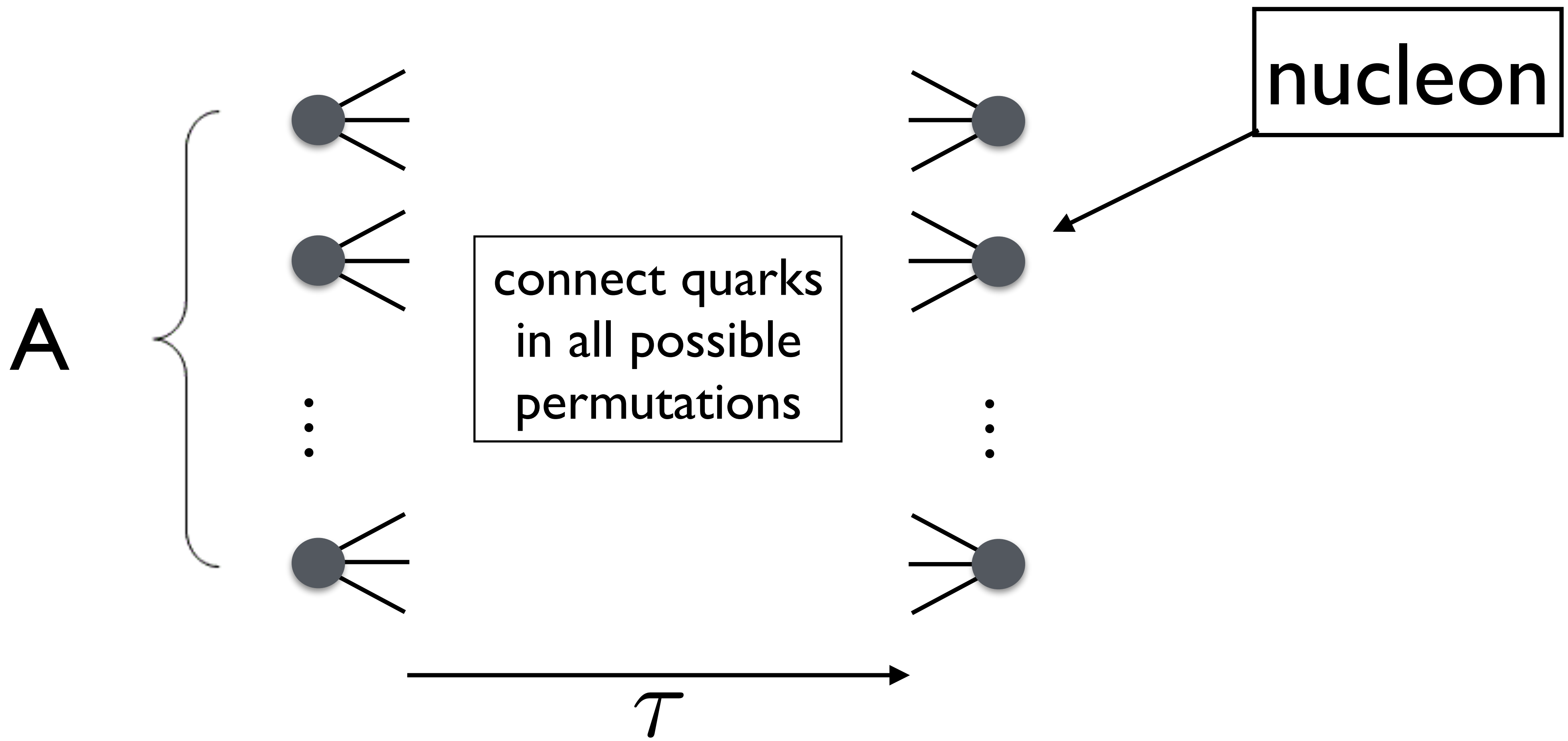
Signal/noise in correlation functions

$$C_p(\tau) \sim e^{-m_p \tau}$$

$$\theta_p(\tau) \sim C_p(\tau)/\sigma_p(\tau) \sim e^{-\left(m_p - \frac{3}{2} m_\pi\right)\tau}$$



Signal/noise at late times



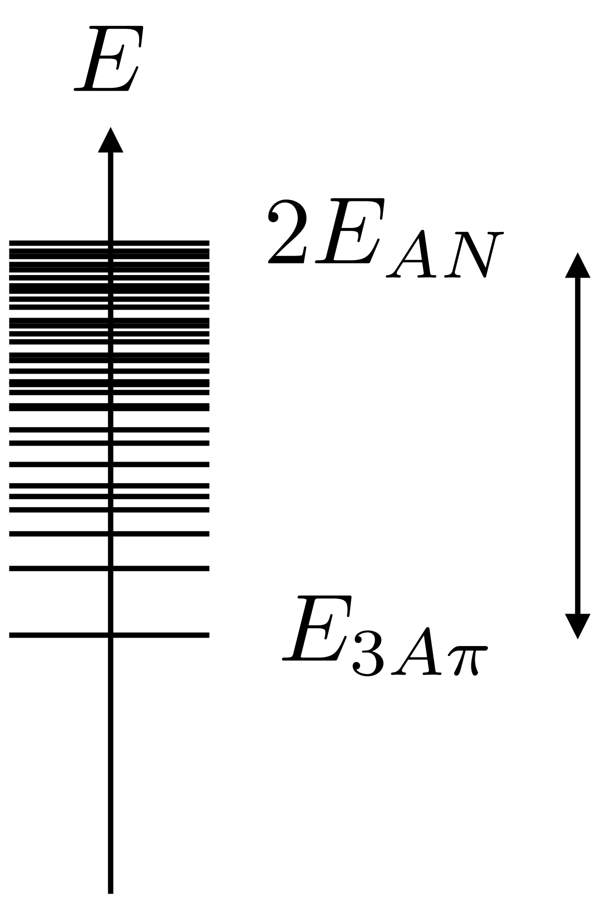
$$\theta_{AN} \sim e^{-\left(E_{AN} - \frac{1}{2}E_{3A\pi}\right)\tau}$$

— degradation scales exponentially with A
— becomes more severe as m_π approaches physical value
— closely related to the “sign problem” at finite μ

A look at “noise states”

Suppose we could choose sources such that they are orthogonal to the lightest “noise states”…

$$\Sigma^2_{ik;jl}(\tau) = \sum_n \tilde{Z}'_{ik,n} \tilde{Z}^*_{jl,n} e^{-\tilde{E}_n \tau}$$



…how many states do we need to orthogonalize against for A nucleons in a finite volume?

A look at "noise states"

- Assume large but finite volume, ignore pion interactions
- Ignore isospin (further multiplicative exponential enhancement)
- Assume zero total momentum

$$\hat{\mathbf{p}}_{3A} = -\sum_{i=1}^{3A-1} \hat{\mathbf{p}}_i$$

$$n(\Delta E^2) = \sum_{\hat{\mathbf{p}}_1 \cdots \hat{\mathbf{p}}_{3A-1}} \theta\left(\Delta E^2 - \sum_{i=1}^{3A} \hat{\mathbf{p}}_i^2\right)$$

$$\Delta E^2 \equiv 4E_{AN}^2 - E_{3A\pi}^2$$

$$\hat{\mathbf{p}}_i = 2\pi \mathbf{n}_i / L$$

A look at “noise states”

- Assume large but finite volume, ignore pion interactions
- Ignore isospin (further multiplicative exponential enhancement)
- Assume zero total momentum

$$n(\Delta E^2) \sim \left(\frac{4\pi}{3A}\right)^{3/2} \frac{\pi^{\frac{9A}{2}}}{\Gamma\left(\frac{9A-1}{2}\right)} \left(\frac{L\sqrt{\Delta E^2}}{2\pi}\right)^{9A-3}$$

$$\Delta E^2 \equiv 4E_{AN}^2 - E_{3A\pi}^2$$

scales exponentially in A

A look at “noise states”

- Exponential proliferation of “noise states” with A seems to make a connection with the “sign problem”
- In principle and in practice, one cannot perform such orthogonalization to remove lowest states from the variance
  - would need exponentially large operator basis
  - noise source and sink vectors are actually constrained

$$\sigma^2(\psi', \psi) = \overbrace{\left(\psi' \otimes \psi'^*\right)}^{\dagger} \Sigma^2 \overbrace{\left(\psi \otimes \psi^*\right)}$$

Signal/noise at late times

At sufficiently late times:

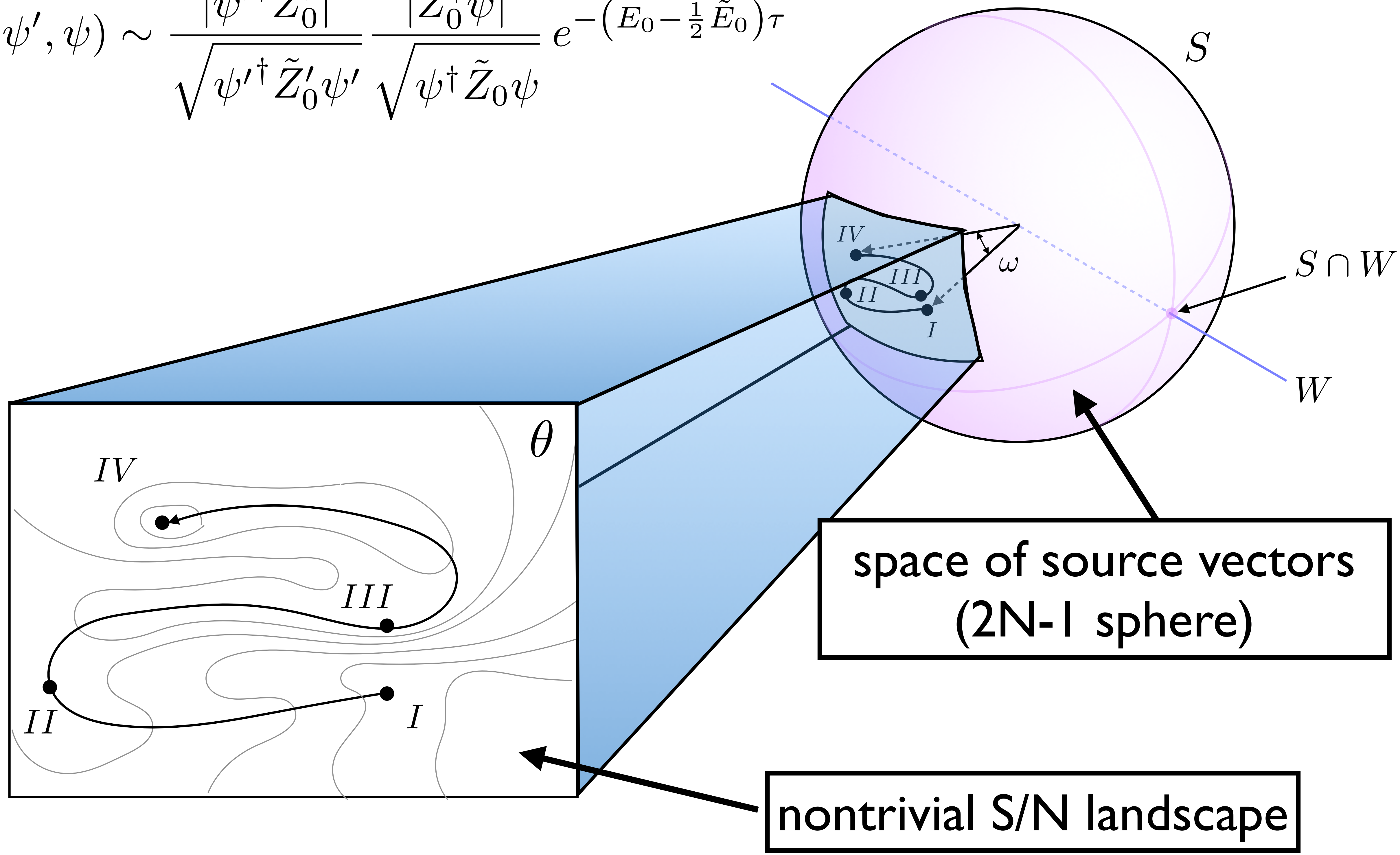
$$\theta(\psi', \psi) \sim \boxed{\frac{|\psi'^{\dagger} Z_0'|}{\sqrt{\psi'^{\dagger} \tilde{Z}_0' \psi'}} \frac{|Z_0^{\dagger} \psi|}{\sqrt{\psi^{\dagger} \tilde{Z}_0 \psi}}} \boxed{e^{-\left(E_0 - \frac{1}{2}\tilde{E}_0\right)\tau}}$$

Although exponential degradation is an inherent and unavoidable property of the system…

…we nonetheless retain some control over signal/noise via the interplay between ratios of overlap factors!

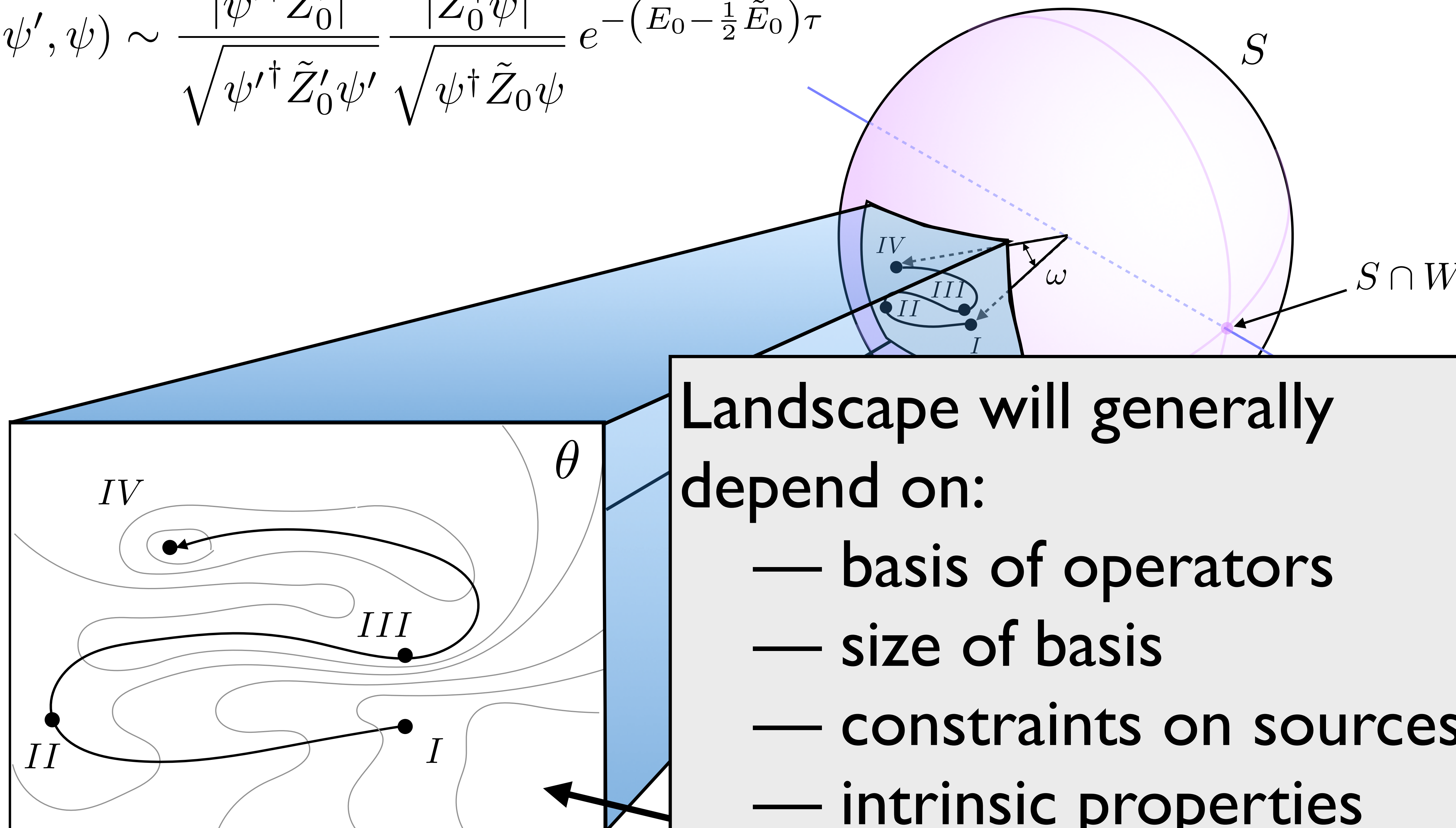
Signal/noise in correlation functions

$$\theta(\psi', \psi) \sim \frac{|\psi'^\dagger Z_0'|}{\sqrt{\psi'^\dagger \tilde{Z}_0' \psi'}} \frac{|Z_0^\dagger \psi|}{\sqrt{\psi^\dagger \tilde{Z}_0 \psi}} \, e^{-\left(E_0 - \frac{1}{2}\tilde{E}_0\right)\tau}$$



Signal/noise in correlation functions

$$\theta(\psi', \psi) \sim \frac{|\psi'^{\dagger} Z_0'|}{\sqrt{\psi'^{\dagger} \tilde{Z}_0' \psi'}} \frac{|Z_0^{\dagger} \psi|}{\sqrt{\psi^{\dagger} \tilde{Z}_0 \psi}} e^{-\left(E_0 - \frac{1}{2}\tilde{E}_0\right)\tau}$$



Landscape will generally depend on:

— basis of operators
— size of basis
— constraints on sources
— intrinsic properties of the system

Signal/noise at late times

At sufficiently late times:

$$\theta(\psi', \psi) \sim \frac{|\psi'^{\dagger} Z_0'|}{\sqrt{\psi'^{\dagger} \tilde{Z}_0' \psi'}} \frac{|Z_0^{\dagger} \psi|}{\sqrt{\psi^{\dagger} \tilde{Z}_0 \psi}} \, e^{-\left(E_0 - \frac{1}{2}\tilde{E}_0\right)\tau}$$

Maximum signal/noise occurs when:

$$\psi_0' \propto (\tilde{Z}_0')^{-1} Z_0' \qquad \psi_0 \propto (\tilde{Z}_0)^{-1} Z_0$$

Signal/noise at late times

At sufficiently late times:

$$\theta(\psi', \psi) \sim \frac{|\psi'^{\dagger} Z_0'|}{\sqrt{\psi'^{\dagger} \tilde{Z}_0' \psi'}} \frac{|Z_0^{\dagger} \psi|}{\sqrt{\psi^{\dagger} \tilde{Z}_0 \psi}} \, e^{-\left(E_0 - \frac{1}{2}\tilde{E}_0\right)\tau}$$

Maximum signal/noise given by:

$$\theta(\psi_0', \psi_0) \sim \sqrt{Z_0'^{\dagger} (\tilde{Z}_0')^{-1} Z_0'} \sqrt{Z_0^{\dagger} (\tilde{Z}_0)^{-1} Z_0} \, e^{-\left(E_0 - \frac{1}{2}\tilde{E}_0\right)\tau}$$

What conditions are required of this?

Signal/noise optimization

- *A priori* it is unclear whether "source optimization" yields a signal/noise comparable to the maximum or whether it is substantially degraded by comparison
- Suggests a new avenue for correlator optimization that has never before been explored: *signal/noise optimization*
- Many considerations:
  - signal/noise optimization produces correlators with minimal uncertainties, but what really matters is the uncertainties on the energies extracted from them
  - nontrivial interplay between signal/noise reduction and excited state contamination

Toy model: a two state system

Toy model: a two state system

Assume without loss of generality:

$$C \propto \begin{pmatrix} 1 & 0 \\ 0 & \Delta \end{pmatrix}$$

$$\Delta = e^{-(E_1 - E_0)\tau}$$

$$\Sigma^2 \sim \tilde{Z}_0 \tilde{Z}_0^\dagger e^{-\tilde{E}_0 \tau} + \mathcal{O}(\tilde{\Delta})$$

$$\tilde{\Delta} = e^{-(\tilde{E}_1 - \tilde{E}_0)\tau}$$

$$\tilde{Z}_0 = \begin{pmatrix} a & b \\ b^* & c \end{pmatrix}$$

Noise Z-factor is positive matrix:

$$ac > |b|^2 \quad a > 0 \quad c > 0$$

Toy model: a two state system

Assume without loss of generality:

$$C \propto \begin{pmatrix} 1 & 0 \\ 0 & \Delta \end{pmatrix} \qquad \Delta = e^{-(E_1 - E_0)\tau}$$

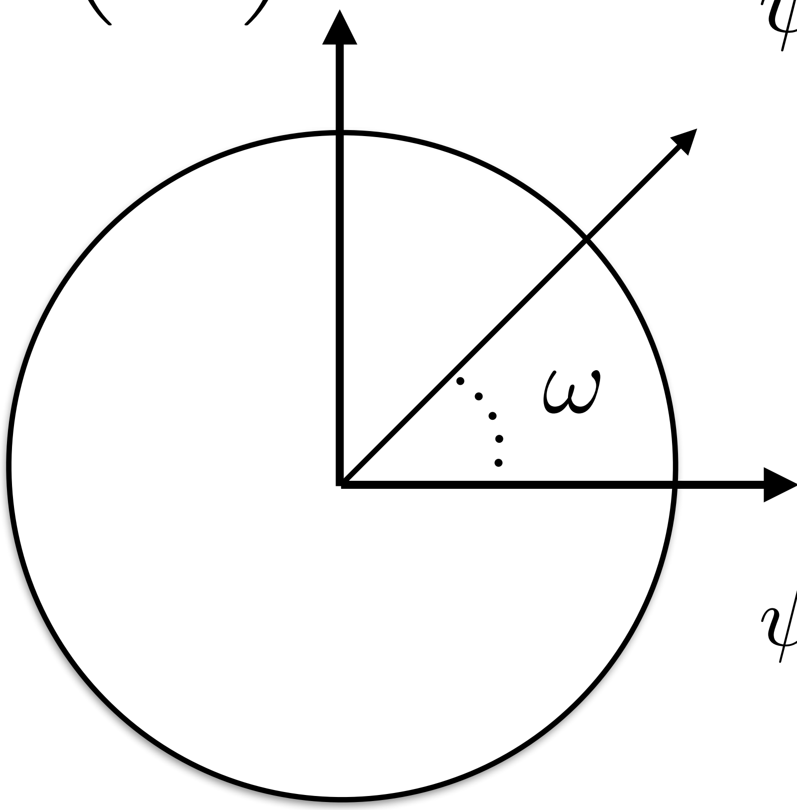
$$\Sigma^2 \sim \tilde{Z}_0 \tilde{Z}_0^\dagger e^{-\tilde{E}_0 \tau} + \mathcal{O}(\tilde{\Delta}) \qquad \tilde{\Delta} = e^{-(\tilde{E}_1 - \tilde{E}_0)\tau}$$

$$\tilde{Z}_0 = \begin{pmatrix} a & b \\ b^* & c \end{pmatrix}$$

4 system-dependent parameters

Two state system (eigenstate source)

$$\psi_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



$$\psi'(\omega, \delta) = \begin{pmatrix} \cos\omega \\ \sin\omega\, e^{i\delta} \end{pmatrix}$$

(overall phase is irrelevant)

$$\delta \in [-\pi/2, \pi/2)$$

$$\omega \in [0, \pi)$$

$$\psi_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Consider the correlator:

$$\psi'(\omega, \delta)^{\dagger} C \psi_n \propto e^{-E_n \tau}$$

Pure exponential: no contamination from the other state!

Two state system (eigenstate source)

Signal/noise, normalized by optimal signal/noise, can be fully parameterized (3 parameters) by the formula:

$$\hat{\theta}_n(\omega,\delta) = \frac{1}{\sqrt{R_n + (R_n - 1)x_n(\omega)\left[x_n(\omega) - 2\cos(\delta - \delta_n)\right]}}$$

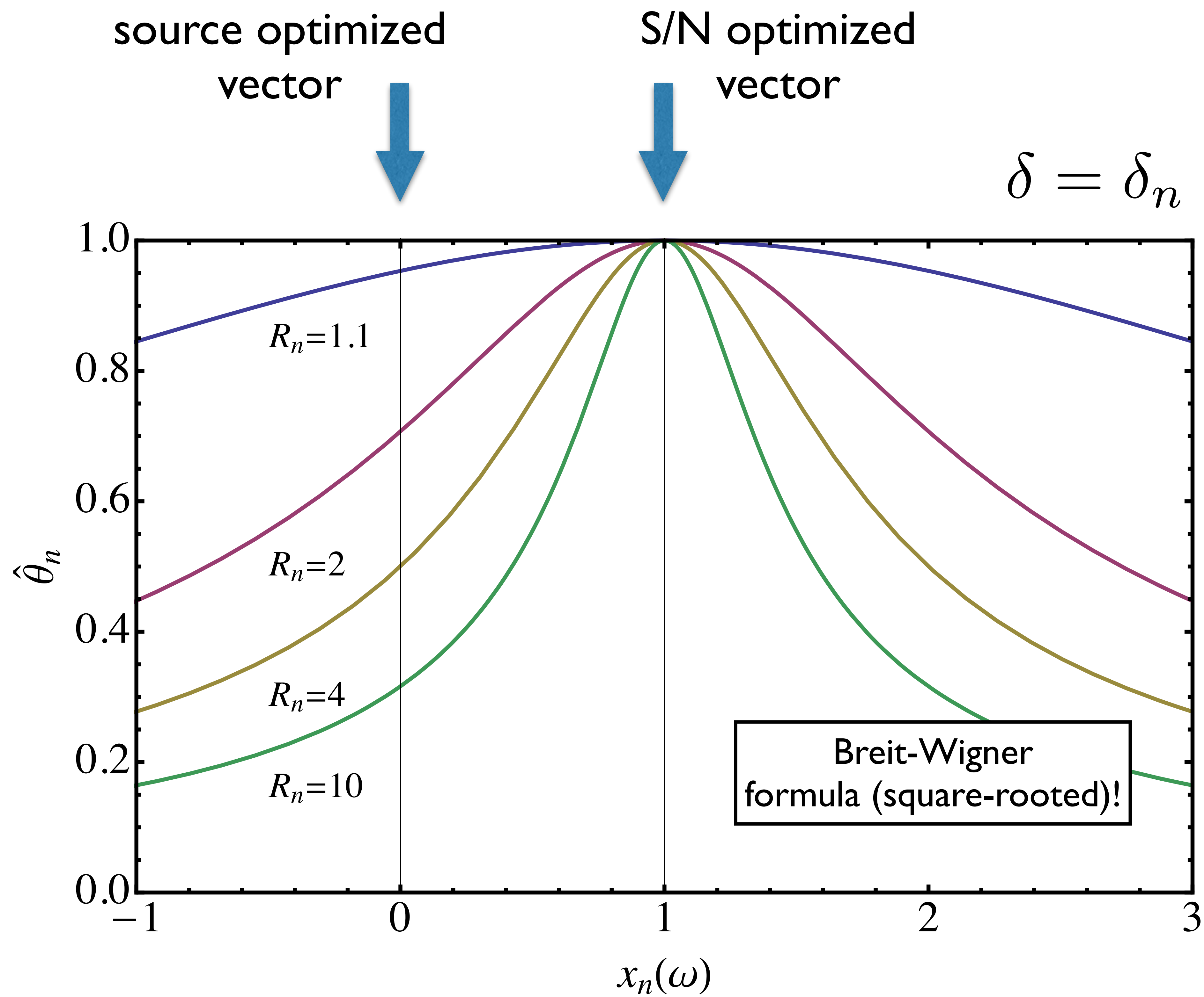
$$x_0(\omega) = \frac{\tan\omega}{\tan\omega_0} \qquad x_1(\omega) = \frac{\cot\omega}{\cot\omega_1}$$

$$\sqrt{R_n} = \text{enhancement factor } (\geq 1)$$

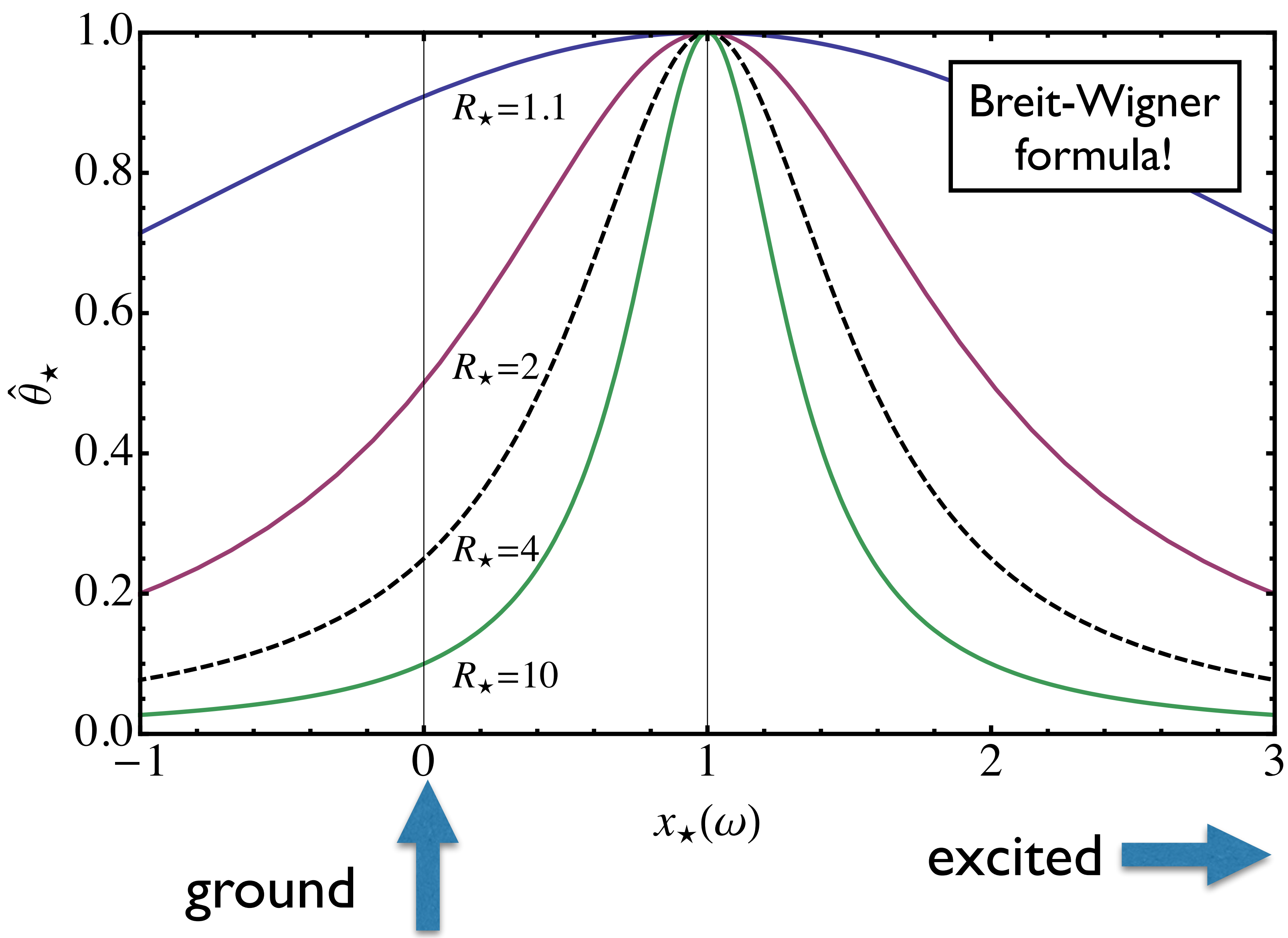
$$\omega_n, \delta_n = \text{optimal angles}$$

System- and basis dependent parameters

Two state system (eigenstate source)



Two state system (source = sink)



$$x_\star(\omega) = \frac{\tan\omega}{\tan\omega_\star}$$

optimal mixing angle

Similar result for equal sources and sinks at late times:

— roughly power of two increase in enhancement
— excited state contamination enters at earlier times
— optimal mixing angle can be small

Application to realistic systems

Signal/noise optimization: fixed source

Lagrange multiplier

$$\Xi(\psi', \psi) = \log \theta^2(\psi', \psi) + \xi' \left(\psi'^\dagger \psi' - 1\right)$$

unconstrained (up to a unit normalization)

fixed

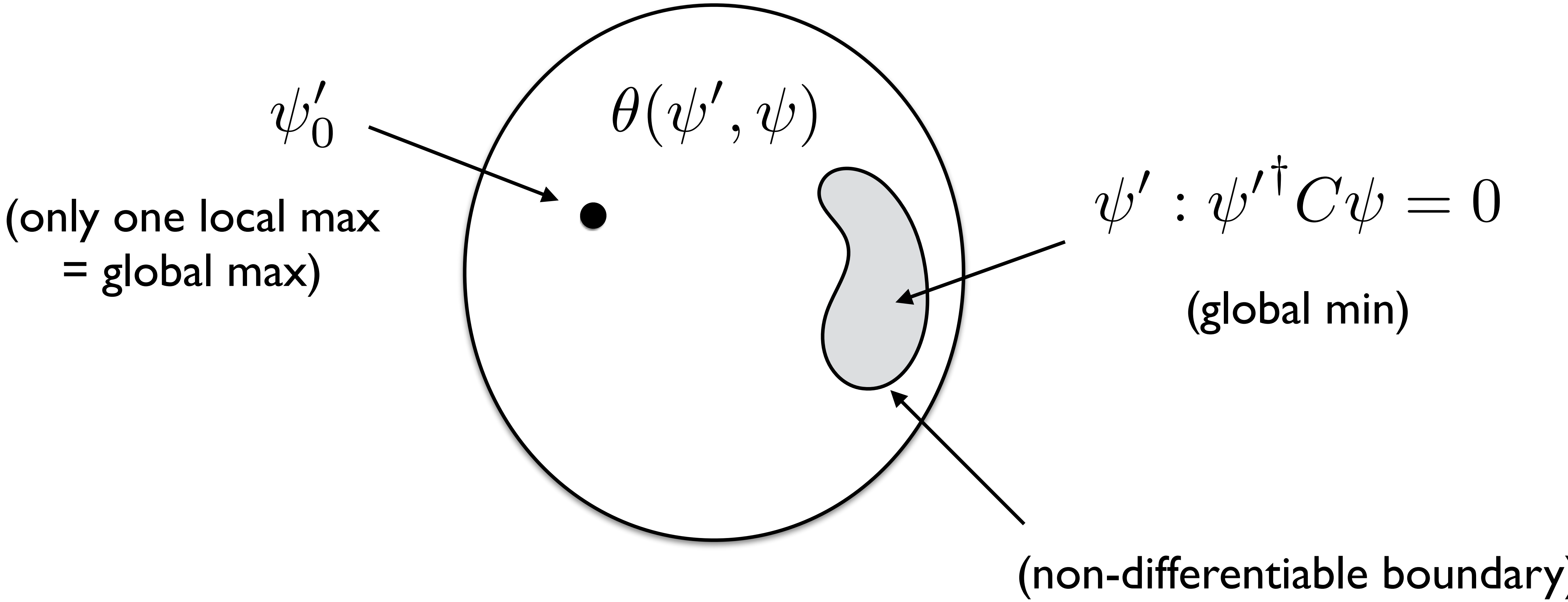
$$\theta(\psi', \psi) = \frac{\left|\psi'^\dagger C \psi\right|}{\sigma(\psi', \psi)}$$

Single solution:

$$\psi'_0 = A'_0(\psi) \sigma_\psi^{-2} C \psi \qquad \sigma_\psi^2 = \langle \mathcal{C} \psi \psi^\dagger \mathcal{C}^\dagger \rangle$$

determined by normalization condition

Signal/noise optimization: fixed source



Single solution:

$$\psi'_0 = A'_0(\psi) \sigma_\psi^{-2} C \psi \qquad \sigma_\psi^2 = \langle \mathcal{C} \psi \psi^\dagger \mathcal{C}^\dagger \rangle$$

determined by normalization condition

Signal/noise optimization: equal source/sink

Lagrange multiplier

$$\Xi(\psi',\psi) = \log\theta^2(\psi',\psi) + \xi'\left(\psi'^{\dagger}\psi' - 1\right) + \xi\left(\psi^{\dagger}\psi - 1\right)$$

unconstrained (up to a unit normalization)

$$\theta(\psi',\psi) = \frac{\left|\psi'^{\dagger} C\psi\right|}{\sigma(\psi',\psi)}$$

Solution (coupled):

$$\psi'_0 = A'_0(\psi_0)\sigma_{\psi_0}^{-2} C\psi_0 \qquad \sigma_{\psi_0}^2 = \langle \mathcal{C}\psi_0\psi_0^{\dagger}\mathcal{C}^{\dagger}\rangle$$

$$\psi_0 = A_0(\psi'_0)\sigma_{\psi'_0}^{-2} C^{\dagger}\psi'_0 \qquad \sigma_{\psi'_0}^2 = \langle \mathcal{C}^{\dagger}\psi'_0{\psi'_0}^{\dagger}\mathcal{C}\rangle$$

Signal/noise optimization: equal source/sink

Iteratively solve:

$$\psi'^{[n+1]} = A_0'(\psi^{[n]})\sigma^{-2}_{\psi^{[n]}} C\psi^{[n]}$$
$$\psi^{[n+1]} = A_0(\psi'^{[n]})\sigma^{-2}_{\psi'^{[n]}} C^\dagger\psi'^{[n]}$$

(at late times, solution found after single iteration)

Solution (coupled):

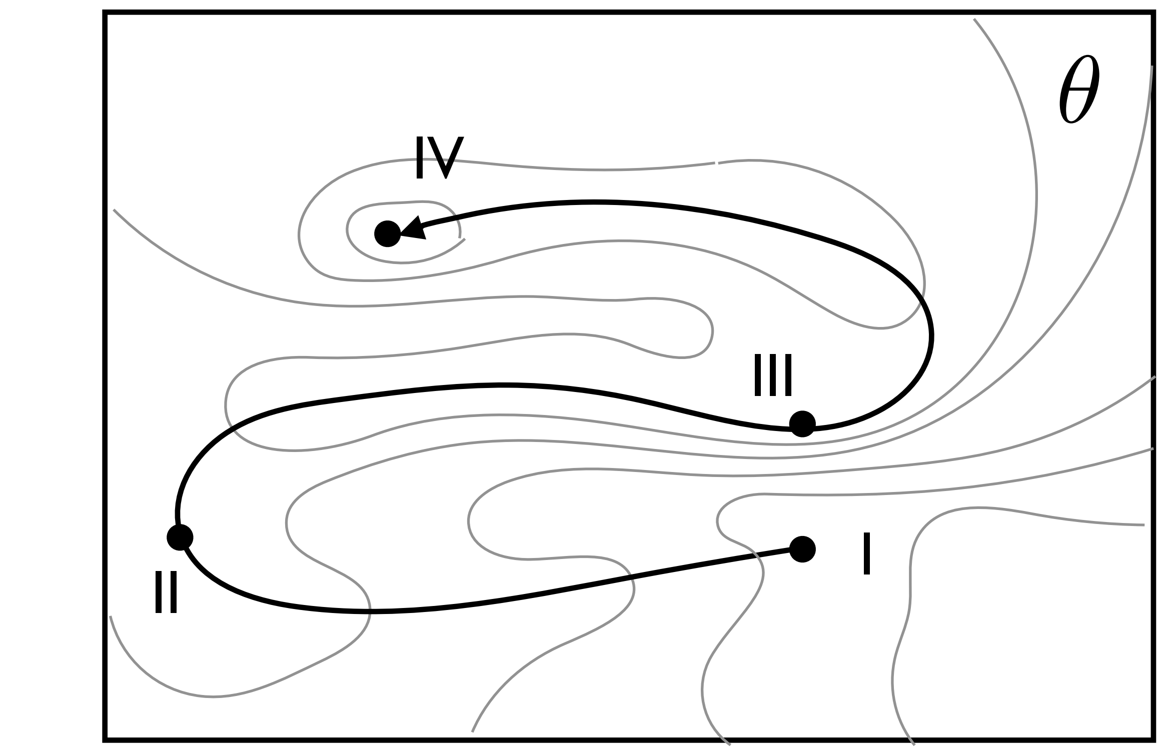
$$\psi_0' = A_0'(\psi_0)\sigma^{-2}_{\psi_0} C\psi_0 \qquad \sigma^2_{\psi_0} = \langle \mathcal{C}\psi_0\psi_0^\dagger\mathcal{C}^\dagger\rangle$$

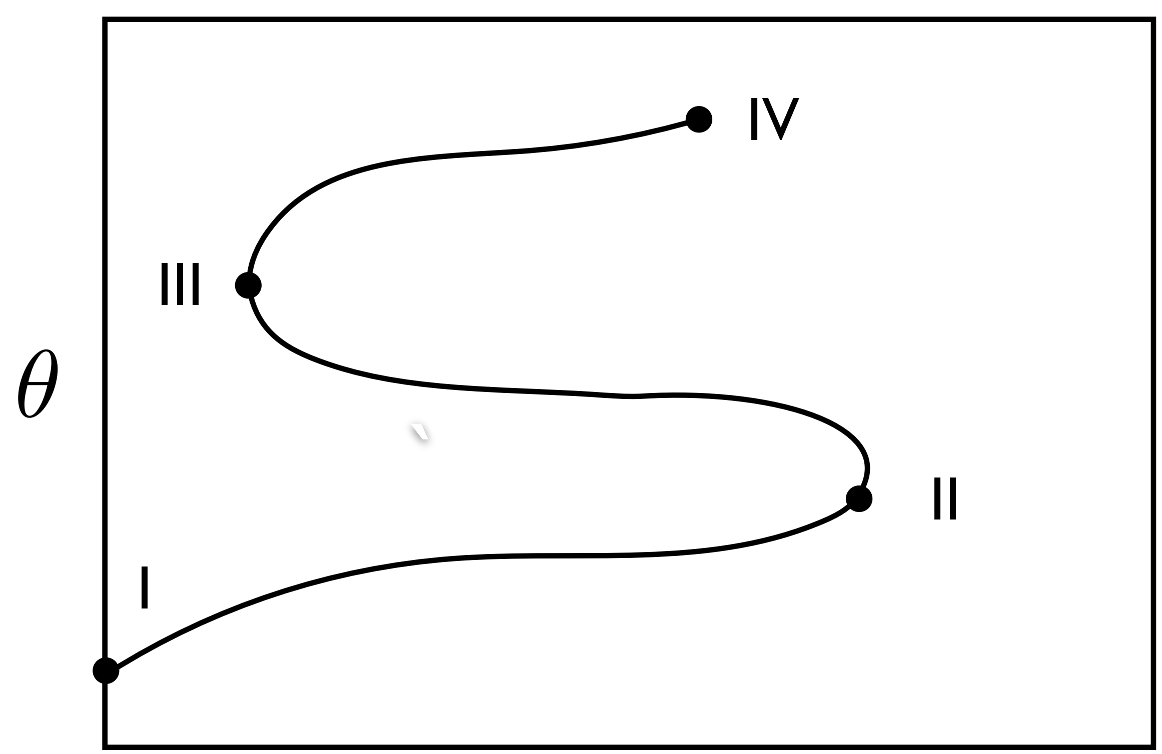
$$\psi_0 = A_0(\psi_0')\sigma^{-2}_{\psi_0'} C^\dagger\psi_0' \qquad \sigma^2_{\psi_0'} = \langle \mathcal{C}^\dagger\psi_0'\psi_0'^\dagger\mathcal{C}\rangle$$

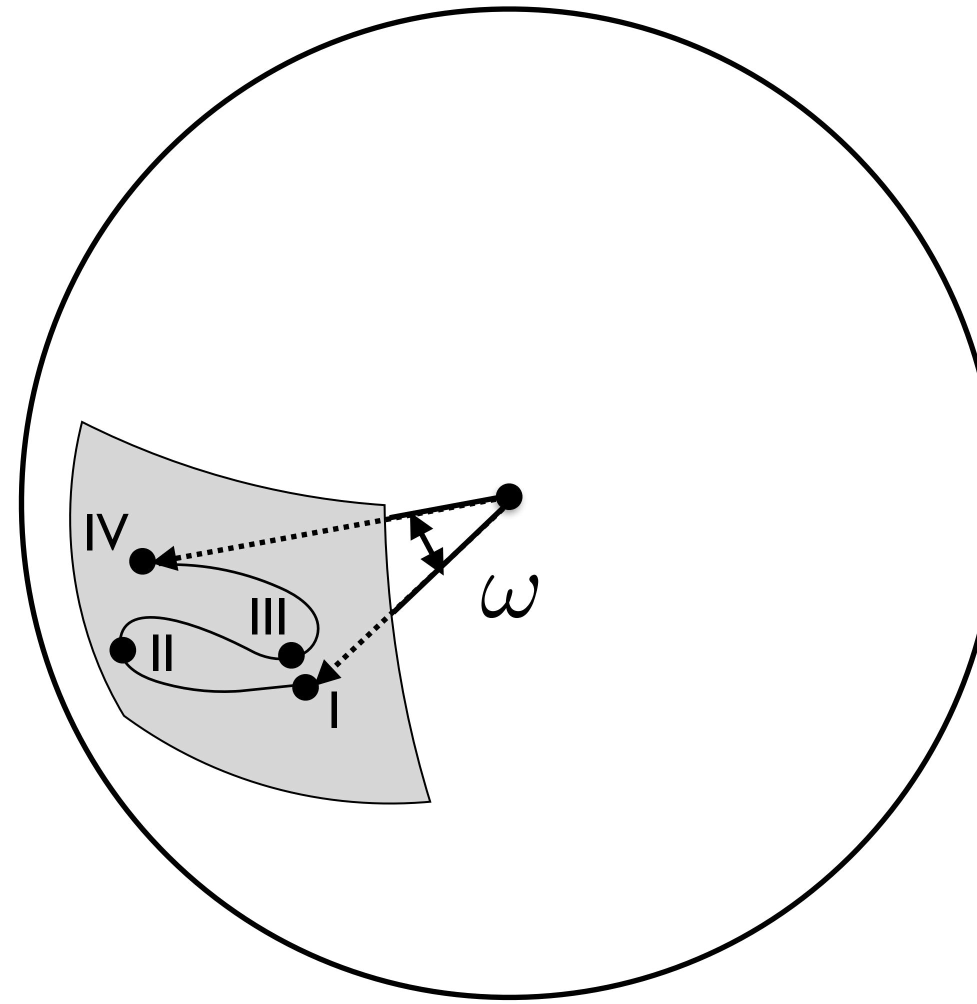
Further extensions

- √ Impose constraints on the sources and sinks
- √ Include correlations between time slices
- √ Construction of a "signal/noise basis"
  - classification of noise in correlator matrix
  - potentially useful when combined with variational methods to excise spurious noisy matrix elements (e.g., balancing statistical and systematic uncertainties)
- √ Steepest ascent: interpolate between source optimized and signal/noise optimized vectors

Path of steepest ascent







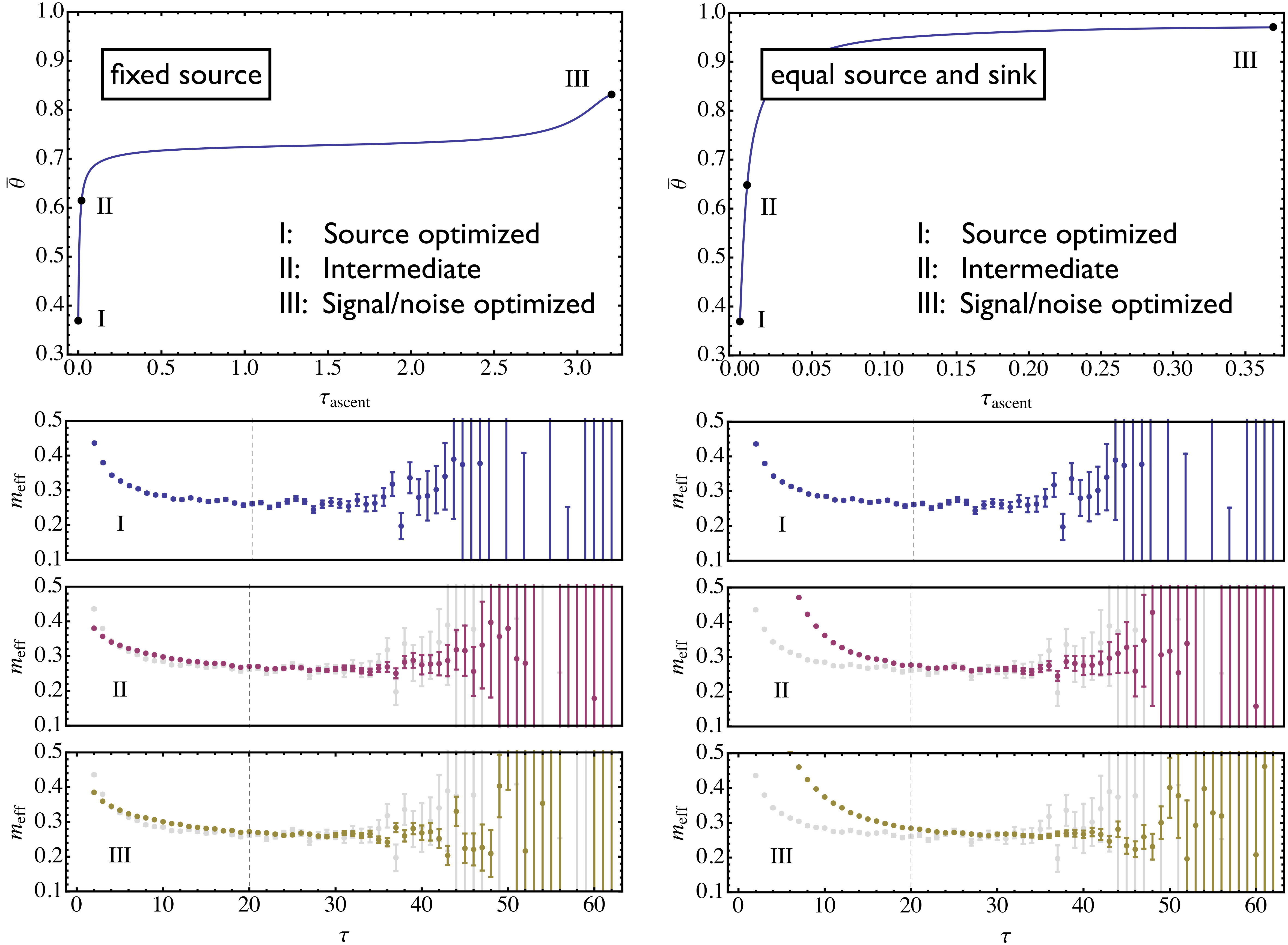
Continuous interpolation between:

I: Source optimized vector
II, III: Intermediate vectors
IV: Signal/noise optimized vector

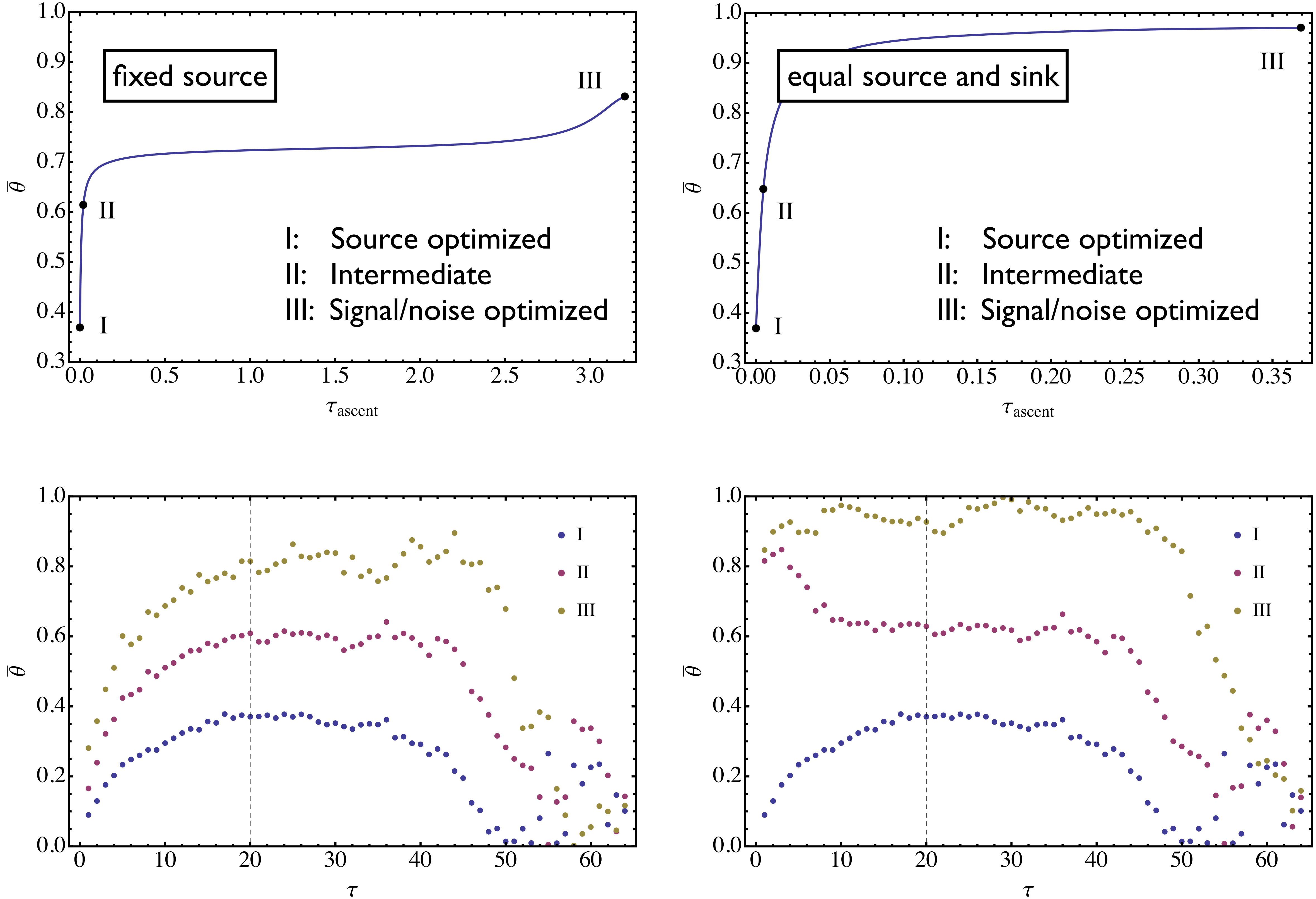
Application to QCD: single hadrons

- Looked at single hadron correlator matrices
  - pion, nucleon, delta baryon and rho
- For this talk, I'll focus on a 5x5 delta baryon correlator
  - 305 anisotropic field configurations (2+1 flavors)
    - courtesy of William & Mary
  - 20^3x128 lattice, 390 MeV pions
  - 30 randomly placed Gaussian smeared sources (quark-level), and zero-momentum projected Gaussian smeared sinks (hadron level)

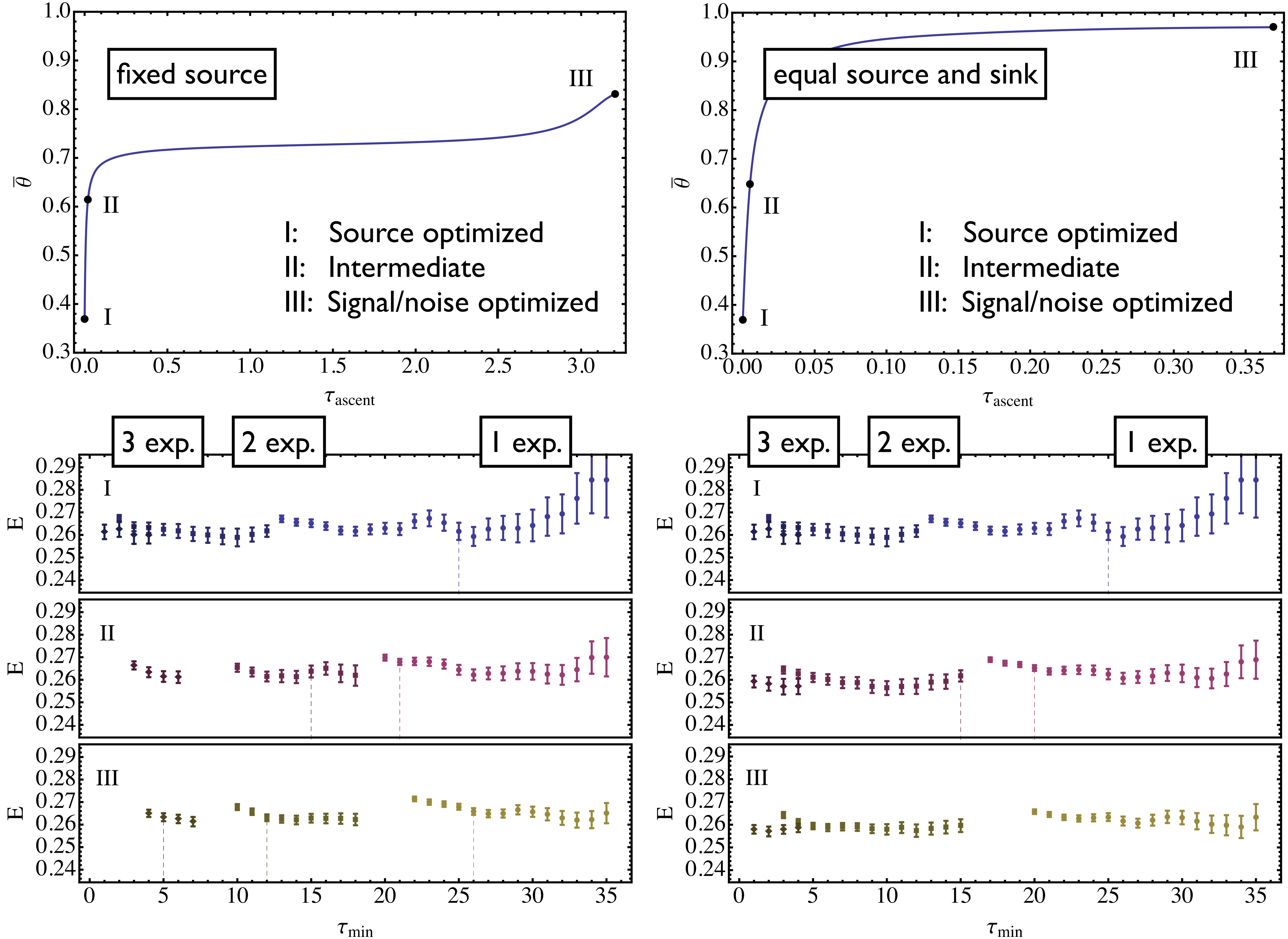
Application to QCD: delta baryon



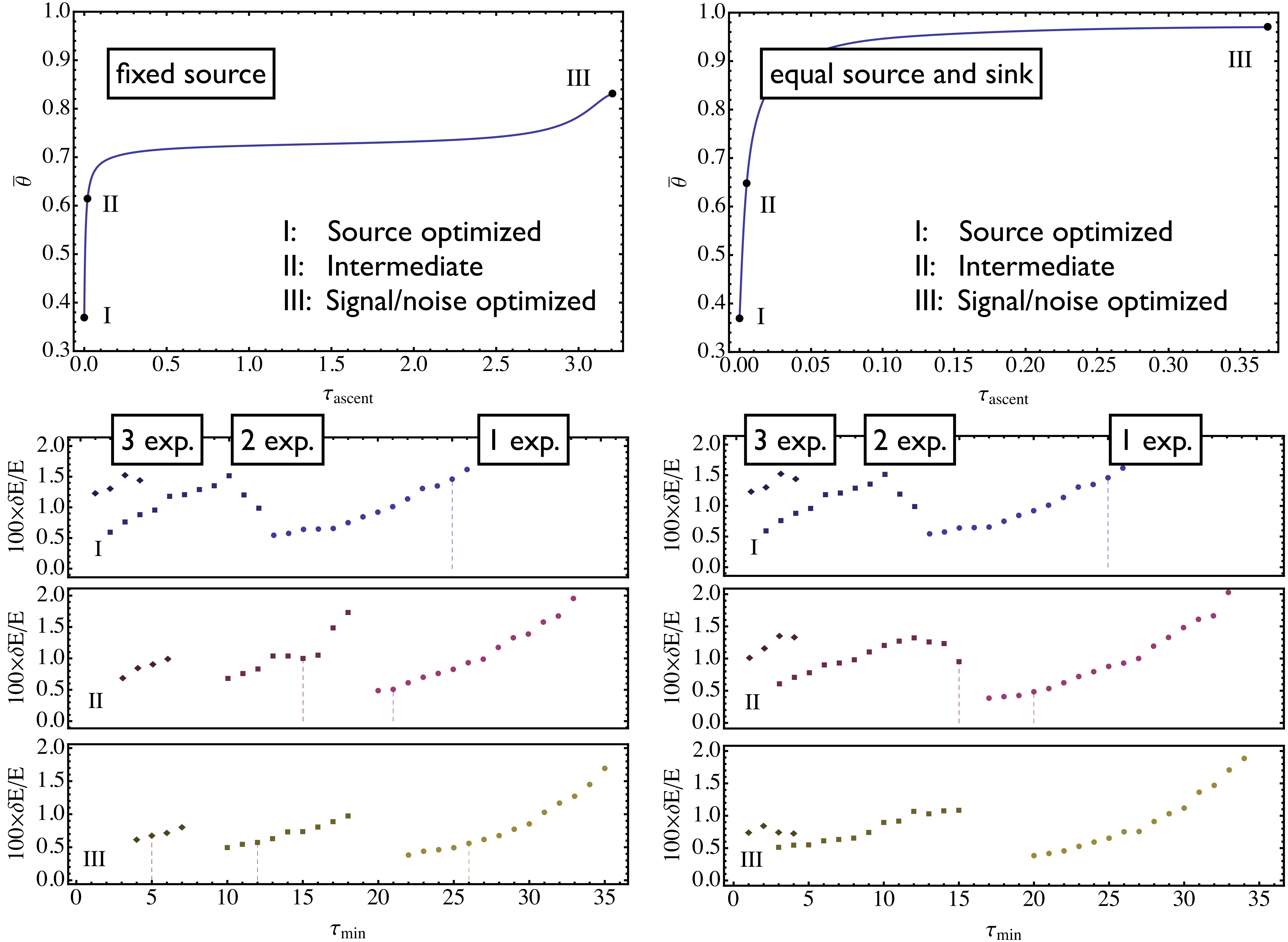
Application to QCD: delta baryon



Application to QCD: delta baryon

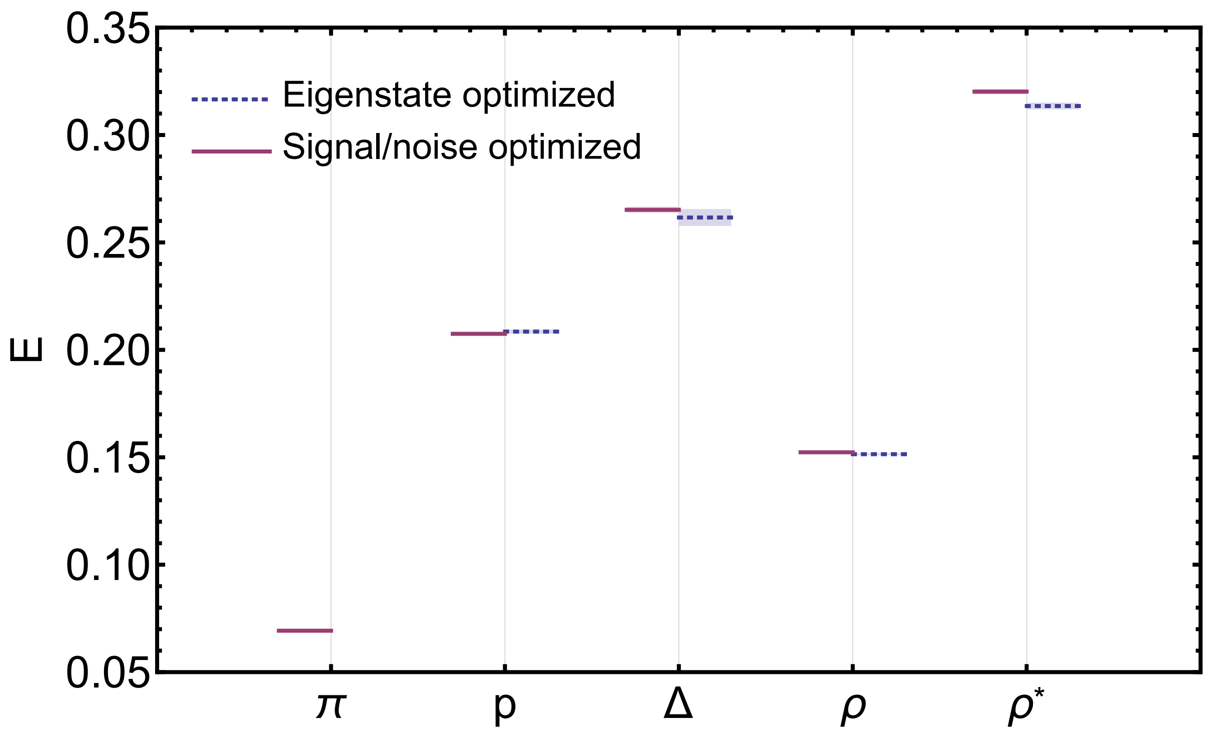


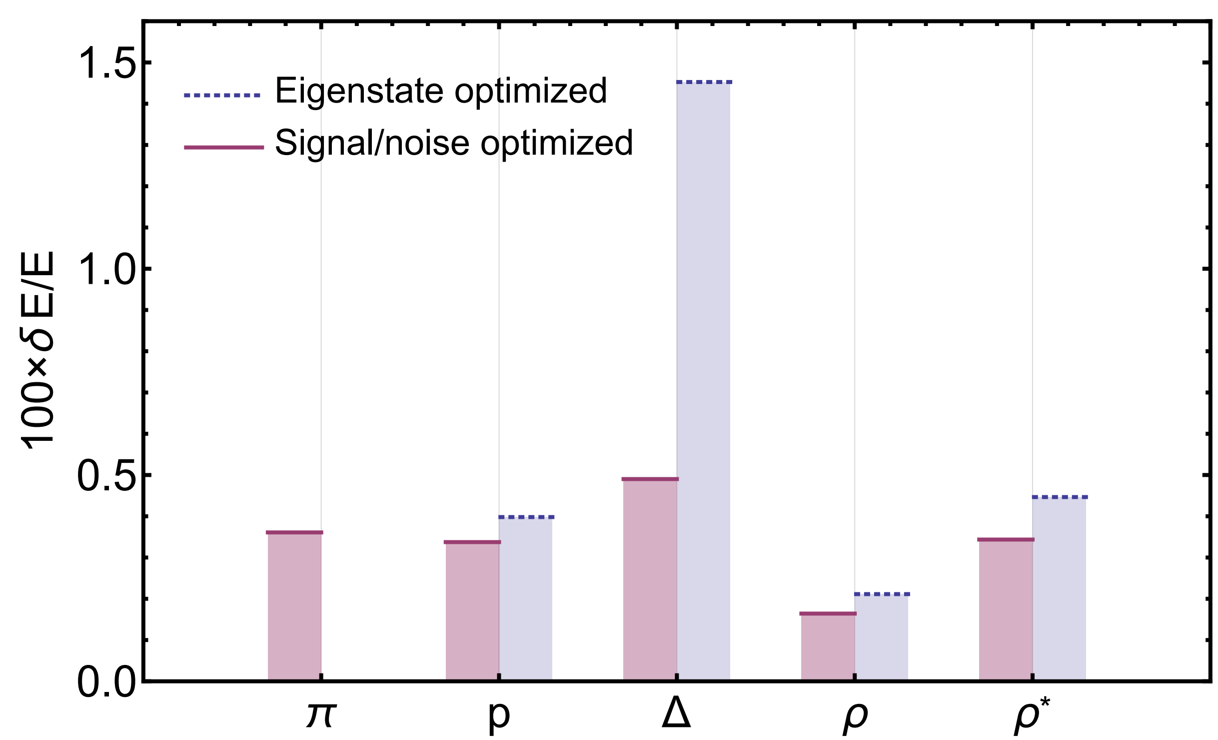
Application to QCD: delta baryon



Signal/noise in correlation functions

Single hadron correlators:
— some cases only result in modest enhancement
— delta baryon ~x3 enhancement





obtained with χ^2/dof threshold of 1.1

Possibilities for further enhancement

- Use the fact that sinks are cheap
  - variational method to obtain a source with good eigenstate overlap
  - create correlators using an enormous basis of operators at sink and the good source, then signal/noise optimize sink
  - if a source exists which can project out lowest energy noise states, this strategy will find them
- Allow mixing of quantum numbers at sink
  - no effect on the signal, no excited state contamination
  - nontrivial off-diagonal contributions to the noise correlator

Conclusion and future directions

- Proposed a new avenue for correlator optimization:
  - many possibilities not discussed (see paper)
  - idea is general, applicable to systems beyond QCD
  - applicable to excited states
- Many unexplored directions:
  - multi-nucleon systems
  - disconnected diagrams
  - three-point functions

Thank you for your attention!