

Analysis of nucleon excited states from lattice QCD with the Bayesian Reconstruction



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Collaborators: Raza Sabbir Sufian, Jian Liang, Terrence Draper, Keh-Fei Liu
(χ QCD collaboration)

Inverse Problems and UQ in Nuclear Physics
INT Workshop 24-88W
July 10th, 2024

Outline

- Introduction
 - Finite-volume spectrum from lattice QCD
- How to extract finite-volume spectrum from lattice QCD
 - Multi-exponential fit
 - Variational methods (GEVP)
 - An example: Roper state from lattice QCD
- Application of the Bayesian Reconstruction
- Conclusion and outlook

The path integral in the Euclidean space - lattice QCD

- Observables from the path integral (Minkowski):

Perturbative expansions

$$\langle O \rangle = \frac{\int \mathcal{D}\phi O e^{iS_M(\phi)}}{\int \mathcal{D}\phi e^{iS_M(\phi)}} \longleftarrow Z_M(J) = \int \mathcal{D}\phi e^{i \int d^4x \mathcal{L}_M}$$

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Wick rotation

$$t \rightarrow -i\tau$$

$$k^0 \rightarrow ik_0^E$$

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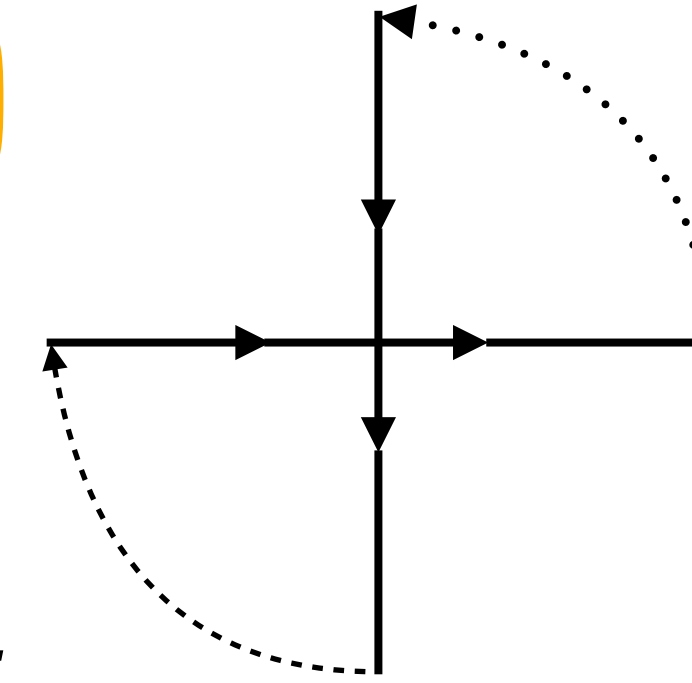
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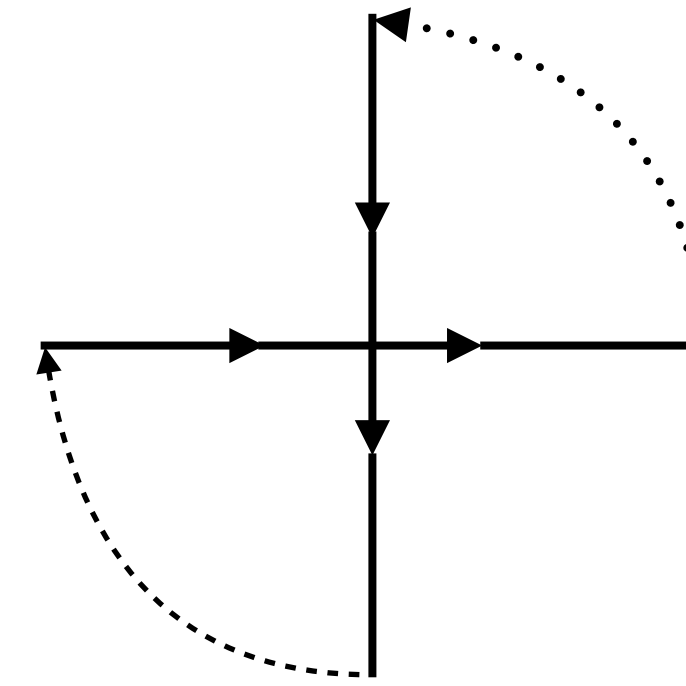
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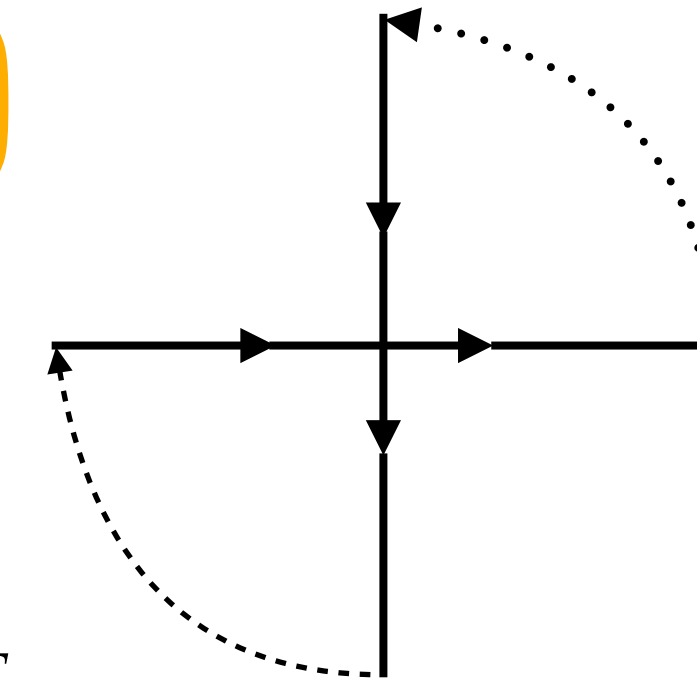
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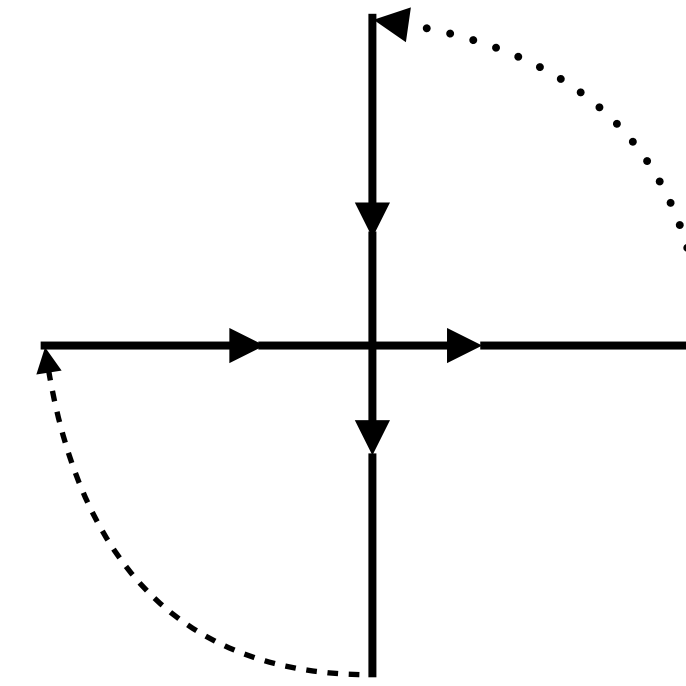
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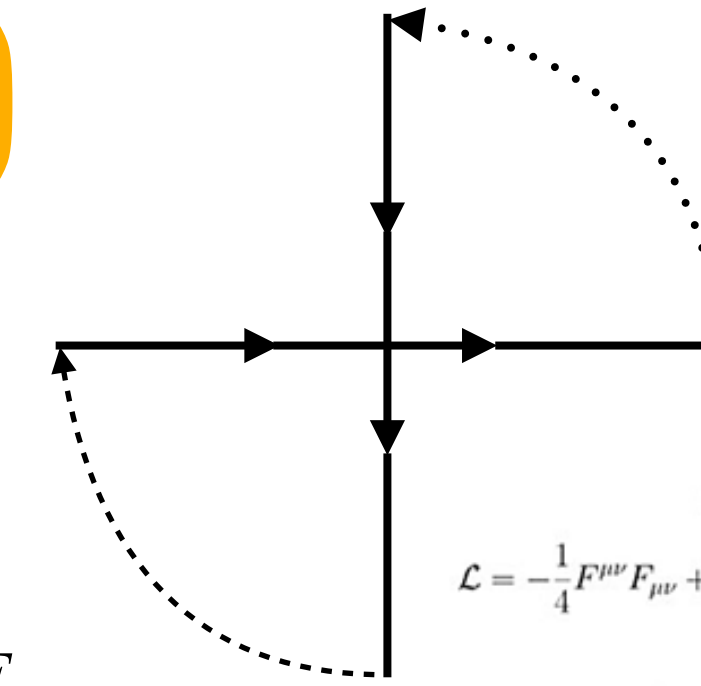
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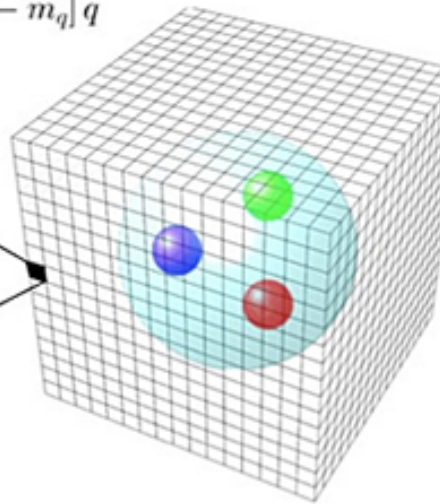
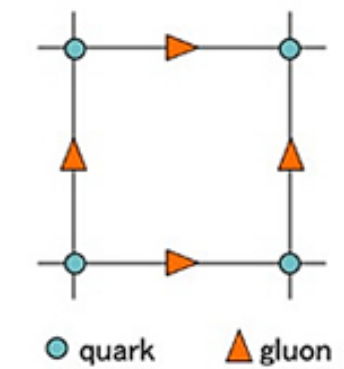
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QCD Lagrangian

$$\mathcal{L} = -\frac{1}{4} F^{\mu\nu} F_{\mu\nu} + \sum_{q=u,d,s,c,b,t} \bar{q} [i\gamma^\mu (\partial_\mu - igA_\mu) - m_q] q$$



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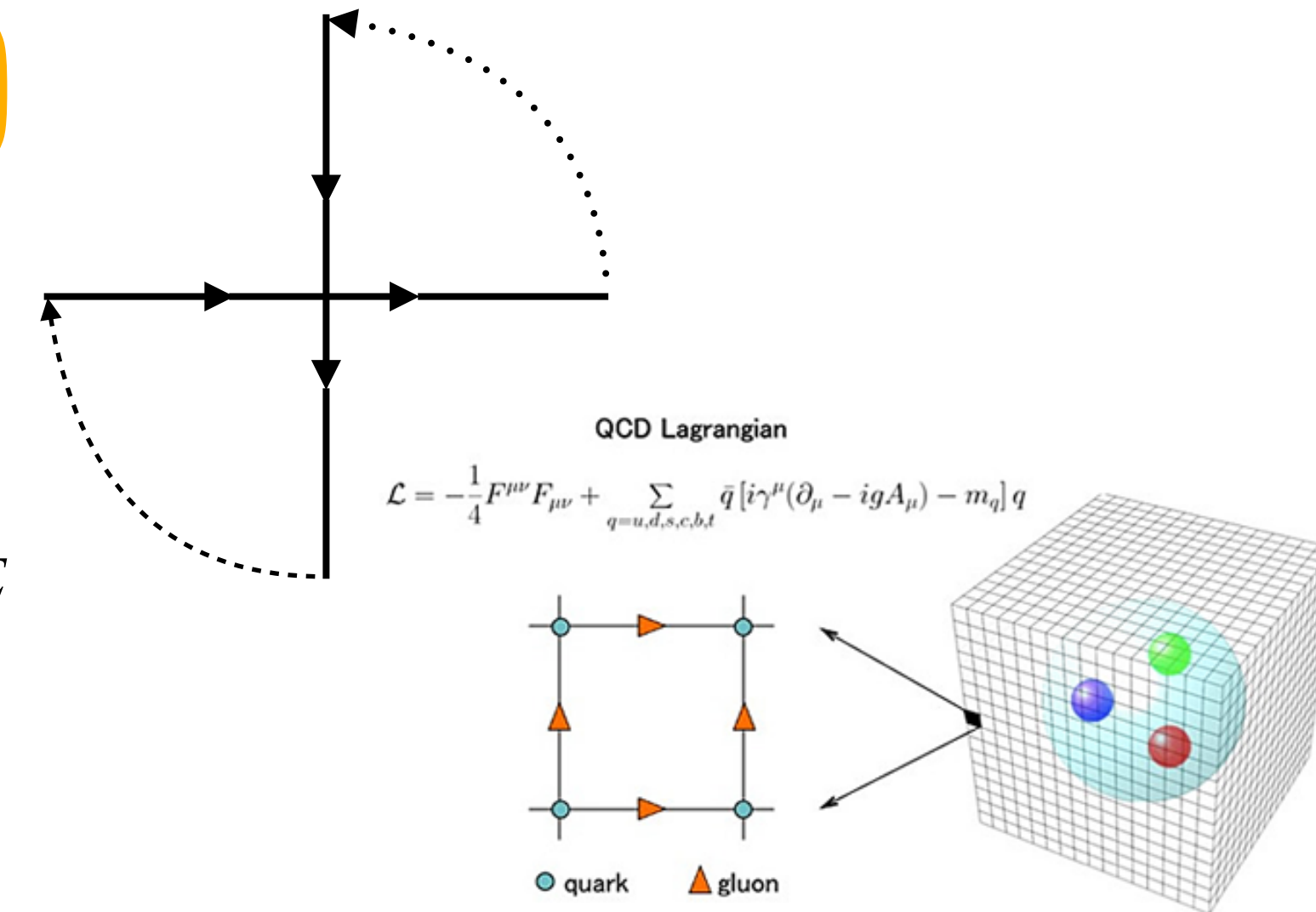
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Non-perturbative

Input parameters

$$a, m_q, \dots, \alpha_s, \dots$$

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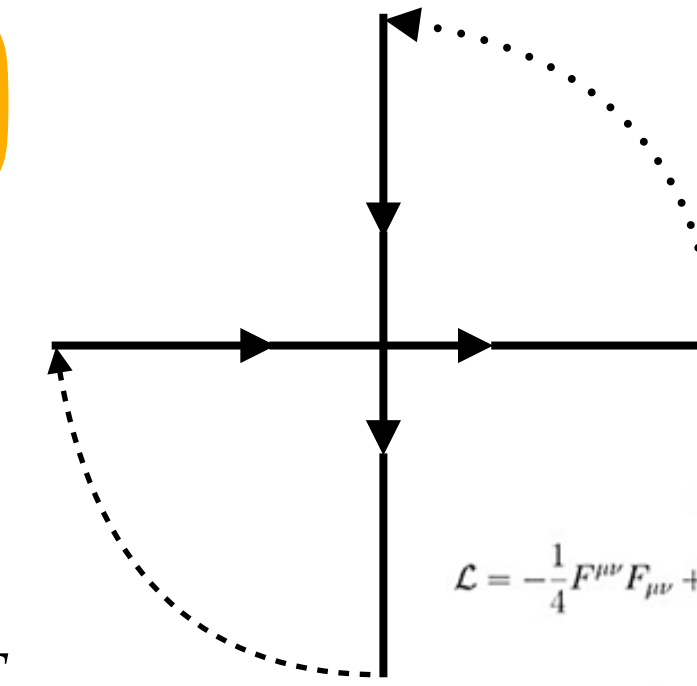
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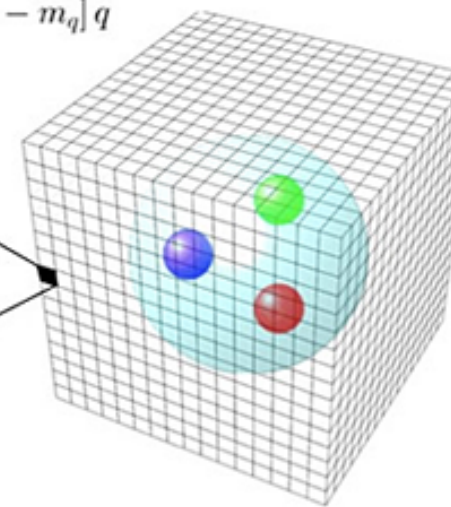
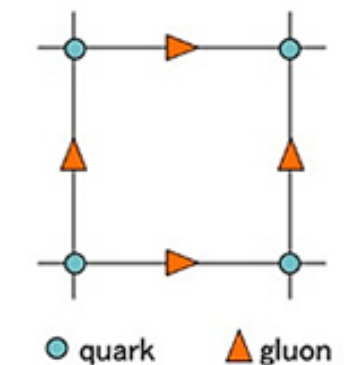
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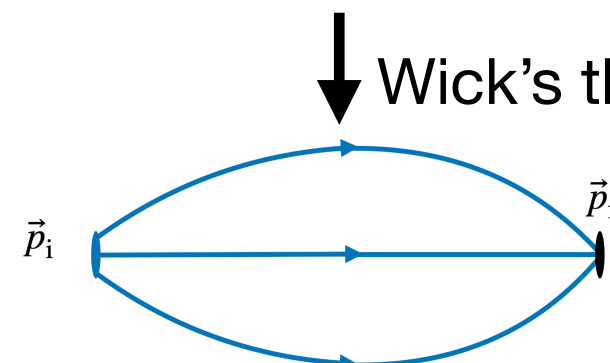
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E.g. n -point correlation functions

$$\langle \Omega | T \phi(x_1) \dots \phi(x_n) | \Omega \rangle$$

Wick's theorem



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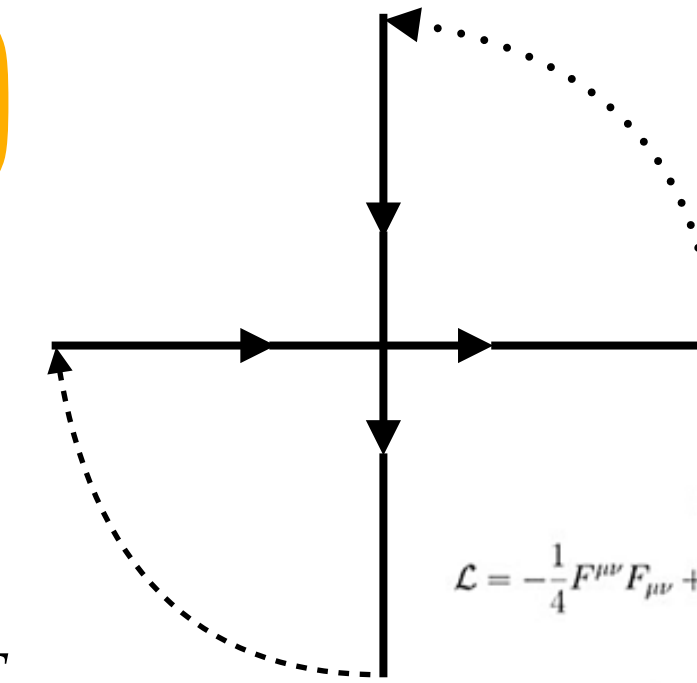
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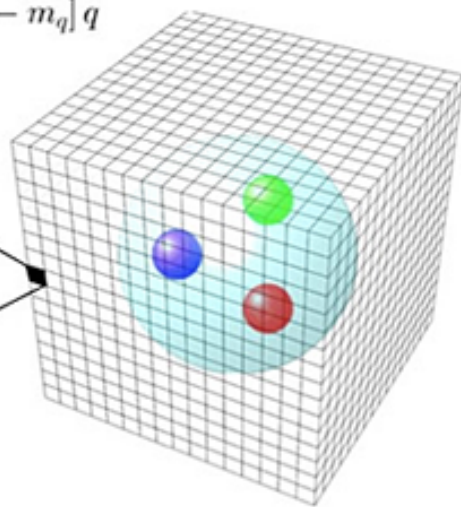
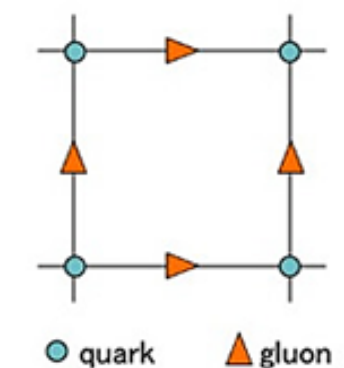
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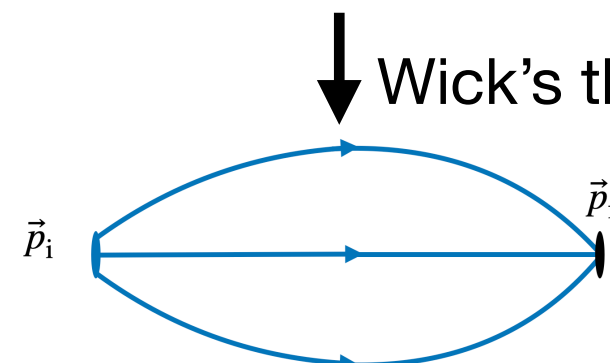
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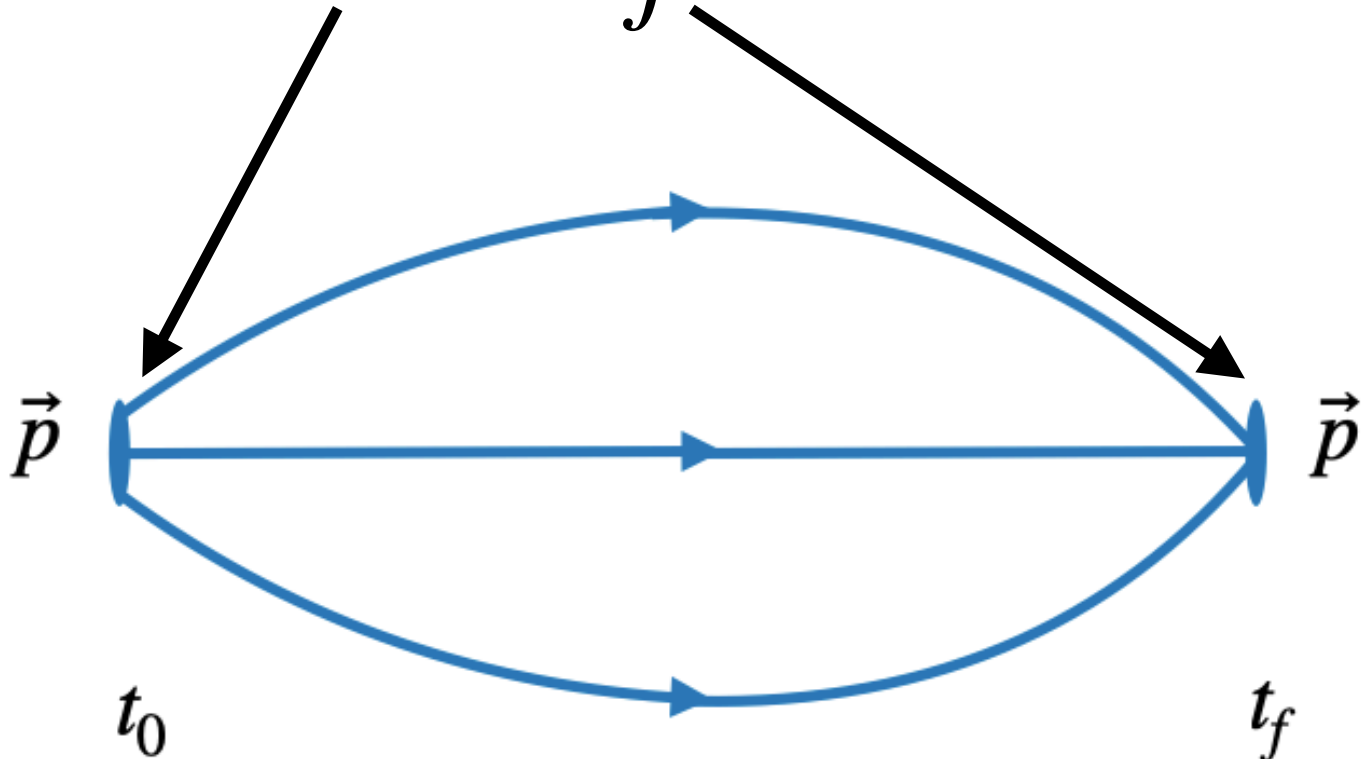
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Finite-volume spectrum, matrix elements ...

Extracting finite-volume spectrum

- What kind of observables do we measure on the lattice?
- To extract the finite-volume spectrum
 - Two-point correlation functions

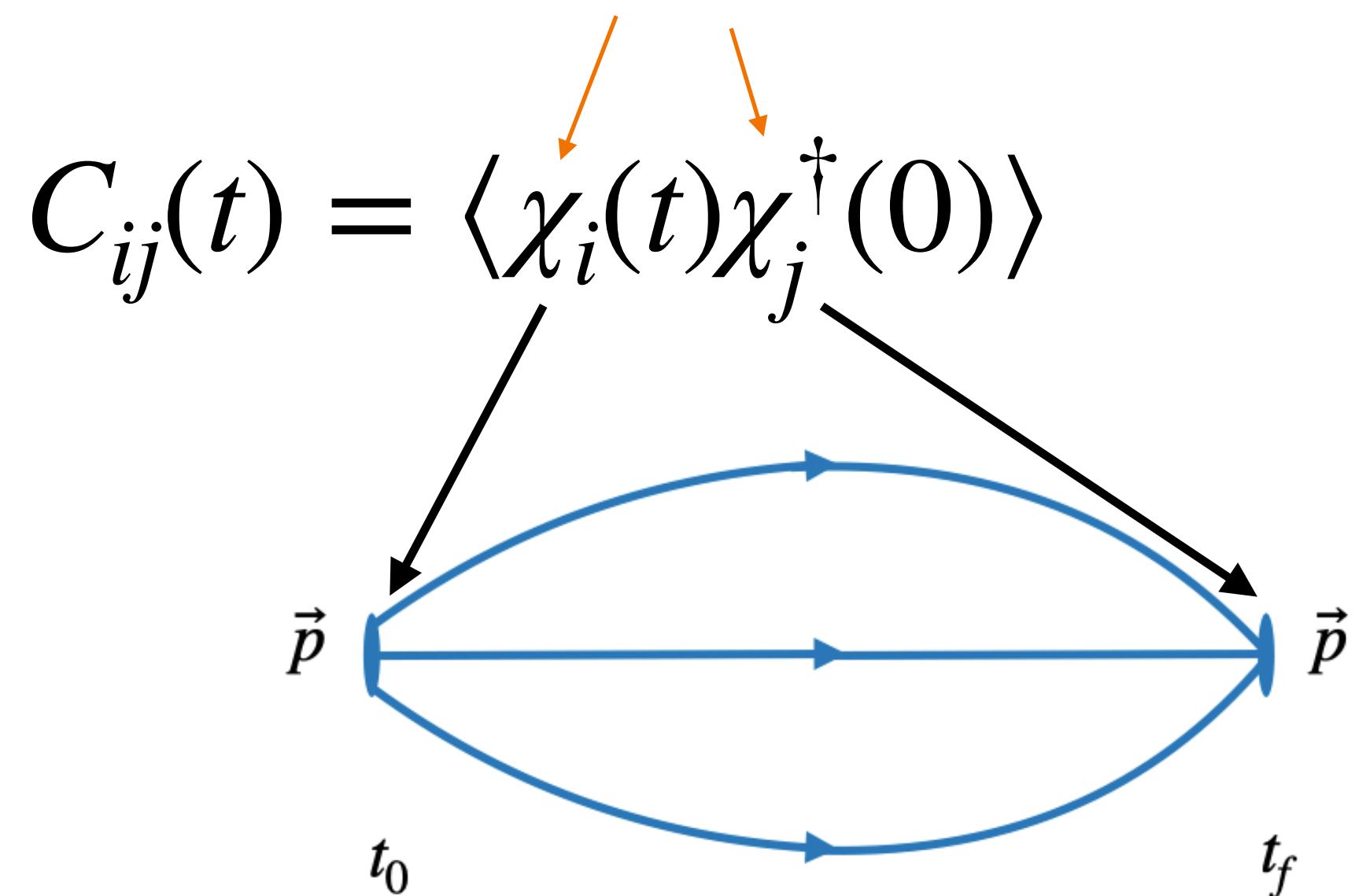
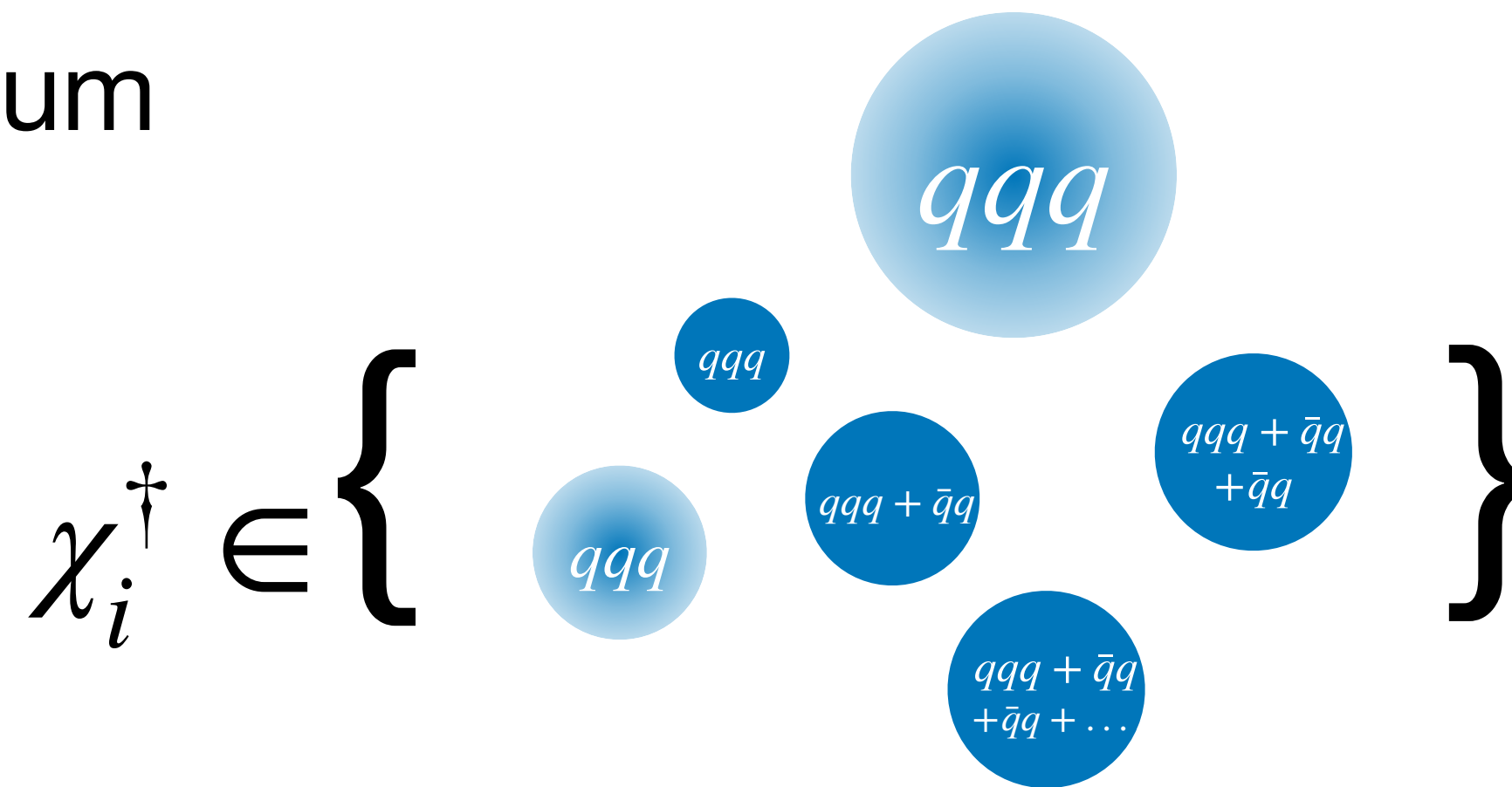
$$C_{ij}(t) = \langle \chi_i(t) \chi_j^\dagger(0) \rangle$$


The diagram illustrates a two-point correlation function on a lattice. It shows two time slices, t_0 and t_f , with momentum vectors \vec{p} . A central horizontal arrow points from t_0 to t_f . Two curved arrows, one above and one below the horizontal one, also point from t_0 to t_f . Arrows from the equation above point to the top and bottom curved arrows, indicating they represent the operators $\chi_i(t)$ and $\chi_j^\dagger(0)$ respectively.

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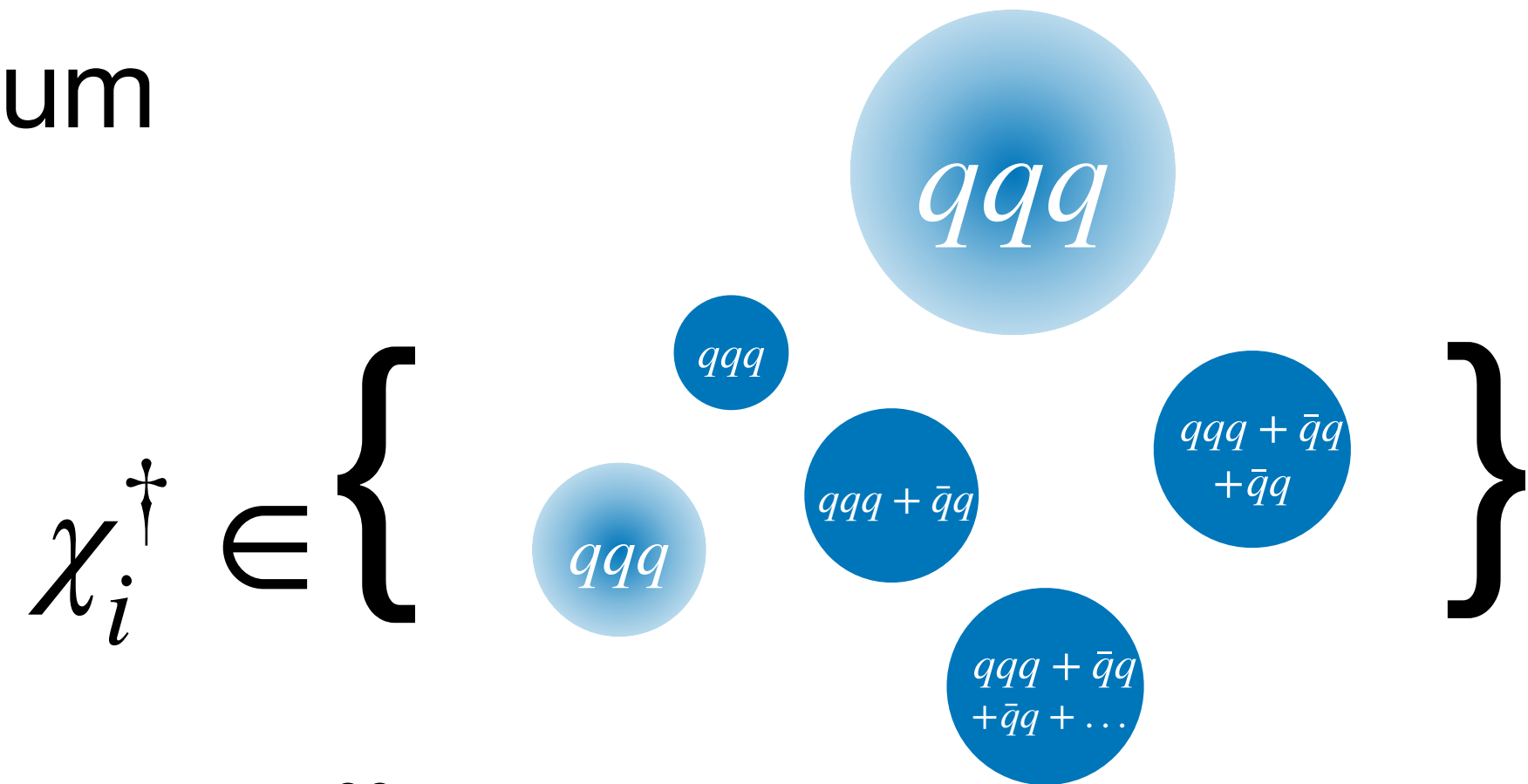
interpolating operators with the same quantum numbers as the hadron state



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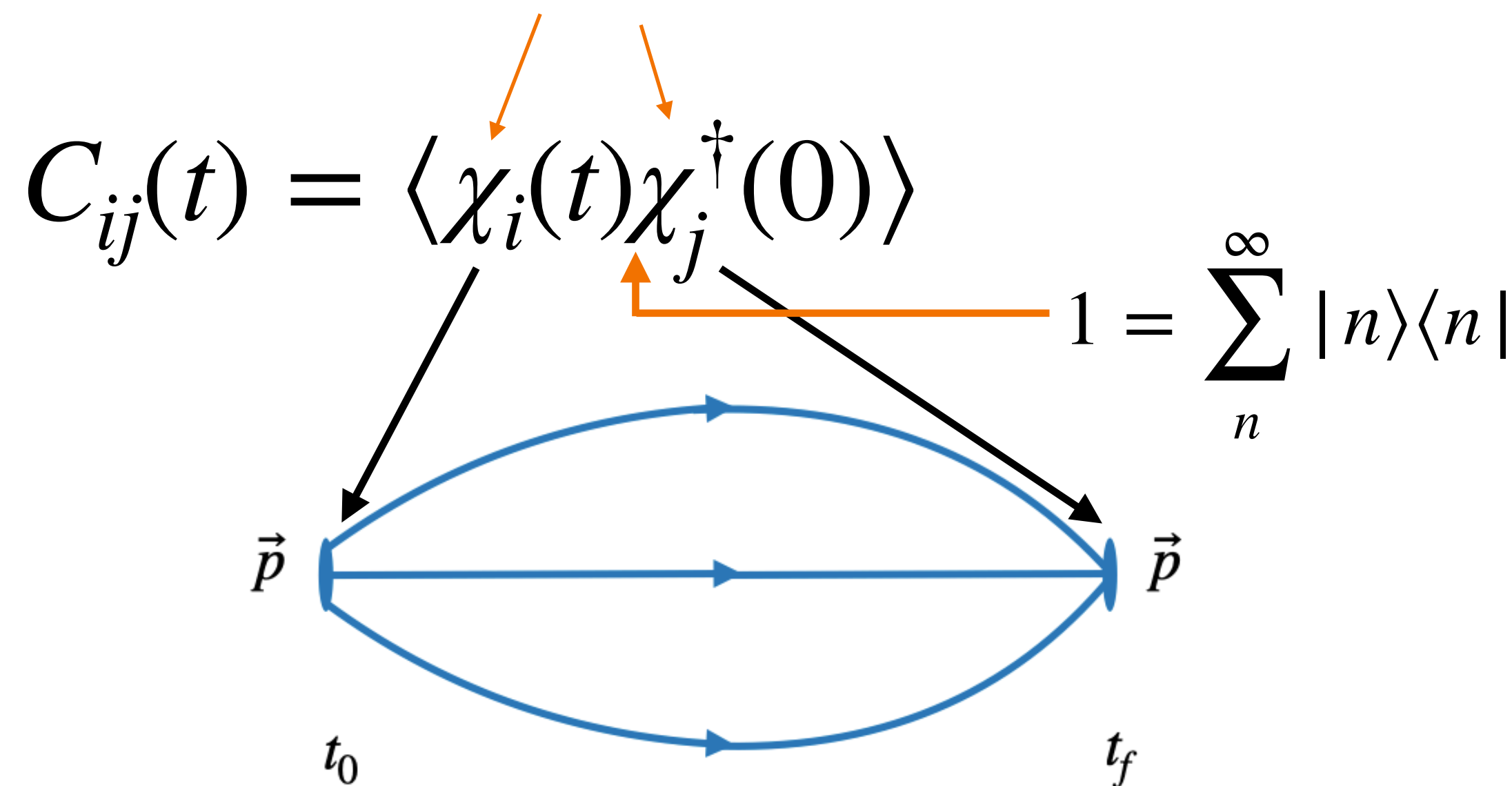
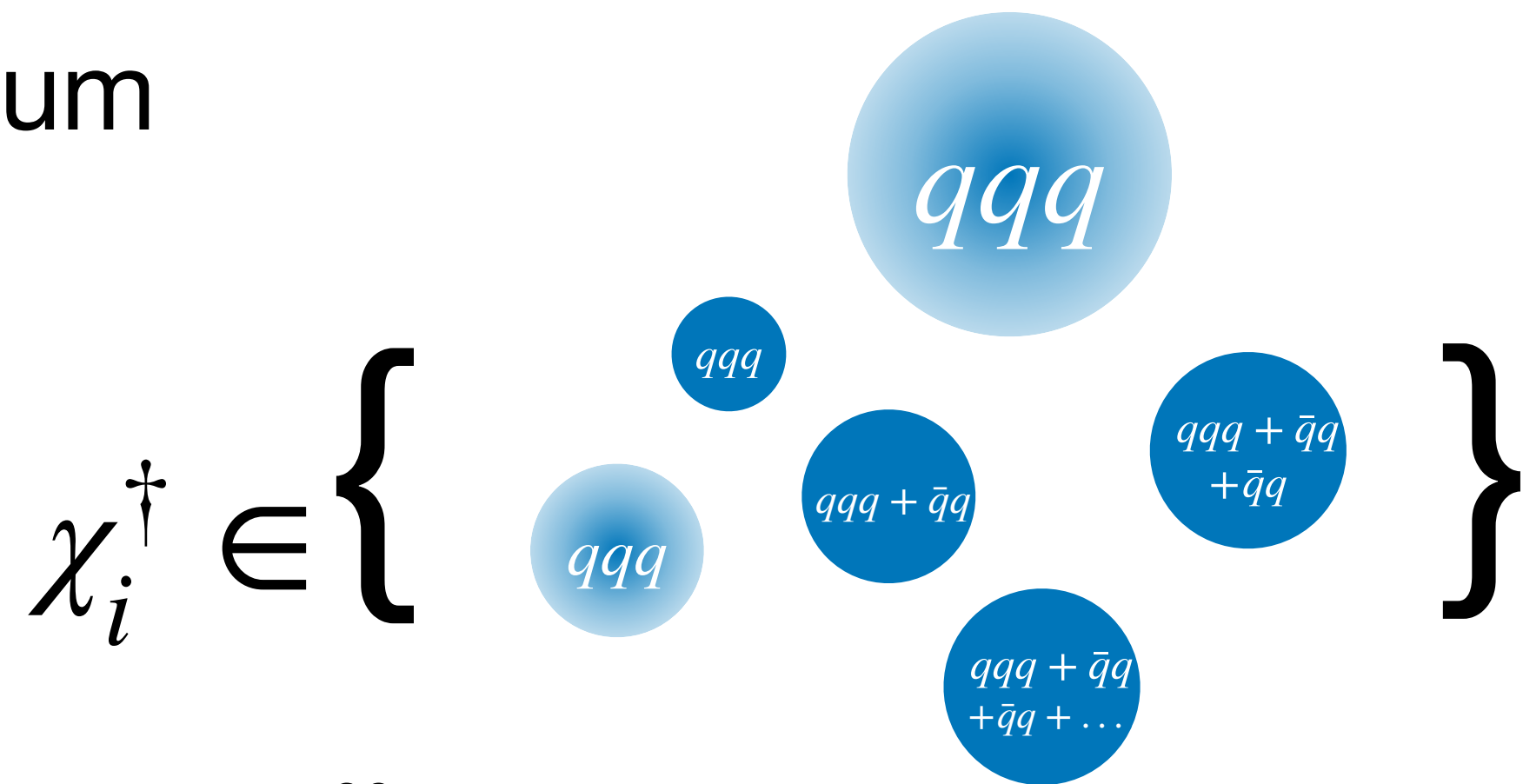
$$C_{ij}(t) = \langle \chi_i(t) \chi_j^\dagger(0) \rangle \rightarrow \sum_{n=0}^{\infty} \langle \Omega | \chi_N | n \rangle \langle n | \chi_N^\dagger | \Omega \rangle e^{-E_n t}$$

$1 = \sum_n |n\rangle \langle n|$

Extracting finite-volume spectrum

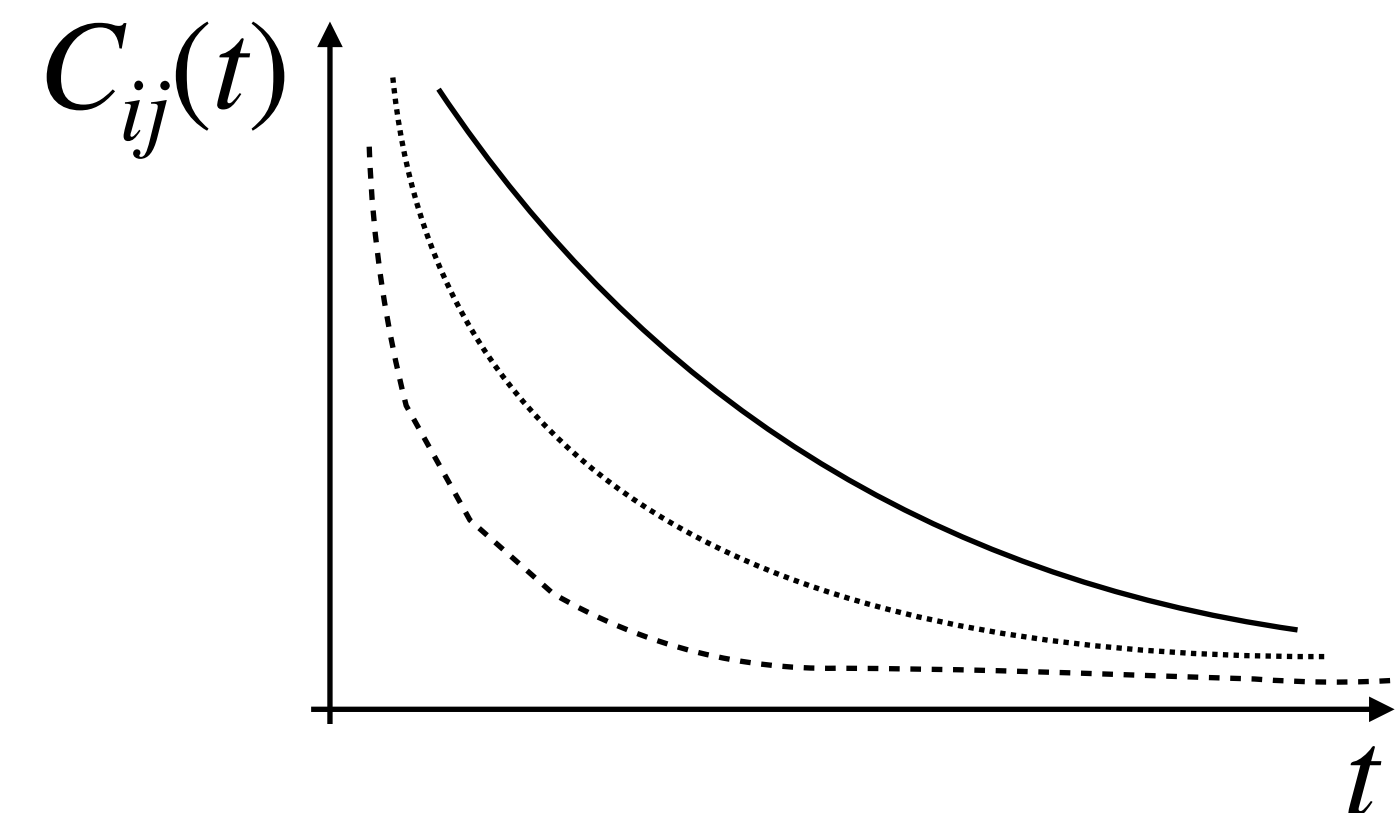
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$$\rightarrow \sum_{n=0}^{\infty} \langle \Omega | \chi_N | n \rangle \langle n | \chi_N^\dagger | \Omega \rangle e^{-E_n t}$$

$$\rightarrow \sum_{n=0}^{\infty} W_n e^{-E_n t}$$



Multi-exponential fit

- To extract the finite-volume spectrum

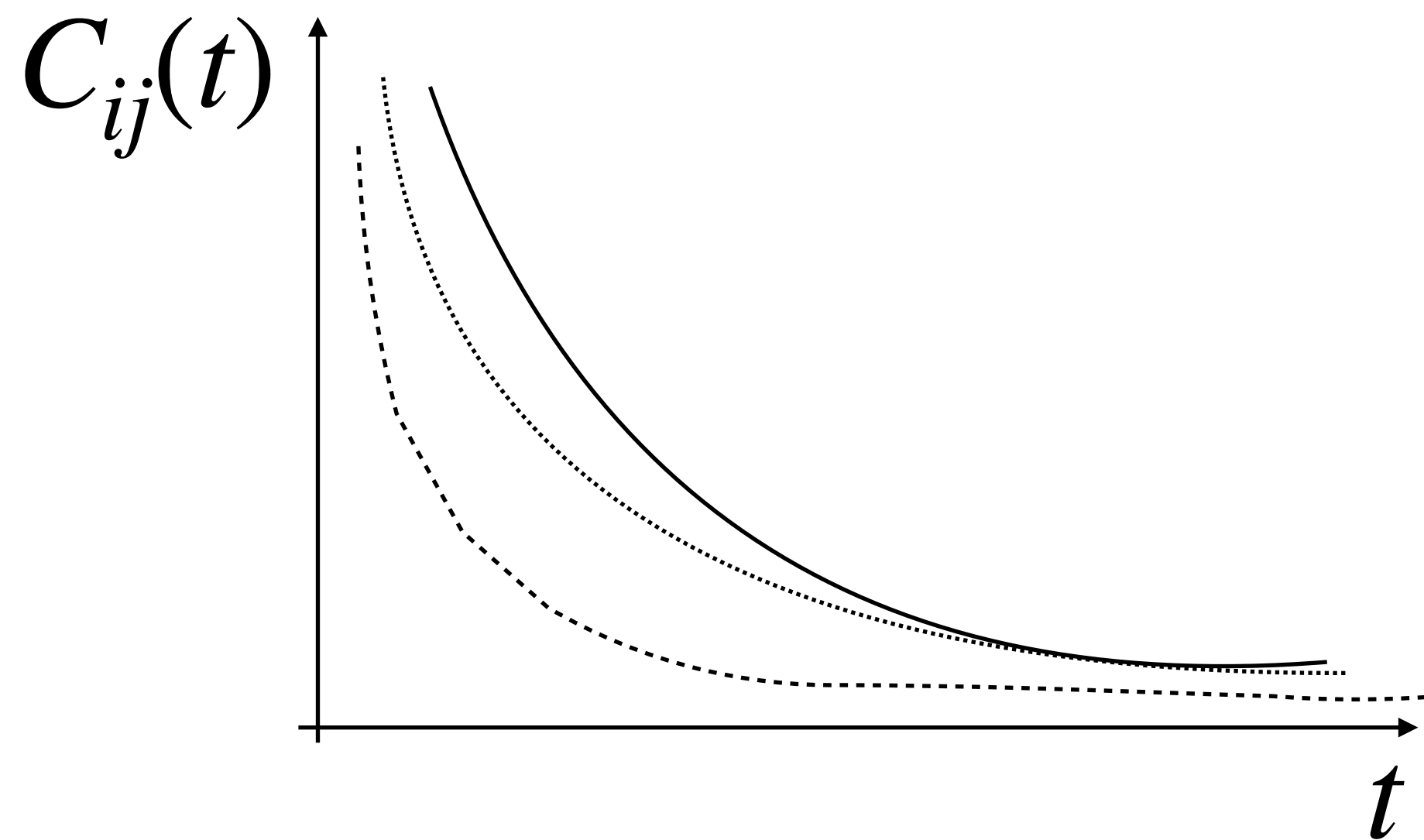
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Constraint 1

$t \gg 0$

$$C_{N,2\text{pt}}(t) = W_0 e^{-E_0 t}$$



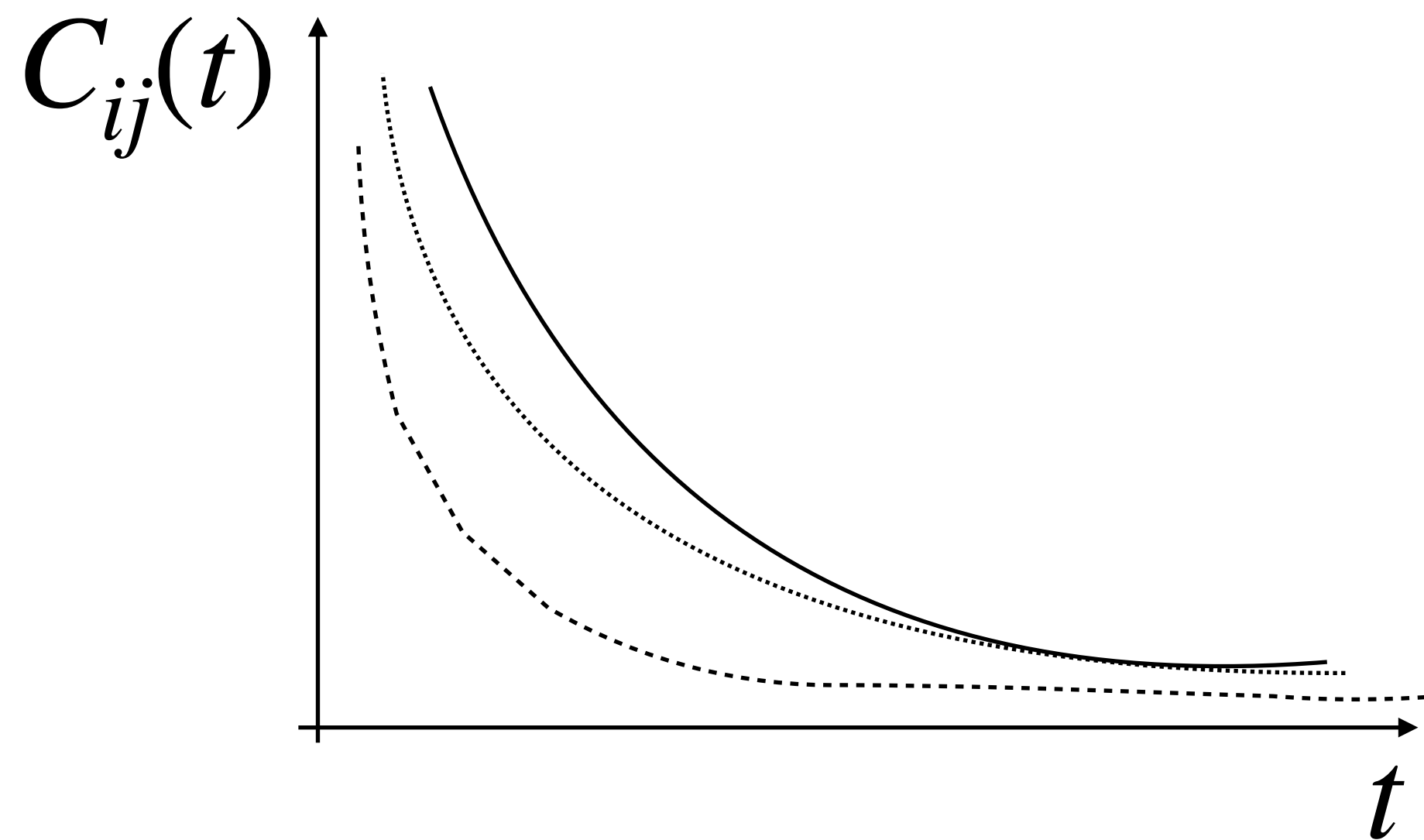
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Strongly stable hadrons
(bound states):

$\pi, K, D, \dots, n, p, \dots$

Find E_0

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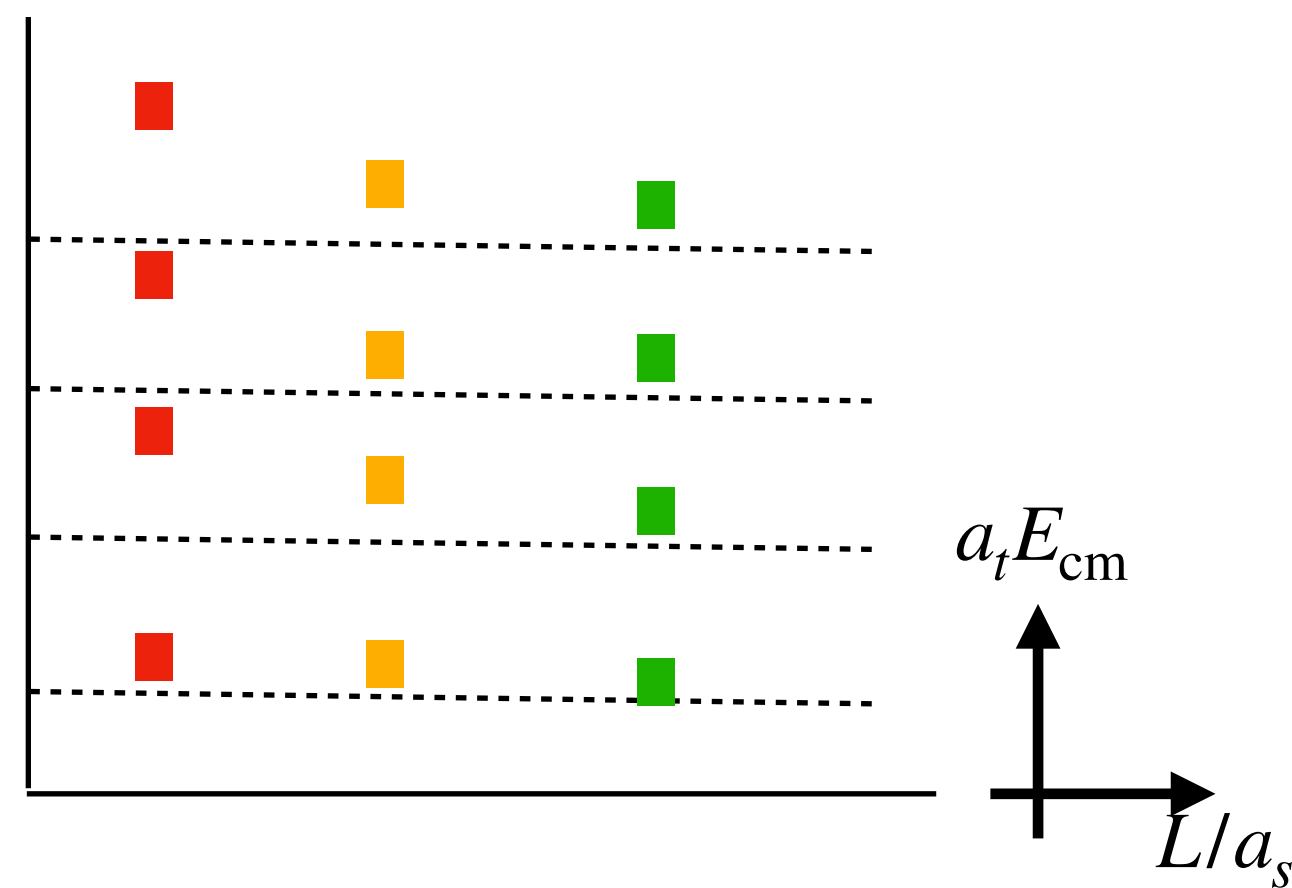
Finite-volume spectrum from lattice QCD

Finite-volume
2pt Correlation
Functions

$$C_{N,2pt}(t; \vec{p})$$

Finite-volume
spectrum

$$E_n$$



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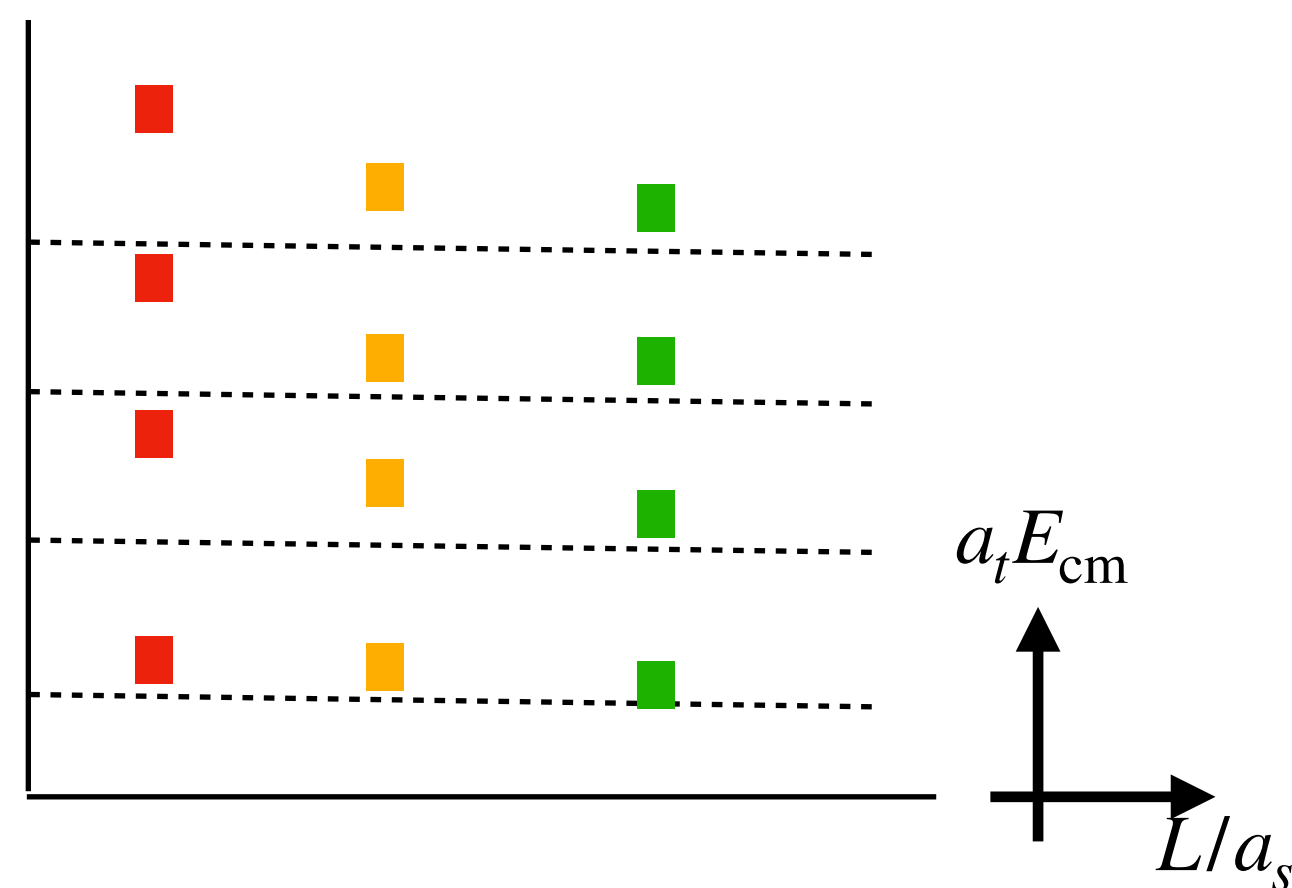
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$$E_n$$

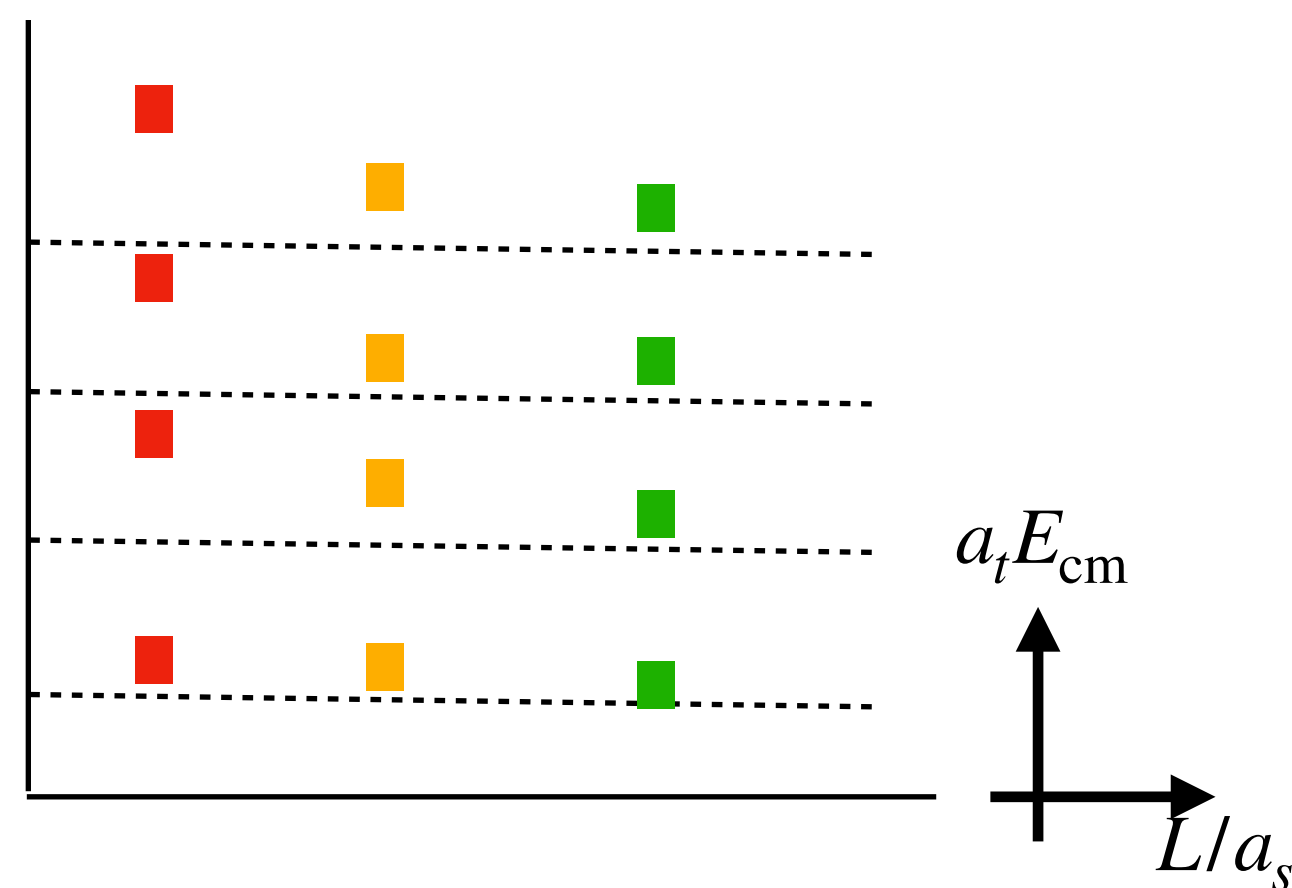
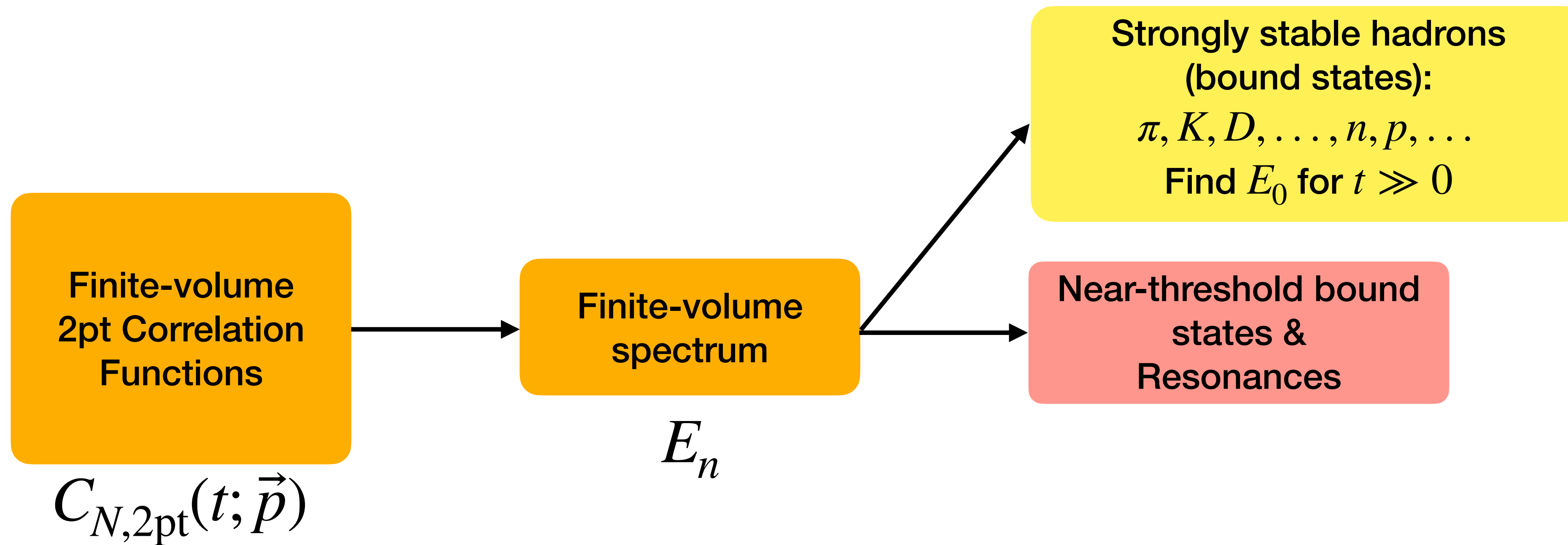
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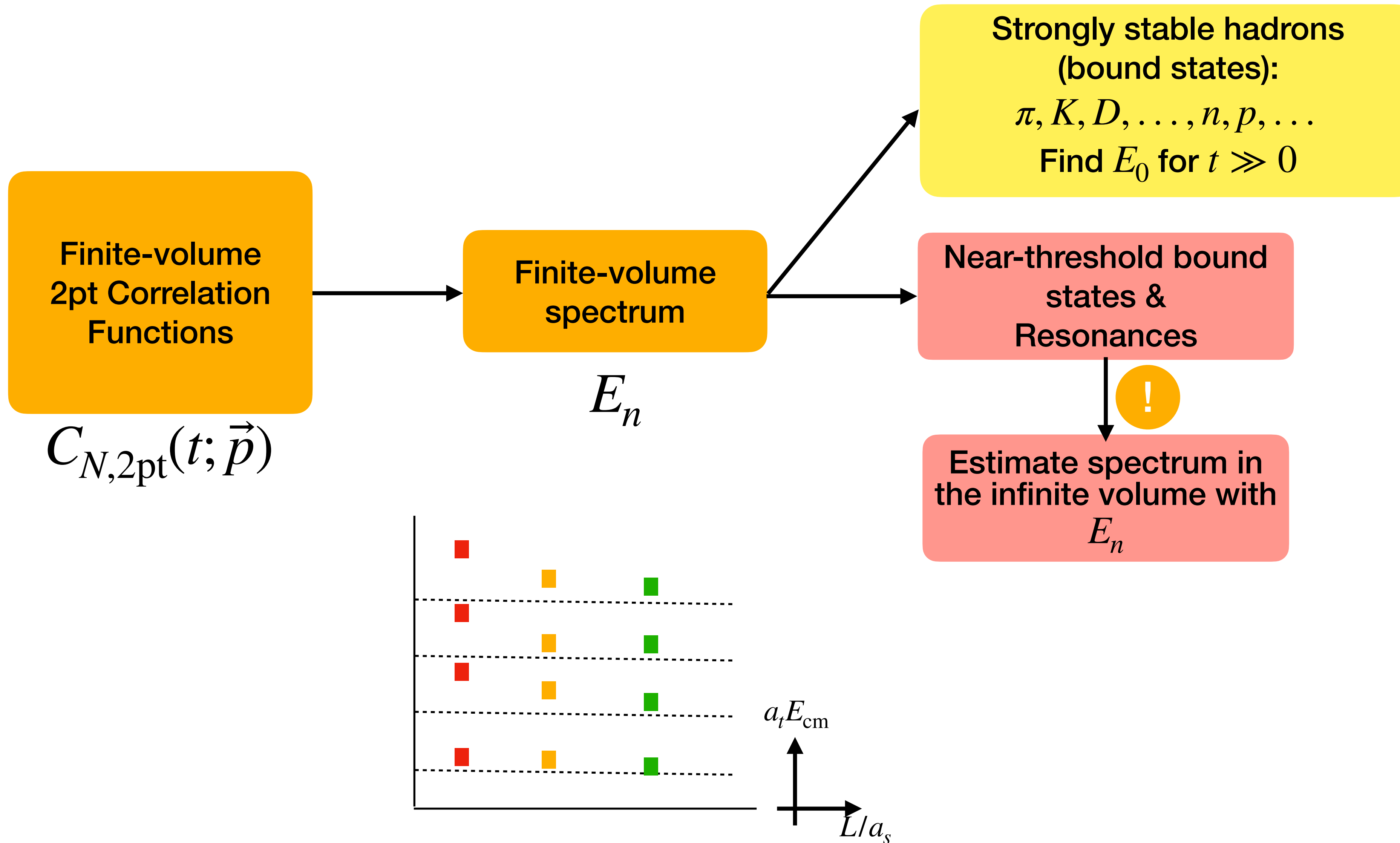
Find E_0 for $t \gg 0$



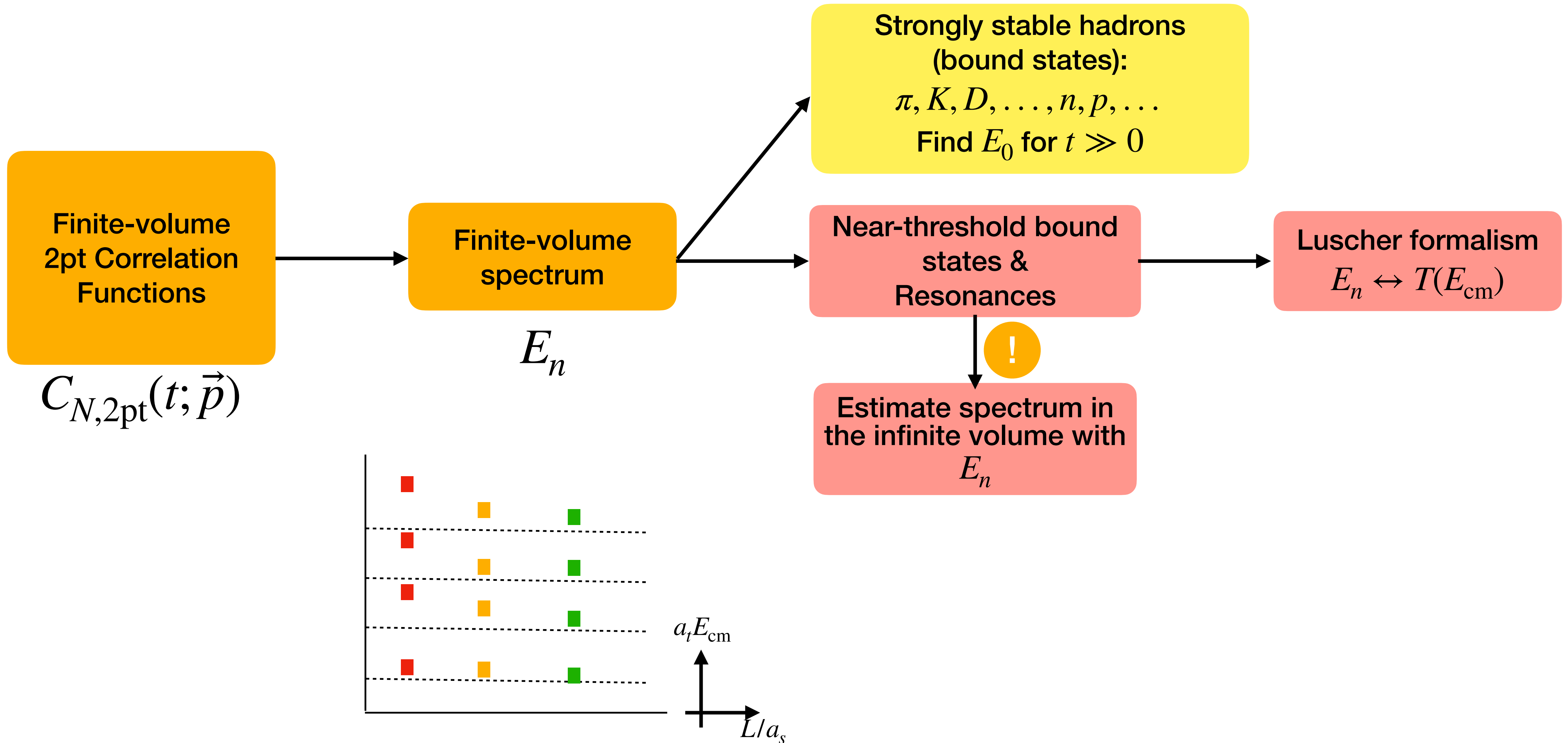
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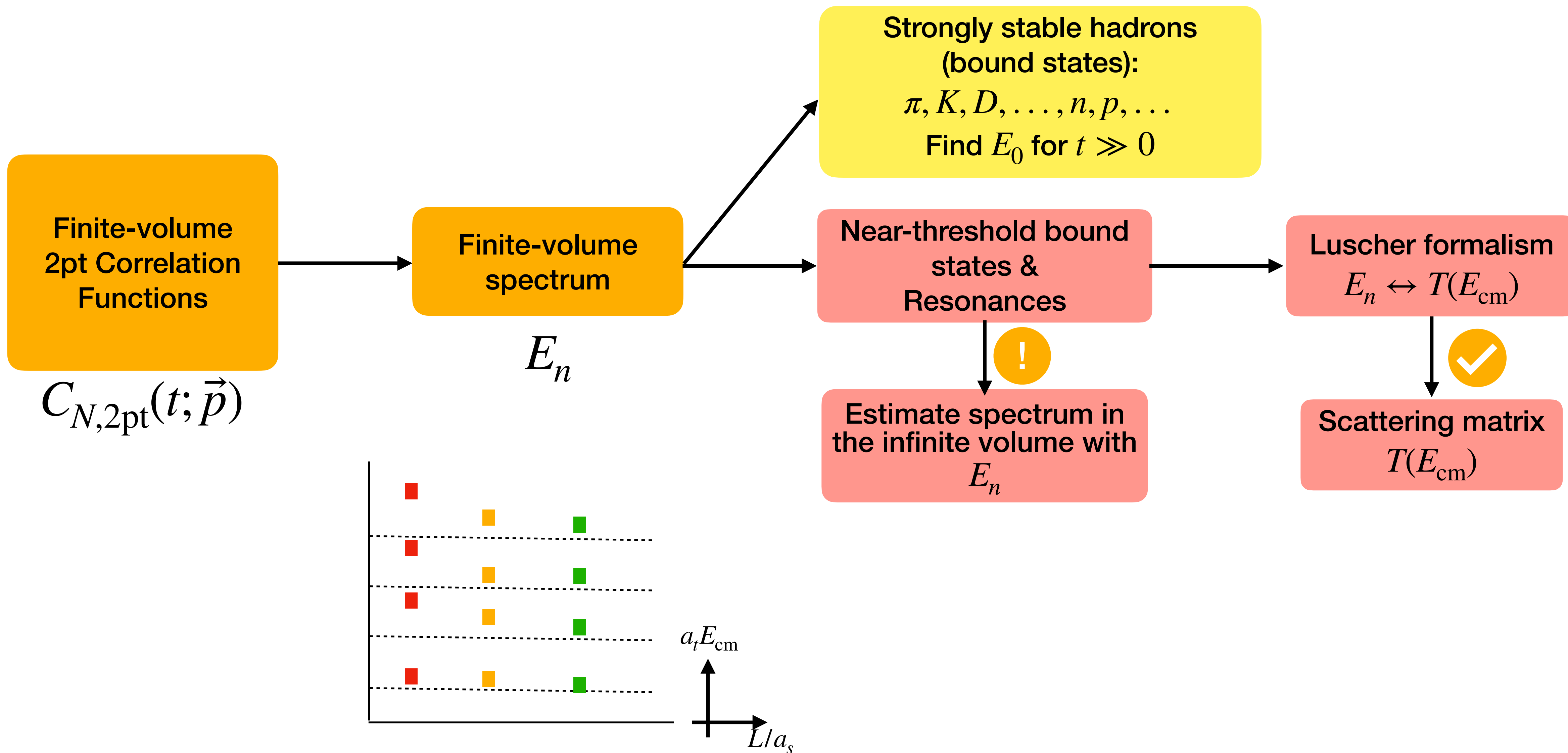
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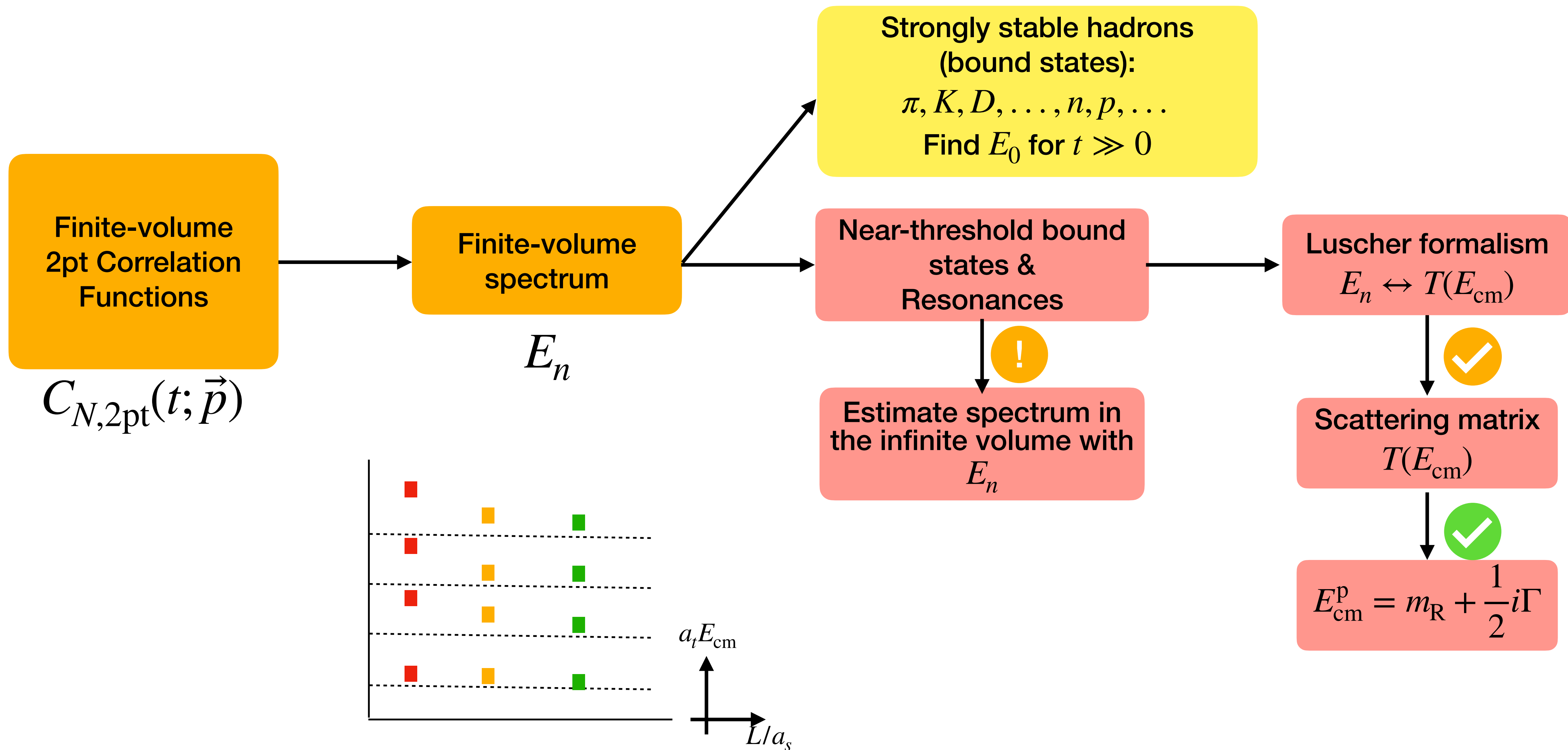
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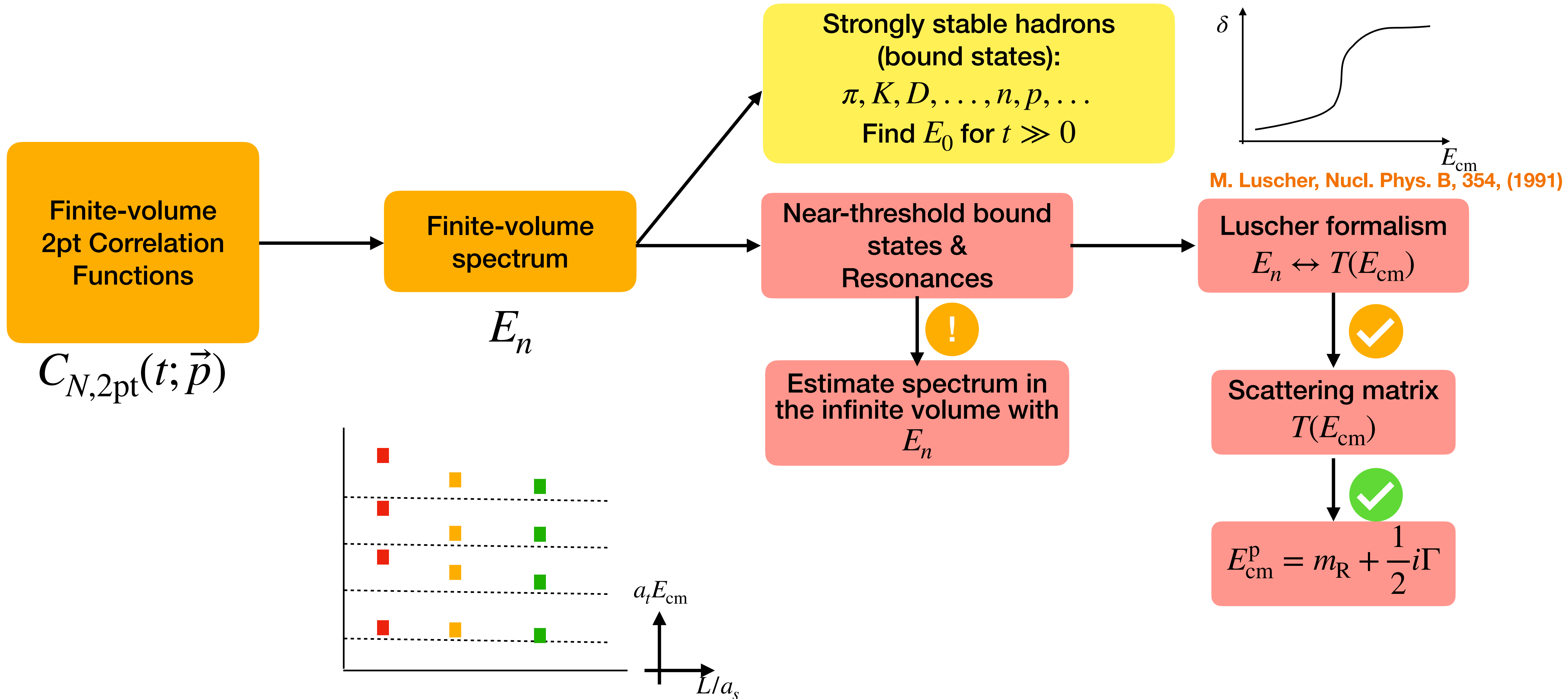
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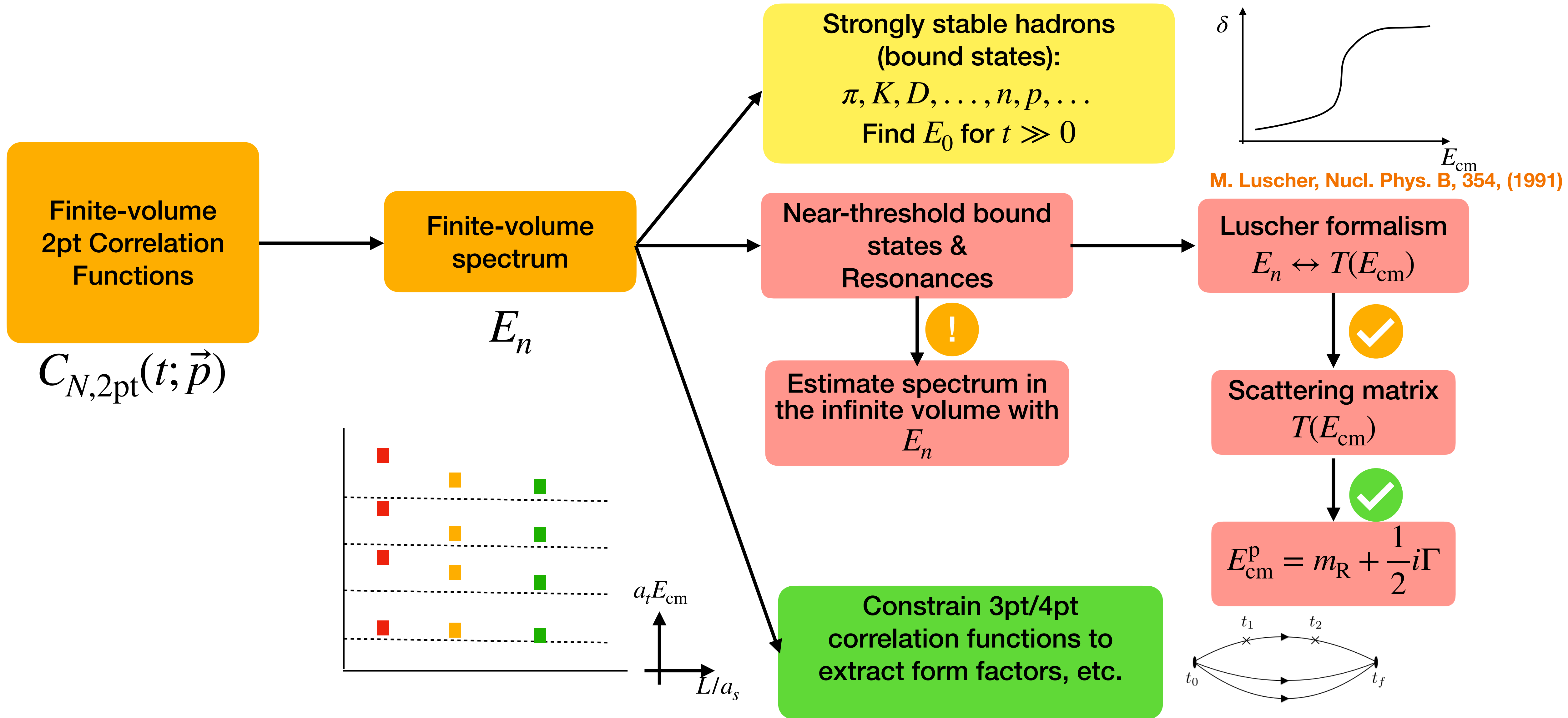
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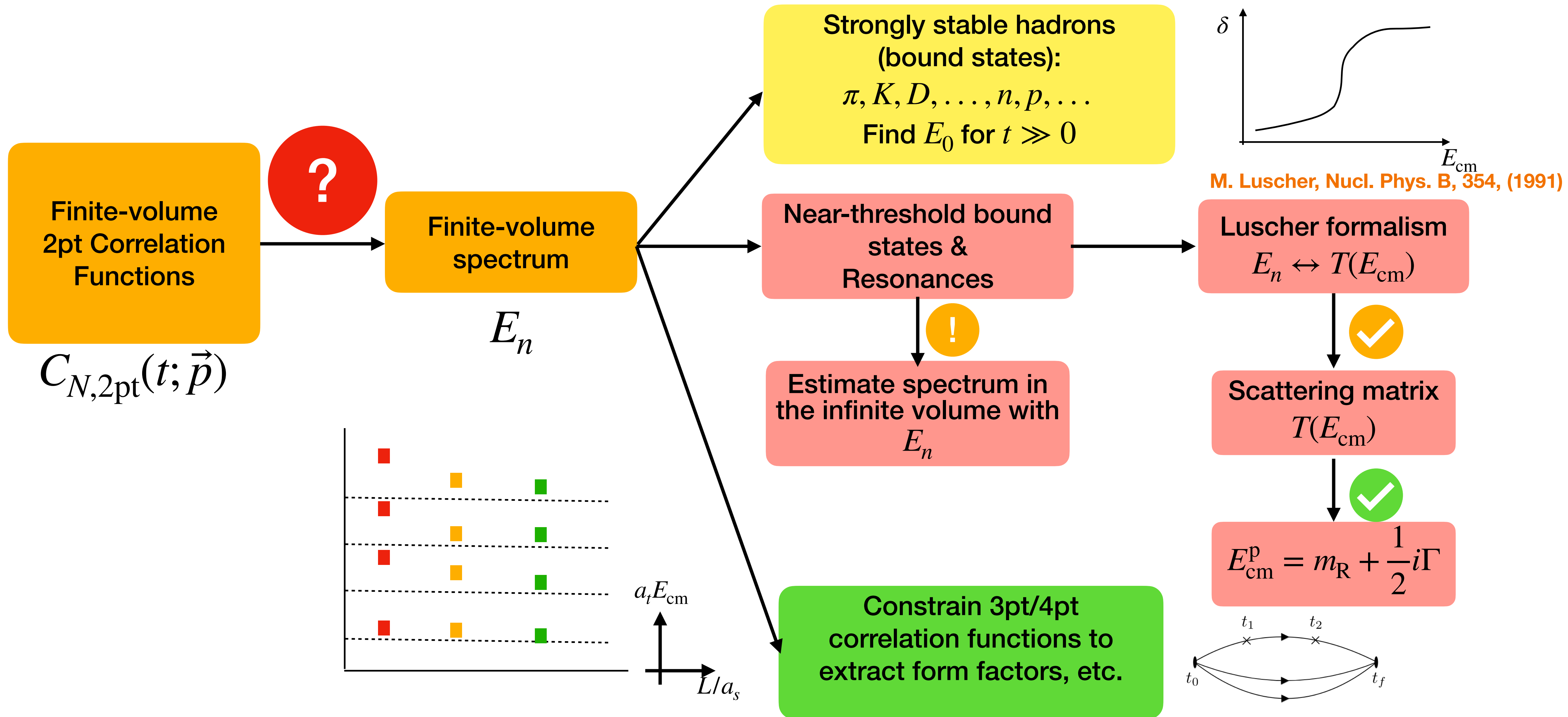
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Multi-exponential fit

- To extract the finite-volume spectrum

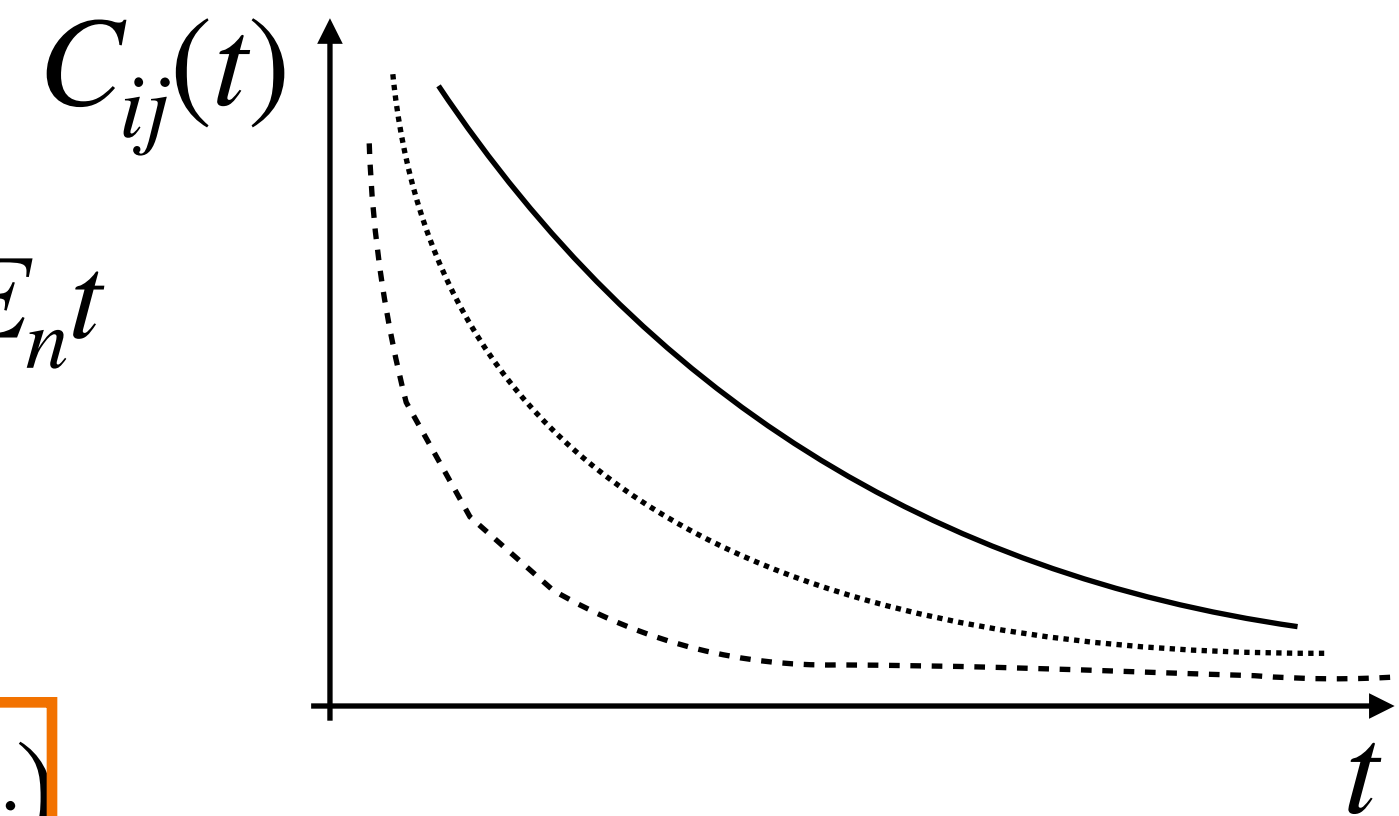
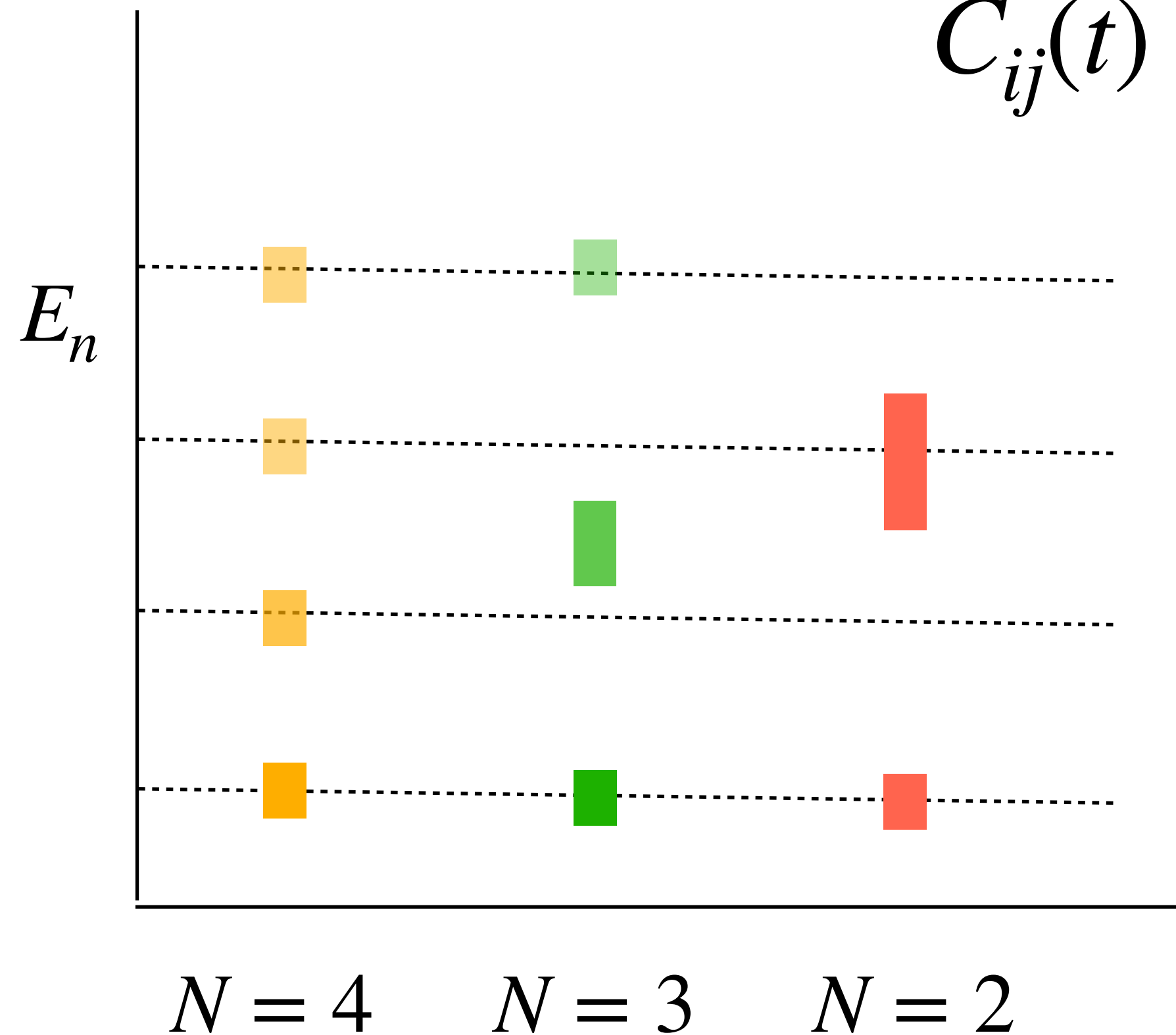
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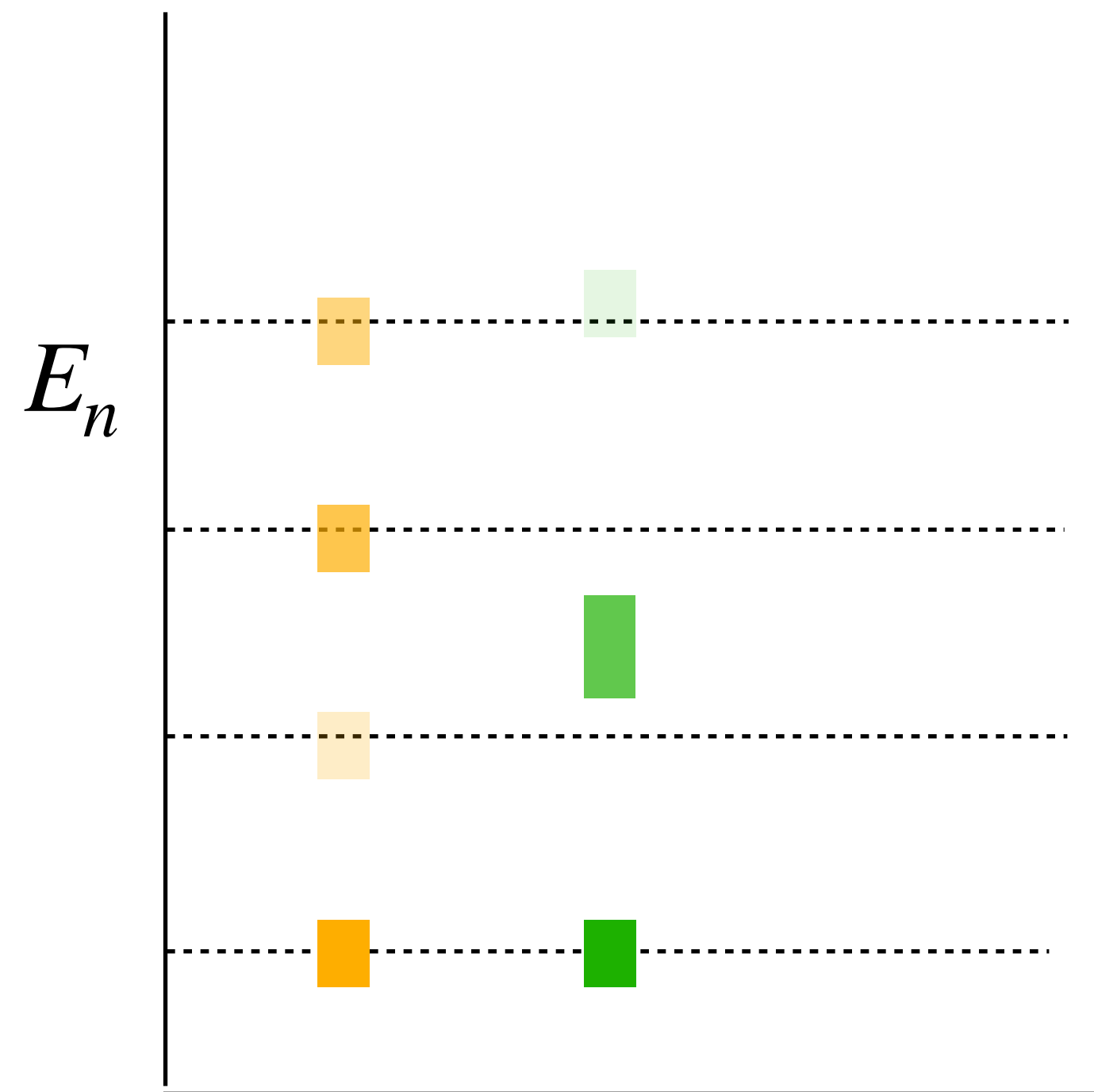
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Multi-exponential fit

- To extract the finite-volume spectrum
 - Two-point correlation functions



$N = 4$ $N = 3$

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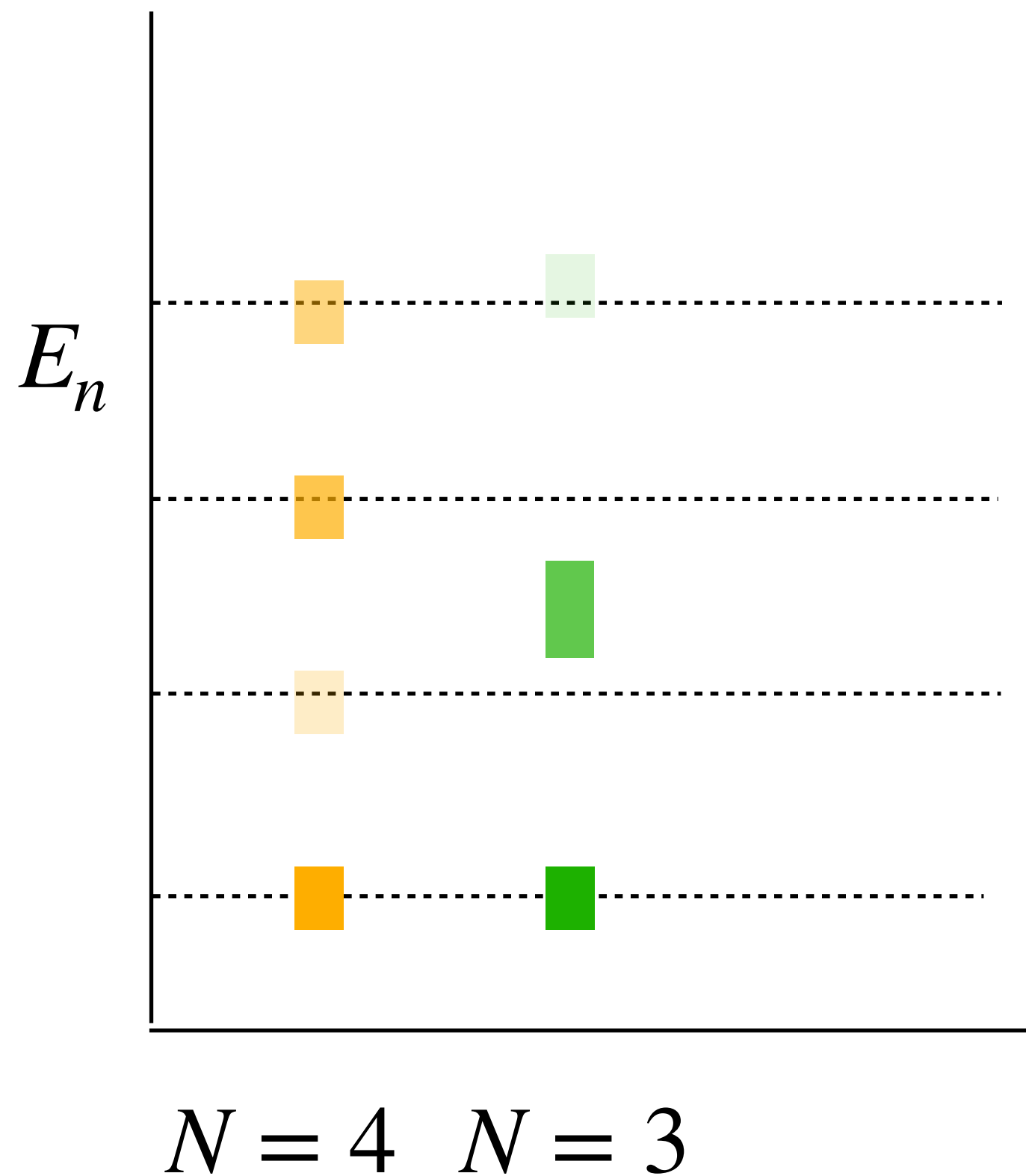
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$$\chi^2 \equiv \sum_{ij} (D_i - \tilde{D}_i) C_{ij}^{-1} (D_j - \tilde{D}_j)$$

Multi-exponential fit

- To extract the finite-volume spectrum
 - Two-point correlation functions



$$C_{ij}(t) = \langle \chi_i(t) \chi_j^\dagger(0) \rangle = \sum_{n=0}^{\infty} W_n e^{-E_n t}$$

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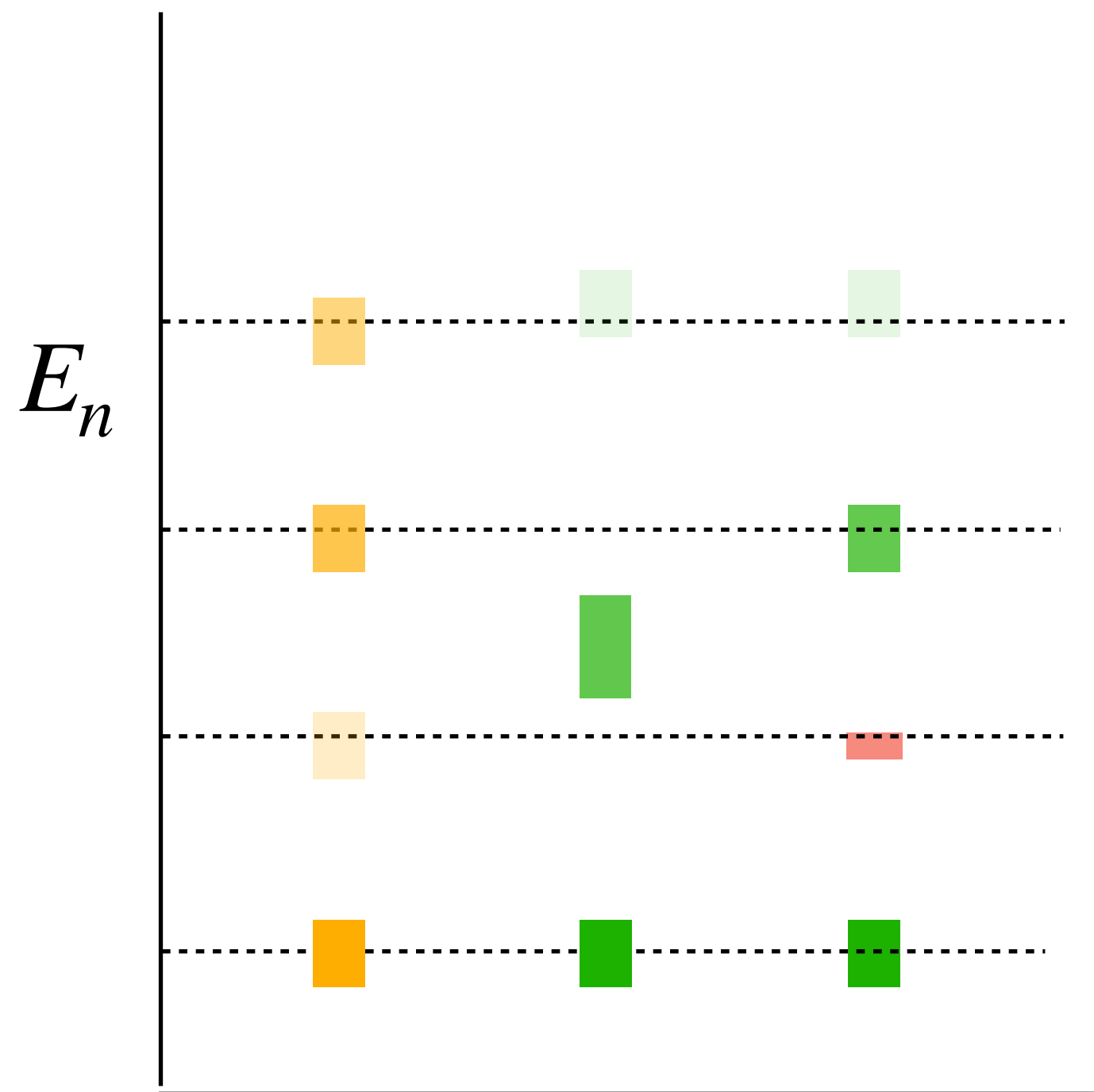
G. P. Lepage et al., arXiv: hep-lat/0110175

+

$$\chi^2_{\text{prior}} \equiv \sum_n \frac{(W_n - \tilde{W}_n)^2}{\tilde{\sigma}_{W_n}^2} + \sum_n \frac{(E_n - \tilde{E}_n)^2}{\tilde{\sigma}_{E_n}^2}$$

Multi-exponential fit

- To extract the finite-volume spectrum
 - Two-point correlation functions



$N = 4$ $N = 3$ +Add prior

$$C_{ij}(t) = \langle \chi_i(t) \chi_j^\dagger(0) \rangle = \sum_{n=0}^{\infty} W_n e^{-E_n t}$$

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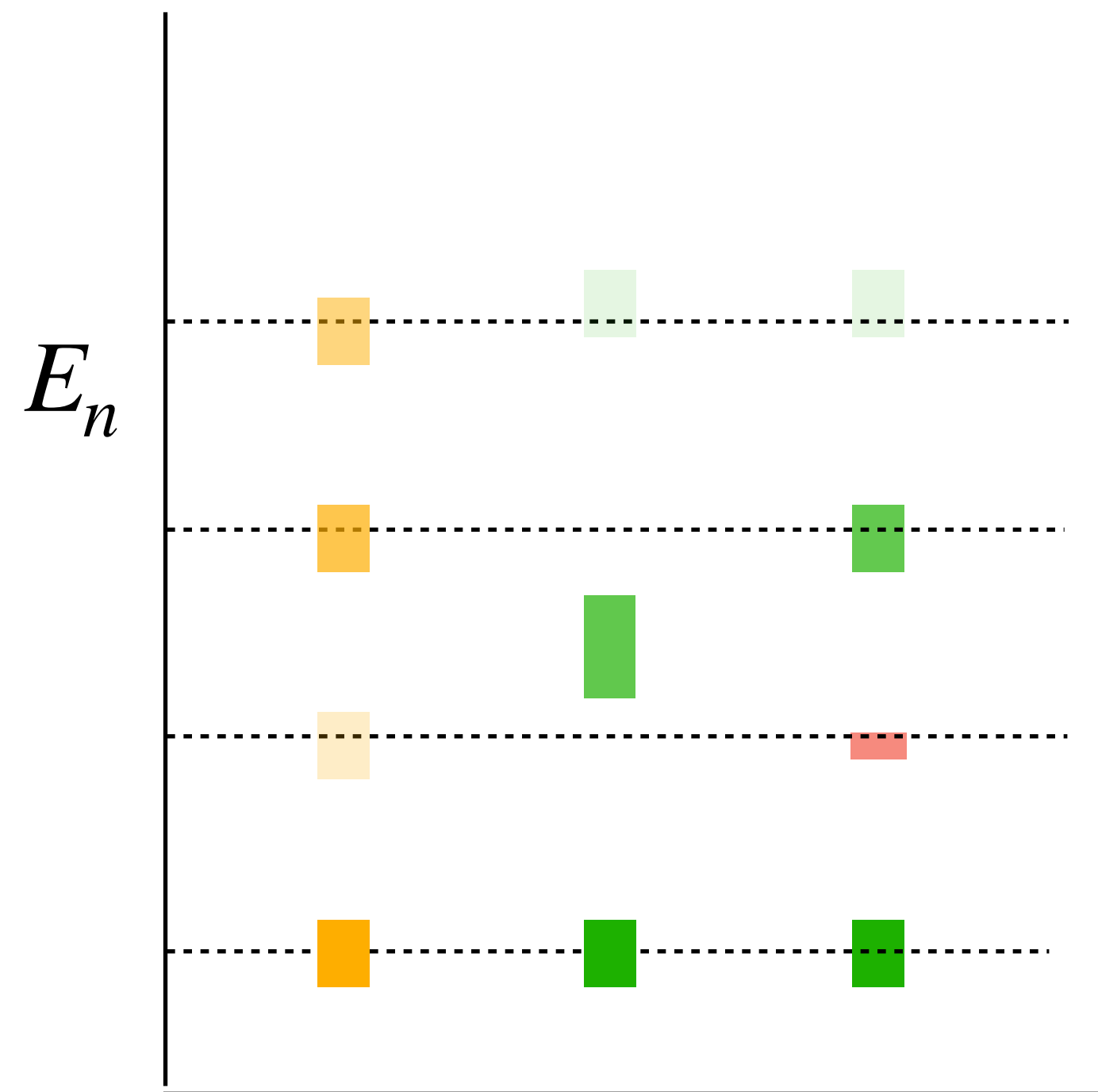
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Q1: How to choose N , \tilde{W}_n , $\tilde{\sigma}_{W_n}$, \tilde{E}_n , $\tilde{\sigma}_{E_n}$?

$$\chi^2 \equiv \sum_{ij} (D_i - \tilde{D}_i) C_{ij}^{-1} (D_j - \tilde{D}_j)$$

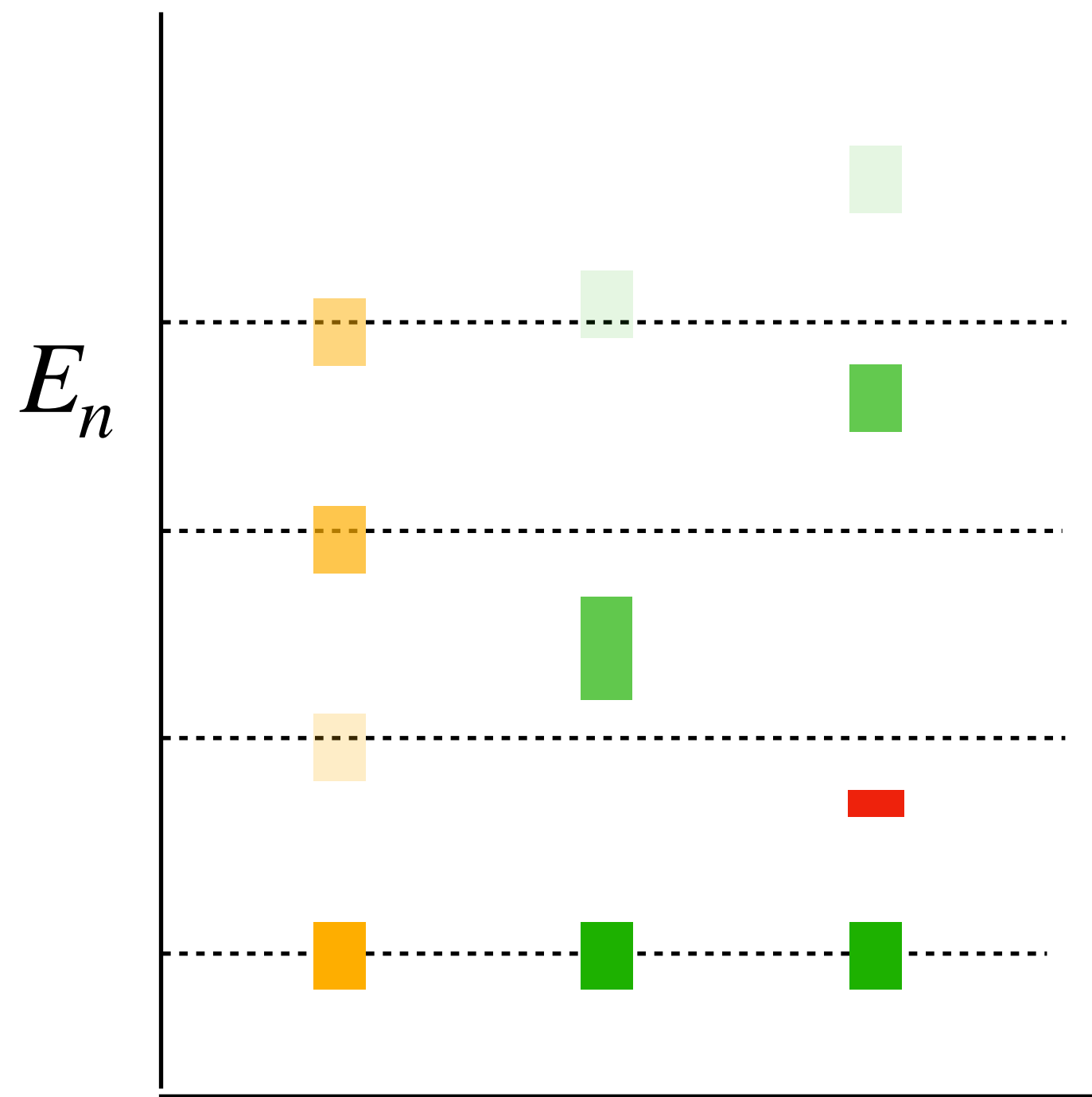
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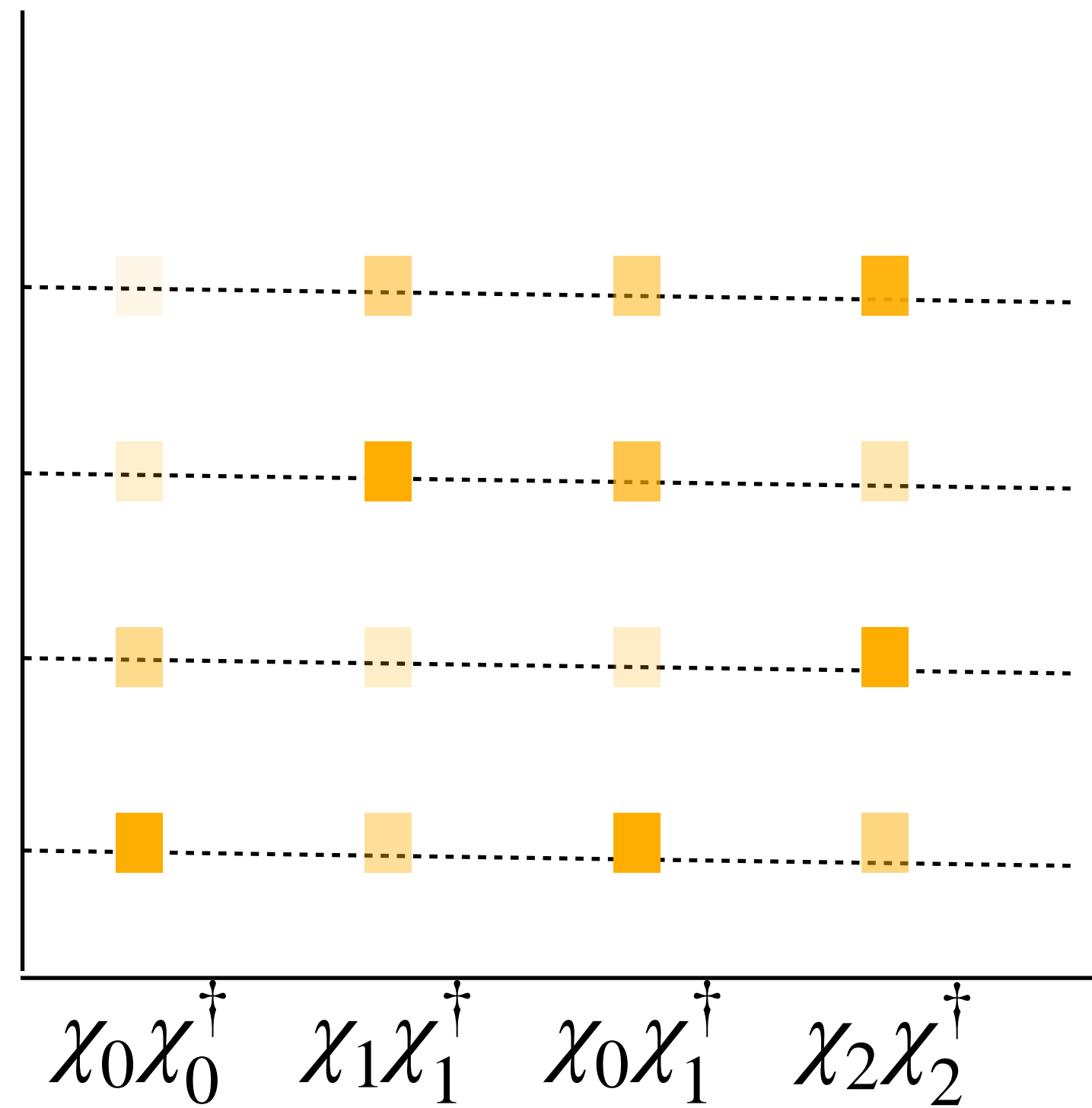
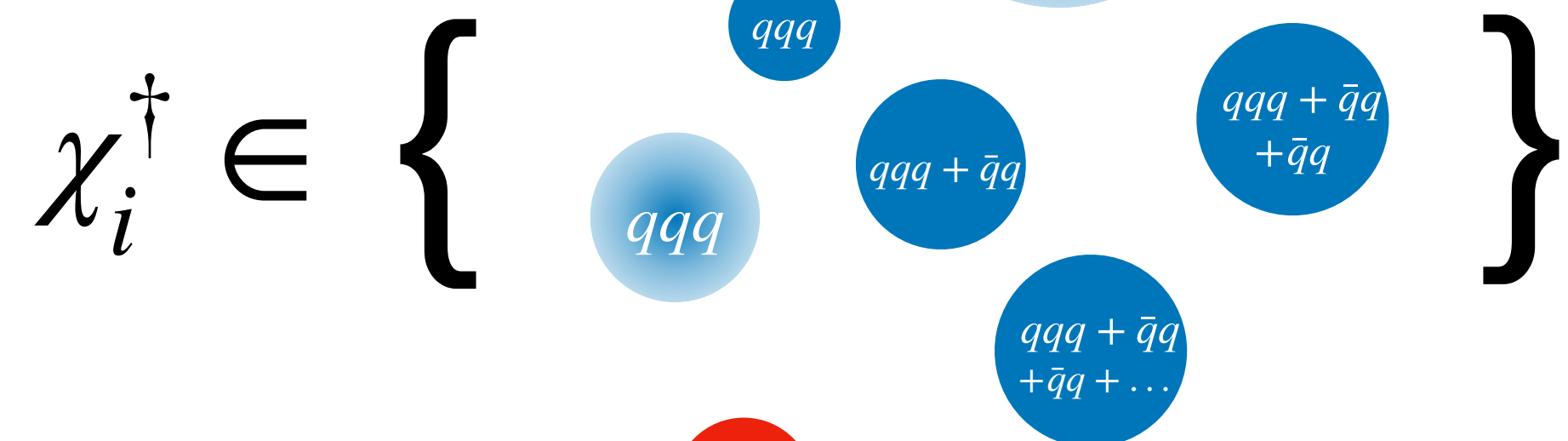
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Multi-exponential fit

- To extract the finite-volume spectrum
- Two-point correlation functions

interpolating operators with the same quantum numbers as the hadron state



$$C_{ij}(t) = \langle \chi_i(t) \chi_j^\dagger(0) \rangle$$

Constraint 1

Why not find linear combinations of χ_i^\dagger 's with the maximum overlap to the states n 's?

$$= \sum_{n=0}^{\infty} W_n e^{-E_n t}$$

$$\downarrow$$

$$\sum_{n=0}^N W_{ij,n} e^{-E_n t}$$

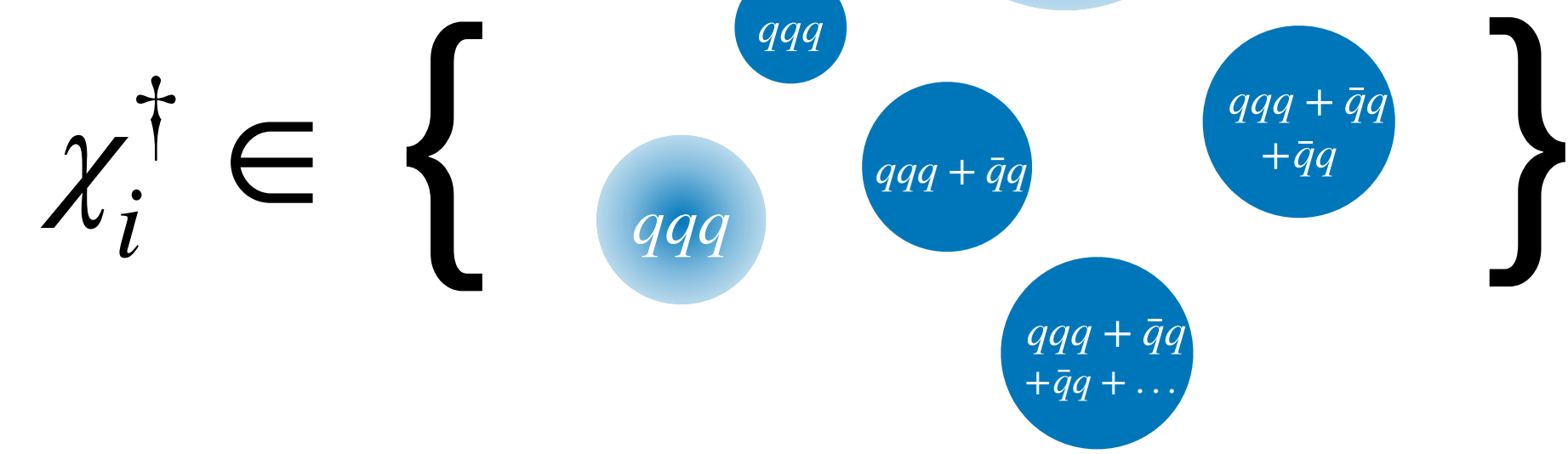
Multi-exponential fit

- To extract the finite-volume spectrum

Choose N basis operators: χ_i^\dagger

- Two-point correlation functions N ✓

$$C_{ij}(t) = \langle \chi_i(t) \chi_j^\dagger(0) \rangle \rightarrow \sum_{n=0} W_{ij,n} e^{-E_n t}$$



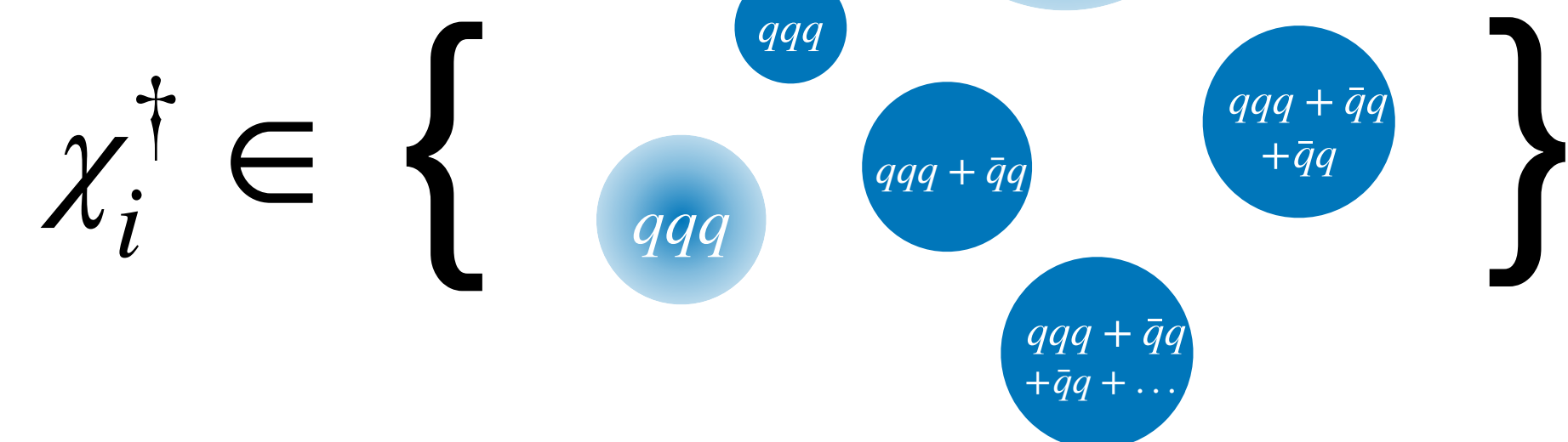
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Find linear combinations of χ_i^\dagger 's

$$X_n^\dagger = \sum_i v_i^{(n)} \chi_i^\dagger$$

Multi-exponential fit

- To extract the finite-volume spectrum

Choose N basis operators: χ_i^\dagger

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Find linear combinations of χ_i^\dagger 's

$$X_n^\dagger = \sum_i v_i^{(n)} \chi_i^\dagger$$

with the maximum overlap to the states n 's

$$\tilde{C}_{2pt}^{(n)}(t) = \langle X^{(n)}(t) X^{(n)\dagger}(0) \rangle = 1 \times e^{-E_n t} + \sum_{k \neq n} |w_k|^2 e^{-E_k t}$$

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$$\mathbf{C}(t) = \begin{pmatrix} C_{00}(t) & C_{01}(t) & \dots & C_{0N}(t) \\ C_{10}(t) & C_{11}(t) & \dots & C_{1N}(t) \\ \dots & \dots & \dots & \dots \\ C_{N0}(t) & C_{N1}(t) & \dots & C_{NN}(t) \end{pmatrix}$$

$$v_i^{(n)*} C_{ij}(t_0) v_j^{(n')} = \delta_{n,n'}$$

Multi-exponential fit

- To extract the finite-volume spectrum

- Two-point correlation functions

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Choose N basis operators: χ_i^\dagger

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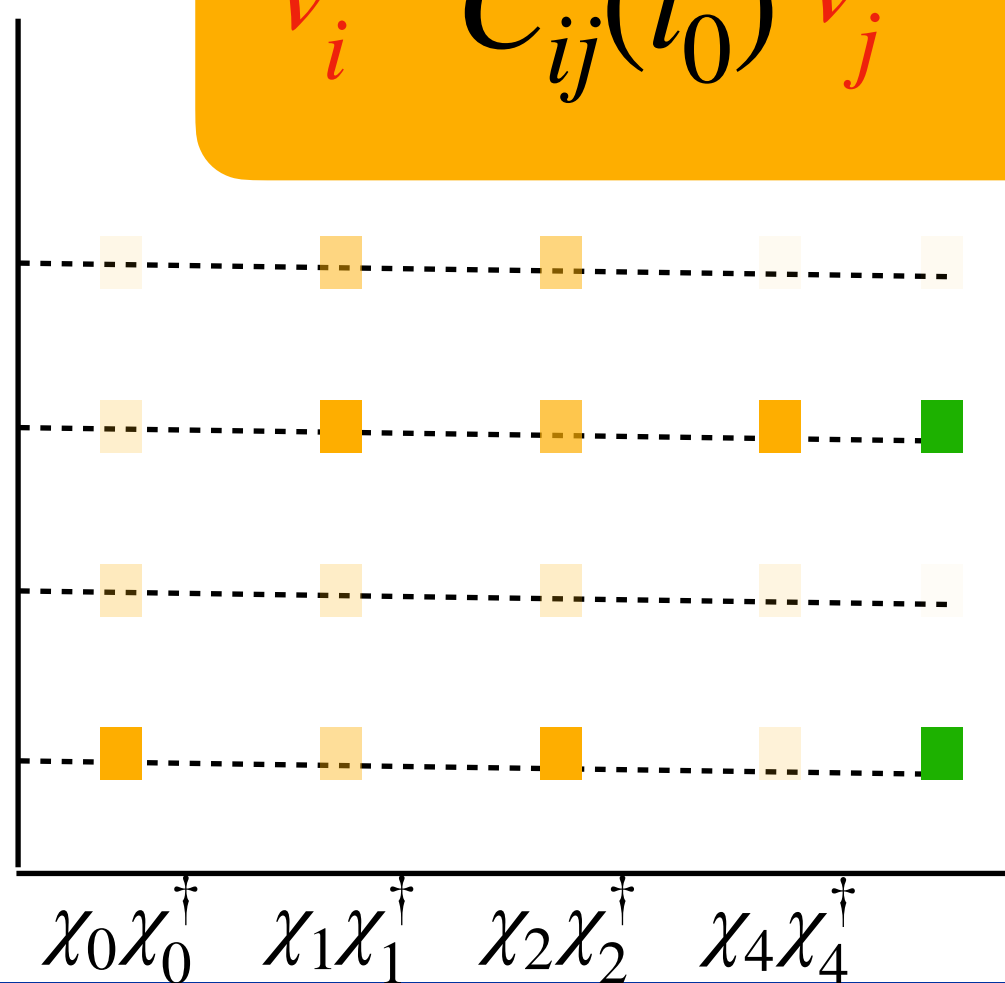
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$$v_i^{(n)*} C_{ij}(t_0) v_j^{(n')} = \delta_{n,n'}$$

$$C(t) v^{(n)} = \lambda^{(n)}(t) C(t_0) v^{(n)} \\ \uparrow \\ = e^{-E_n t}$$

generalized eigenvalue problem (GEVP)



Q2: How to make sure we are not missing some of the E_i 's ?

Multi-exponential fit

- To extract the finite-volume spectrum

- Two-point correlation functions

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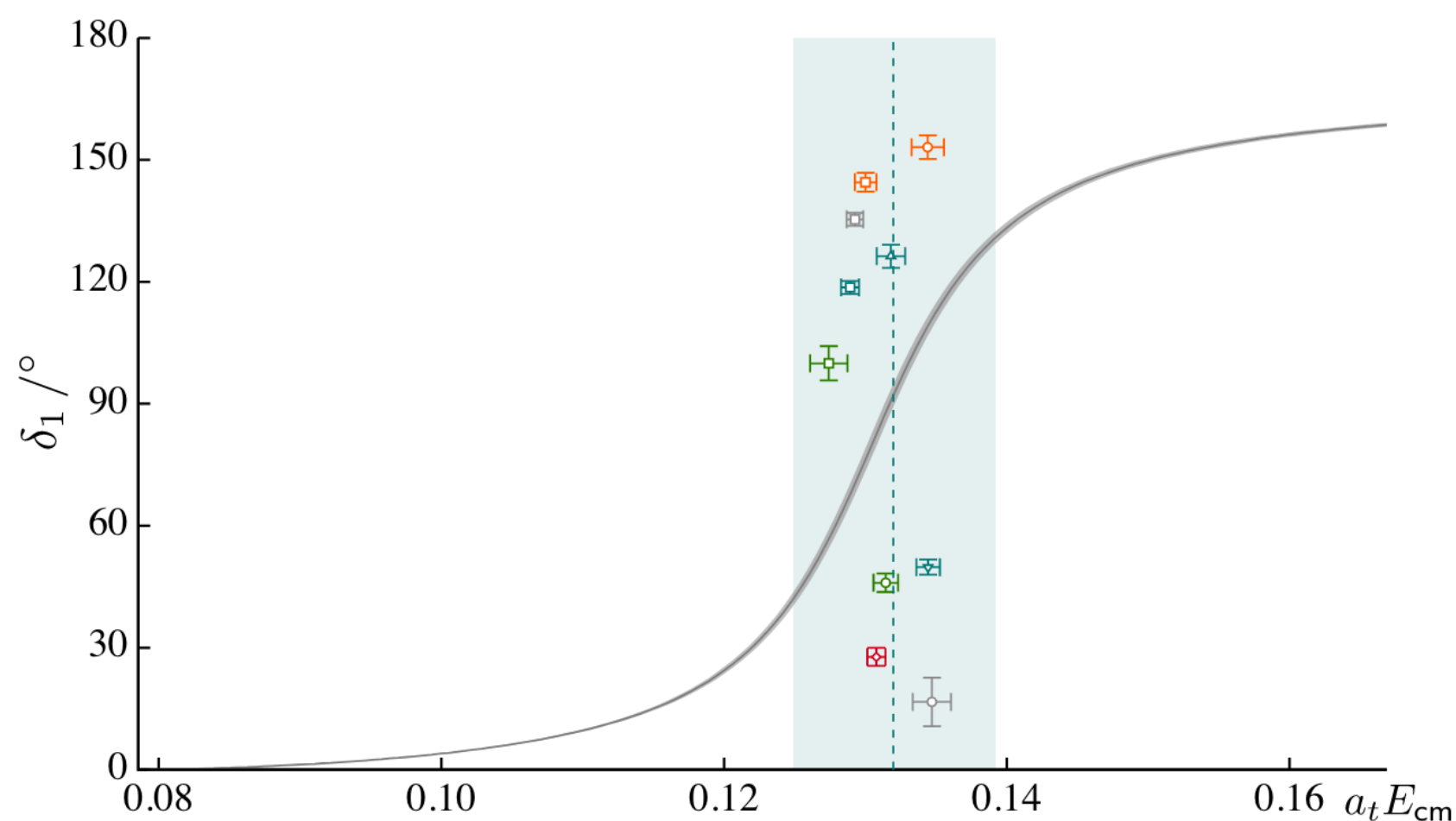
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M. Luscher, Nucl. Phys. B, 354, (1991)

Q2: How to make sure we are not missing some of the E_i 's ?

Wilson et al., Phys. Rev. D, vol. 92, no. 9, p. 094502, Nov. 2015



Multi-exponential fit

- To extract the finite-volume spectrum

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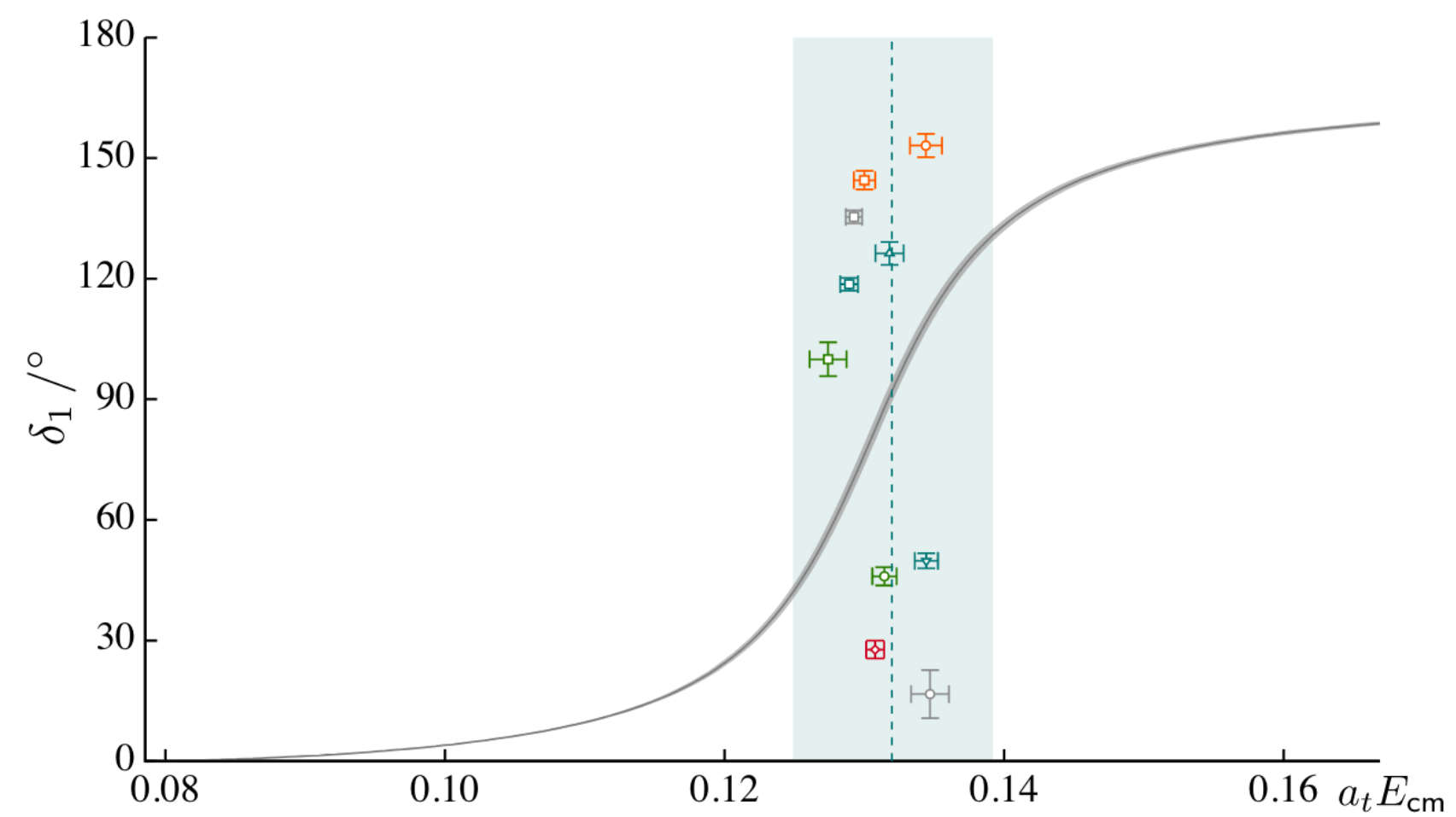
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Luscher formalism
 $E_n \leftrightarrow T(E_{cm})$

Wilson et al., Phys. Rev. D, vol. 92, no. 9, p. 094502, Nov. 2015

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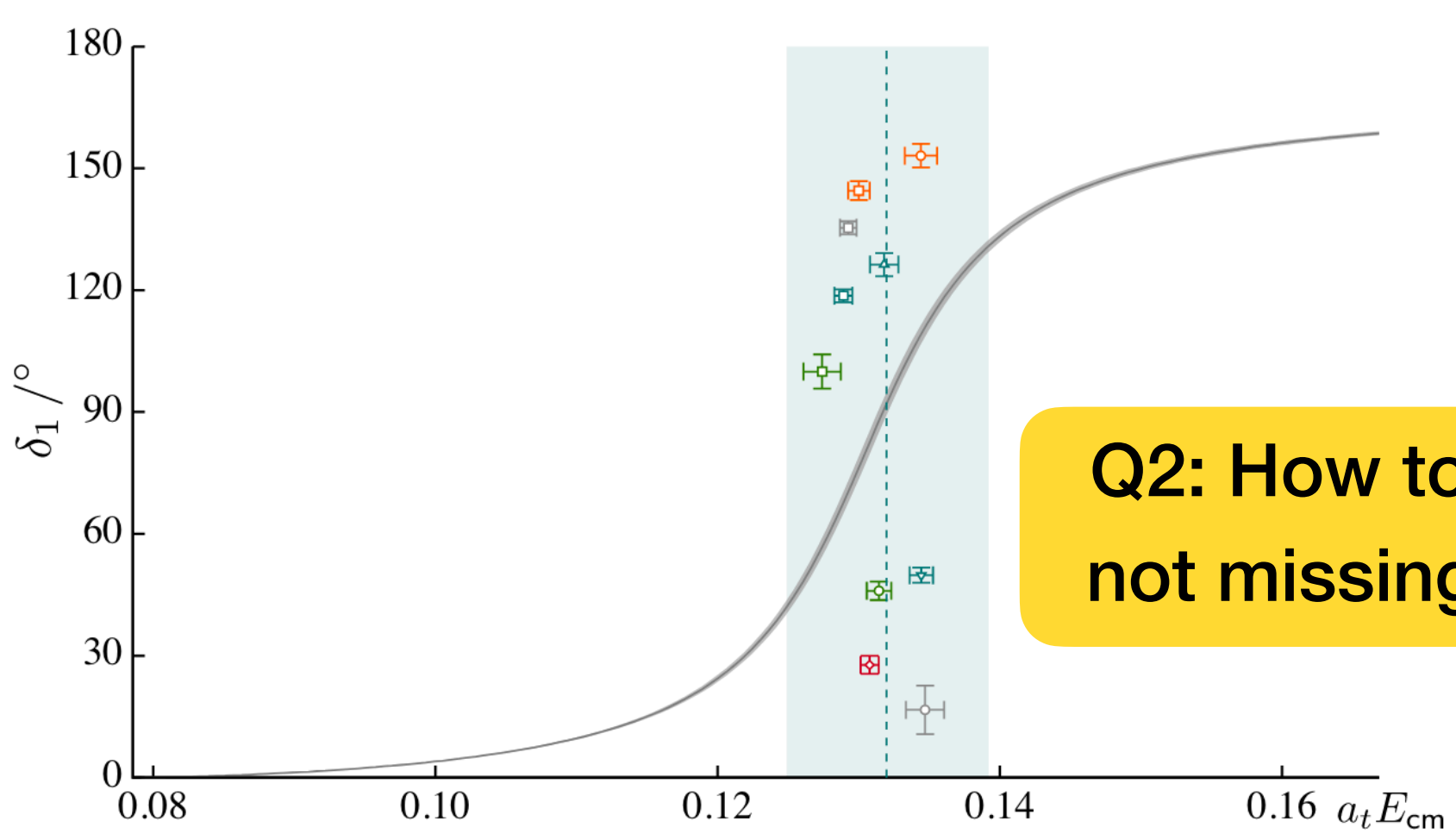
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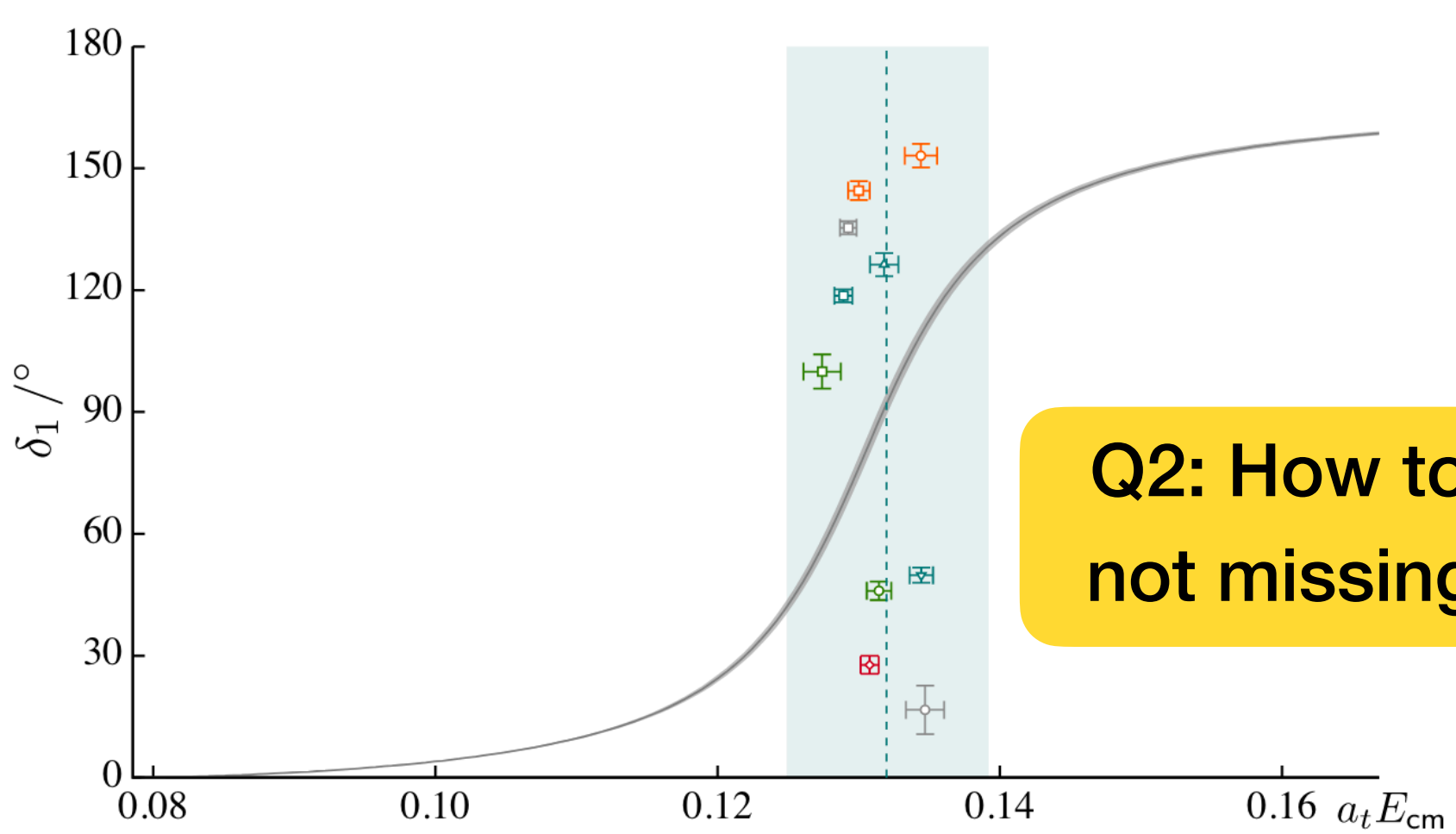
More operators!
"distillation"

M. Luscher, Nucl. Phys. B, 354, (1991)

Luscher formalism
 $E_n \leftrightarrow T(E_{cm})$

M. Peardon et al. (Hadron Spectrum), Phys.Rev. D80, 054506 (2009)

Cost for GEVP is high!!!



Q2: How to make sure we are not missing some of the E_i 's ?

Wilson et al., Phys. Rev. D, vol. 92, no. 9, p. 094502, Nov. 2015

Finite-volume spectrum from lattice QCD

Q2*: Do we really need to make sure we are not missing (resolve) some of the E'_i 's ?

Finite-volume
2pt Correlation
Functions

$$C_{N,2pt}(t; \vec{p})$$



Finite-volume
spectrum

$$E_n$$

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Strongly stable hadrons
(bound states):

$\pi, K, D, \dots, n, p, \dots$

Find E_0 for $t \gg 0$

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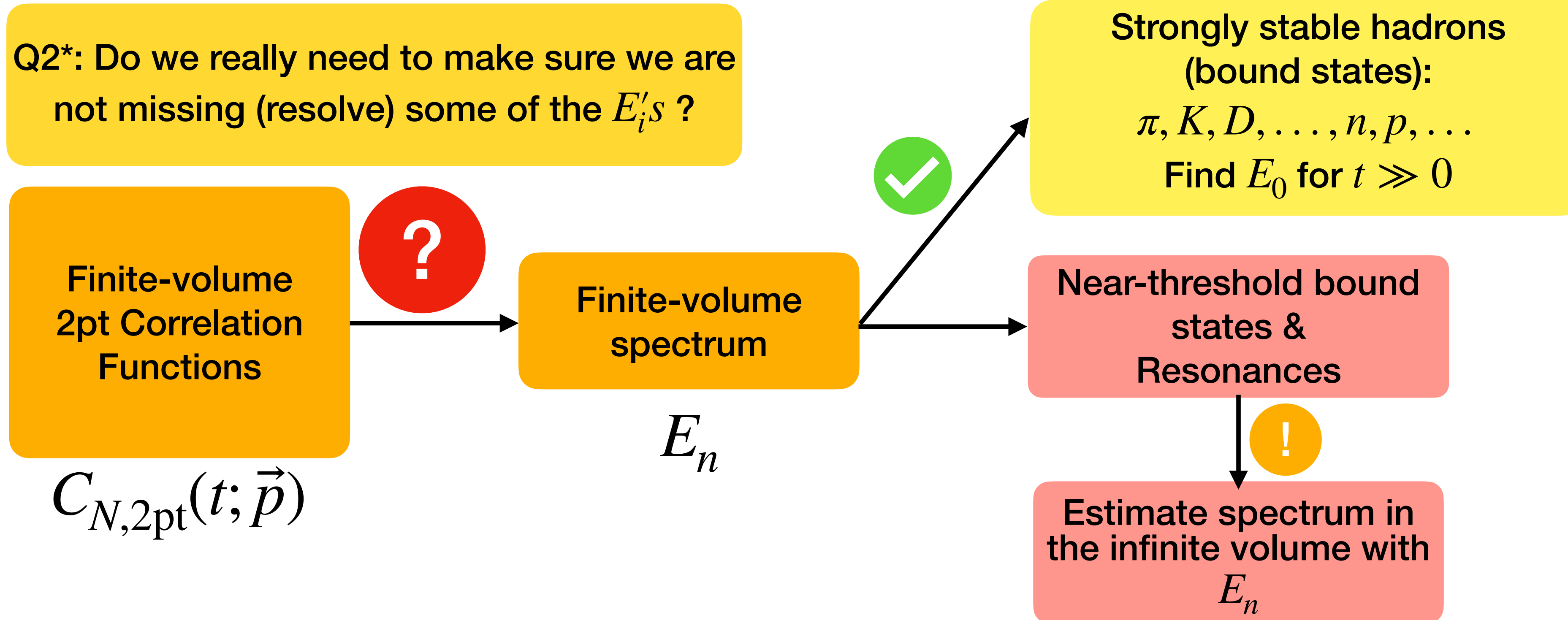
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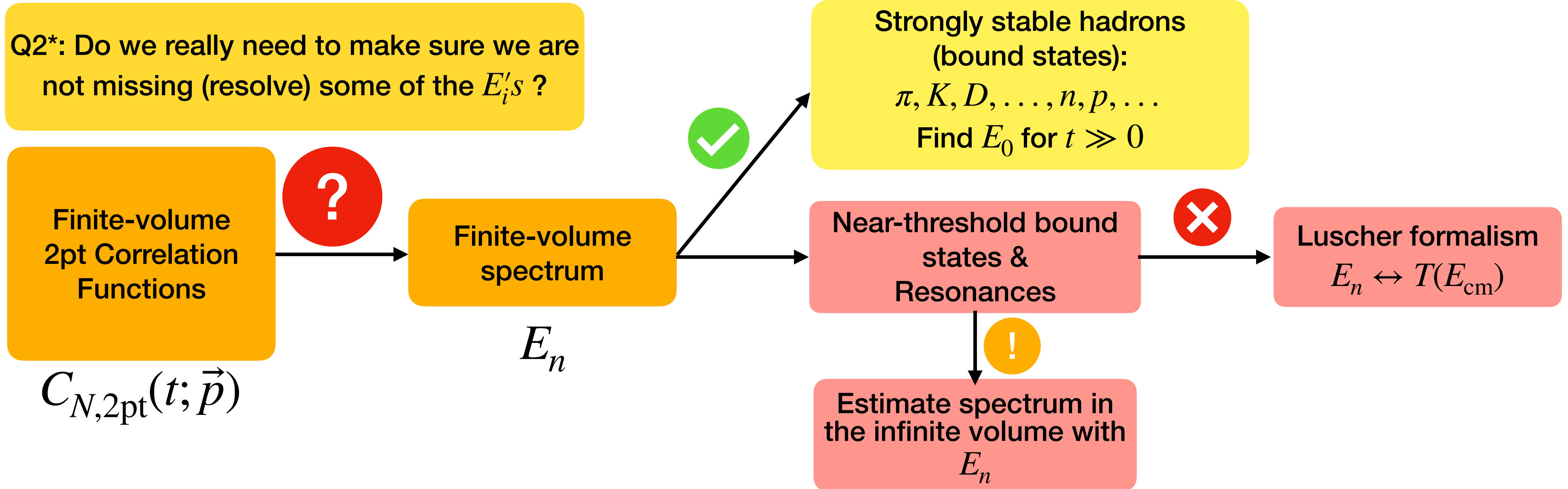
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Near-threshold bound
states &
Resonances

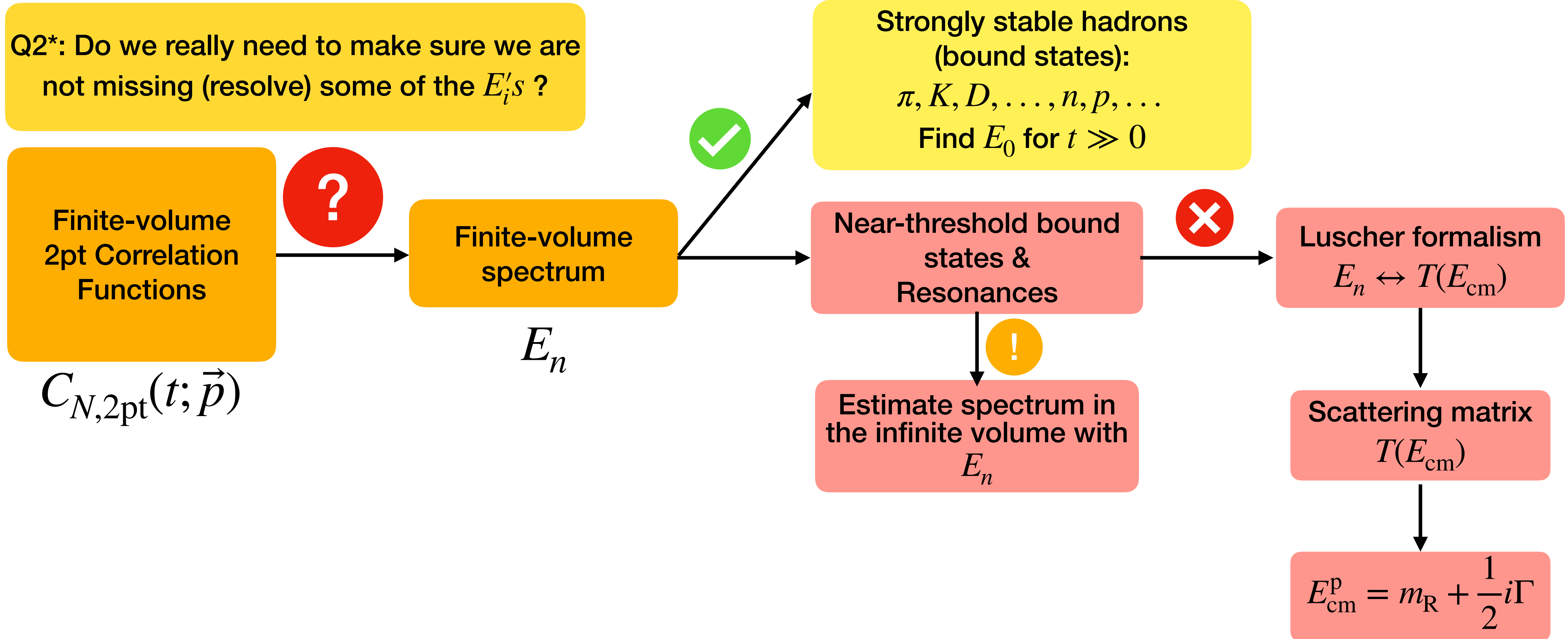
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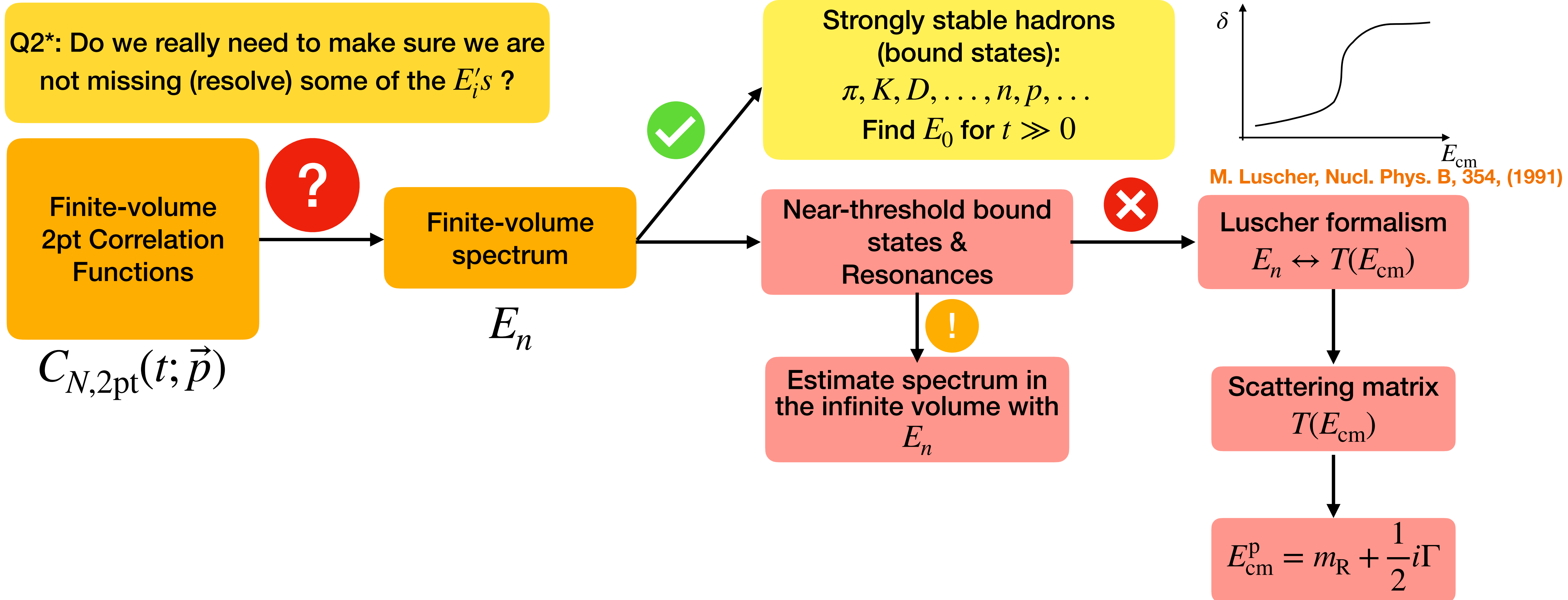
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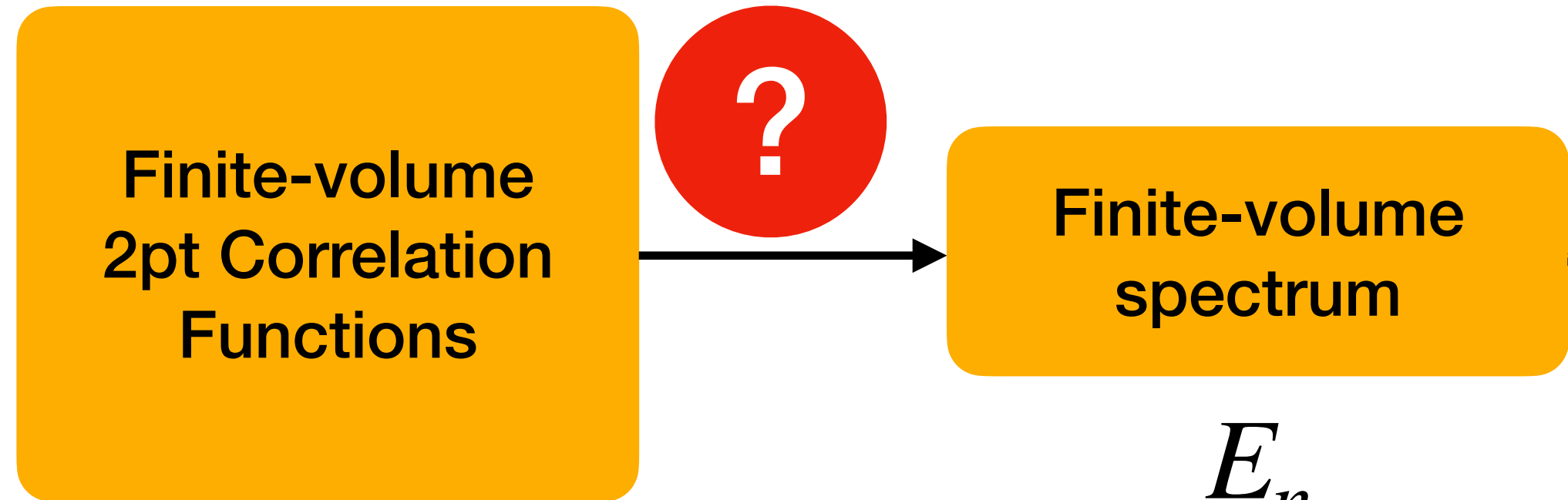


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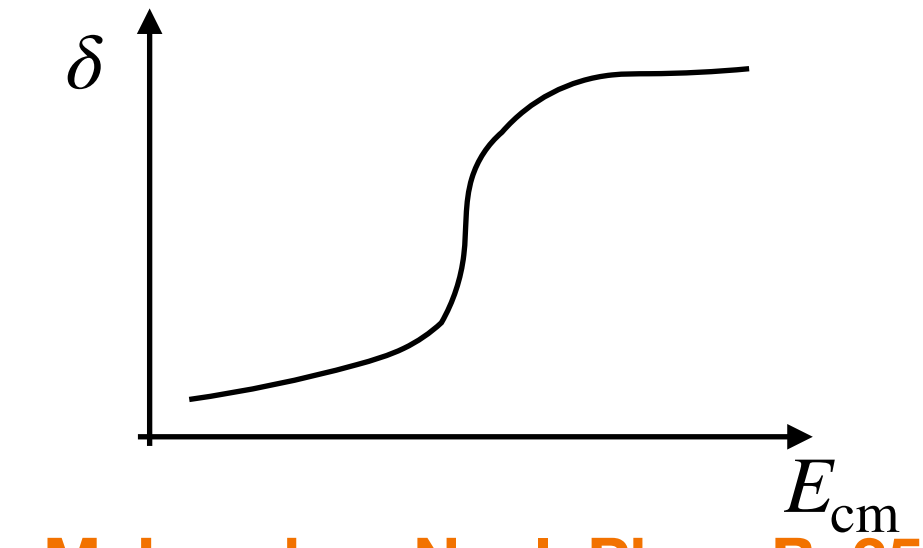
$$C_{N,2pt}(t; \vec{p})$$

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Strongly stable hadrons (bound states):
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 Find E_0 for $t \gg 0$

Near-threshold bound states & Resonances

Estimate spectrum in the infinite volume with E_n

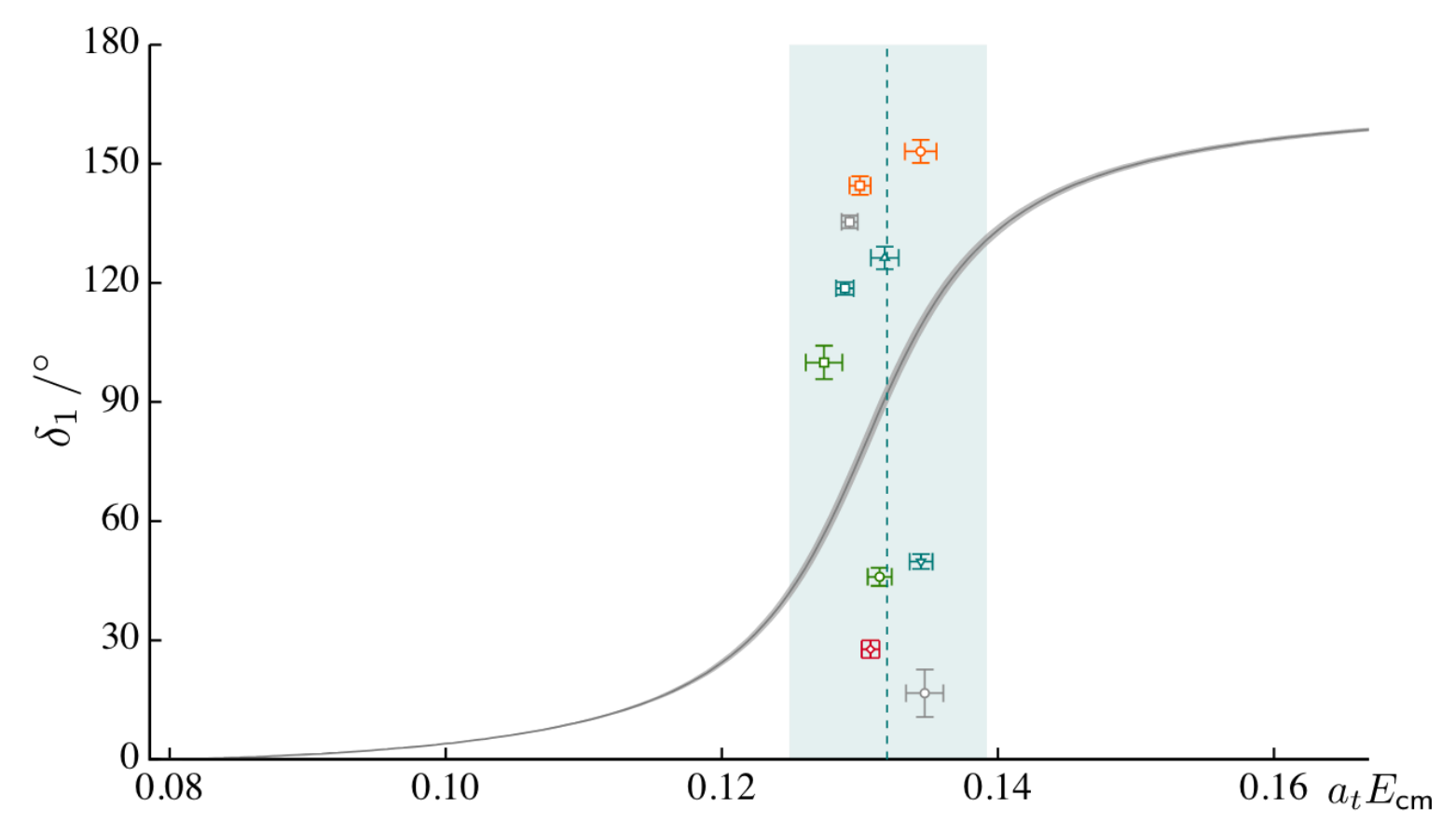


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Scattering matrix
 $T(E_{cm})$

$$E_{cm}^p = m_R + \frac{1}{2}i\Gamma$$



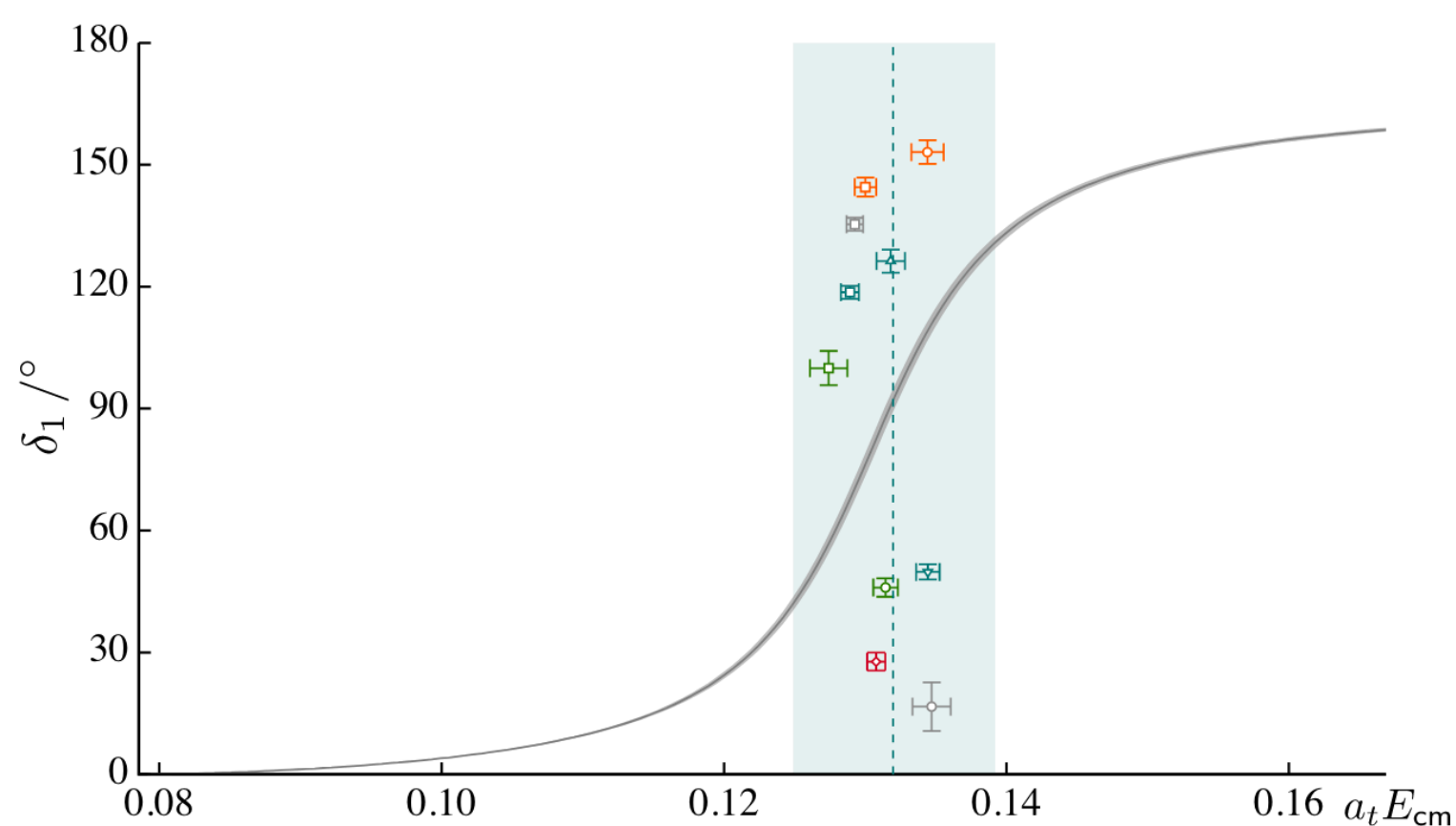
Wilson et al., Phys. Rev. D, vol. 92, no. 9, p. 094502, Nov. 2015

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Finite-volume 2pt Correlation Functions

$$C_{N,2pt}(t; \vec{p})$$



Wilson et al., *Phys. Rev. D*, vol. 92, no. 9, p. 094502, Nov. 2015



Finite-volume spectrum

$$E_n$$



Strongly stable hadrons (bound states):
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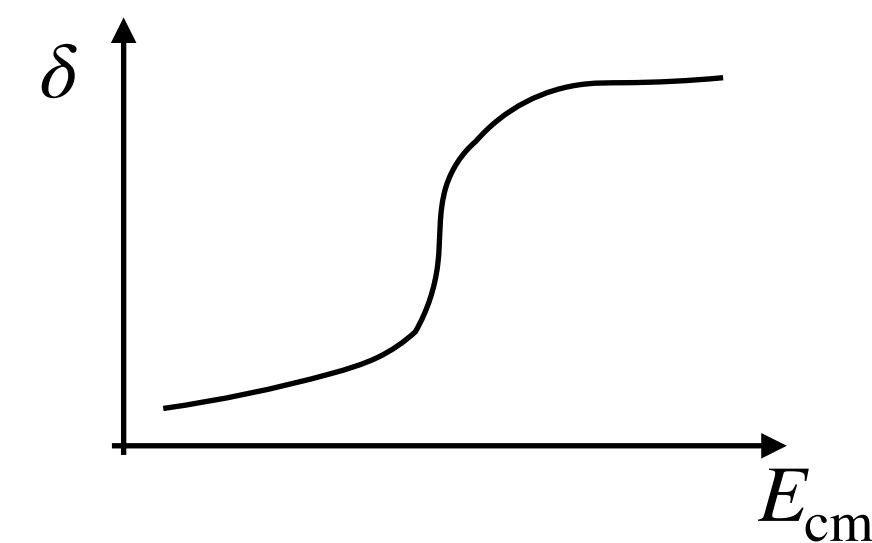
Near-threshold bound states & Resonances



Estimate spectrum in the infinite volume with E_n



Constrain 3pt/4pt correlation functions to extract form factors, etc.

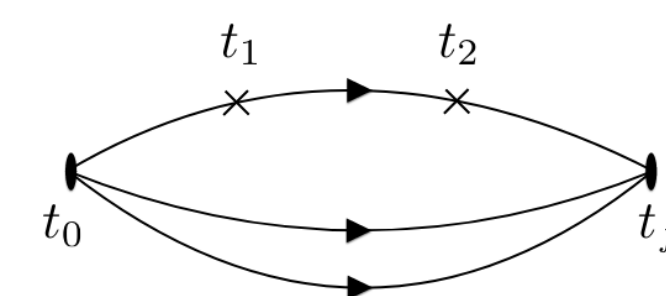


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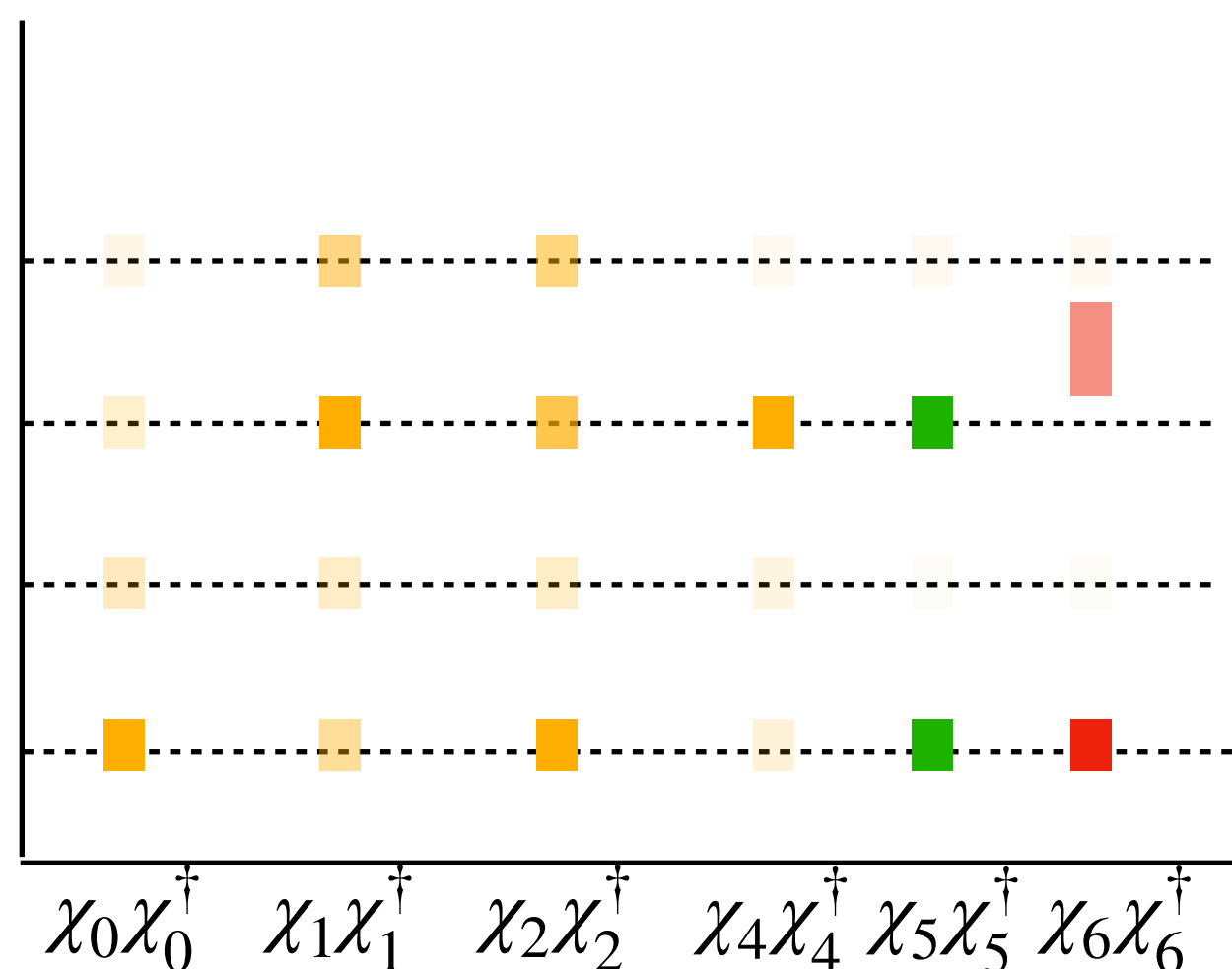


Finite-volume spectrum from lattice QCD

Q2**: Can we choose the basis wisely/efficiently, if we are not interested in resolving all the E'_i 's?

Finite-volume 2pt Correlation Functions

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Finite-volume spectrum

E_n

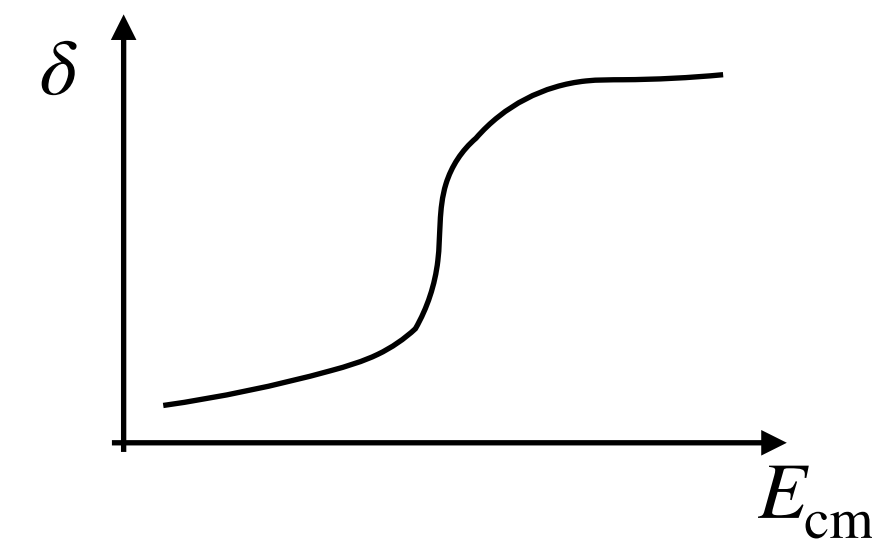


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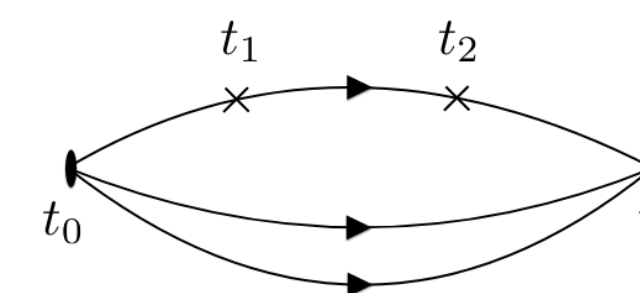


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Talk by Liu



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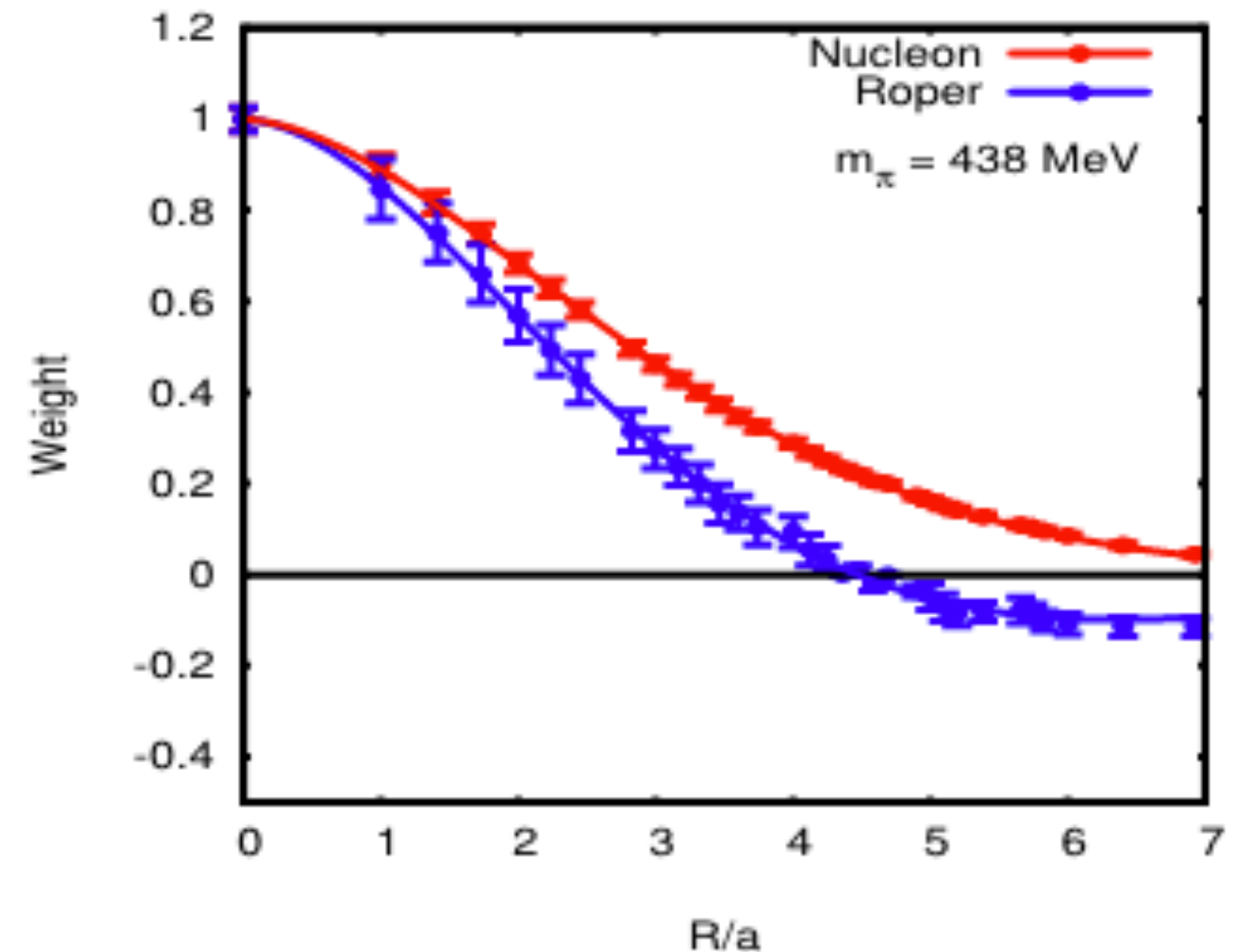
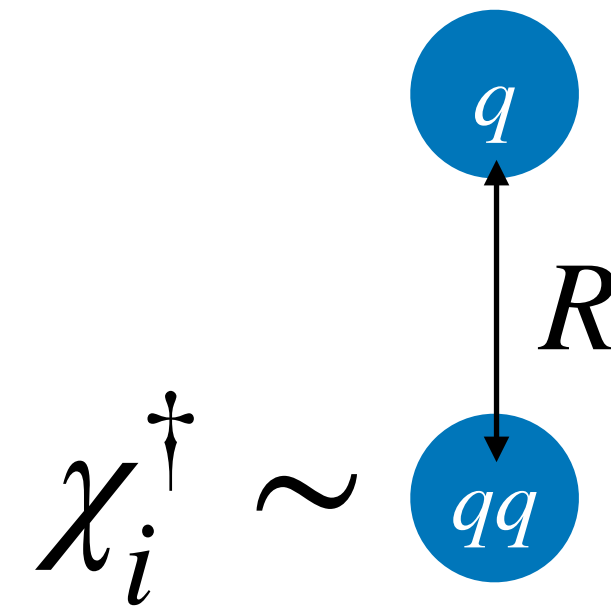
Example: Roper State from Overlap Fermions

$N(1440) 1/2^+$

$$I(J^P) = \frac{1}{2}(\frac{1}{2}^+)$$

Re(pole position) = 1360 to 1380 (≈ 1370) MeV
 $-2\text{Im}(\text{pole position}) = 180$ to 205 (≈ 190) MeV
 Breit-Wigner mass = 1410 to 1470 (≈ 1440) MeV
 Breit-Wigner full width = 250 to 450 (≈ 350) MeV

$N(1440)$ DECAY MODES	Fraction (Γ_i/Γ)	p (MeV/c)
$N\pi$	55–75 %	398
$N\eta$	<1 %	†
$N\pi\pi$	17–50 %	347
$\Delta(1232)\pi$, P -wave	6–27 %	147
$N\sigma$	11–23 %	–
$p\gamma$, helicity=1/2	0.035–0.048 %	414
$n\gamma$, helicity=1/2	0.02–0.04 %	413



Sensitive to the **size**
 of the 3-quark interpolating operator

Nucleon and Roper wavefunctions
 in the Coulomb gauge

M. Sun et al., “Roper State from Overlap Fermions,” [PhysRevD.101.054511](https://arxiv.org/abs/1905.05451)

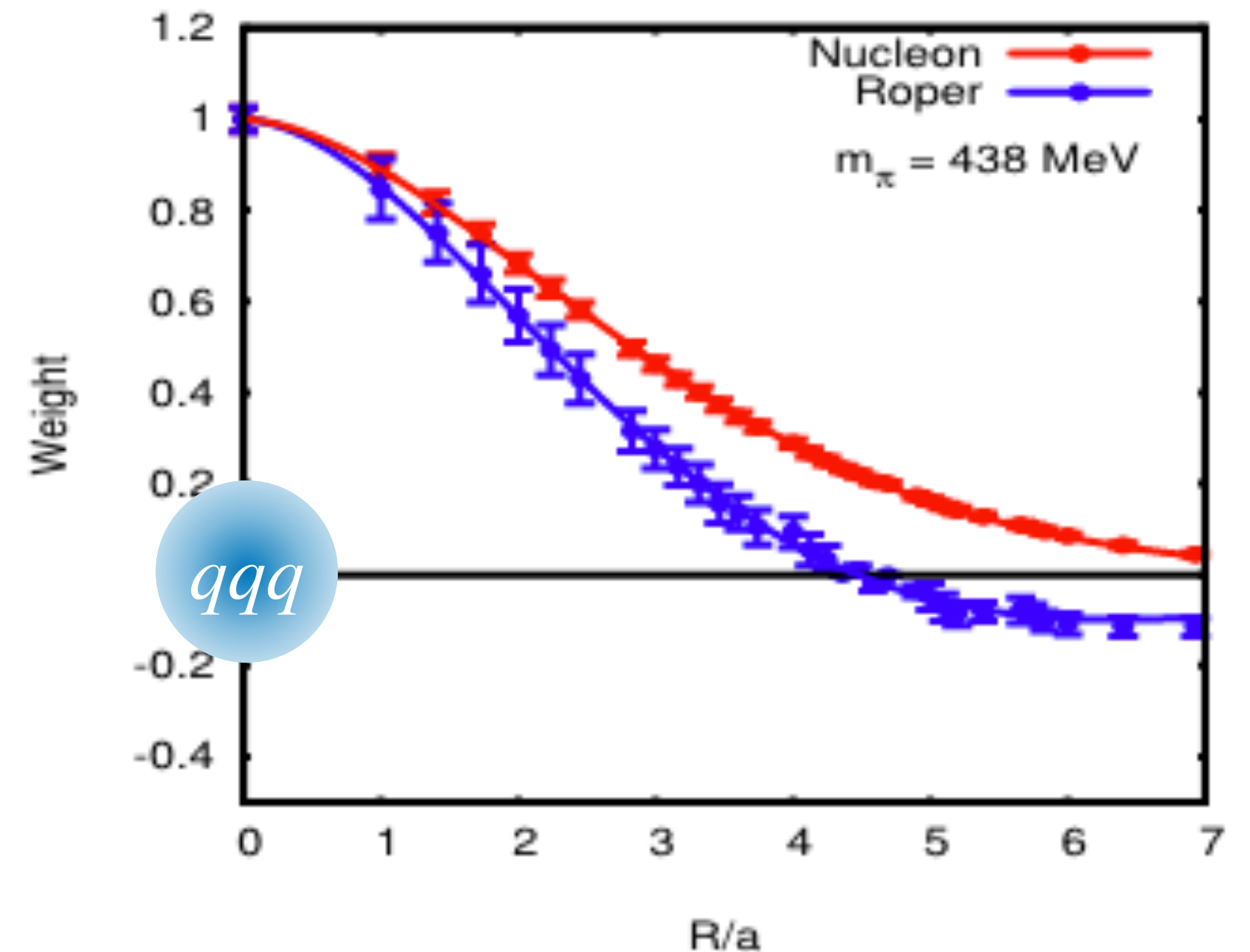
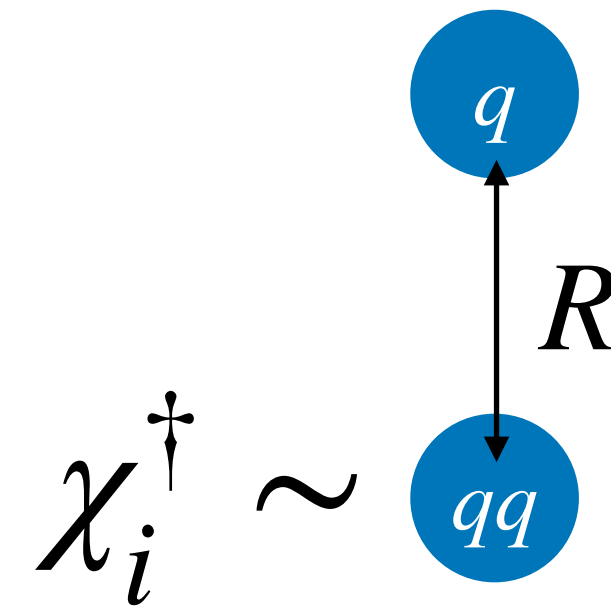
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 Breit-Wigner full width = 250 to 450 (≈ 350) MeV

$N(1440)$ DECAY MODES	Fraction (Γ_i/Γ)	p (MeV/c)
$N\pi$	55–75 %	398
$N\eta$	<1 %	†
$N\pi\pi$	17–50 %	347
$\Delta(1232)\pi$, P -wave	6–27 %	147
$N\sigma$	11–23 %	–
$p\gamma$, helicity=1/2	0.035–0.048 %	414
$n\gamma$, helicity=1/2	0.02–0.04 %	413



Sensitive to the **size**
 of the 3-quark interpolating operator

Nucleon and Roper wavefunctions
 in the Coulomb gauge

M. Sun et al., “Roper State from Overlap Fermions,” [PhysRevD.101.054511](https://arxiv.org/abs/1905.05451)

Example: Roper State from Overlap Fermions

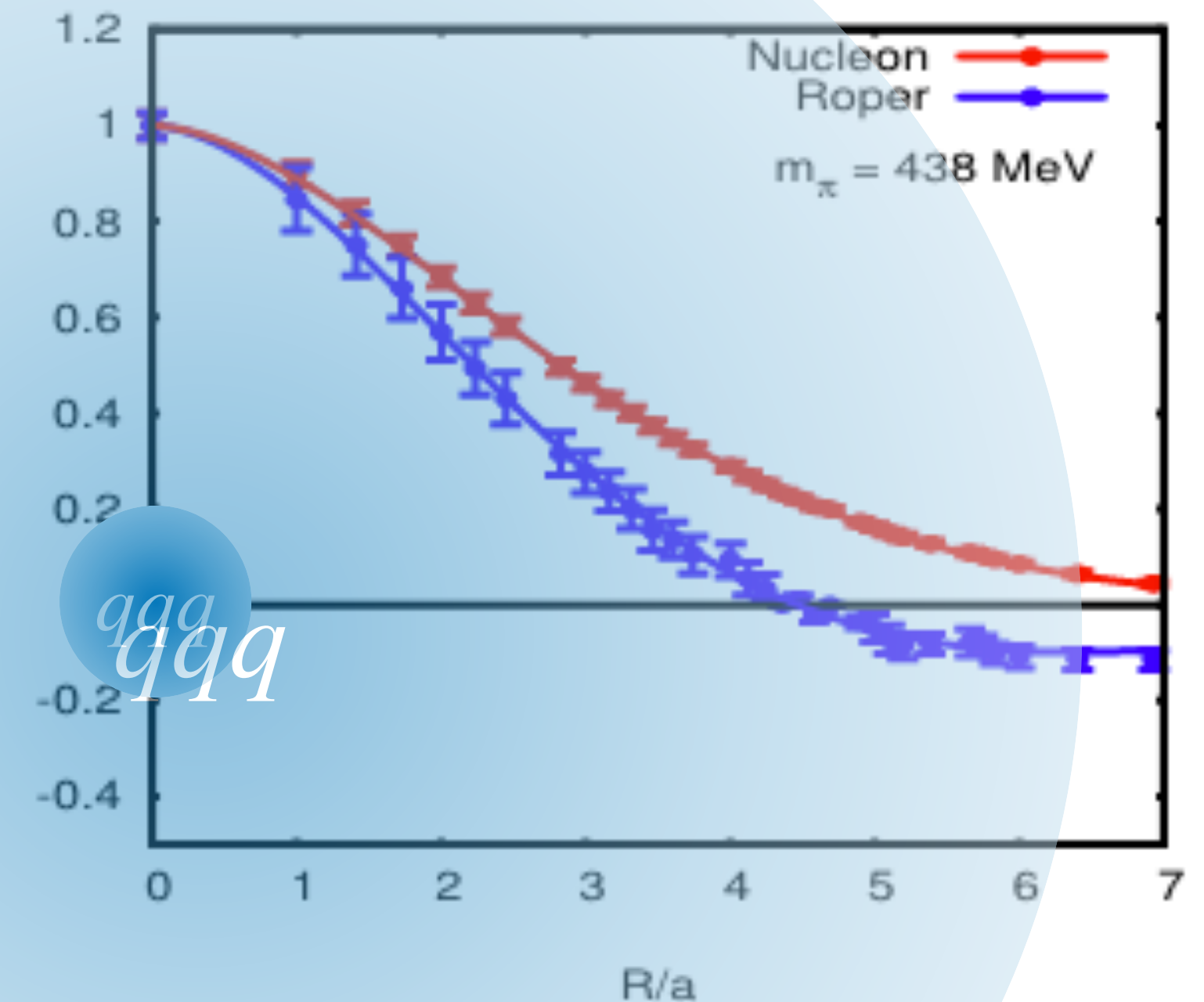
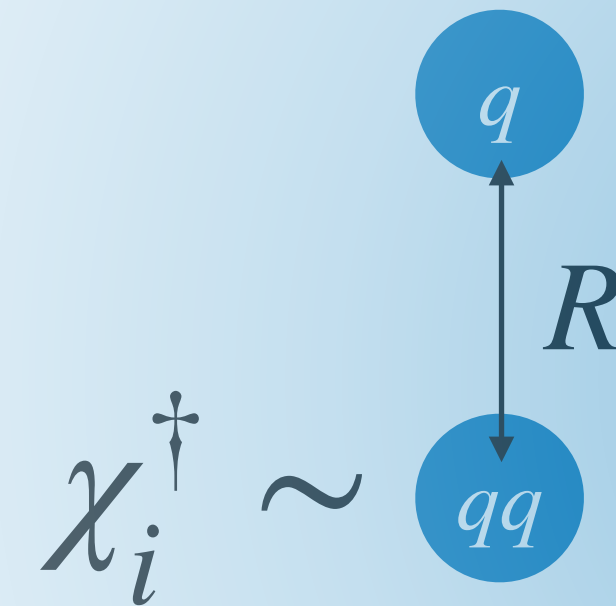
$N(1440) 1/2^+$

$$I(J^P) = \frac{1}{2}(\frac{1}{2}^+)$$

Re(pole position) = 1360 to 1380 (≈ 1370) MeV
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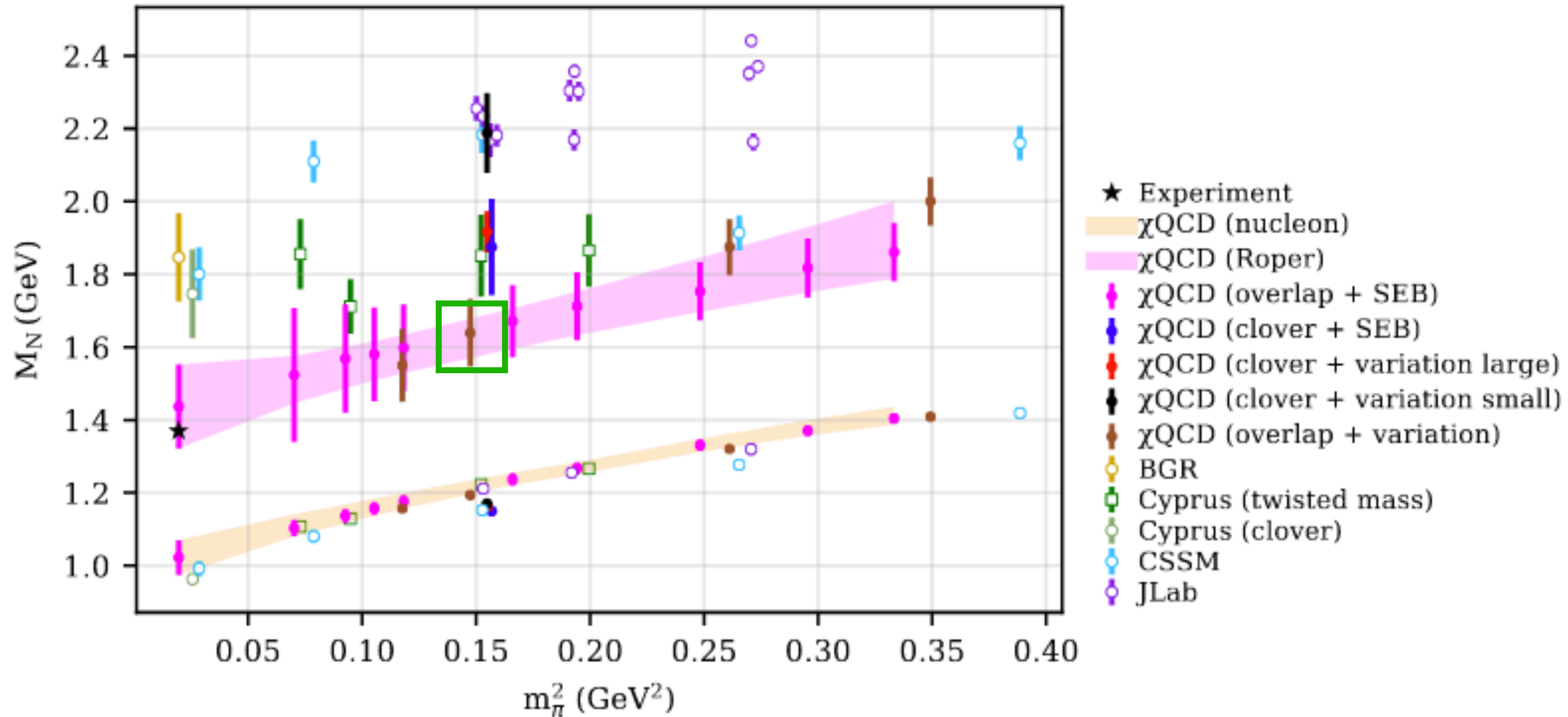


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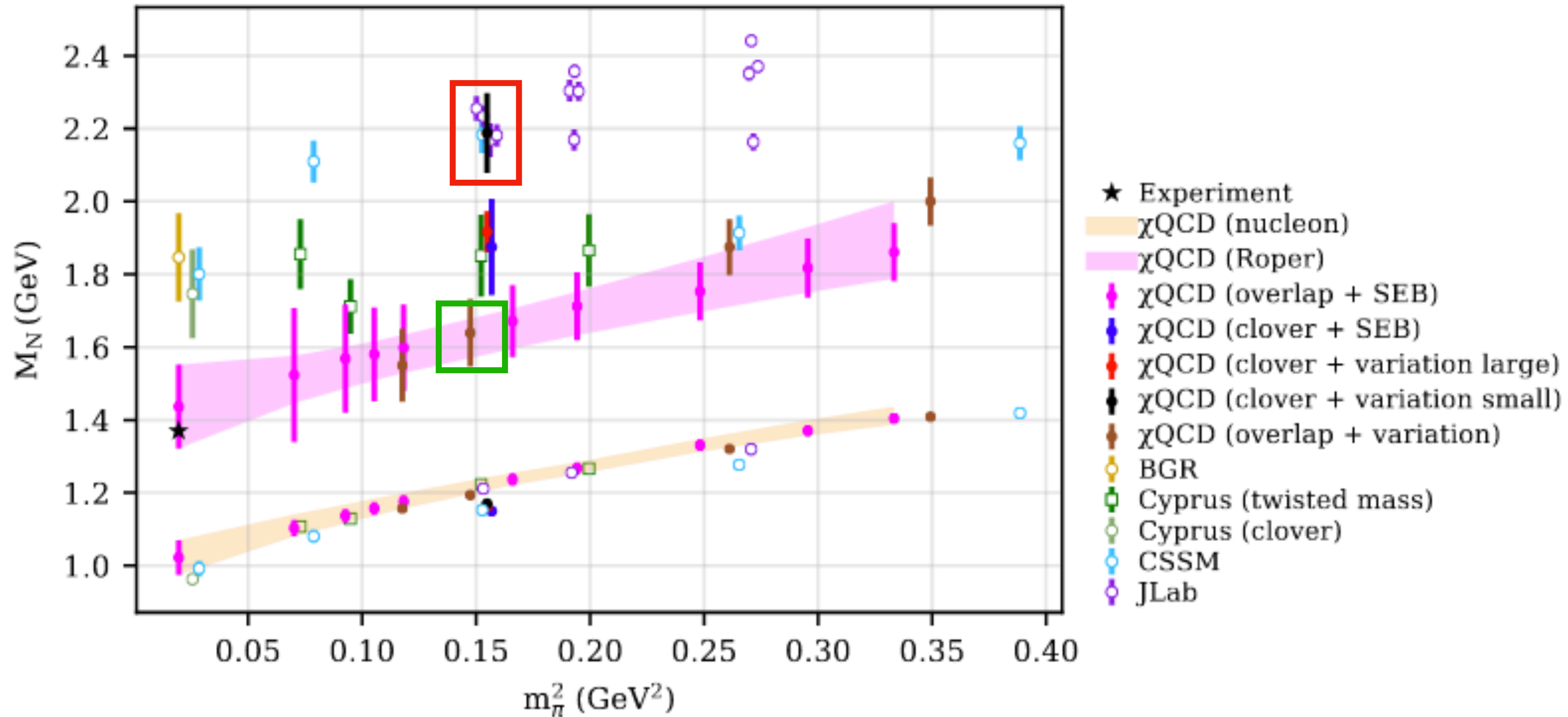
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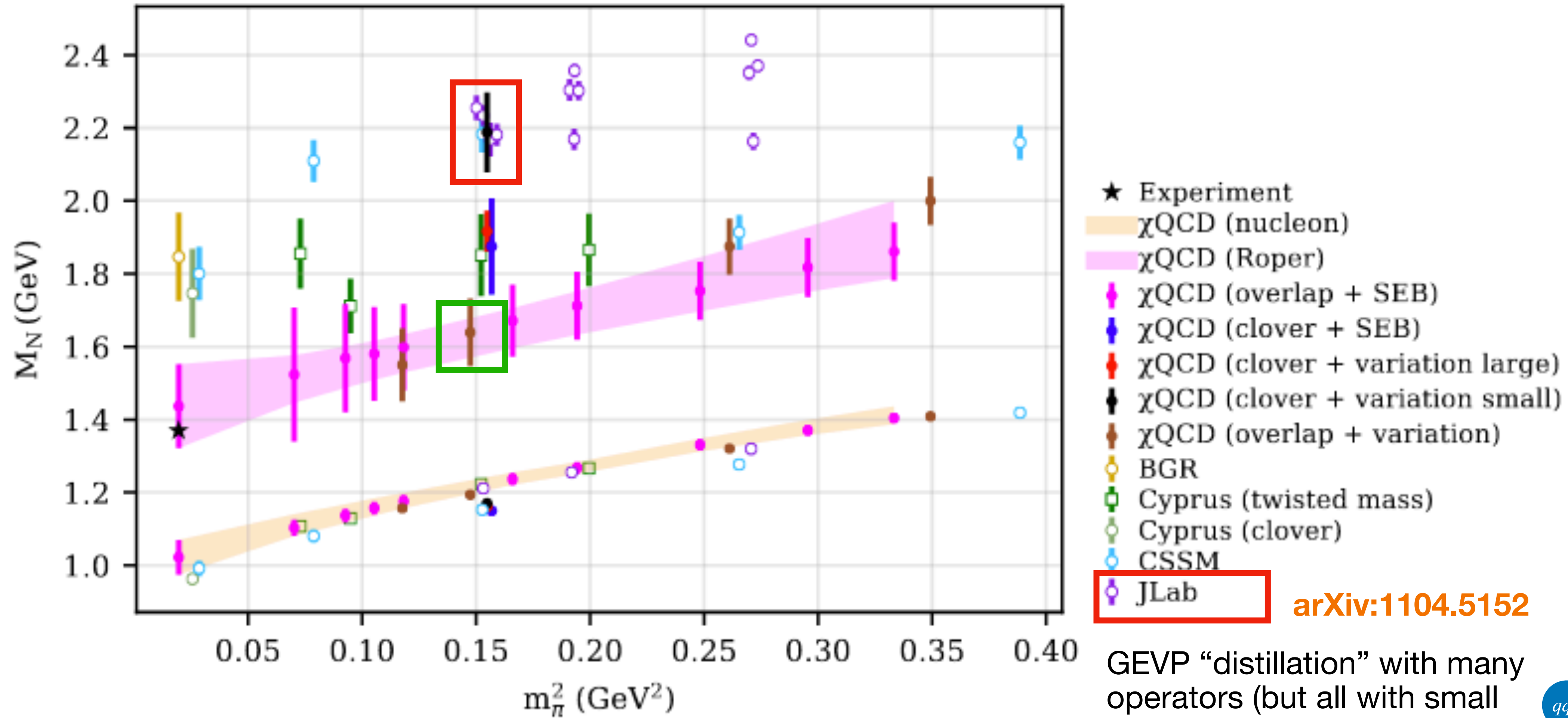
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GEVP "distillation" with many operators (but all with small smearing sizes)

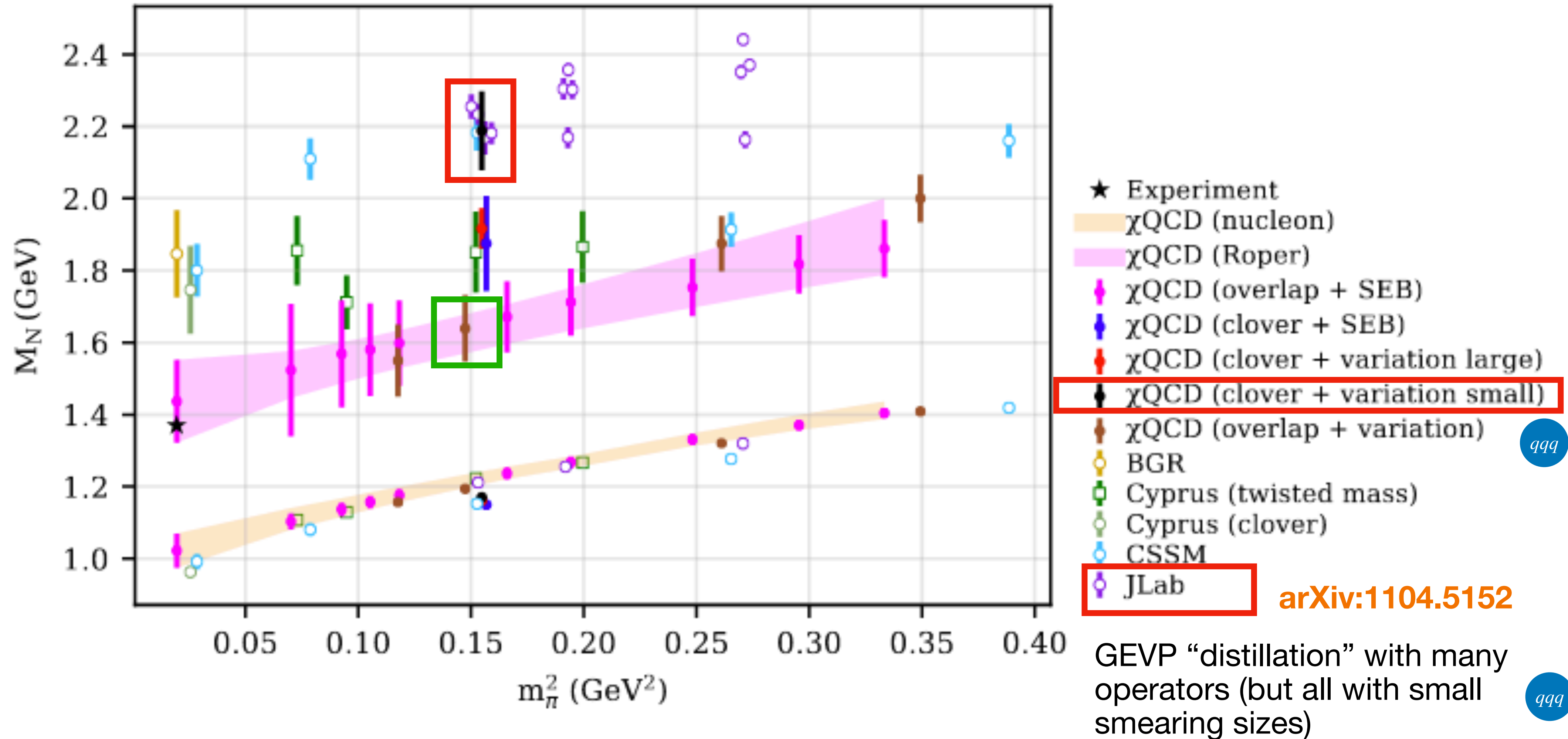
qqq

$qqq + \bar{q}q$

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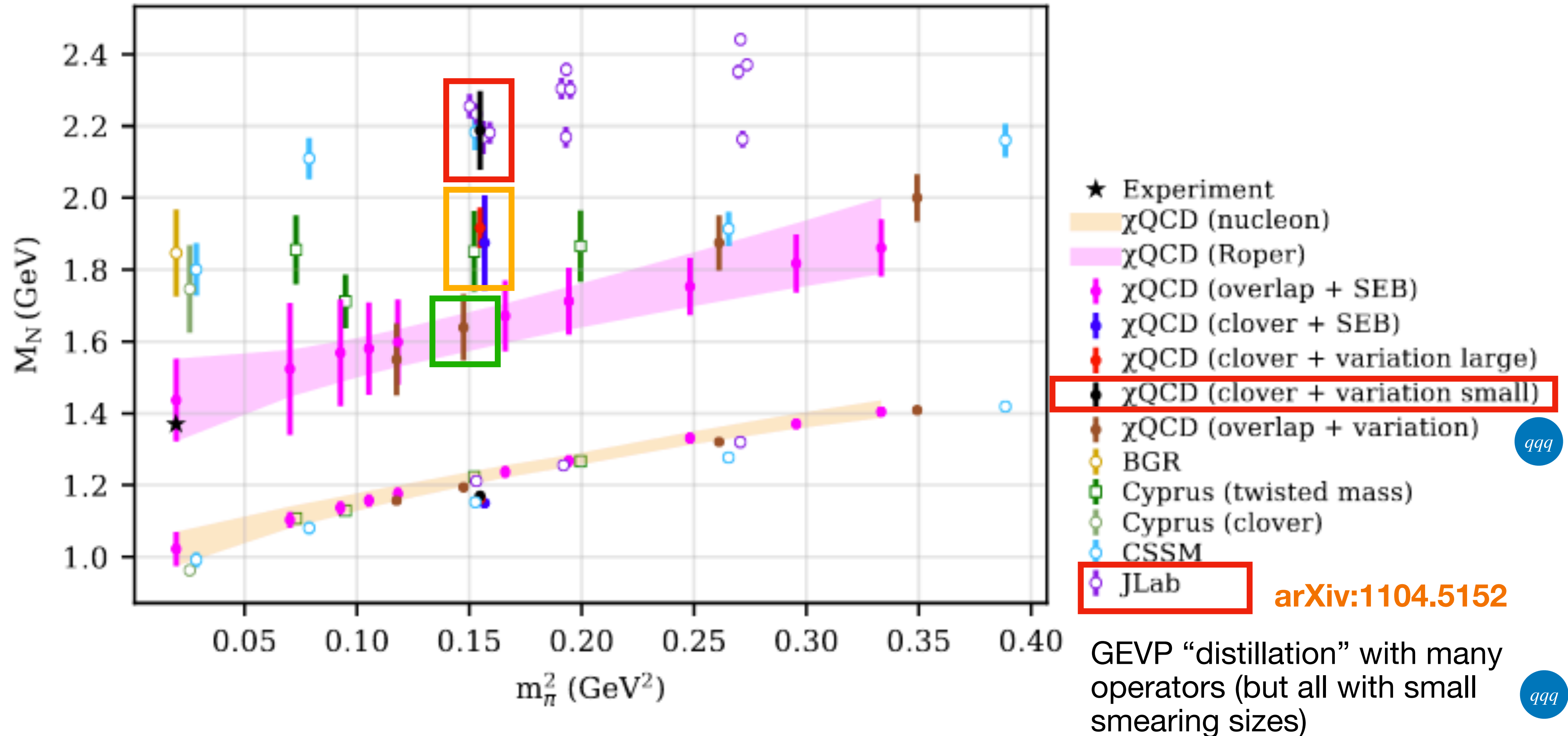
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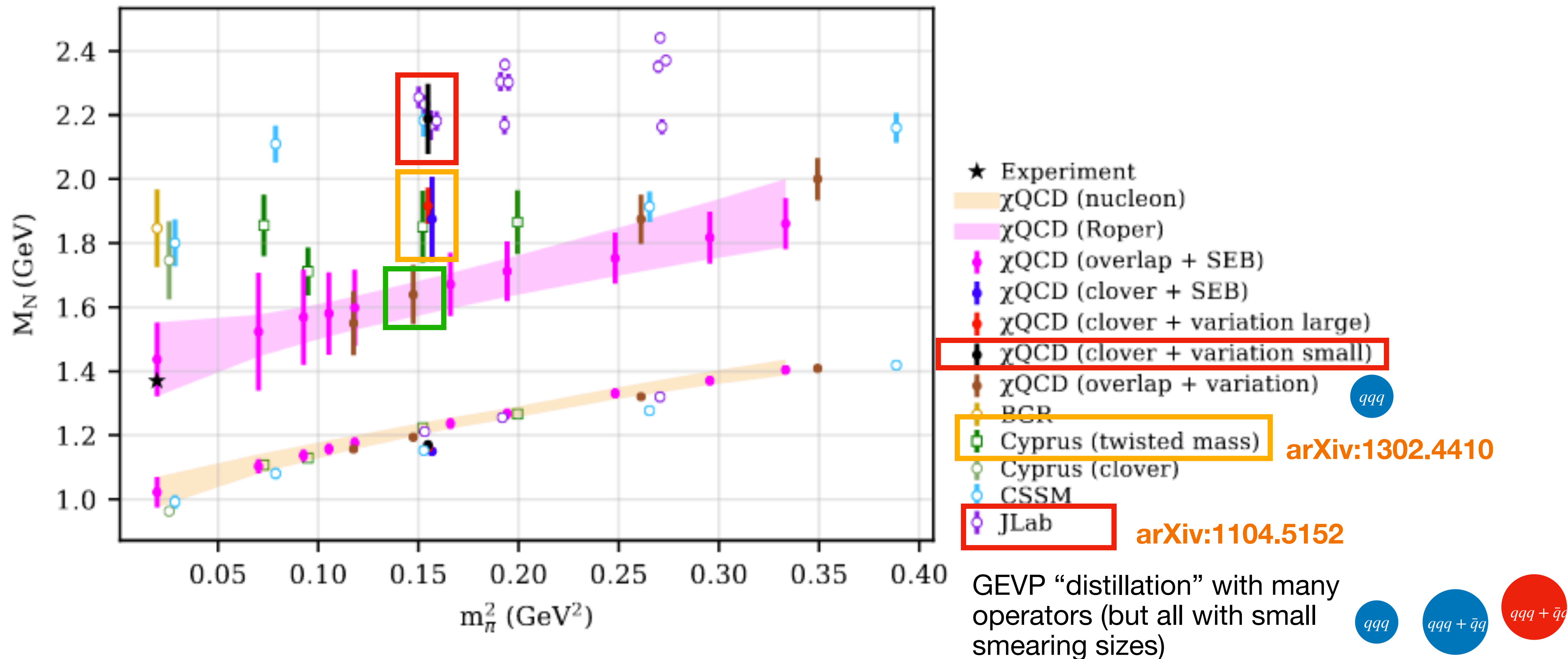
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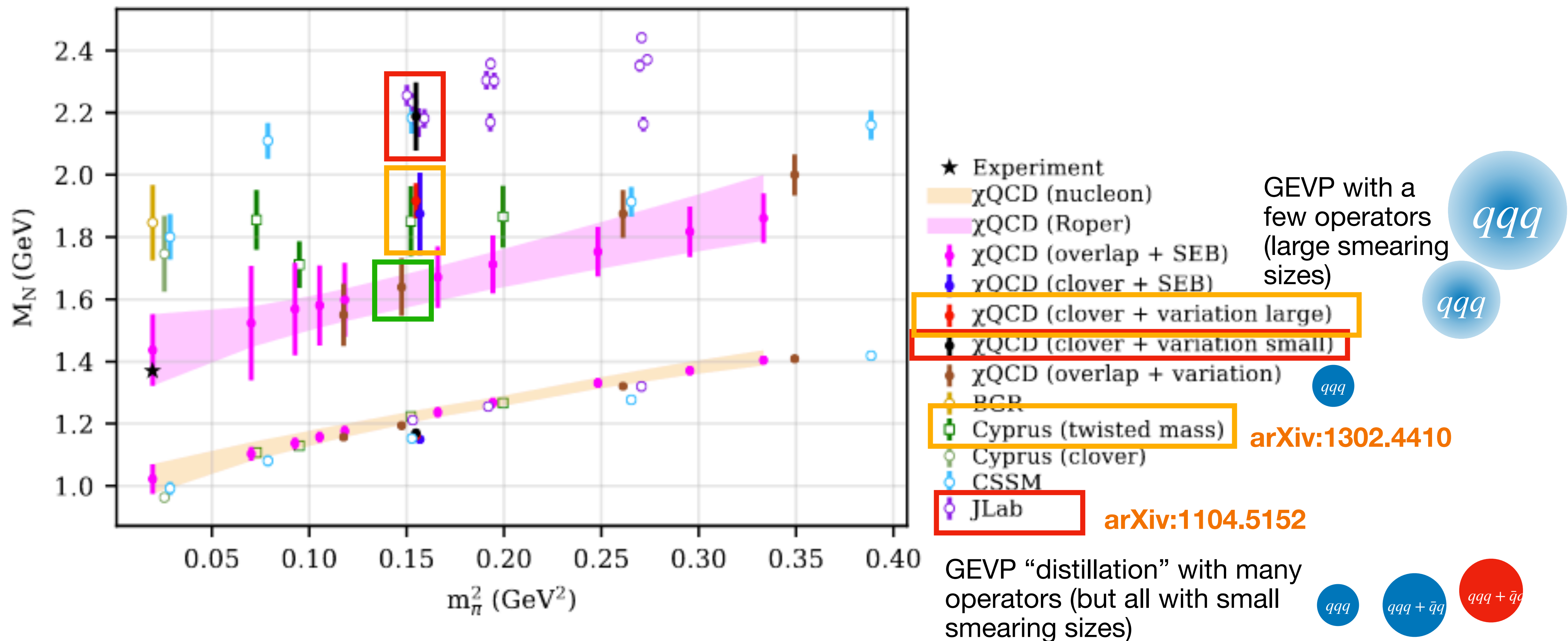
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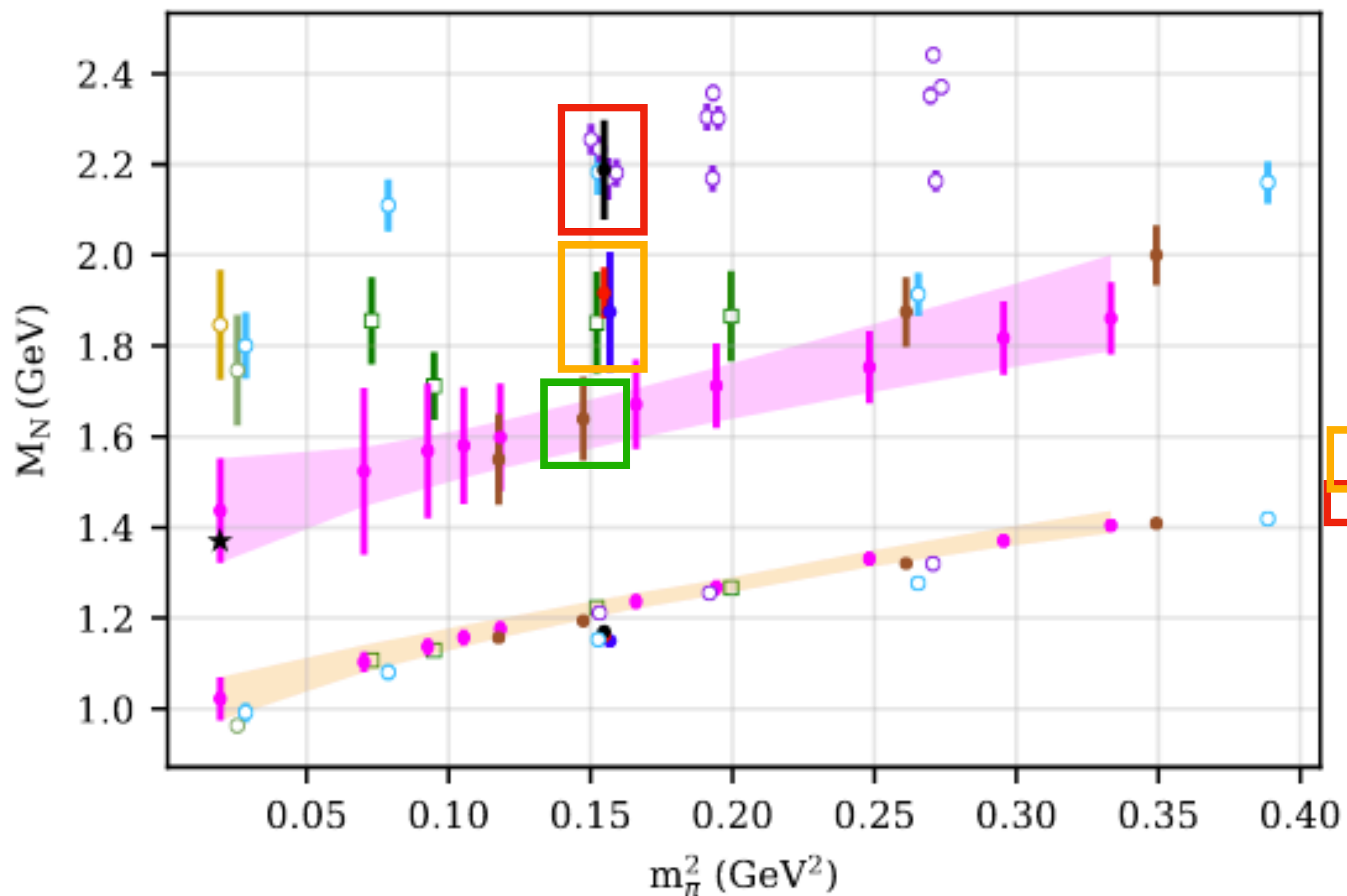
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Q2**: Can we choose the basis wisely and efficiently, if we are not interested in resolving all the E'_i 's? Yes!

- ★ Experiment
- χQCD (nucleon)
- χQCD (Roper)
- χQCD (overlap + SEB)
- χQCD (clover + SEB)
- χQCD (clover + variation large)
- χQCD (clover + variation small)
- χQCD (overlap + variation)
- BCR
- Cyprus (twisted mass)
- Cyprus (clover)
- CSSM
- JLab

GEVP with a few operators (large smearing sizes)

GEVP "distillation" with many operators (but all with small smearing sizes)

arXiv:1302.4410

arXiv:1104.5152

qqq

qqq

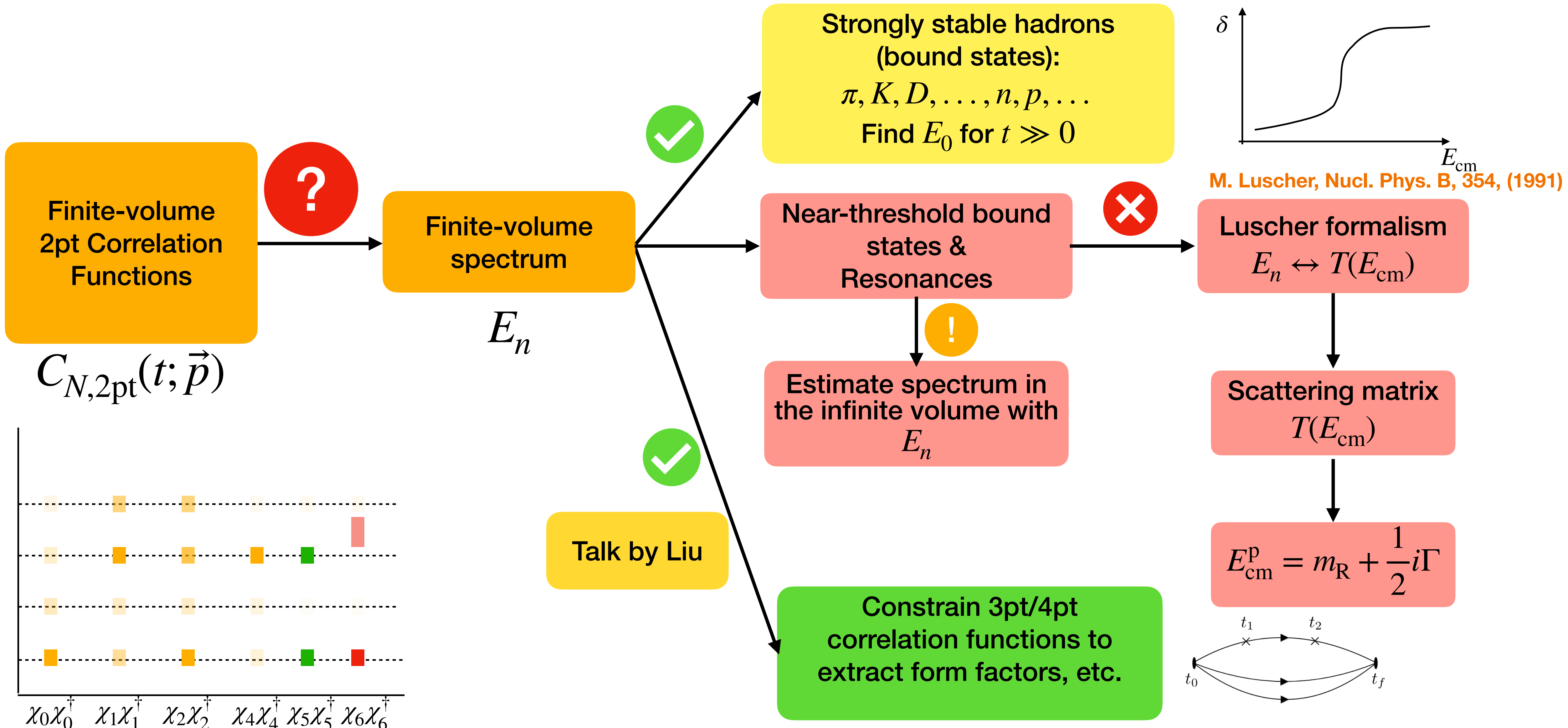
qqq

qqq

qqq + q̄q

qqq + q̄q

Finite-volume spectrum from lattice QCD

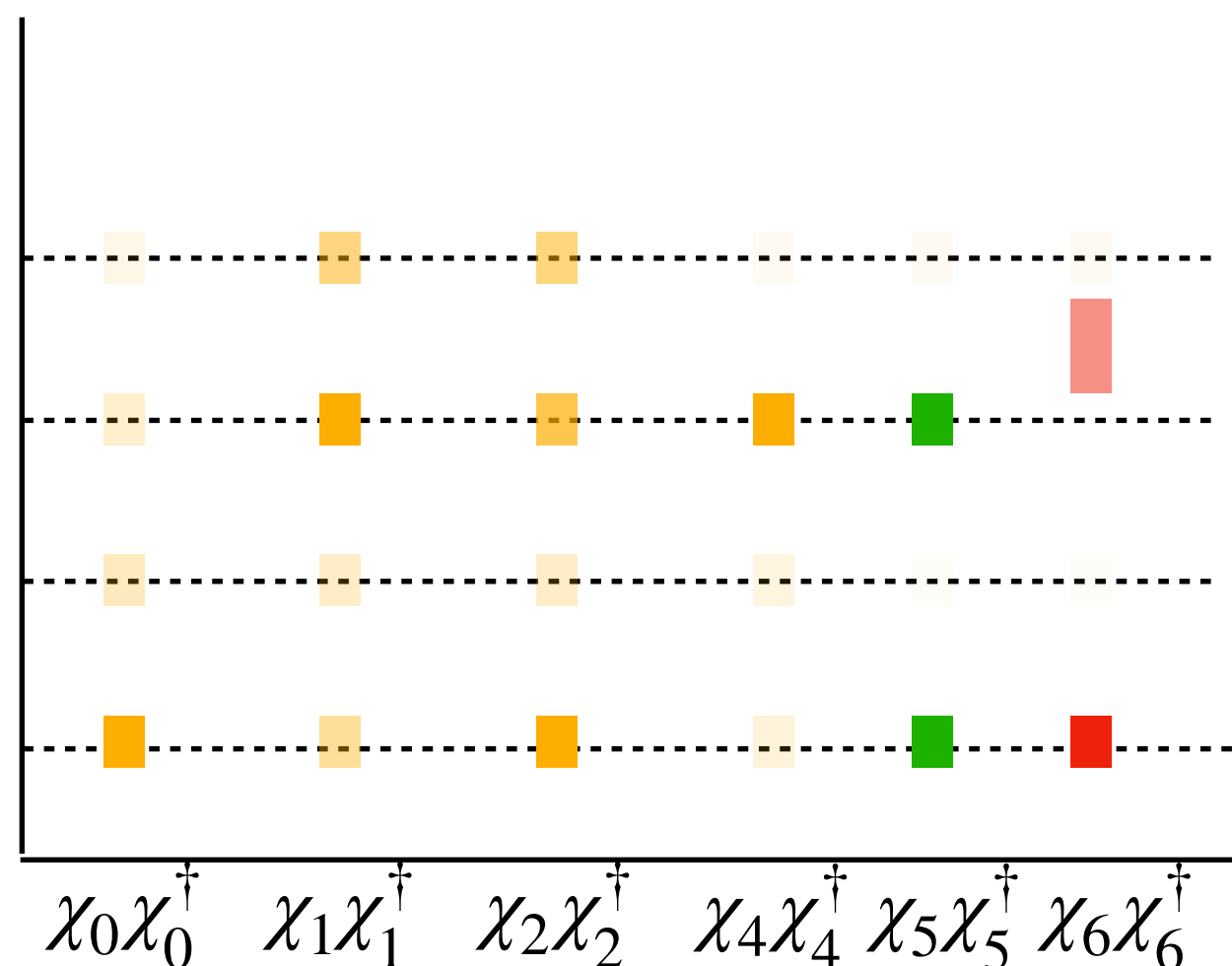


Finite-volume spectrum from lattice QCD

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Finite-volume 2pt Correlation Functions

$$C_{N,2pt}(t; \vec{p})$$



Finite-volume spectrum

E_n



Talk by Liu

Strongly stable hadrons (bound states):
 $\pi, K, D, \dots, n, p, \dots$
Find E_0 for $t \gg 0$

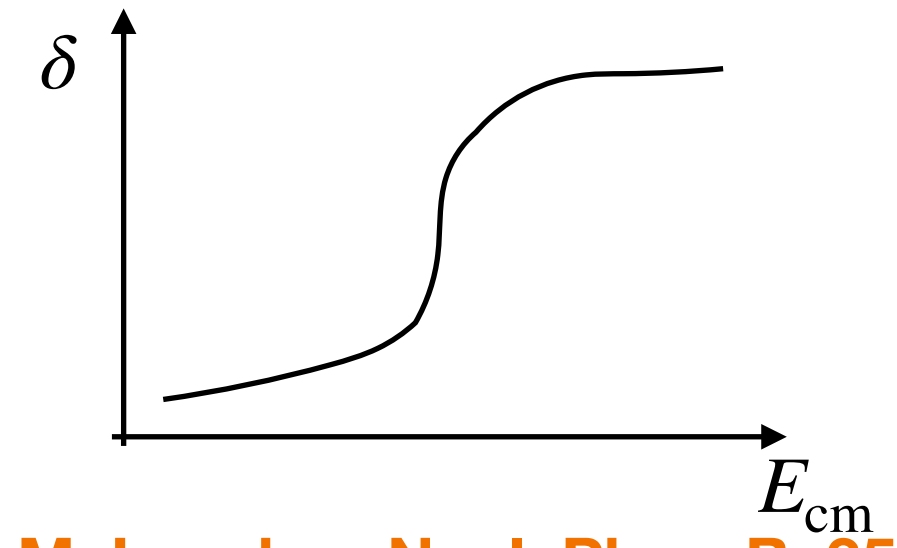
Near-threshold bound states & Resonances



Estimate spectrum in the infinite volume with E_n



Constrain 3pt/4pt correlation functions to extract form factors, etc.

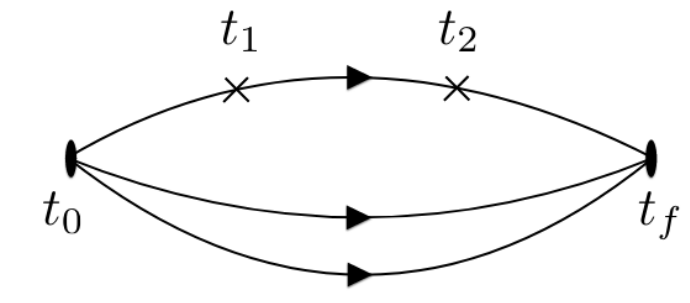


M. Luscher, Nucl. Phys. B, 354, (1991)

Luscher formalism
 $E_n \leftrightarrow T(E_{cm})$

Scattering matrix
 $T(E_{cm})$

$$E_{cm}^p = m_R + \frac{1}{2}i\Gamma$$

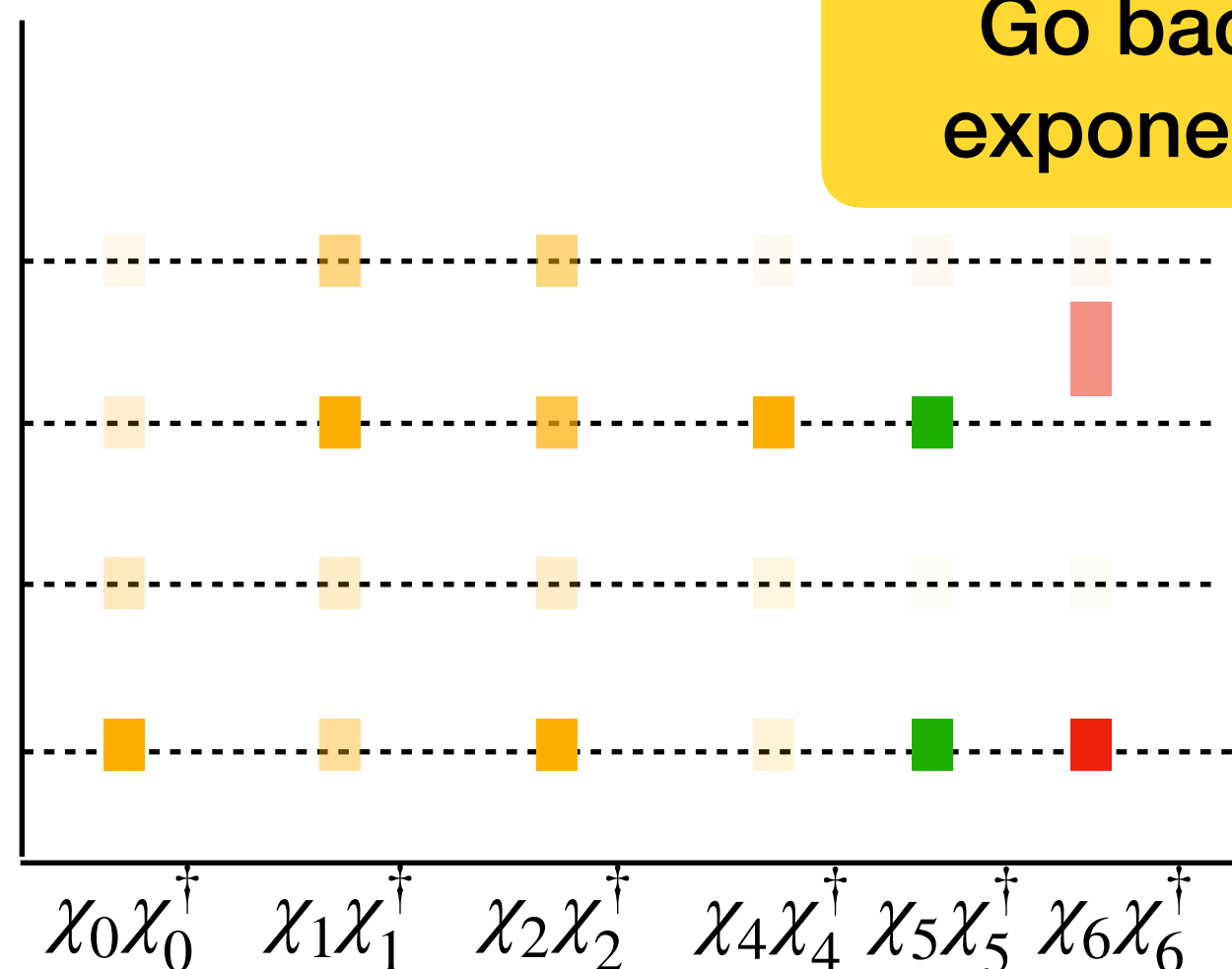


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Finite-volume spectrum

E_n

Only one operator?
Go back to multi-exponential priors?

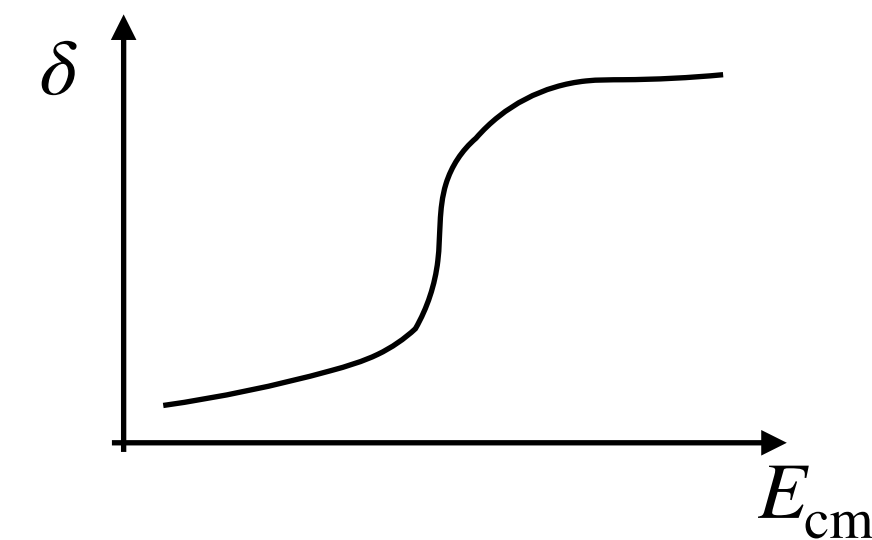
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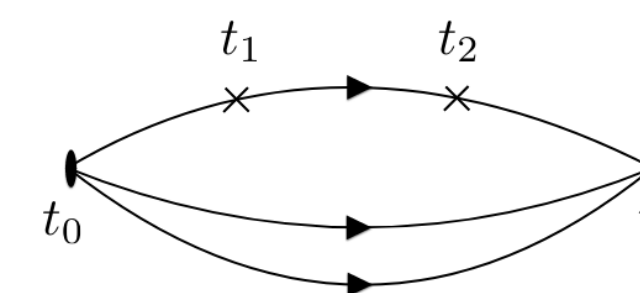


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The Bayesian Reconstruction for inverse problems

A. Rothkopf, "Bayesian inference of real-time dynamics from lattice QCD," Front. Phys., arXiv:2208.13590

Yannis Burnier and Alexander Rothkopf, Phys. Rev. Lett. 111, 182003

Marginalize α_l with $P[\alpha] = 1$

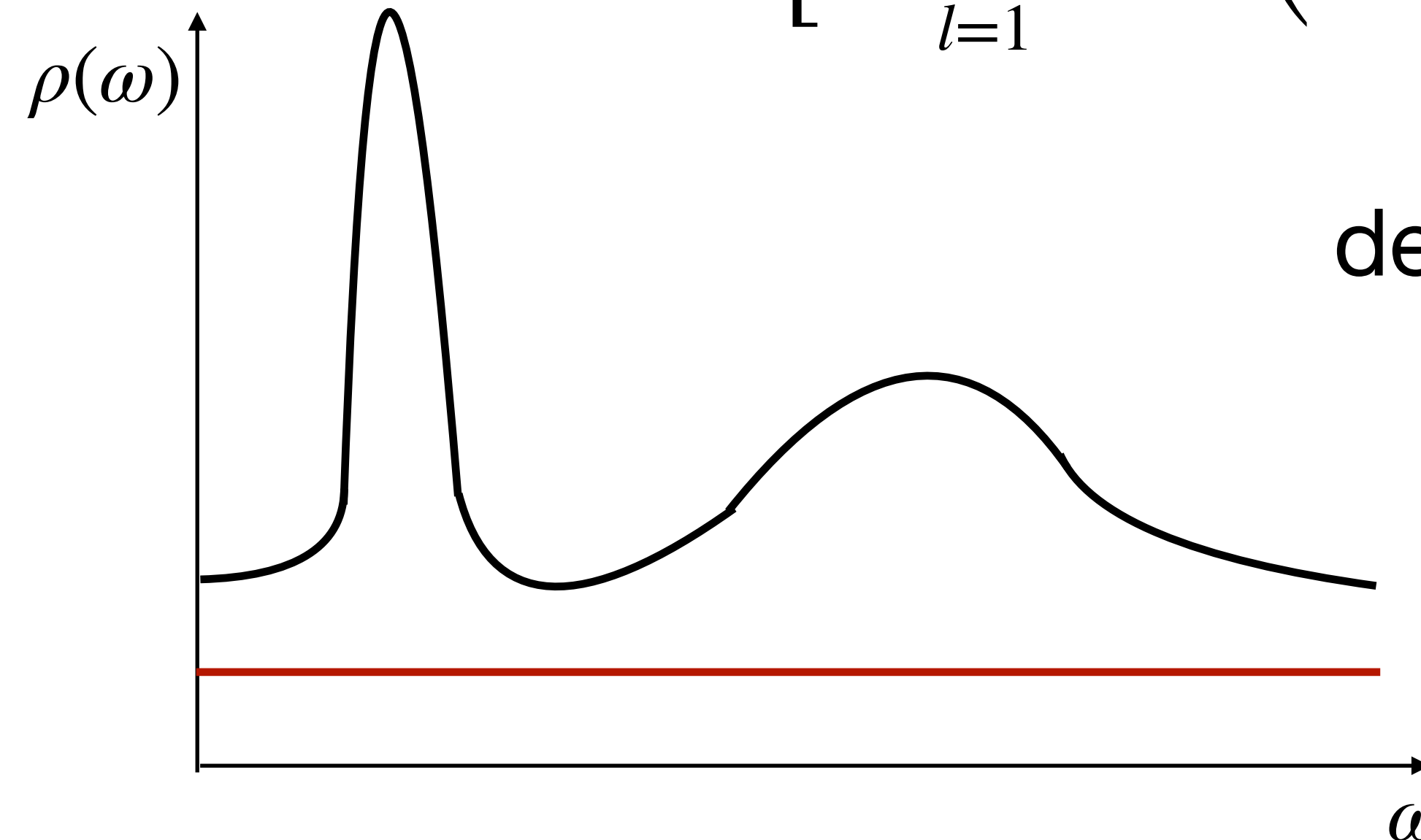
$$\underbrace{P[\rho | D, m]}_{\text{posterior}^*} = \underbrace{P[D | \rho, I]}_{\text{likelihood}} \times \underbrace{\prod_l \int d\alpha_l P[\rho | \alpha, m] P[\alpha]}_{\text{prior}^*} / \underbrace{P[D | m]}_{\text{evidence}}$$

$$e^{-Q} \quad e^{-L} \quad e^S$$

$$P[\rho | \alpha, m] = \exp \left[- \sum_{l=1}^{N_\mu} \alpha_l \Delta\mu \left(1 - \frac{\rho_l}{m_l} - \log \left[\frac{\rho_l}{m_l} \right] \right) \right]$$

fitted spectrum

default model



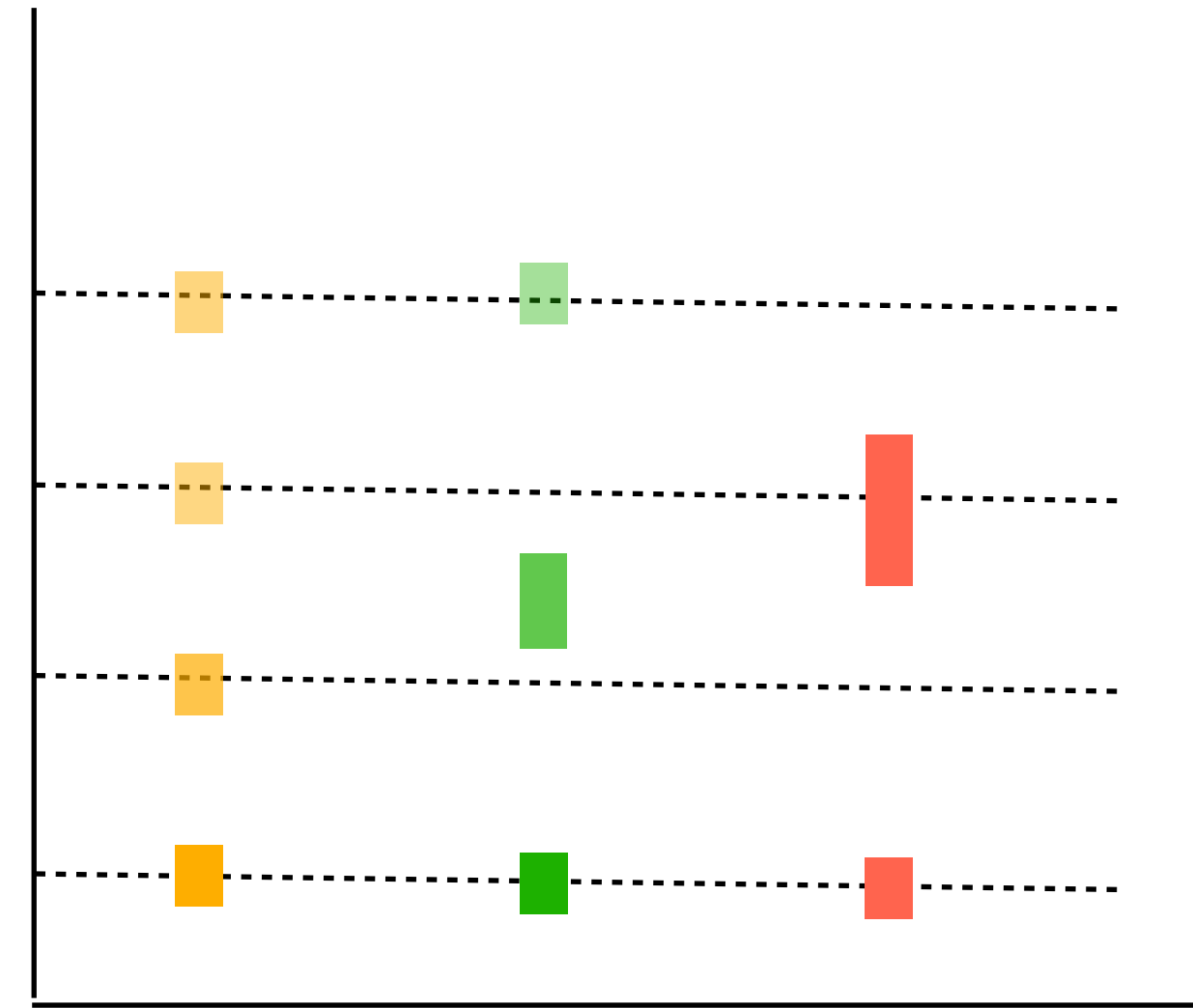
$$Q = L - S + \dots$$

$$\chi^2 \equiv \sum_{ij} (D_i - \tilde{D}_i) C_{ij}^{-1} (D_j - \tilde{D}_j)$$

The Bayesian Reconstruction on nucleon correlators

- To extract the finite-volume spectrum
 - Two-point correlation functions

$$C_{ij}(t) = \langle \chi_i(t) \chi_j^\dagger(0) \rangle = \sum_{n=0}^{\infty} W_n e^{-E_n t}$$



$N = 4$ $N = 3$ $N = 2$

↓

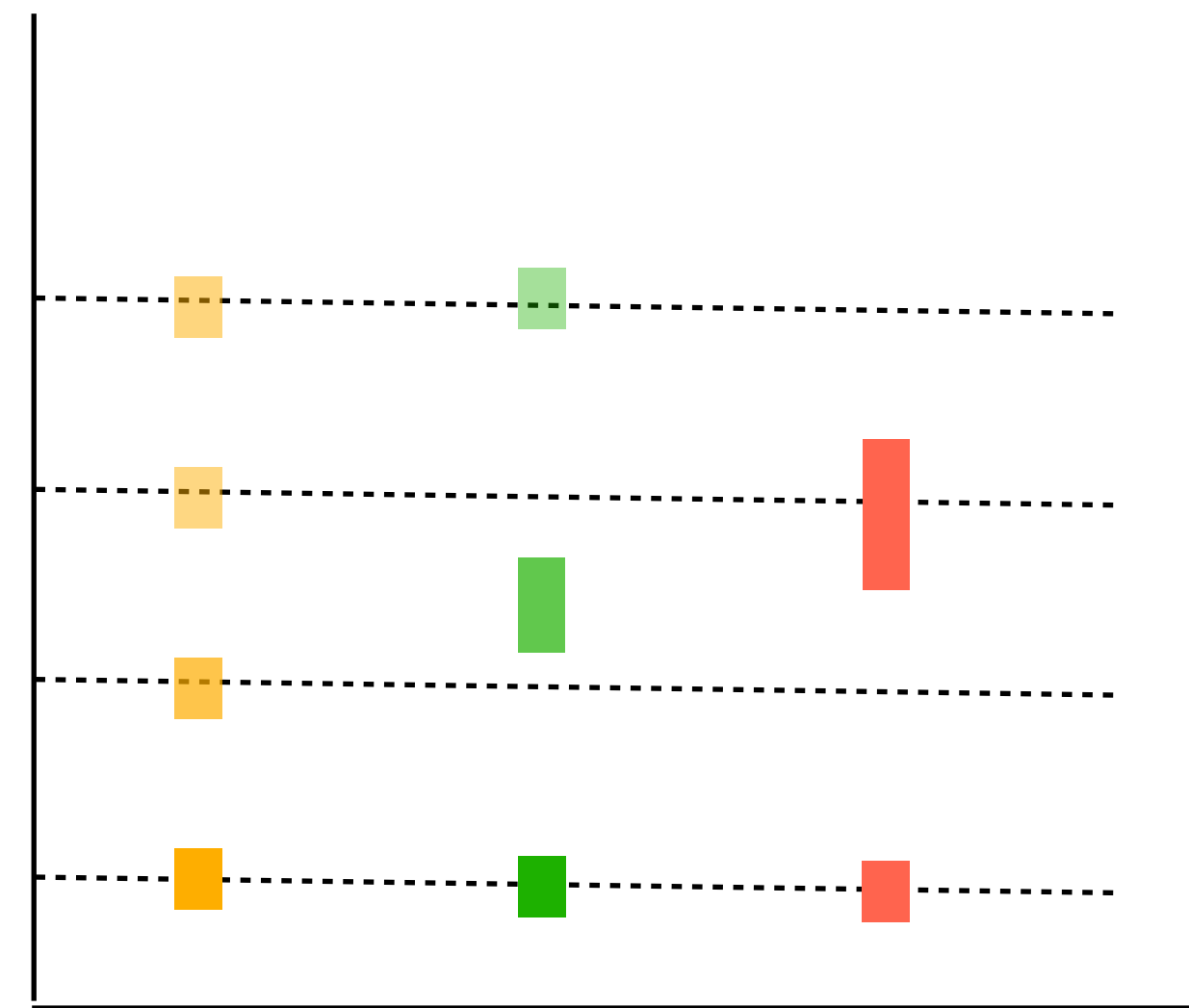
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- Finite-volume spectrum found in terms of spectral function $\rho(\omega)$

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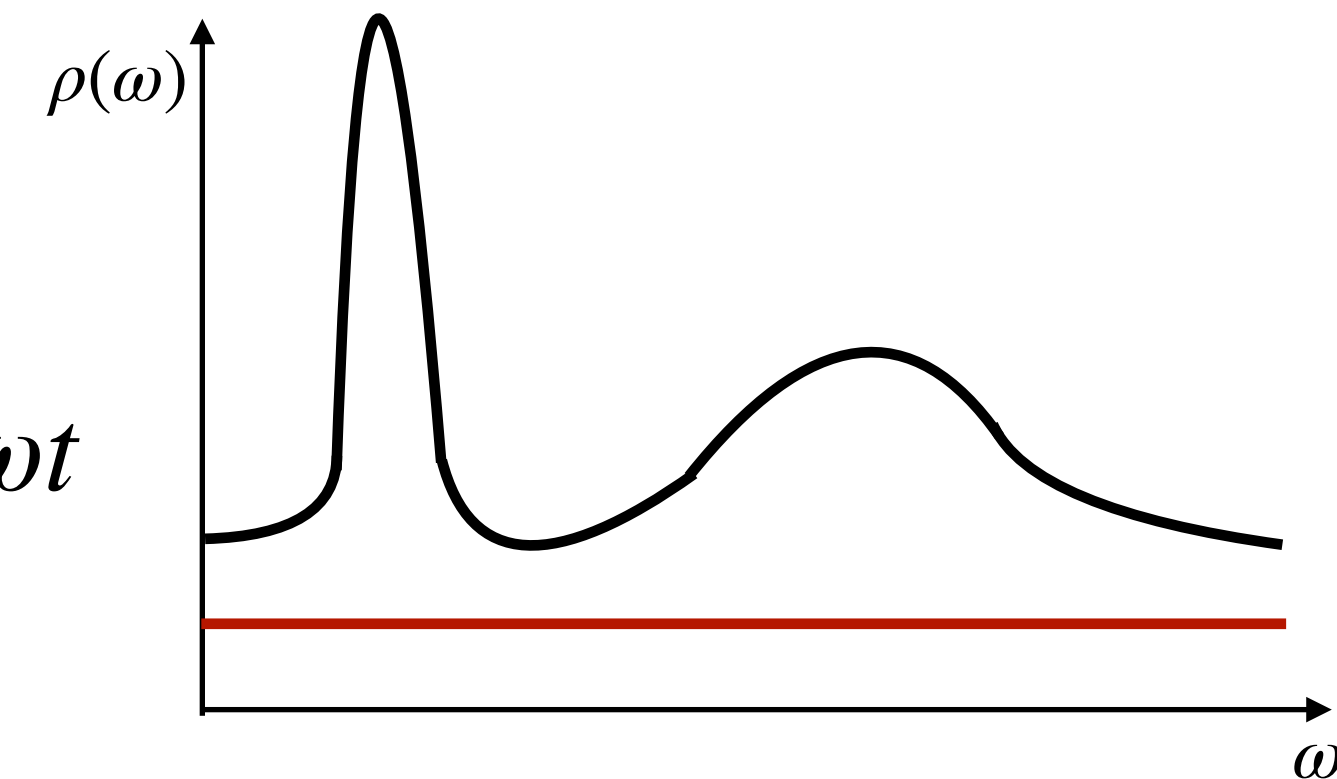
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M. T. Hansen et al.,
Phys. Rev. D 96, 094513 (2017)

Talks by Liang,
Sufian

$$\rightarrow \int d\omega \rho(\omega) e^{-\omega t}$$

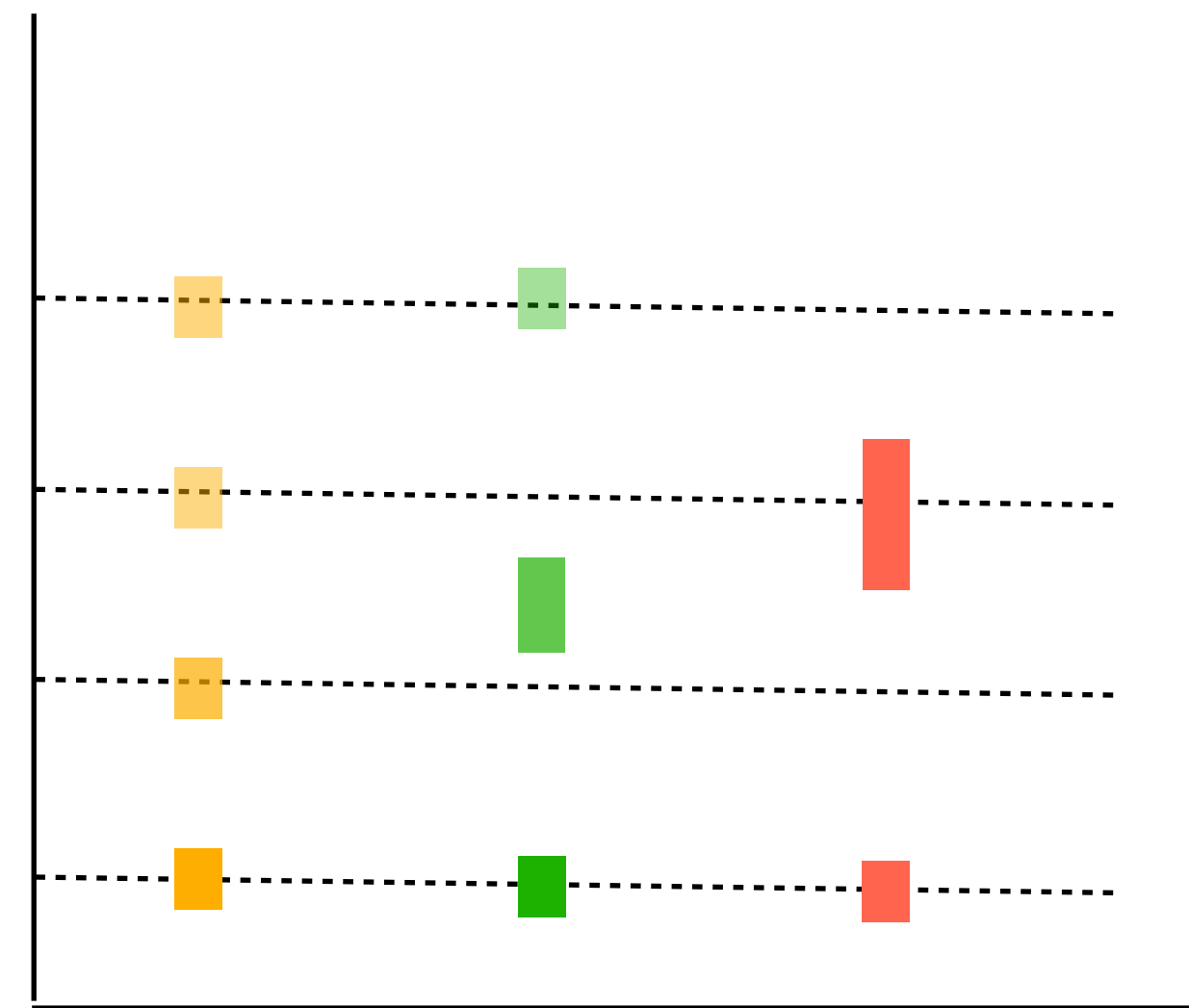


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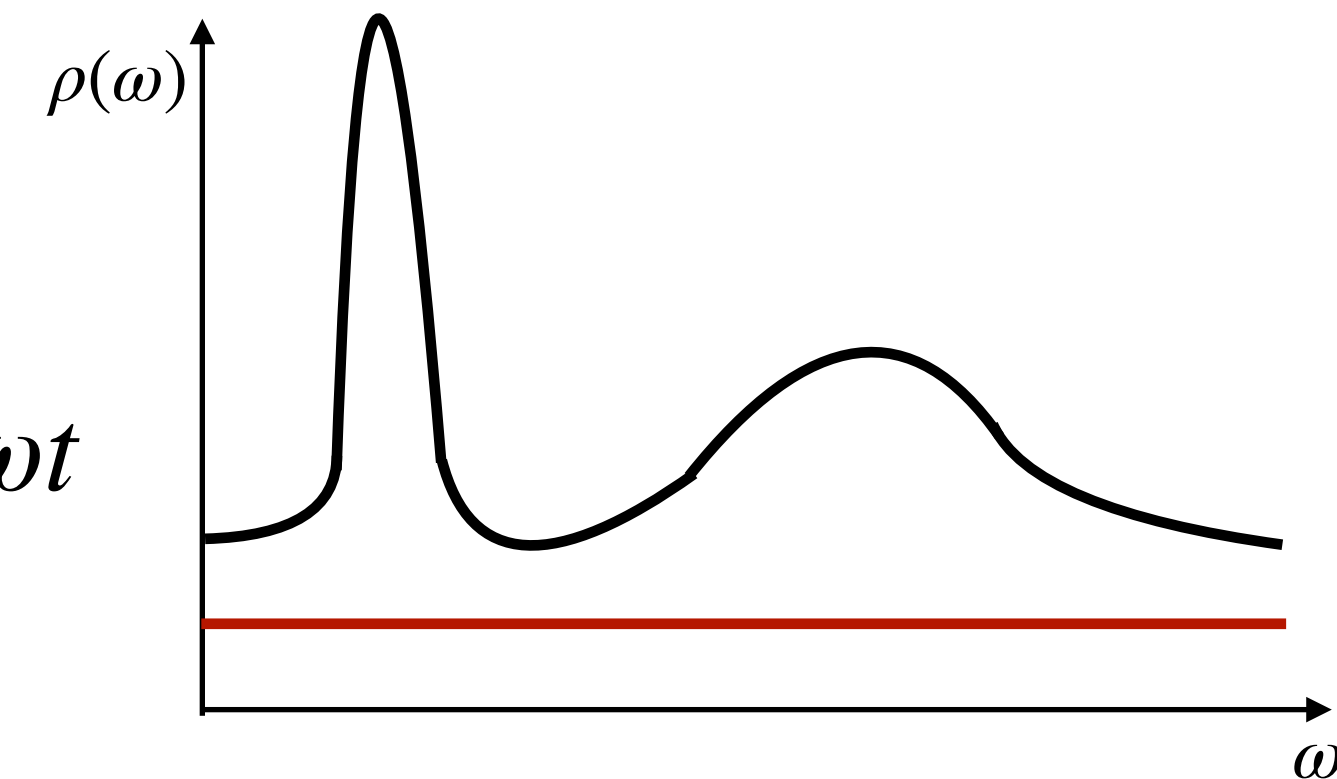
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M. T. Hansen et al.,
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Talks by Liang,
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$$\rightarrow \int d\omega \rho(\omega) e^{-\omega t}$$



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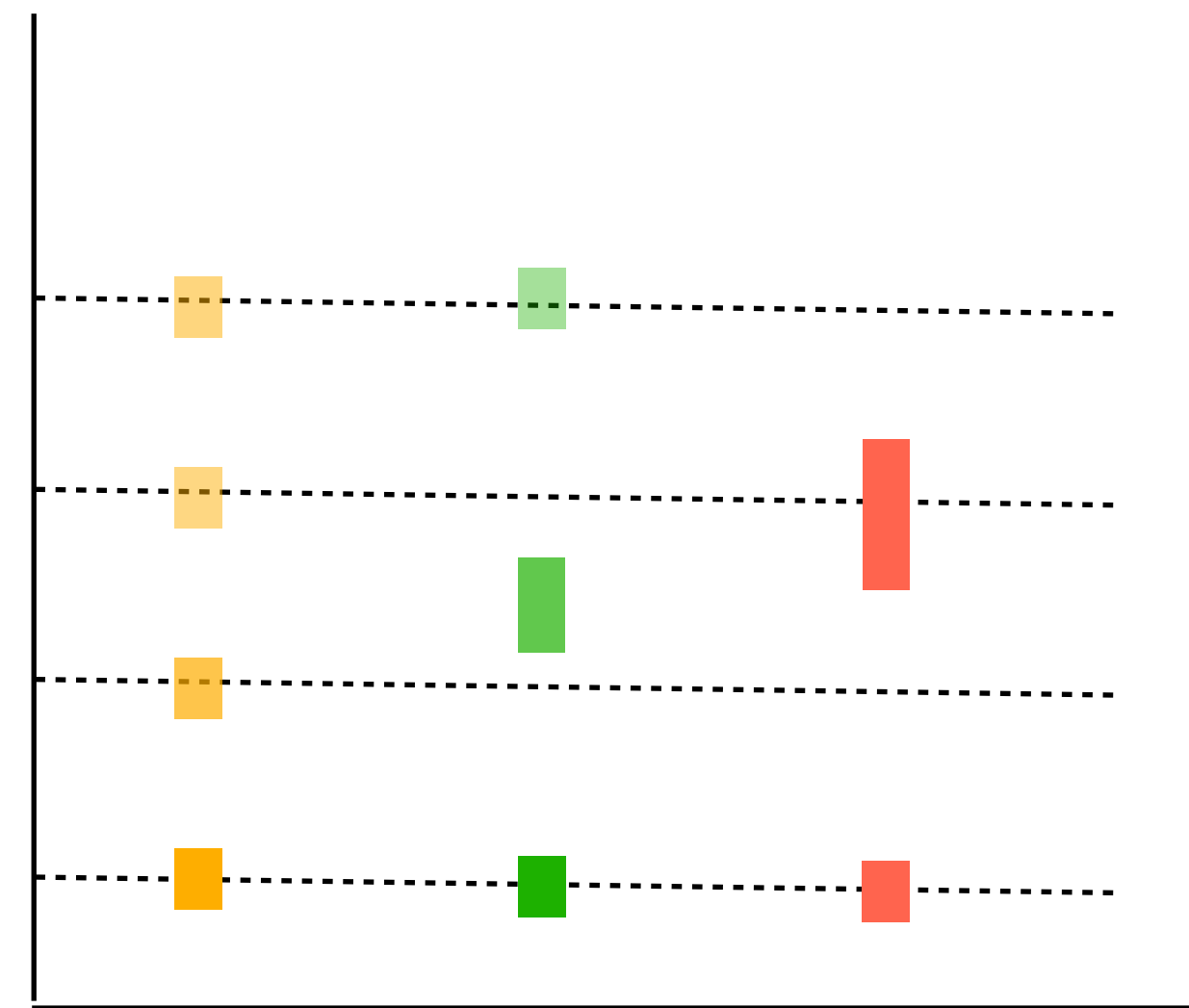
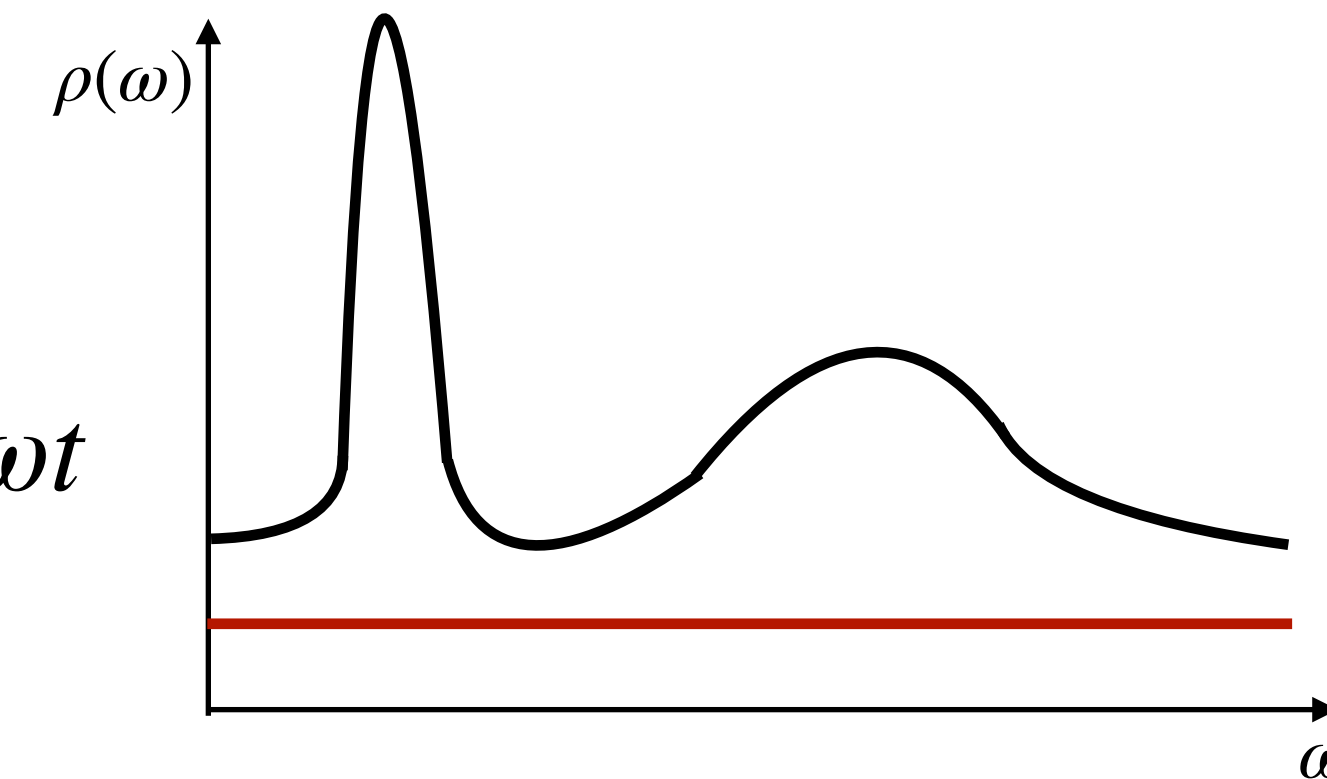
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M. T. Hansen et al.,
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G. P. Lepage et al., arXiv: hep-lat/0110175

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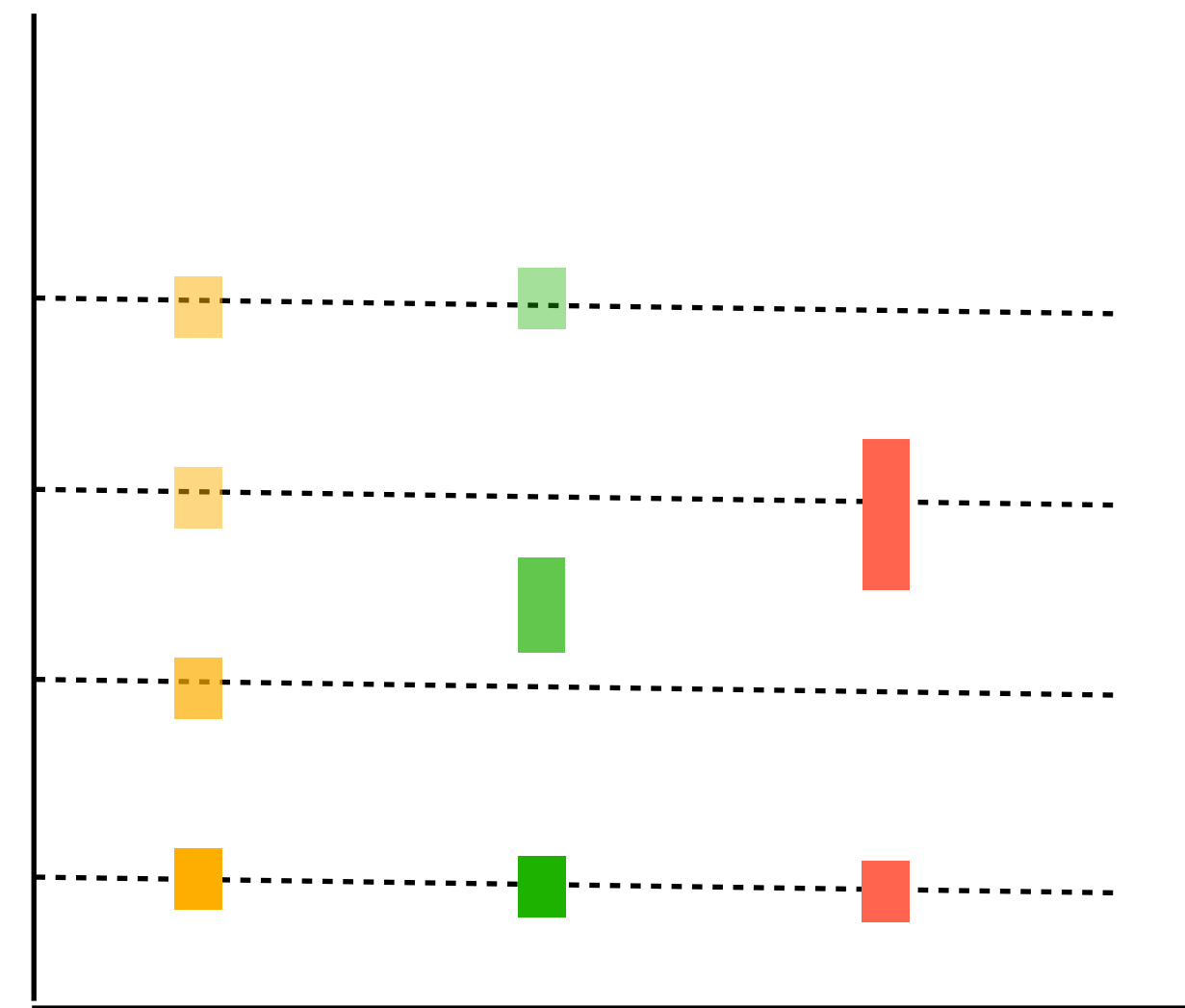
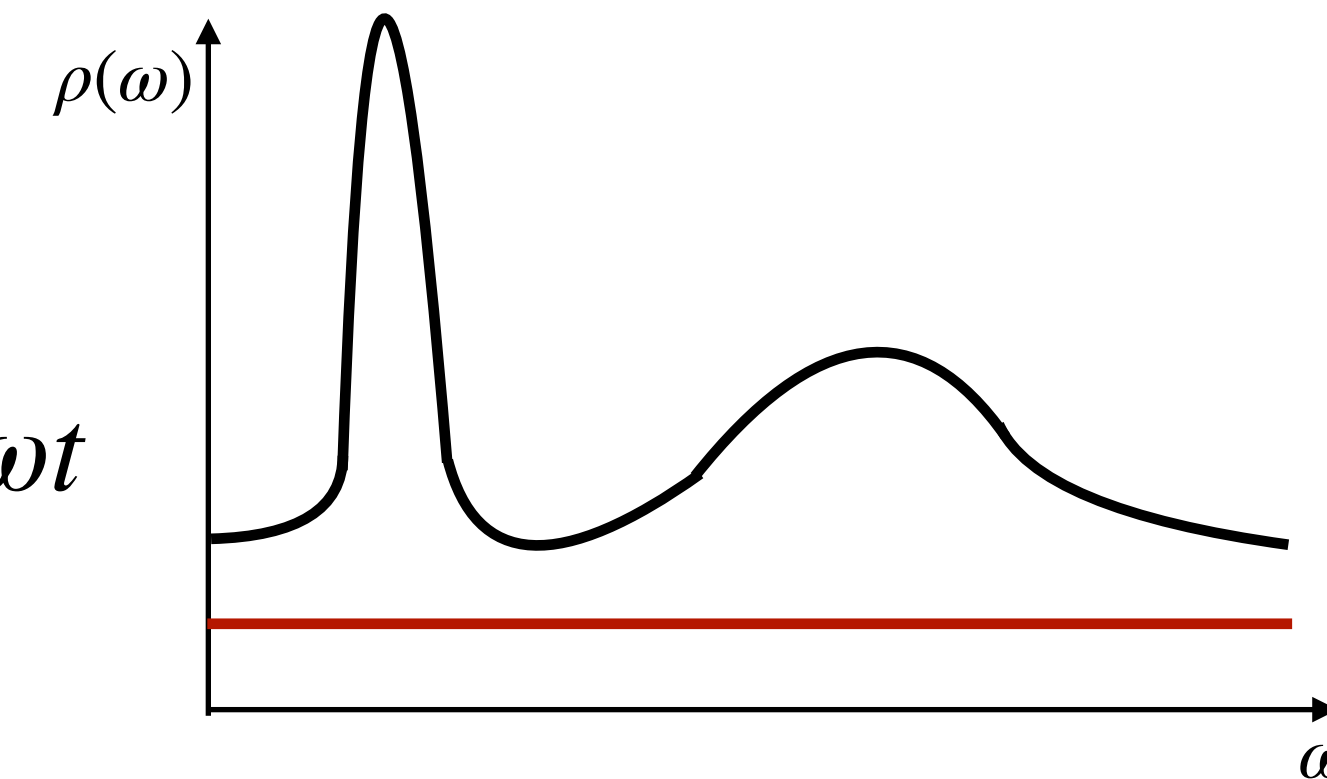
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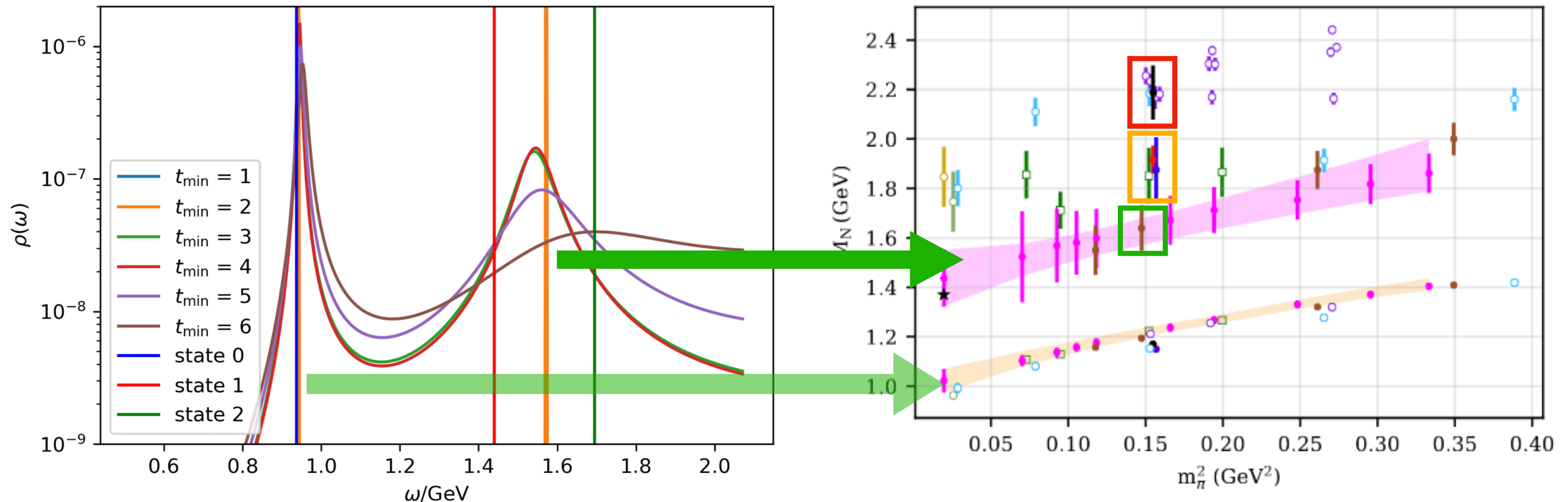
Finite-volume spectrum with BR **preliminary**

Ens.	Action (F+G)	$1/a$ (GeV)	Lattice volume	m_l	m_s	m_{res}	m_π	Size (fm)
				(in lattice units)			(MeV)	(fm)
10	MDWF+I	1.730(4)	$48^3 \times 96 \times 24$	0.00078	0.0362	0.000614	139	5.5

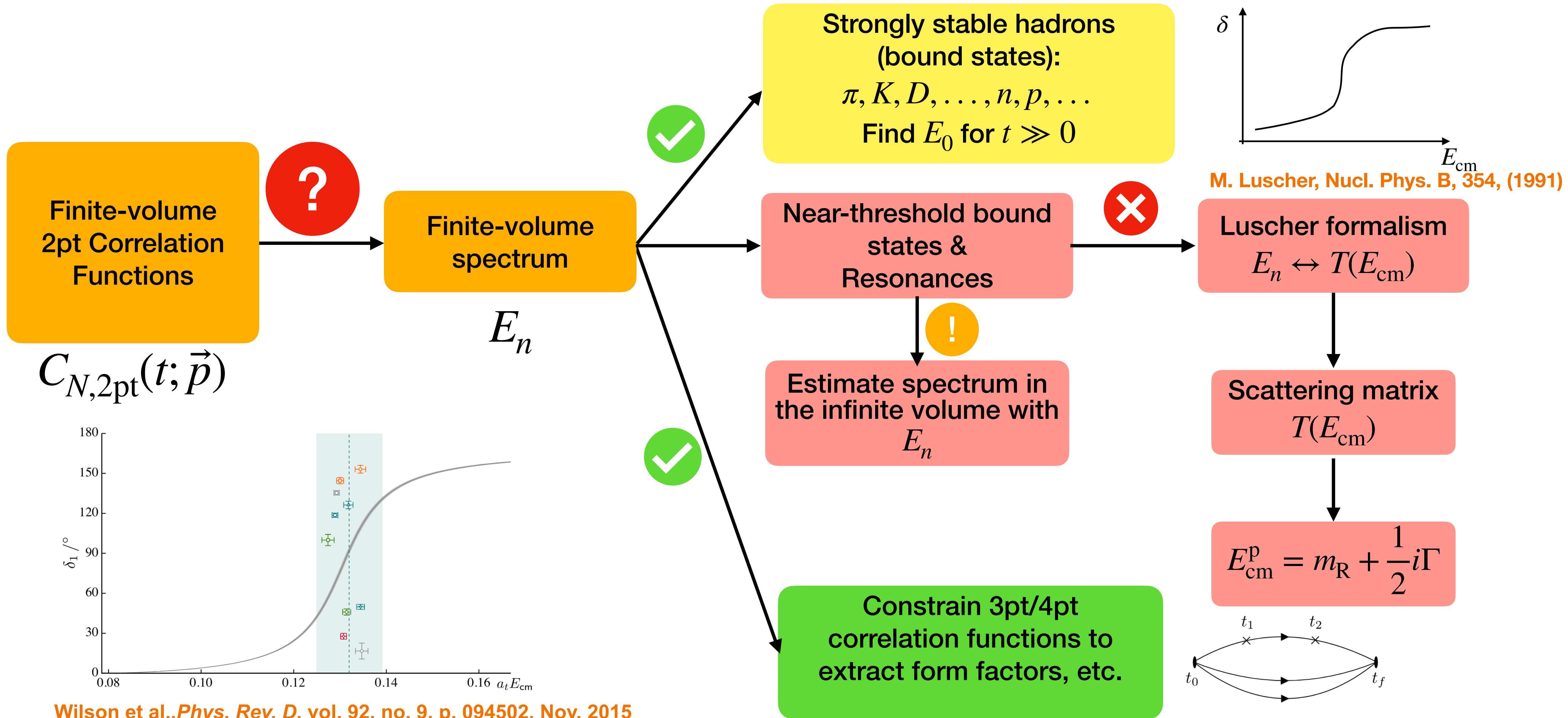
Default model

$$m(\omega) = const.$$

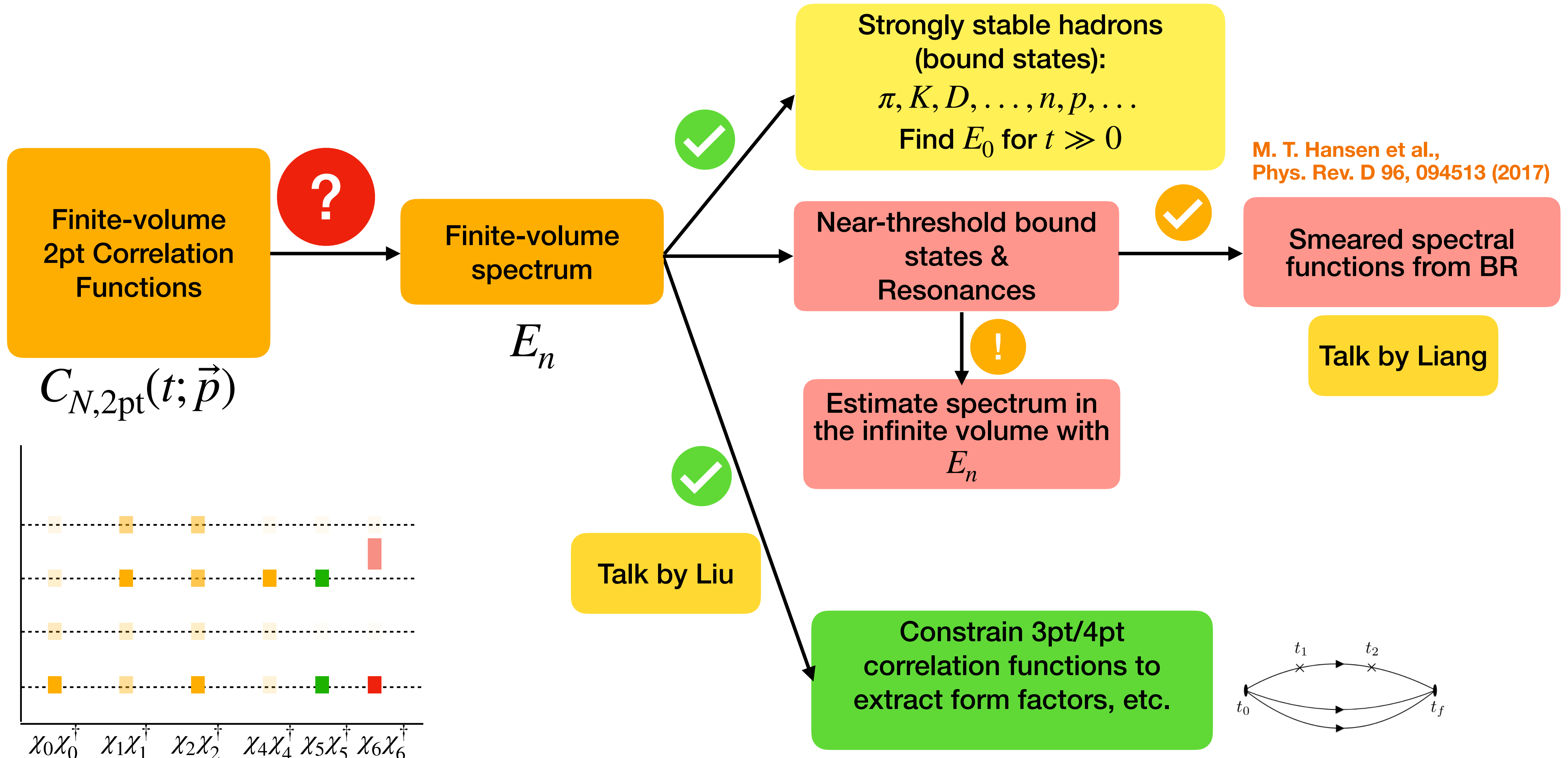
T. Blum et al., Phys. Rev. D 93, 074505



Finite-volume spectrum from lattice QCD



Finite-volume spectrum from lattice QCD with BR



Conclusion and outlook

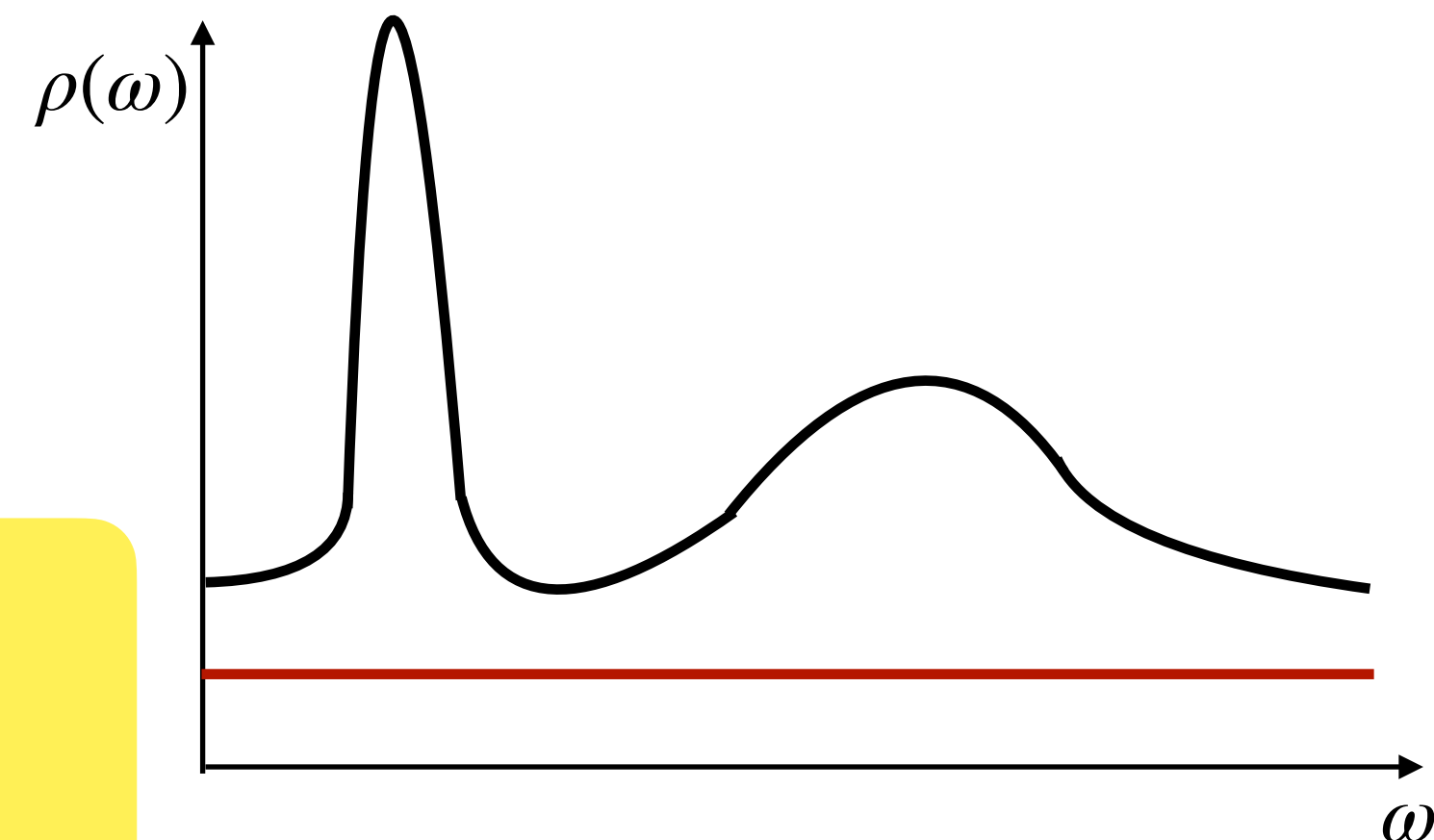
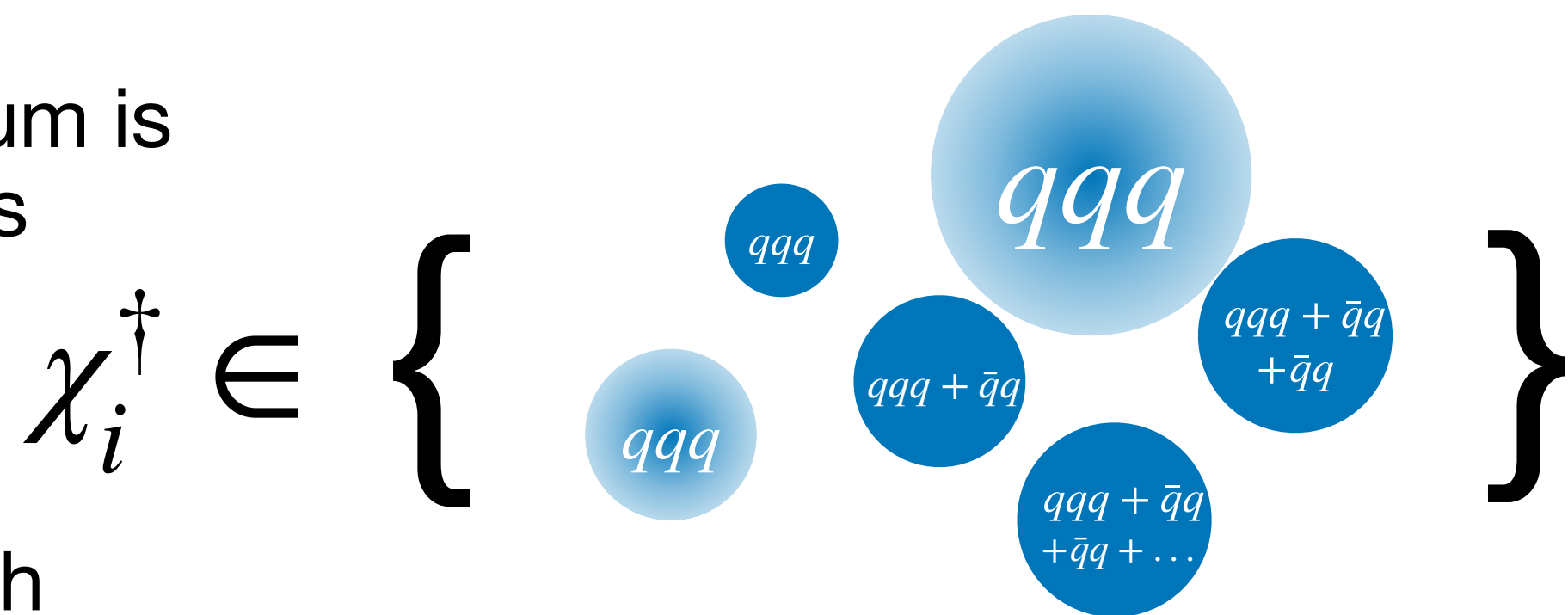
- Extraction of finite-volume spectrum is important in lattice QCD for various physics topics.

- We don't **always** have to use **many interpolating operators** with **high computational cost**.

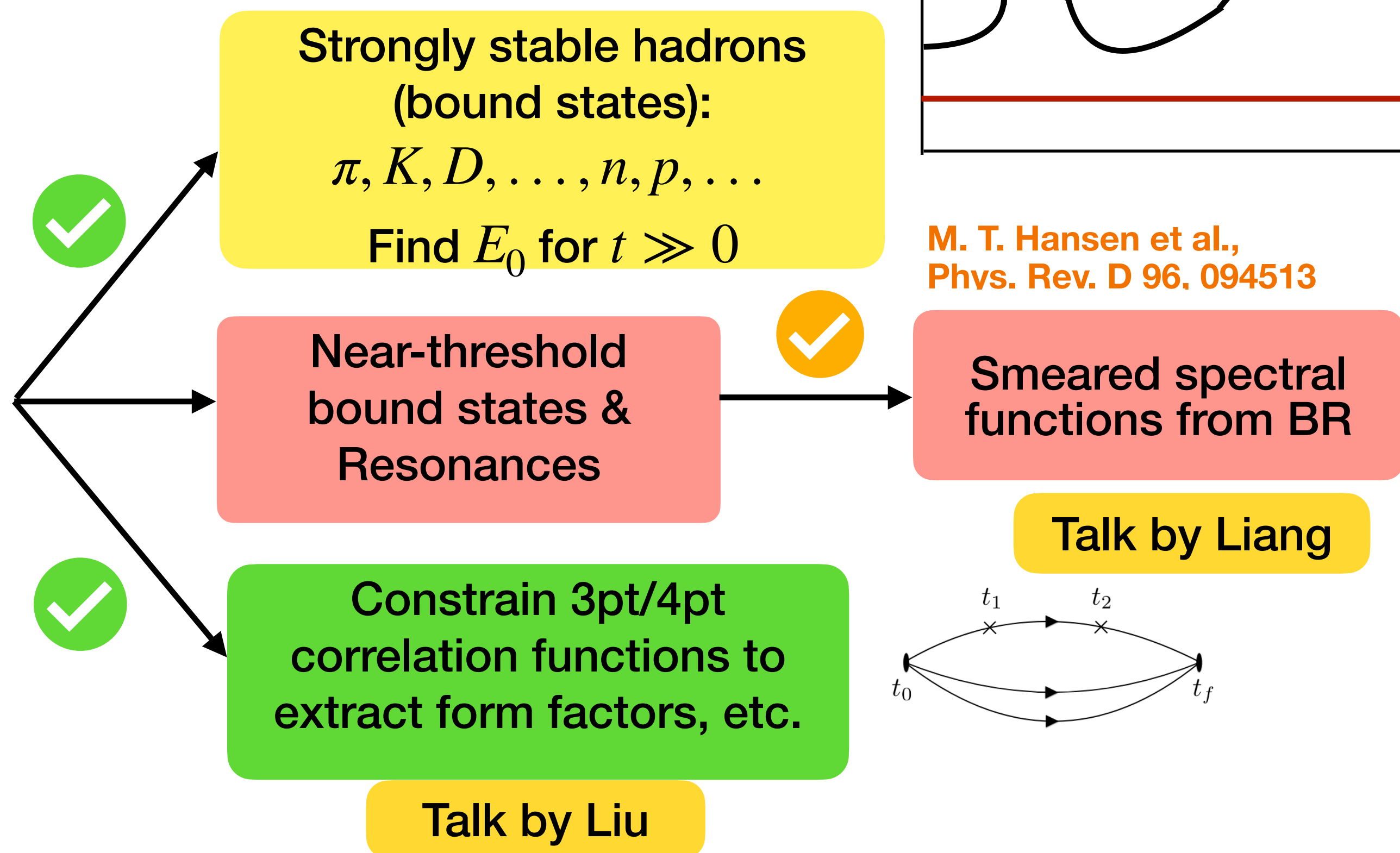
- Theories can help us **choose the basis of interpolating operators wisely/efficiently**.

- **The Bayesian Reconstruction (BR) method can be used** to extract the finite-volume spectrum $\rho(\omega)$.

- More on-going tests of BR
- To be continued ...



M. T. Hansen et al.,
Phys. Rev. D 96, 094513



Thanks for your attention!