THE 2021 NATIONAL NUCLEAR PHYSICS SUMMER SCHOOL

LATTICE QCD
AND
NUCLEON(US) STRUCTURE

ZOHREH DAVOUDI
UNIVERSITY OF MARYLAND AND RIKEN FELLOW

LECTURE I:
LATTICE QCD FORMALISM AND METHODOLOGY

LECTURE II:
NUCLEON STRUCTURE FROM LATTICE QCD

LECTURE III:
TOWARDS NUCLEAR STRUCTURE FROM LATTICE QCD

LECTURE I:
LATTICE QCD FORMALISM AND METHODOLOGY

Quantum chromodynamics (QCD) in continuum:

QCD is a SU(3) Yang-Mills theory augmented with several flavors of massive quarks:

Quark kinetic and mass term

Quark/gluon interactions

$$\mathcal{L}_{QCD} = \sum_{f=1}^{N_f} \left[\bar{q}_f (i\gamma^\mu \partial_\mu - m_f) q_f - g A^i_\mu \bar{q}_f \gamma^\mu T^i q_f\right]$$

$$-\frac{1}{4} F^i_{\mu\nu} F^{i\mu\nu} + \frac{g}{2} f_{ijk} F^i_{\mu\nu} A^{i\mu} A^{j\nu} - \frac{g^2}{4} f_{ijk} f_{klm} A^j_\mu A^k_\nu A^{l\mu} A^{m\nu}$$

Gluons kinetic and interaction terms

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Observe that:

i) There are only $1 + N_f$ input parameters plus QCD coupling. Fix them by a few quantities and all strongly-interacting aspects of nuclear physics is predicted (in principle)!

ii) QCD is asymptotically free such that: $\alpha_s(\mu') = \dfrac{1}{2\underbrace{b_0}_{\text{Positive constant for } N_f \leq 16} \log \frac{\mu'}{\Lambda_{QCD}}}$

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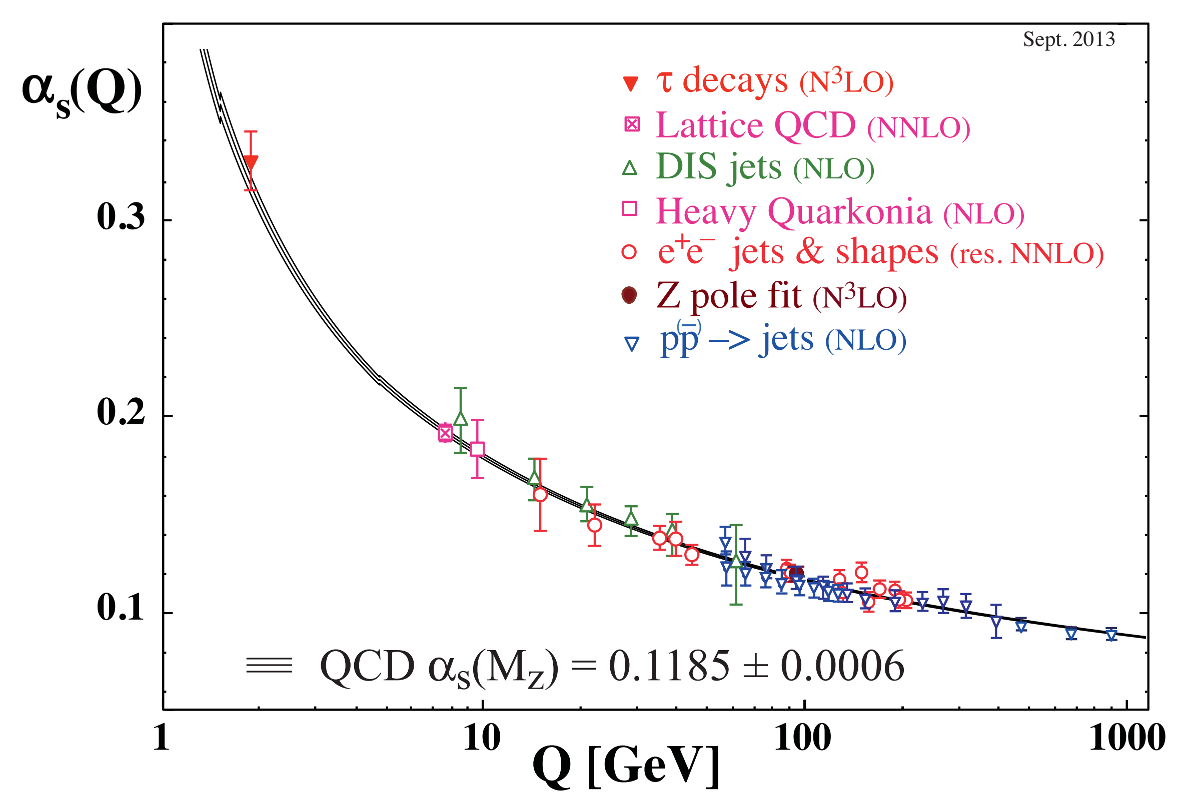

Let’s enumerate the steps toward numerically simulating this theory nonperturbatively…

Step I: Discretize the QCD action in both space and time. Consider a finite hypercubic lattice. Wick rotate to imaginary times.

Step II: Generate a large sample of thermalized decorrelated vacuum configurations.

Step III: Form the correlation functions by contracting the quark fields. Need to specify the interpolating operators for the state under study.

Step IV: Extract energies and matrix elements from correlation functions.

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See e.g., ZD, arXiv:1409.1966 [hep-lat]

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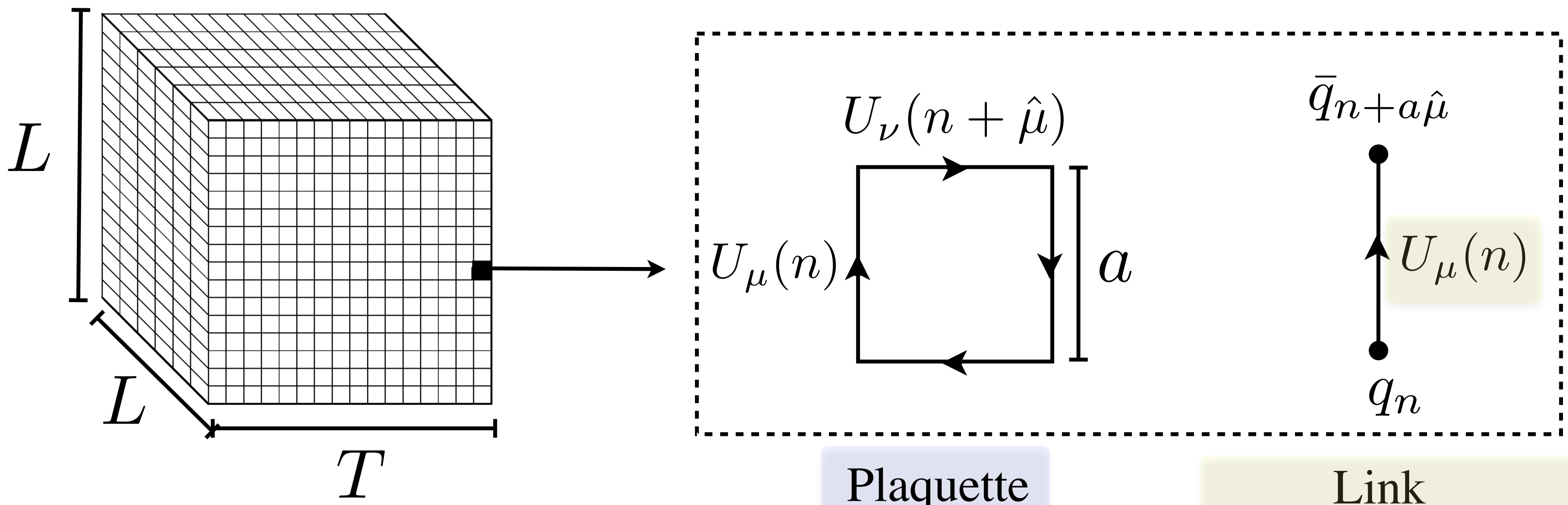

Plaquette

Link
$U_\mu(n) \equiv e^{igA_\mu(n)}$

Two conditions:

$T, L \gg m_\pi^{-1}$ $\qquad$ $a \ll \Lambda_{QCD}^{-1}$

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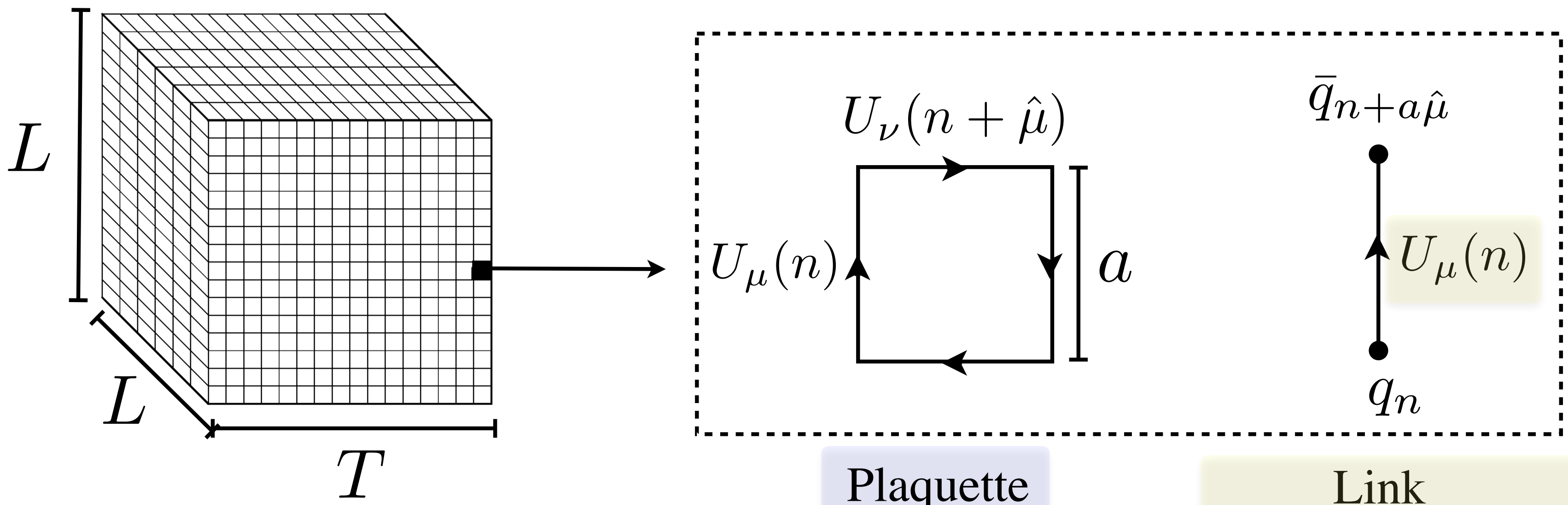

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An example of a discretized action by K. Wilson:

$$S^{(E)}_{\text{Wilson}} = \underbrace{\frac{\beta}{N_c}}_{\beta = 2/g^2} \sum_n \sum_{\mu<\nu} \Re\mathrm{Tr}[\mathbb{1} - P_{\mu\nu;n}] - \sum_n \bar{q}_n[\overline{m}^{(0)} + 4]q_n + \sum_n \sum_\mu \left[\bar{q}_n \frac{r - \gamma_\mu}{2} U_\mu(n) q_{n+\hat{\mu}} + \bar{q}_n \frac{r + \gamma_\mu}{2} U^\dagger_\mu(n-\hat{\mu}) q_{n-\hat{\mu}}\right]$$

Wilson parameter. Gives the naive action if set to zero and has doublers problem.

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For discussions of actions consistent with chiral symmetry of continuum see:
Kaplan, arXiv:0912.2560 [hep-lat].
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Step II: Generate a large sample of thermalized decorrelated vacuum configurations.

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}U_\mu \mathcal{D}q \mathcal{D}\bar{q}\ e^{-S^{(G)}_{\text{lattice}}[U] - S^{(F)}_{\text{lattice}}[U,q,\bar{q}]}\ \hat{\mathcal{O}}[U, q, \bar{q}]$$

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Quark part of expectation values

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Quark part of expectation values

Define: $\langle \hat{\mathcal{O}} \rangle_F = \frac{1}{\mathcal{Z}_F} \int \mathcal{D}q\mathcal{D}\bar{q}\; e^{-S^{(F)}_{\text{lattice}}[U,q,\bar{q}]} \mathcal{O}[q,\bar{q},U]$

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$$\Downarrow$$

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{N} \sum_i^N \langle \hat{\mathcal{O}} \rangle_F [U^{(i)}]$$

N number of $U^{(i)}$ sampled from the distribution: $\frac{1}{\mathcal{Z}} e^{-S^{(G)}_{\mathrm{lattice}}[U]} \prod_f \det D_f$

Steps II is computationally costly…

Example: Consider a lattice with: $L/a = 48,\ T/a = 256$

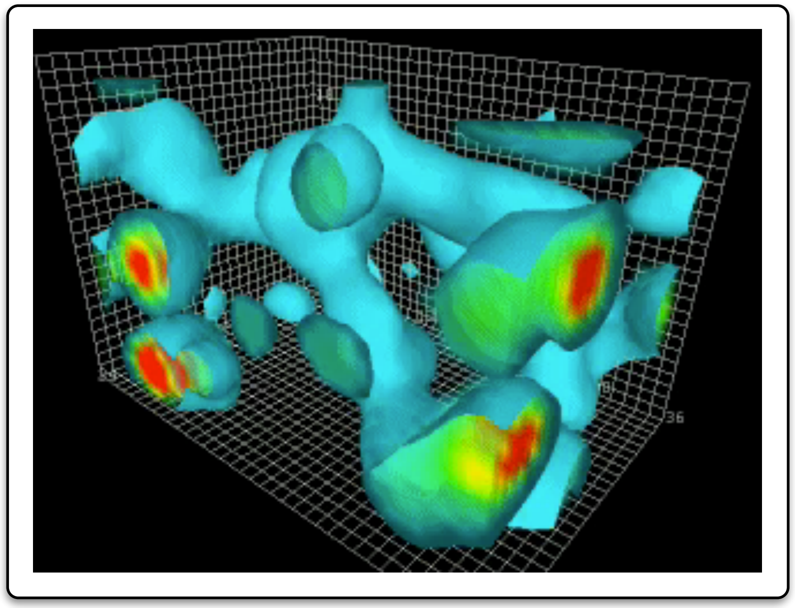
Sampling SU(3) matrices. Already for one sample requires storing

$$8 \times 48^3 \times 256 = 226,492,416$$

c-numbers in the computer!

Requires calculating determinant of a large matrix.

Requires tens of thousands of uncorrelated samples. Molecular-dynamics-inspired hybrid Monte Carlo sampling algorithms often used.



Step III: Form the correlation functions by contracting the quarks. Need to specify the interpolating operators for the state under study.

$$\langle\hat{\mathcal{O}}\rangle_F = \frac{1}{\mathcal{Z}_F}\int \mathcal{D}q\mathcal{D}\bar{q}\; e^{-S^{(F)}_{\text{lattice}}[U,q,\bar{q}]}\mathcal{O}[q,\bar{q},U]$$

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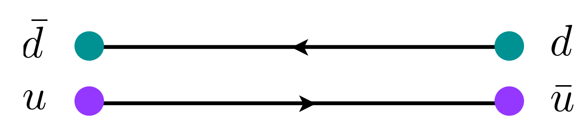
e.g., $\boxed{\hat{O} = \overline{u}\gamma_5 d}$



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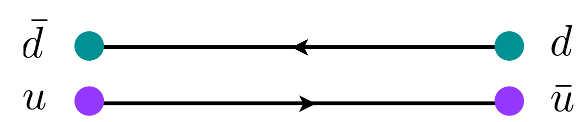
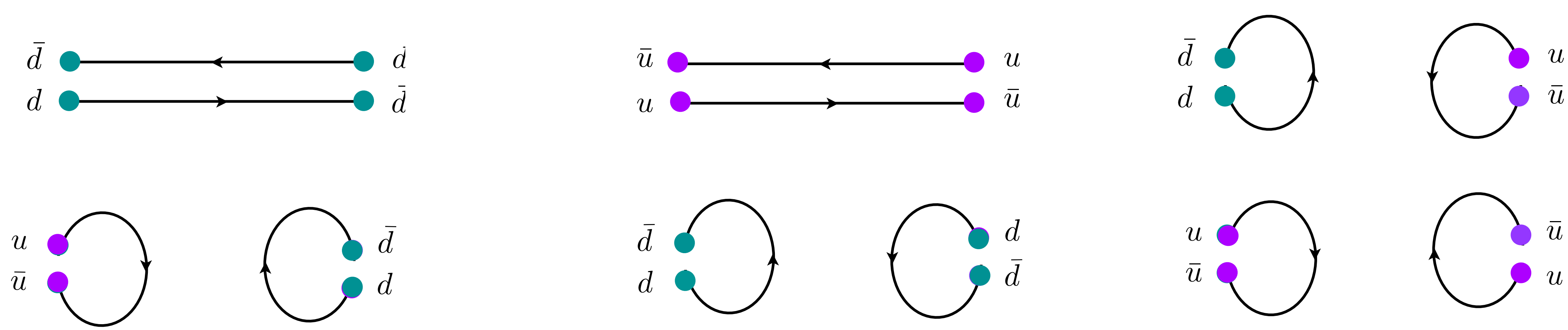


e.g., $\boxed{\hat{O} = \frac{1}{\sqrt{2}}(\overline{u}\gamma^5 u - \overline{d}\gamma^5 d)}$



Quark disconnected diagrams. Require expensive all-to-all propagators.

Steps III is computationally costly…

Example: Consider a lattice with: $L/a = 48,\ T/a = 256$

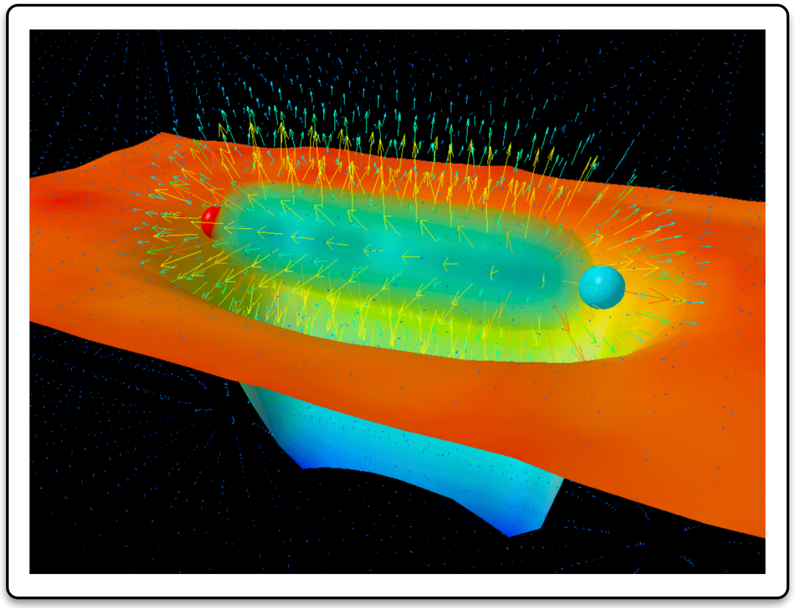
Solving

$$[D(U)]_{X,Y}[S(U)]_{Y,X_0} = G_{X,X_0}$$

Dirac matrix | Quark propagator | Source

Requires taking determinant and inverting a matrix with dimensions:

$$(4 \times 3 \times 48^3 \times 256)^2 =$$
$$339,738,624 \times 339,738,624$$



EXERCISE 1

Show that for the correlation function of the charged pion:

$$\langle \hat{O}^{\pi^+}(n)\hat{O}^{\pi^+\dagger}(0)\rangle_F \quad = \quad -\mathrm{Tr}\left[D_u^{-1}(n,0)D_d^{-1}(n,0)\right]$$

where D_u^{-1} and D_d^{-1} denote the the inverse Dirac matrix (the quark propagator) for the u and d quarks, respectively. Trace is over spin and color degrees of freedom.

BONUS EXERCISE 1

Show that for the correlation function of the neutral pion:

$$\begin{aligned}
\langle \hat{O}^{\pi^0}(n)\hat{O}^{\pi^0\dagger}(0)\rangle_F \quad = \quad & -\frac{1}{2}\mathrm{Tr}\left[\gamma^5 D_u^{-1}(n,0)\gamma^5 D_u^{-1}(0,n)\right] \\
& +\frac{1}{2}\mathrm{Tr}\left[\gamma^5 D_u^{-1}(n,n)\right]\mathrm{Tr}\left[\gamma^5 D_u^{-1}(0,0)\right] \\
& -\frac{1}{2}\mathrm{Tr}\left[\gamma^5 D_u^{-1}(n,n)\right]\mathrm{Tr}\left[\gamma^5 D_d^{-1}(0,0)\right] + \{u \leftrightarrow d\}
\end{aligned}$$

Step IV: Extract energies and matrix elements from correlation functions

$$C_{\hat{\mathcal{O}},\hat{\mathcal{O}}'}(\tau;\mathbf{d}) \ = \ \sum_{\mathbf{x}} e^{2\pi i \mathbf{d}\cdot\mathbf{x}/L} \langle 0|\hat{\mathcal{O}}'(\mathbf{x},\tau)\hat{\mathcal{O}}^{\dagger}(\mathbf{0},0)|0\rangle = \mathcal{Z}_0'\mathcal{Z}_0^{\dagger} e^{-E^{(0)}\tau} + \mathcal{Z}_1'\mathcal{Z}_1^{\dagger} e^{-E^{(1)}\tau} + \ldots$$

Ground state and a tower of excited states are, in principle, accessible!

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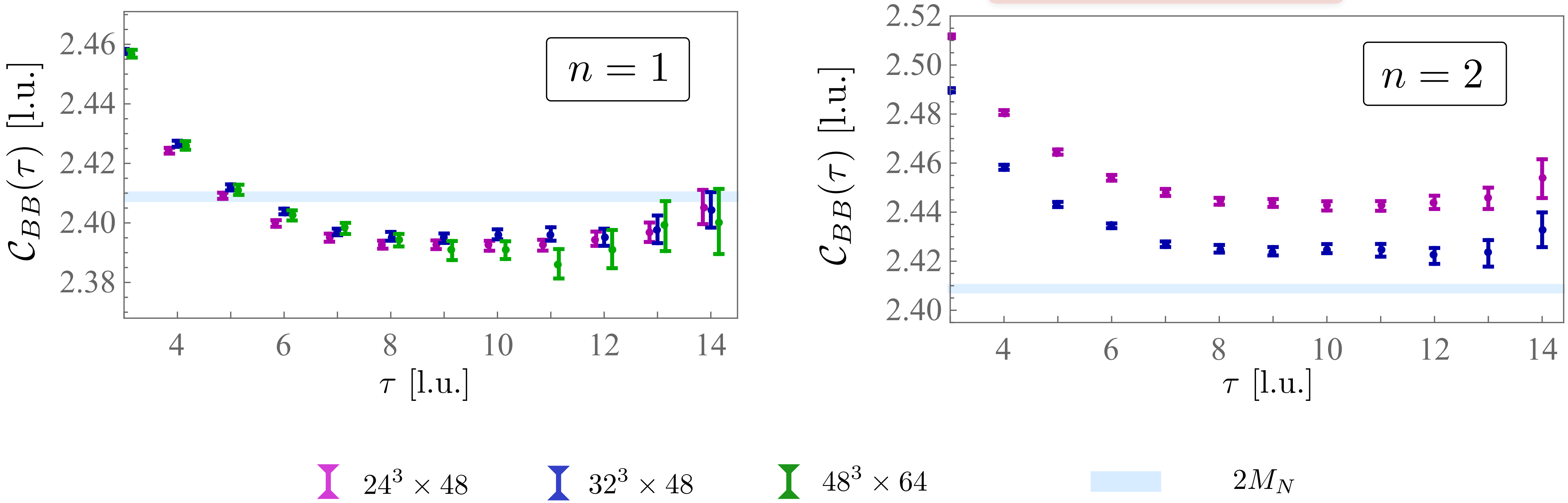
Example: $\boxed{NN\ (^1S_0)}$

What should we make of the volume dependence?



Beane et al (NPLQCD), arXiv:1705.09239, Wagman et al (NPLQCD), arXiv:1706.06550.

[STILL CONTINUING ON] LECTURE I:
LATTICE QCD FORMALISM AND METHODOLOGY

[Recap] Steps involved in any lattice QCD calculation:

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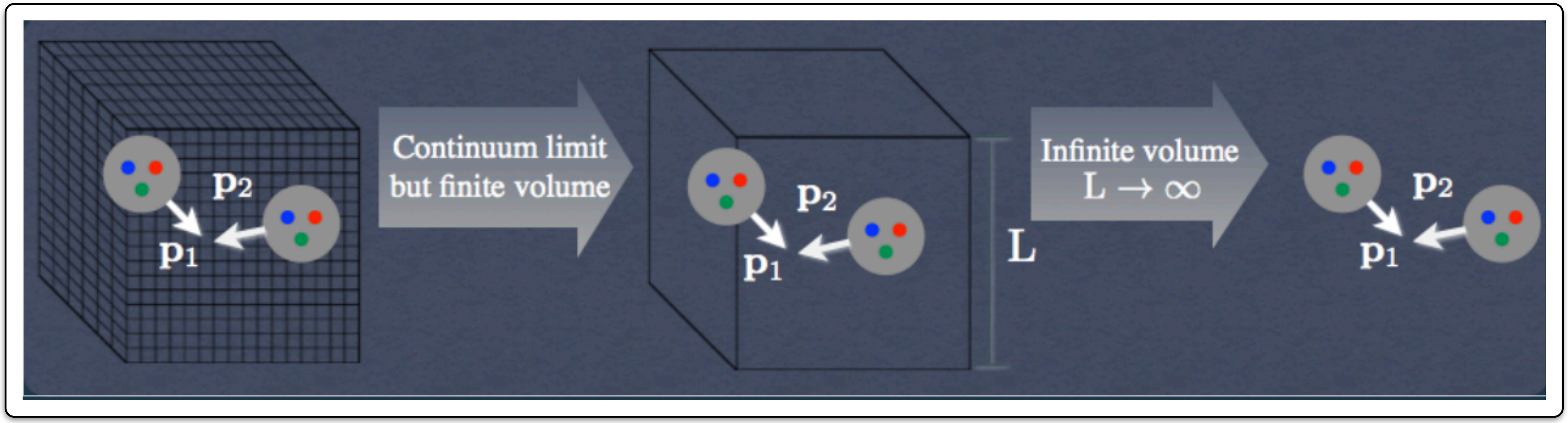
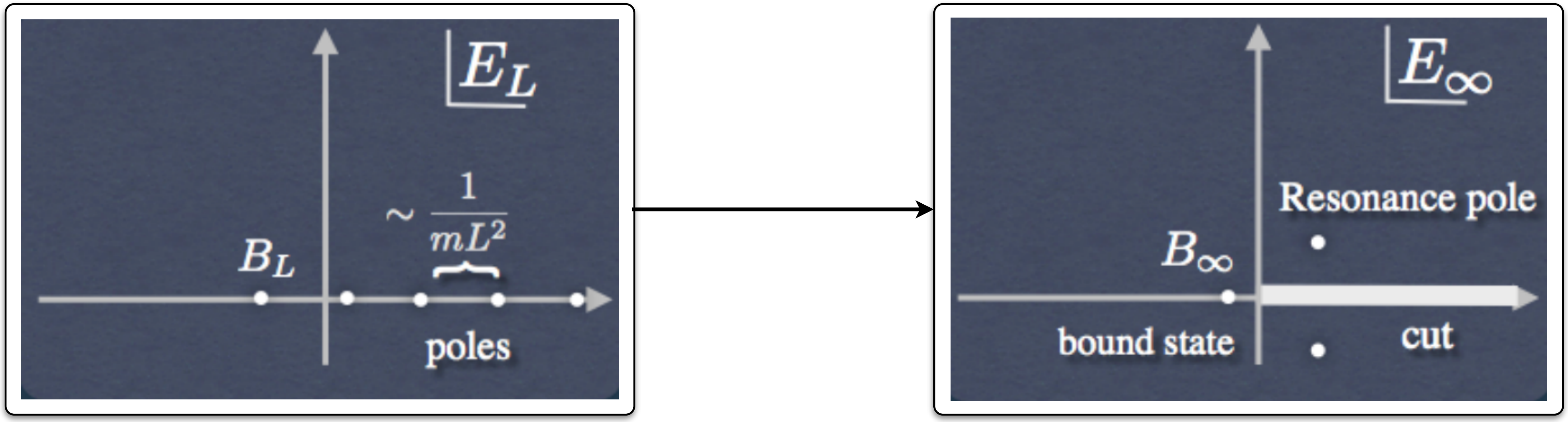
Example: two-hadron scattering





Let’s discuss in greater depth step V:

Step V: make the connection to physical observables, such as scattering amplitudes, decay rates, etc.

i) Finite-volume effects in the single-hadron sector

ii) Finite-volume formalism for two-hadron elastic scattering

iii) Finite-volume formalism for coupled-channel two-hadron inelastic scattering and resonances

iv) Finite-volume formalism for transition amplitudes and resonance form factors

v) Finite-volume formalism for three-hadron scattering and resonances and decays

vi) Finite-volume effects in lattice QED+QCD studies of hadrons

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See e.g., ZD, arXiv:1409.1966 [hep-lat, Briceno, Dudek and Young, Rev. Mod. Phys. 90.025001, Ann. Rev. Nucl. Part. Sci. 69 (2019).

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Kim, Sachrajda and Sharpe, Nucl.Phys.B727(2005)218-243.

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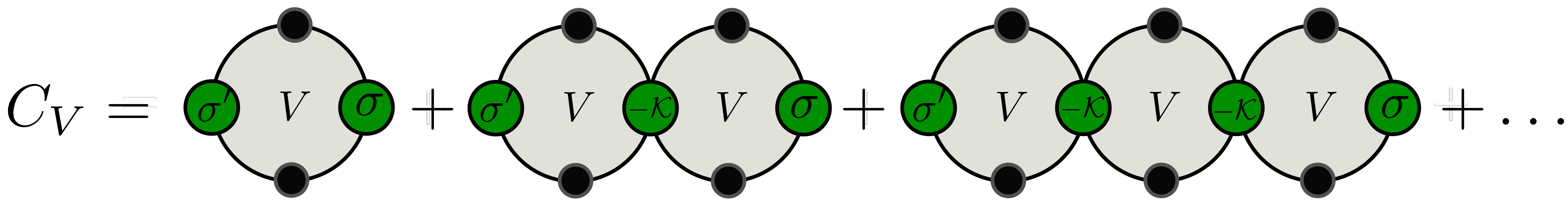

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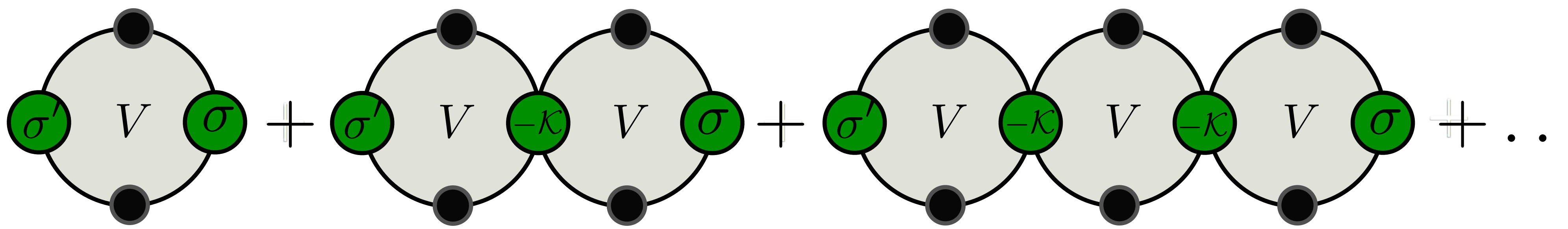
$C_V =$ 

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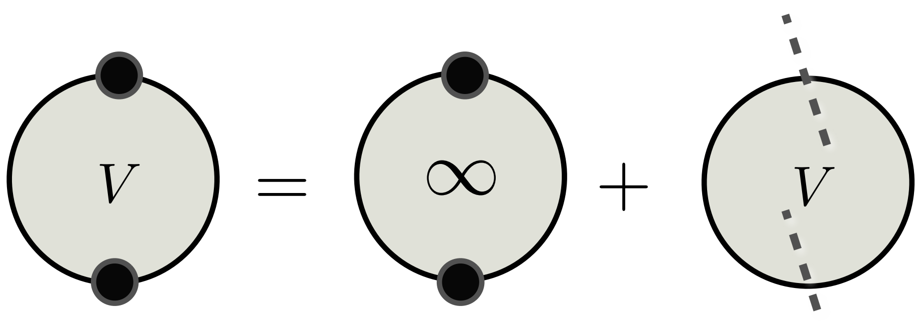
(1) 

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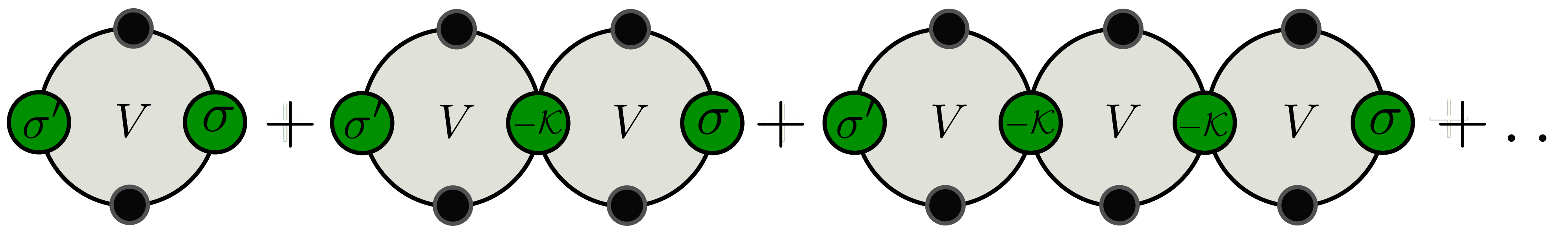
$C_V =$ 

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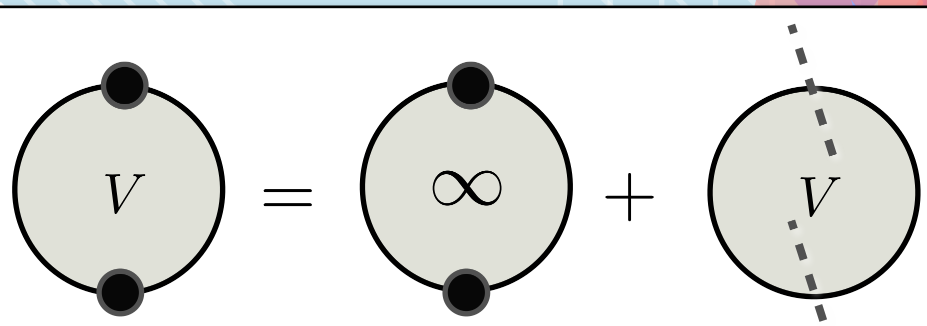
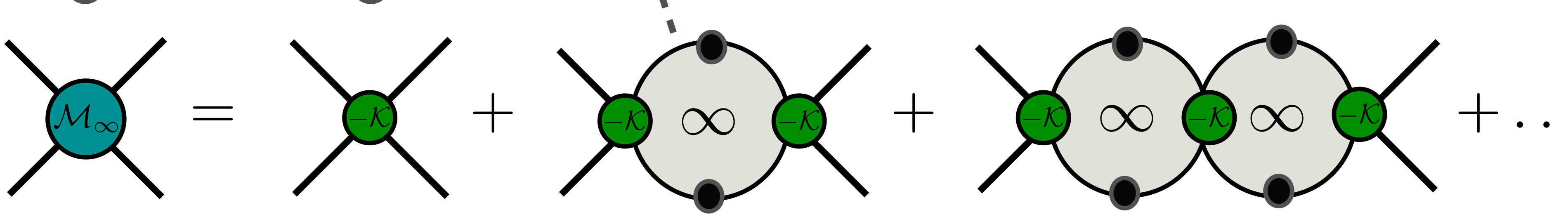
(1) 

(2) 

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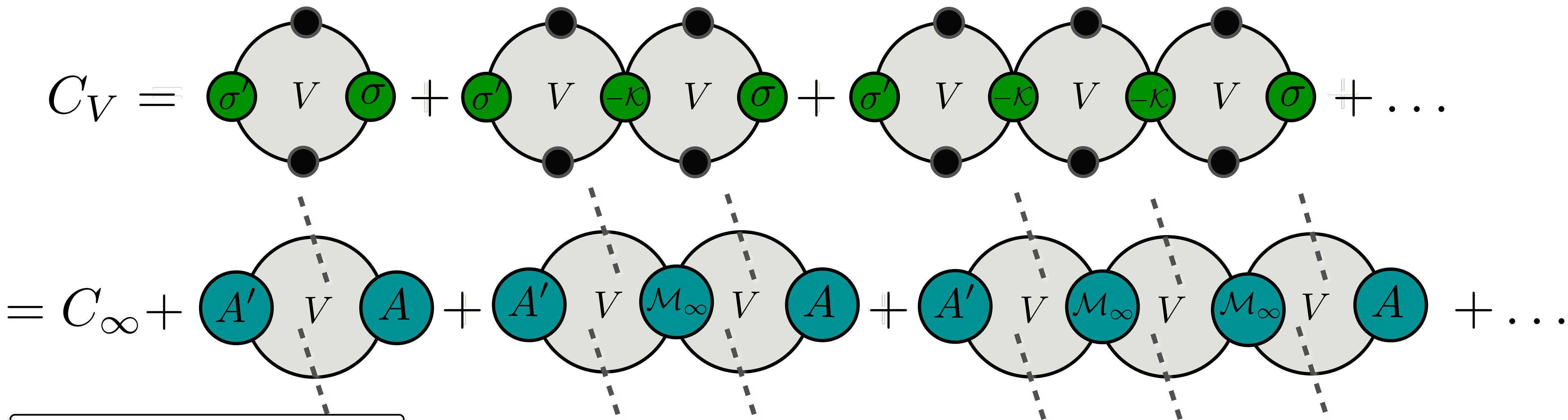

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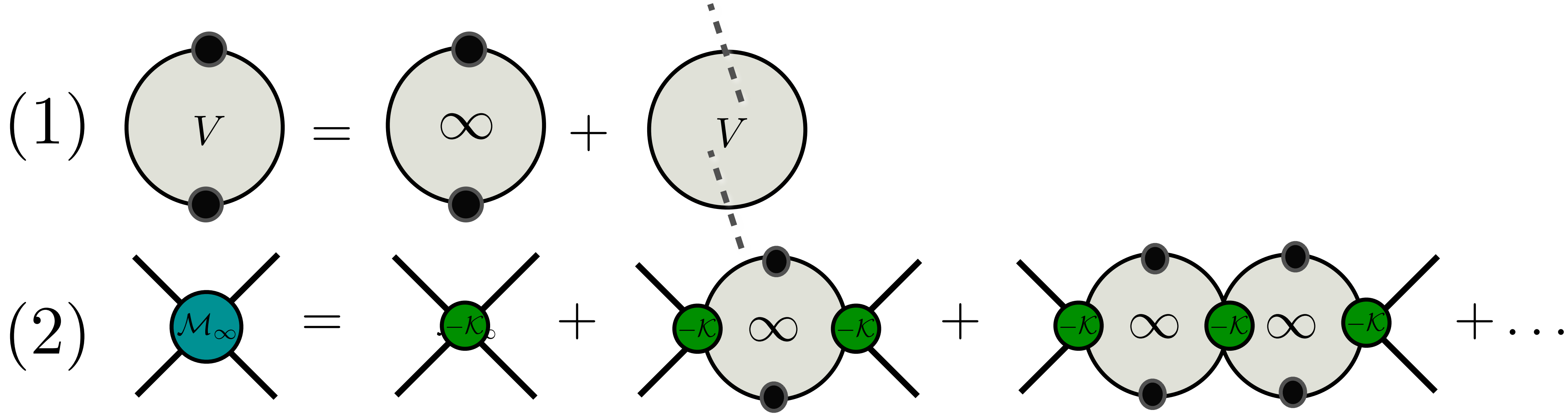

EXERCISE 2

By rearranging the diagrams in C_V (the first line in the upper panel) using the relations in the lower panel, verify the expansion in the second line in the upper panel. What is the relation between $\sigma(\sigma')$ and $A(A')$?

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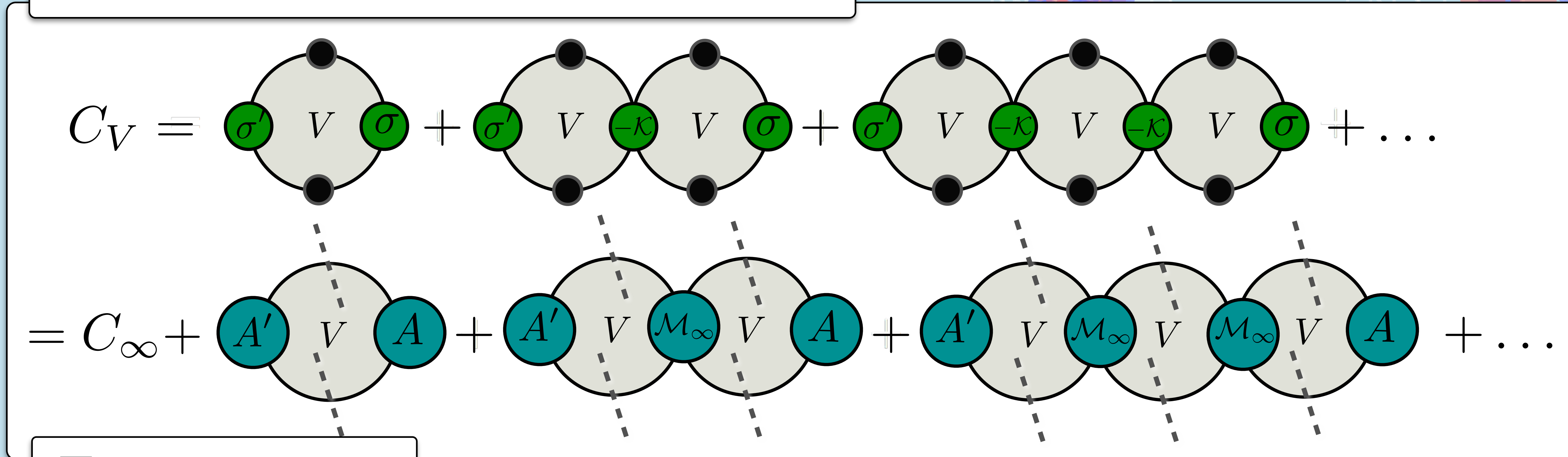

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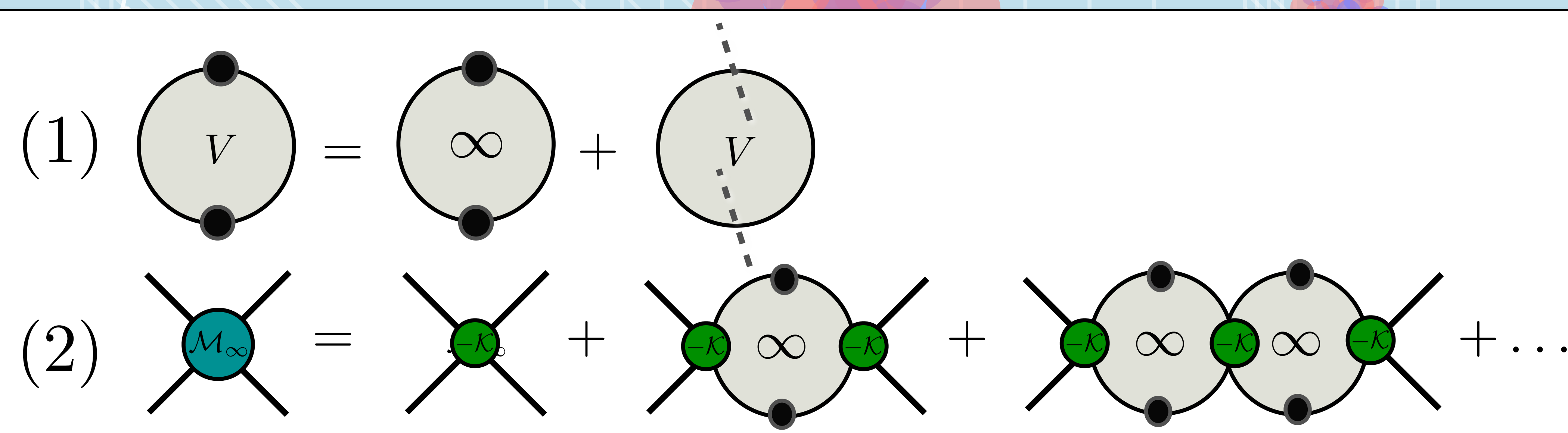

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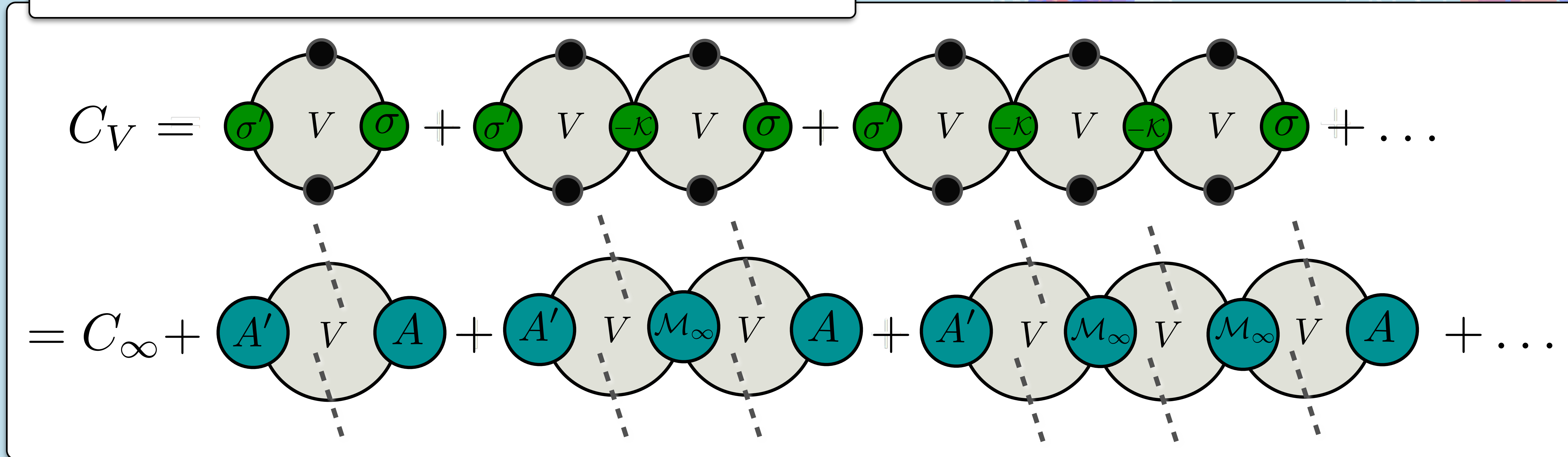


$$\det\left[\delta\mathcal{G}^V(E^*) + \mathcal{M}_\infty^{-1}(E^*)\right] = 0$$

Finite-volume function

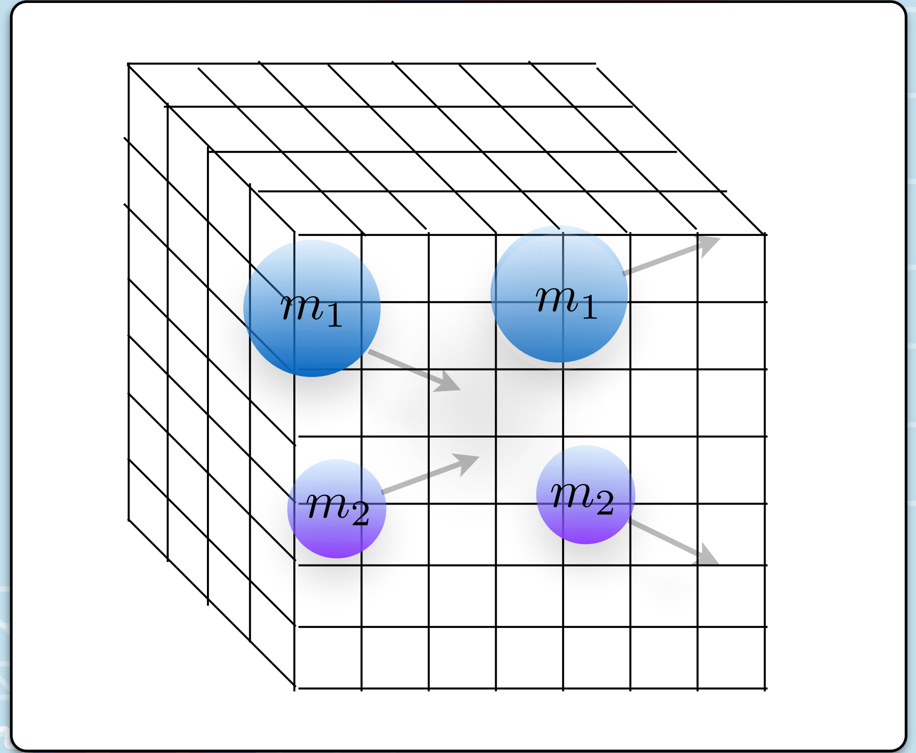
Scattering amplitude

Kim, Sachrajda and Sharpe, Nucl.Phys.B727(2005)218-243.

Poles of C_V which are the finite-volume CM energy eigenvalues.

$$\det\left[\delta\mathcal{G}^V(E^*) + \mathcal{M}_\infty^{-1}(E^*)\right] = 0$$

Luescher (1986, 1991).



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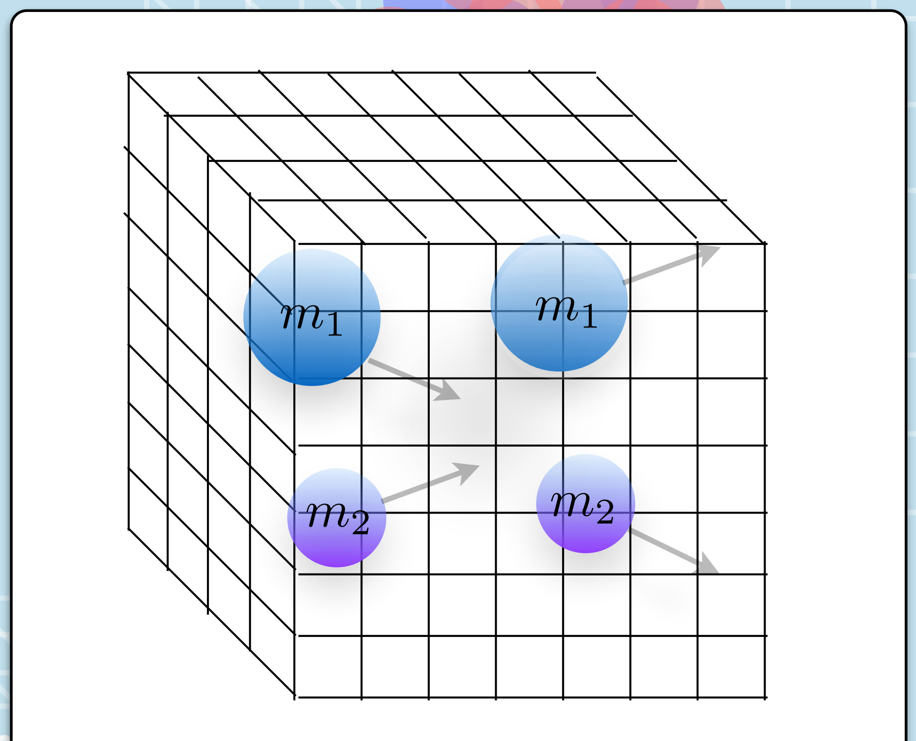


Elastic amplitude more closely…

CM energy

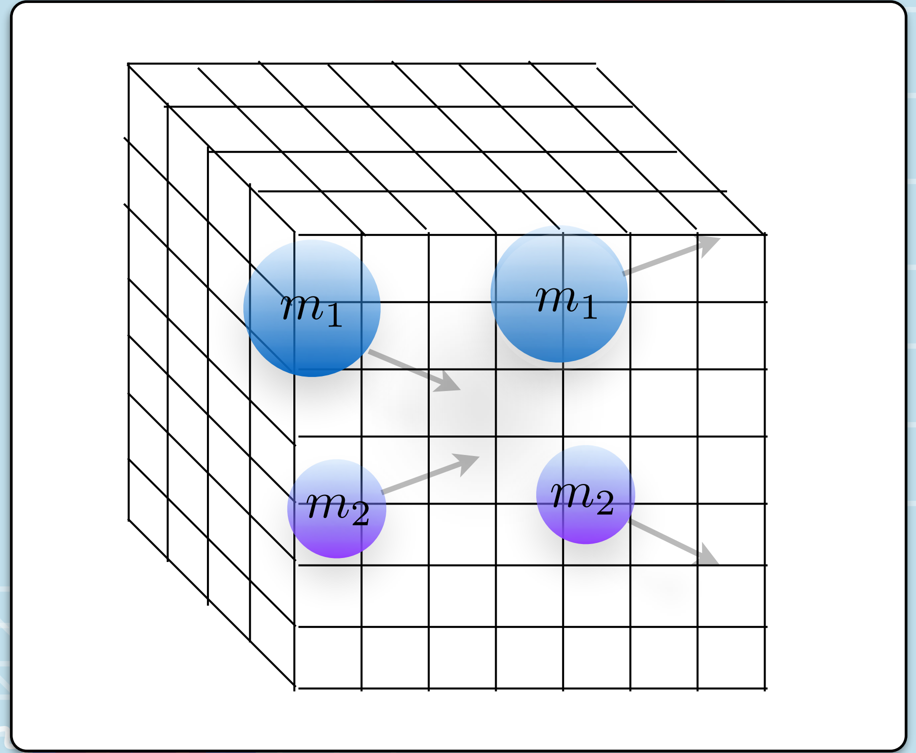
Phase shift

$$(\mathcal{M})_{l_1,m_1;l_2,m_2} = \delta_{l_1,l_2}\delta_{m_1,m_2}\frac{8\pi E^*}{nq^*}\frac{e^{2i\delta^{(l)}(q^*)}-1}{2i}$$

Symmetry factor

$$q^{*2} = \frac{1}{4}\left(E^{*2} - 2(m_1^2+m_2^2) + \frac{(m_1^2-m_2^2)^2}{E^{*2}}\right)$$

$$\det\left[\delta\mathcal{G}^V(E^*) + \mathcal{M}_\infty^{-1}(E^*)\right] = 0$$



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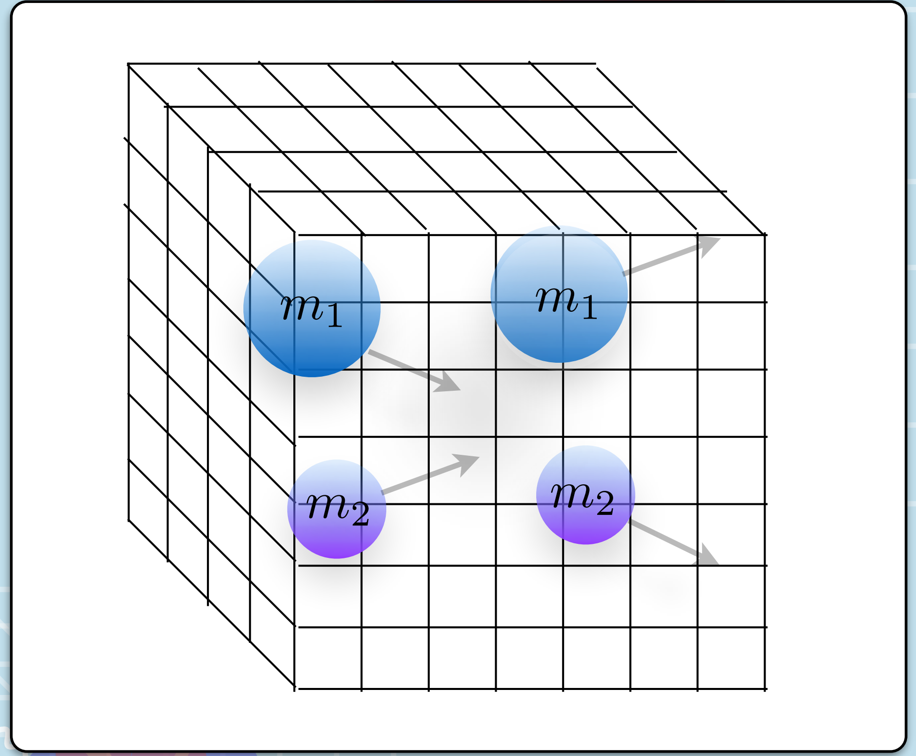


Finite-volume function more closely…

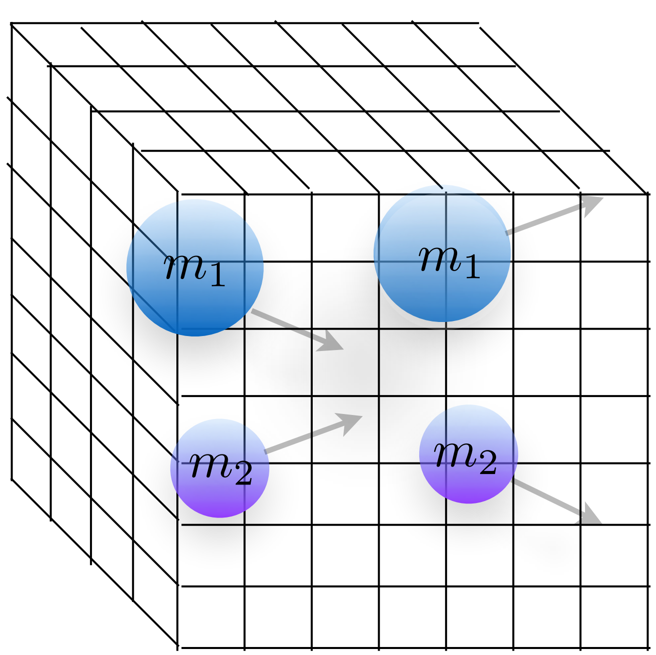
$$(\delta\mathcal{G}^V)_{l_1,m_1;l_2,m_2} = i\frac{q^* n}{8\pi E^*}\left(\delta_{l_1,l_2}\delta_{m_1,m_2} + i\frac{4\pi}{q^*}\sum_{l,m}\frac{\sqrt{4\pi}}{q^{*l}}c^{\mathbf{P}}_{lm}(q^{*2})\int d\Omega^* Y^*_{l_1m_1}Y^*_{lm}Y_{l_2m_2}\right)$$

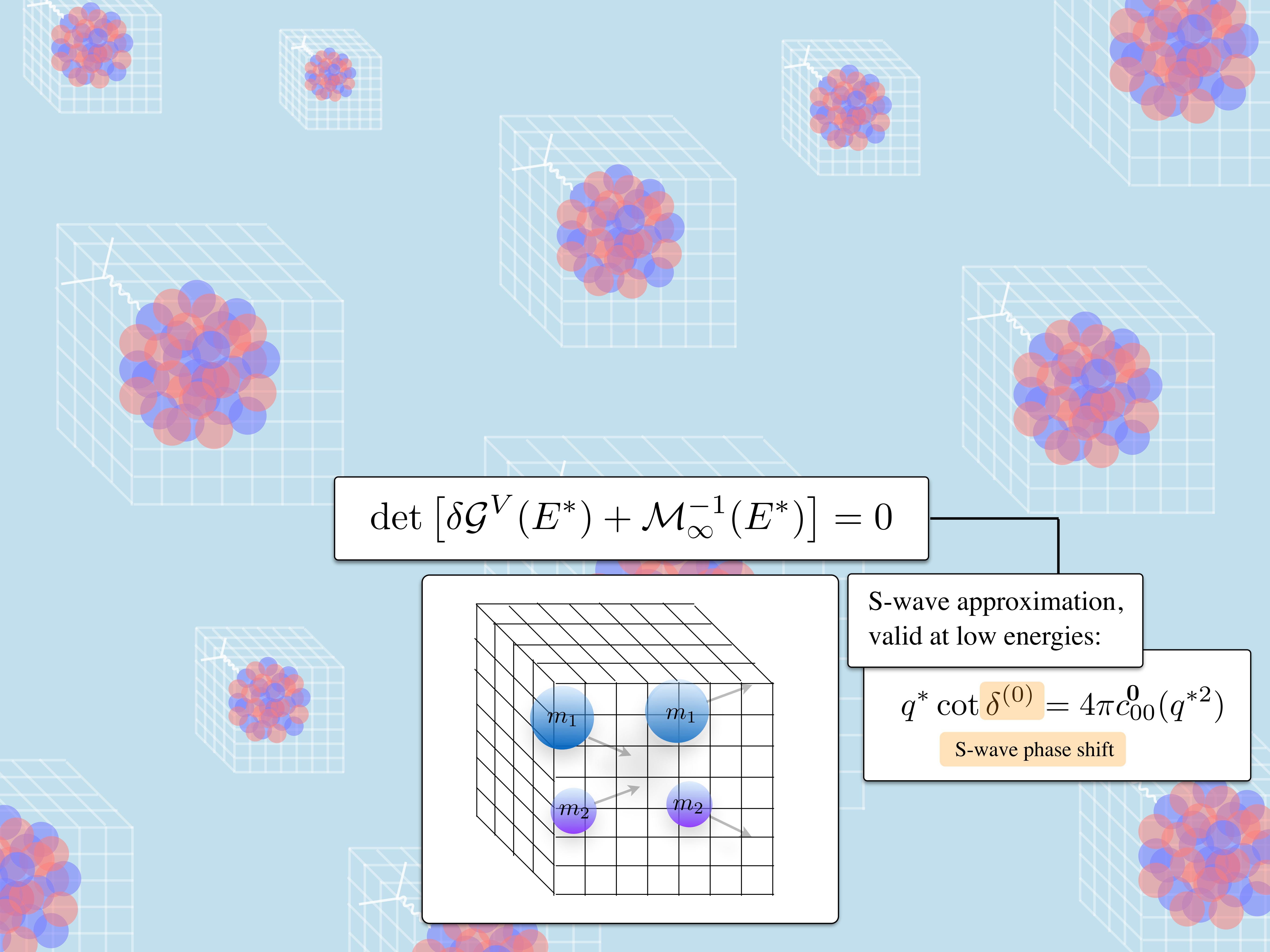
$$c^{\mathbf{P}}_{lm}(x) = \frac{1}{\gamma}\left[\frac{1}{L^3}\sum_{\mathbf{k}} - \mathcal{P}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\right]\frac{\sqrt{4\pi}Y_{lm}(\hat{k}^*)\ k^{*l}}{k^{*2} - x}$$

$$\mathbf{k}^* = \gamma^{-1}\left[\mathbf{k}_{\parallel} - \frac{1}{2}\left(1 + \frac{m_1^2 - m_2^2}{E^{*2}}\right)\mathbf{P}\right] + \mathbf{k}_{\perp}$$

ZD and Savage, Phys. Rev.D84,114502(2011).

$$\det\left[\delta\mathcal{G}^V(E^*) + \mathcal{M}_\infty^{-1}(E^*)\right] = 0$$




$\det\left[\delta\mathcal{G}^{V}(E^*) + \mathcal{M}_{\infty}^{-1}(E^*)\right] = 0$
S-wave approximation, valid at low energies:
$q^* \cot \delta^{(0)} = 4\pi c_{00}^{\mathbf{0}}(q^{*2})$
S-wave phase shift
m_1
m_1
m_2
m_2

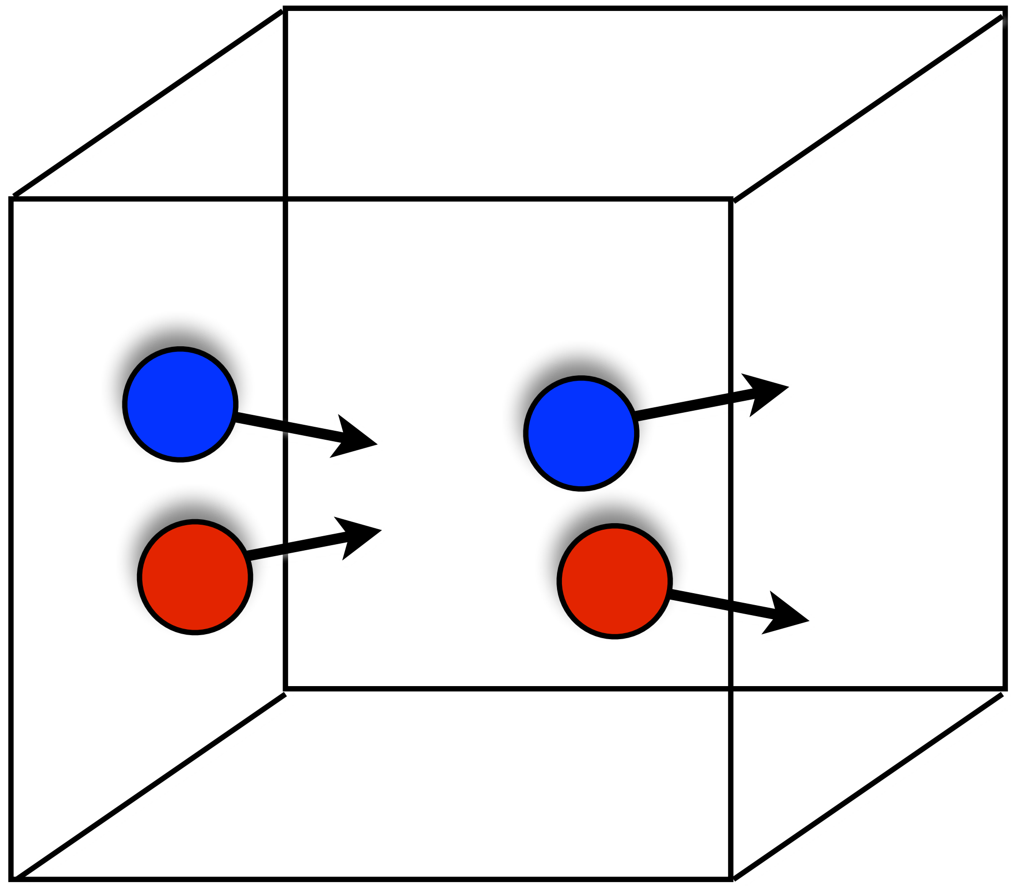
EXERCISE 3

Derive the S-wave limit of Luescher's quantization condition from the master relation.

BONUS EXERCISE 2

Plot the S-wave finite-volume function $c_{00}^{\mathbf{0}}$ for a range of momenta q^{*2}, including negative values. At what values of q^{*2} do you observe singularities? What do these momenta correspond to?

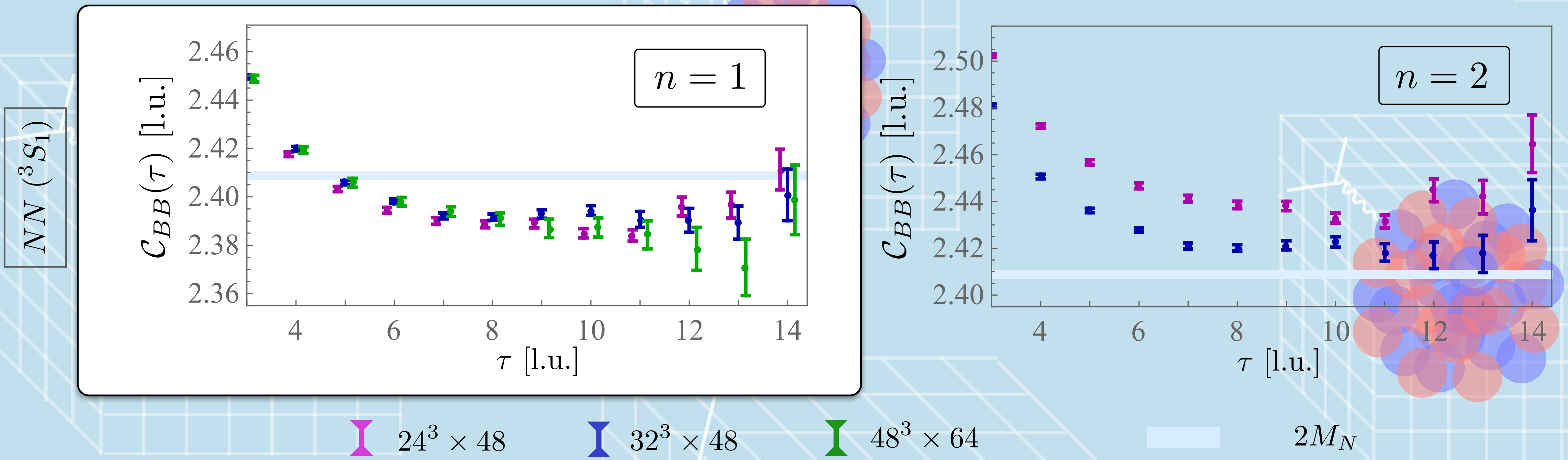
Now let's see an application of Luescher's method to obtain elastic scattering amplitudes of two nucleon from lattice QCD (at a large quark mass!):



Wagman et al.(NPLQCD), Phys.Rev.D 96,114510(2017).

Step 1: Obtain the lowest-lying spectra

$N_f = 3,\ m_\pi = 0.806\ \text{GeV},\ a = 0.145(2)\ \text{fm}$



Beane et al (NPLQCD), arXiv:1705.09239, Wagman et al (NPLQCD), arXiv:1706.06550.

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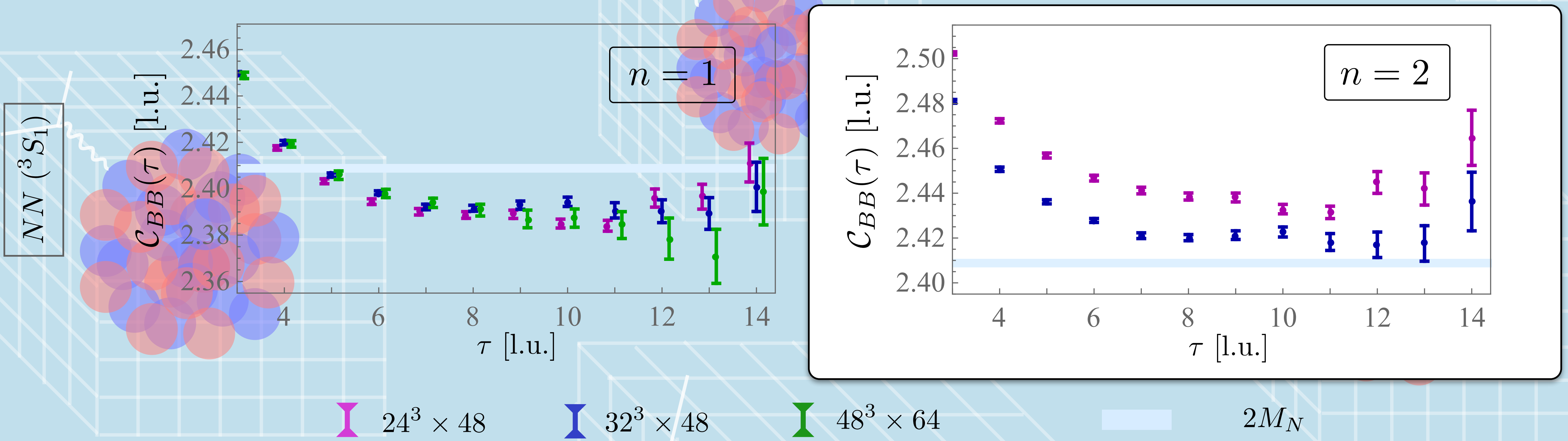

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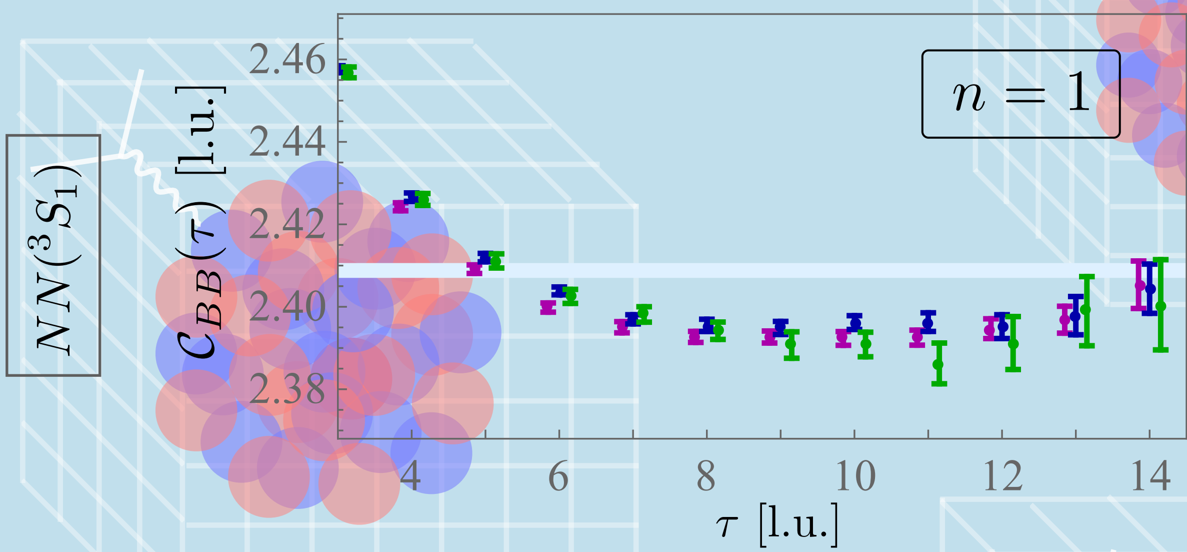
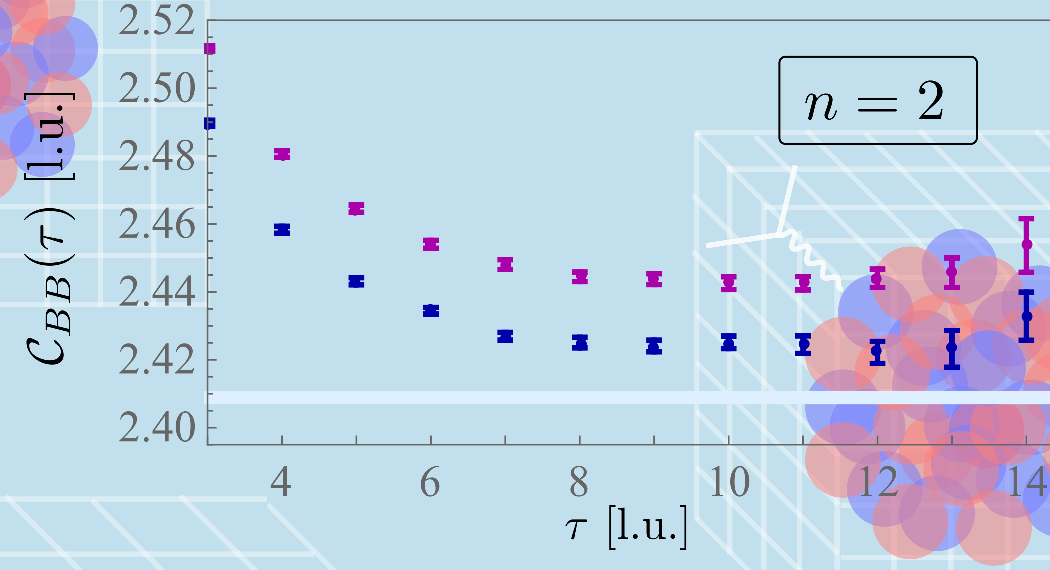
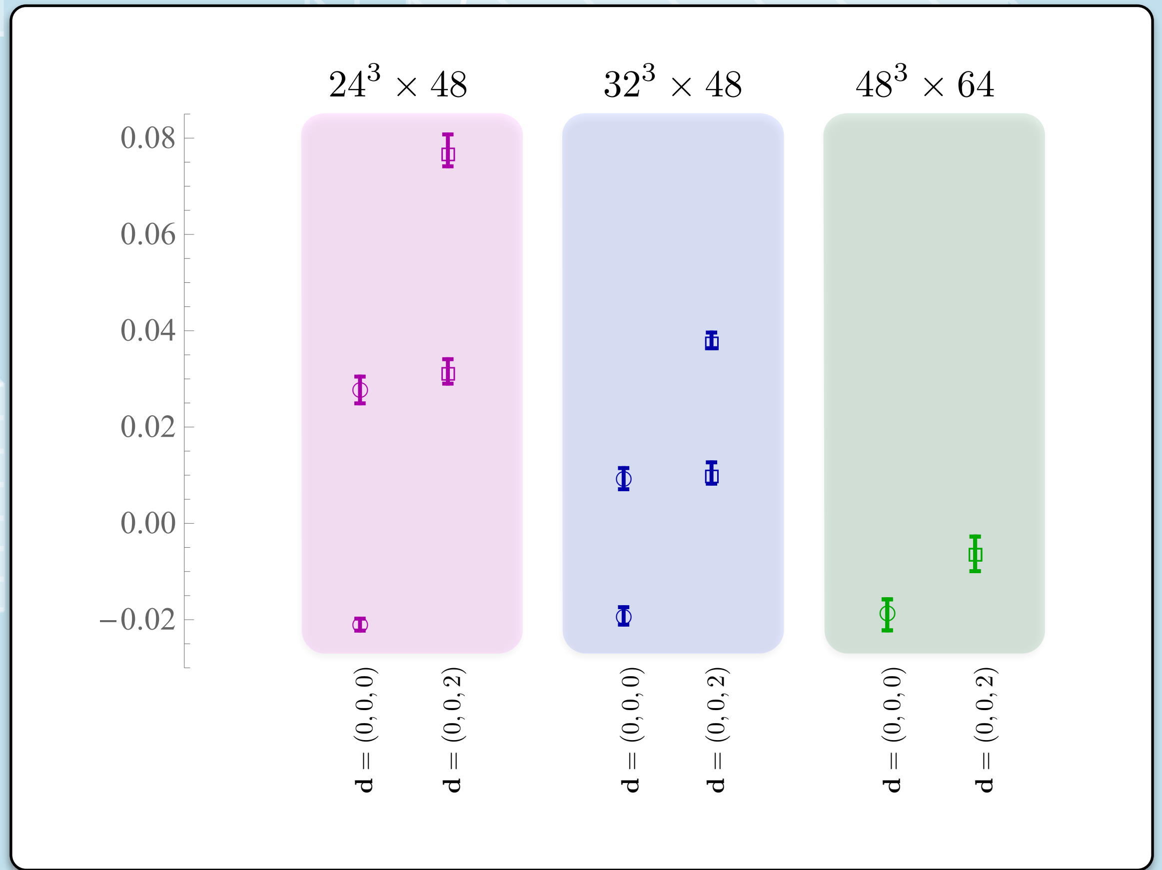




$NN(^3S_1)$



Beane et al (NPLQCD), arXiv:1705.09239, Wagman et al (NPLQCD), arXiv:1706.06550.

Step 2: Feed the energies to the Luescher's equation and obtain the S-wave scattering phase shifts.

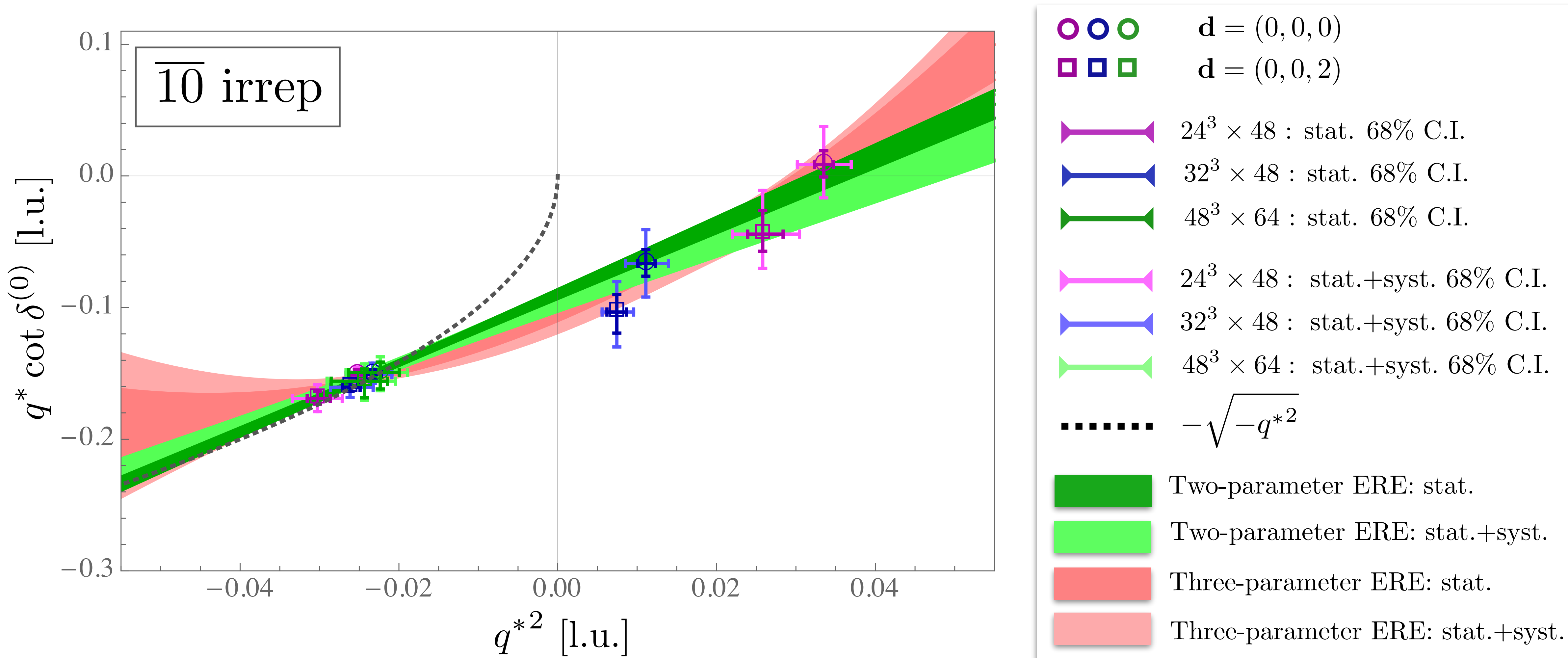
$$q^* \cot \underbrace{\delta^{(0)}}_{\text{S-wave phase shift}} = 4\pi c^{\mathbf{0}}_{00}(q^{*2})$$

Beane et al (NPLQCD), arXiv:1705.09239, Wagman et al (NPLQCD), arXiv:1706.06550.

Step 2: Feed the energies to the Luescher's equation and obtain the S-wave scattering phase shifts.

$N_f = 3,\ m_\pi = 0.806\ \text{GeV},\ a = 0.145(2)\ \text{fm}$

$$q^* \cot \delta^{(0)} = -\frac{1}{a} + \frac{1}{2} r q^{*2} + \cdots$$



$$B = 27.9^{(+3.1)(+2.2)}_{(-2.3)(-1.4)}\ \text{MeV}$$

Beane et al (NPLQCD), arXiv:1705.09239, Wagman et al (NPLQCD), arXiv:1706.06550.

Let's discuss in greater depth step V:

Step V: make the connection to physical observables, such as scattering amplitudes, decay rates, etc.

i) Finite-volume effects in the single-hadron sector

ii) Finite-volume formalism for two-hadron elastic scattering

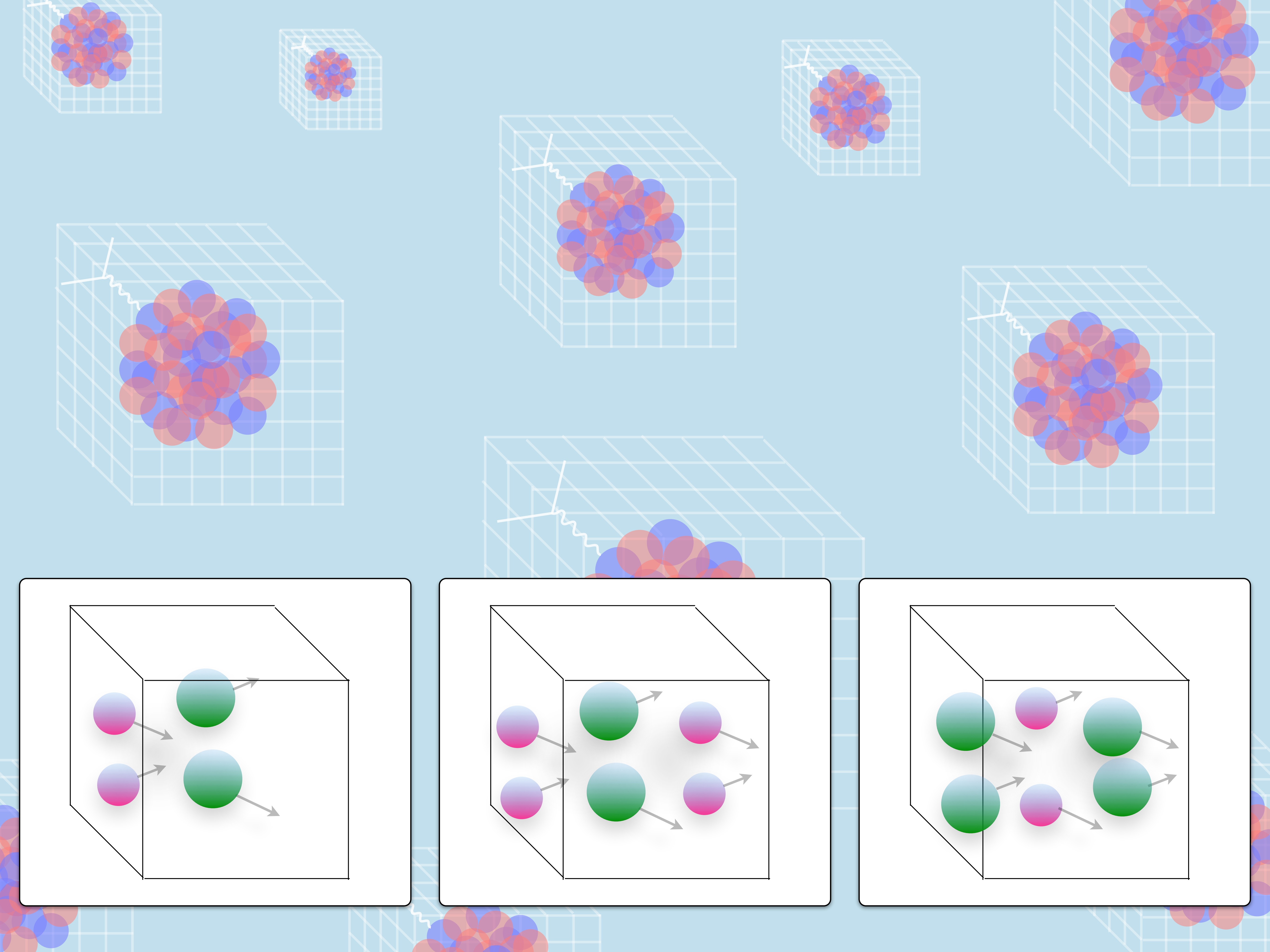
iii) Finite-volume formalism for coupled-channel two-hadron elastic scattering and resonances

iv) Finite-volume formalism for transition amplitudes and resonance form factors

v) Finite-volume formalism for three-hadron scattering and resonances

vi) Finite-volume effects in lattice QED+QCD studies of hadrons

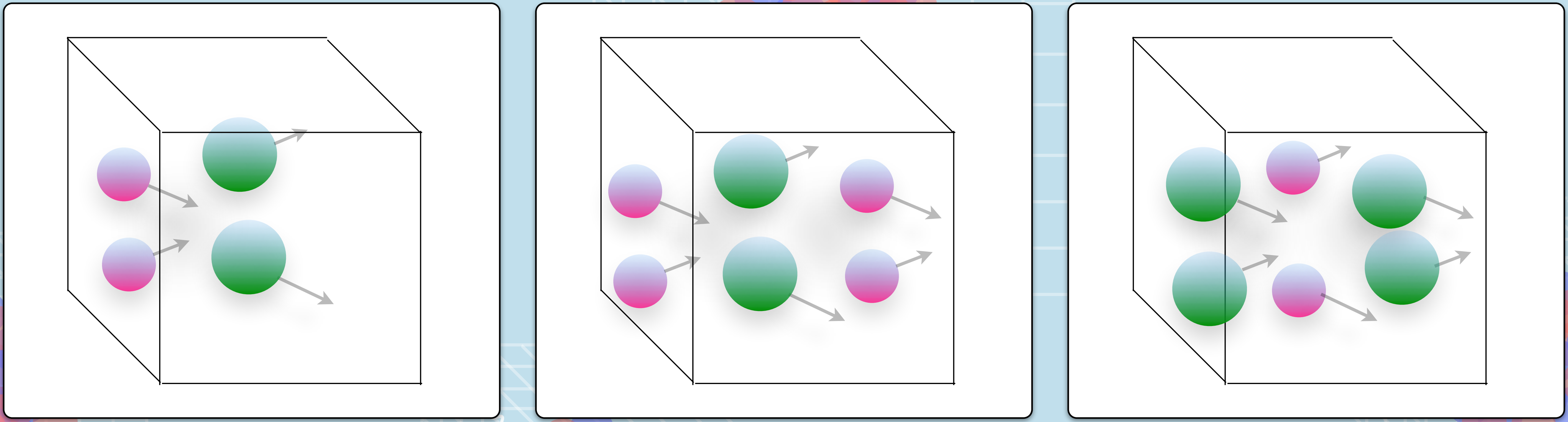
See e.g., ZD, arXiv:1409.1966 [hep-lat, Briceno, Dudek and Young, Rev. Mod. Phys. 90.025001, Ann. Rev. Nucl. Part. Sci. 69 (2019).



Briceno and ZD, Phys. Rev.D88,094507(2013).

Hansen and Sharpe, Phys. Rev. D86, 016007(2012).

$$\mathrm{Det}\left[\delta\mathcal{G}^{V}(E^{*})+\mathcal{M}_{\infty}^{-1}(E^{*})\right]=0$$



Now let's see an application of the coupled-channel formalism: Hunting resonances using lattice QCD in the P-wave coupled $\pi\pi - K\overline{K}$ channel

Wilson et al.(HadSpec), Phys.Rev. D92 (2015), 094502

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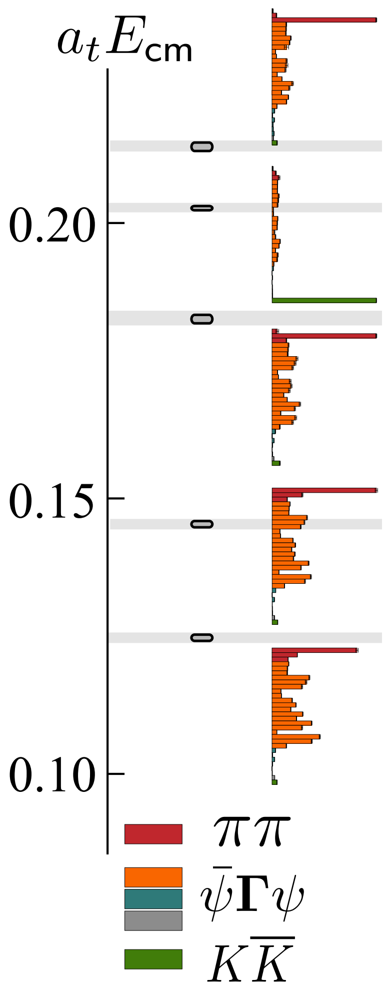
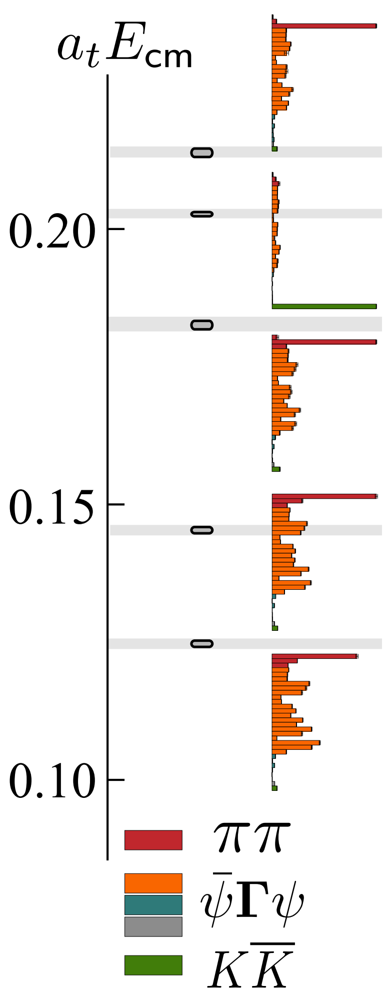


Example: T1 irrep energies

$N_f = 2+1, m_\pi = 236$ MeV, $V \approx (4\text{ fm})^3$

Wilson et al.(HadSpec), Phys.Rev. D92 (2015), 094502



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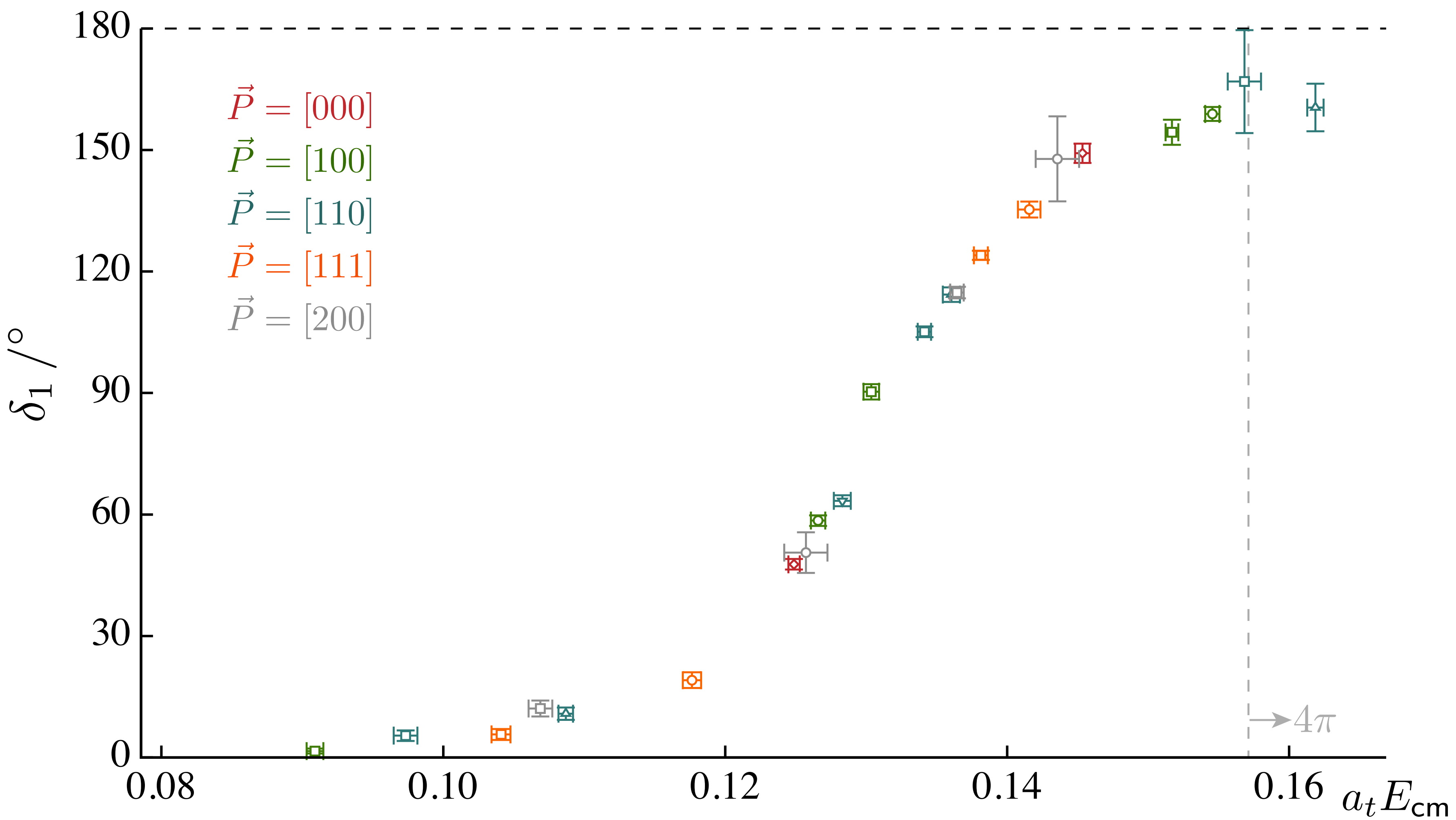
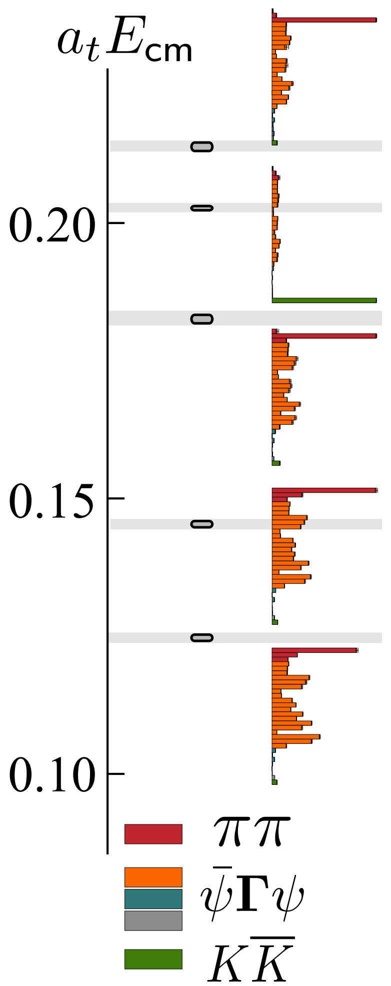


P-wave $\pi\pi$ phase shift as a function of energy

$N_f = 2 + 1, m_\pi = 236$ MeV, $V \approx (4 \text{ fm})^3$

Wilson et al.(HadSpec), Phys.Rev. D92 (2015), 094502



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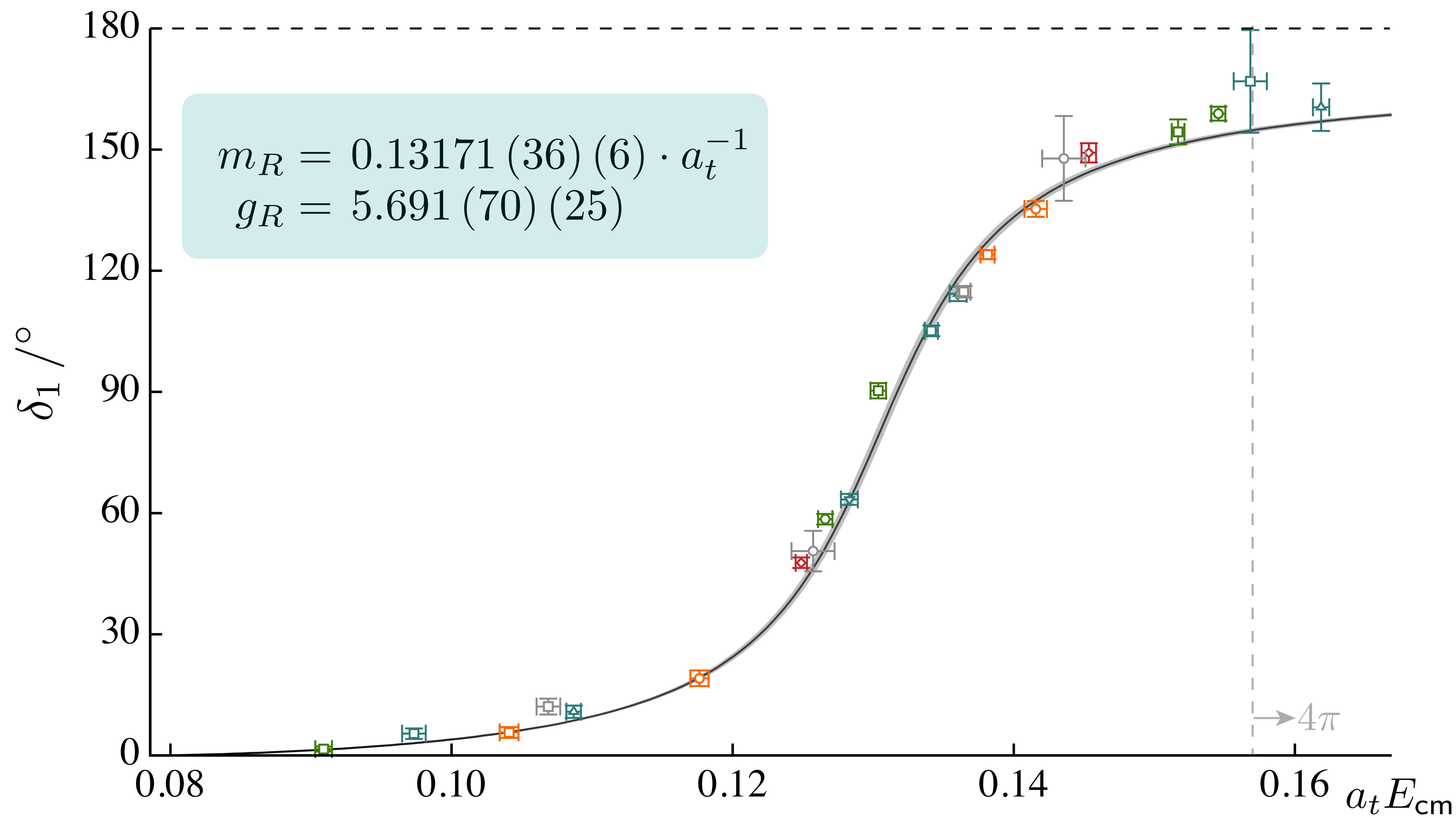


Fit to a Breit-Wigner form

$$\mathcal{M}(s) = \frac{1}{\rho(s)}\,\frac{\sqrt{s}\,\Gamma(s)}{m_R^2 - s - i\sqrt{s}\,\Gamma(s)}$$

$$\rho_i(E_{\mathsf{cm}}) = 2k_i/E_{\mathsf{cm}}$$

$$s = E_{\mathsf{cm}}^2$$

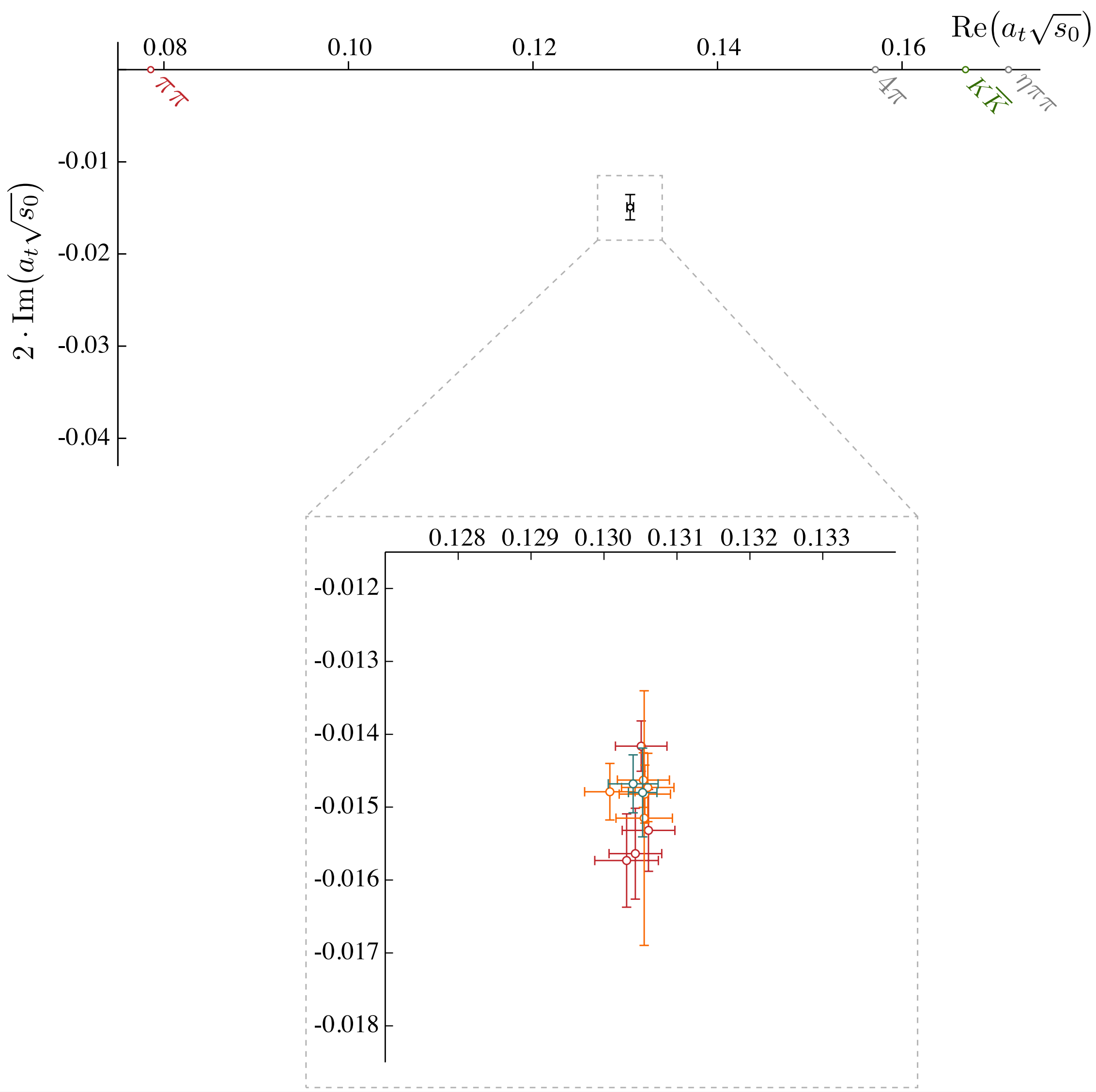
$$\Gamma(s) = \frac{g_R^2}{6\pi}\,\frac{k^3}{s}$$

$$N_f = 2+1, m_\pi = 236\ \text{MeV},\ V \approx (4\ \text{fm})^3$$

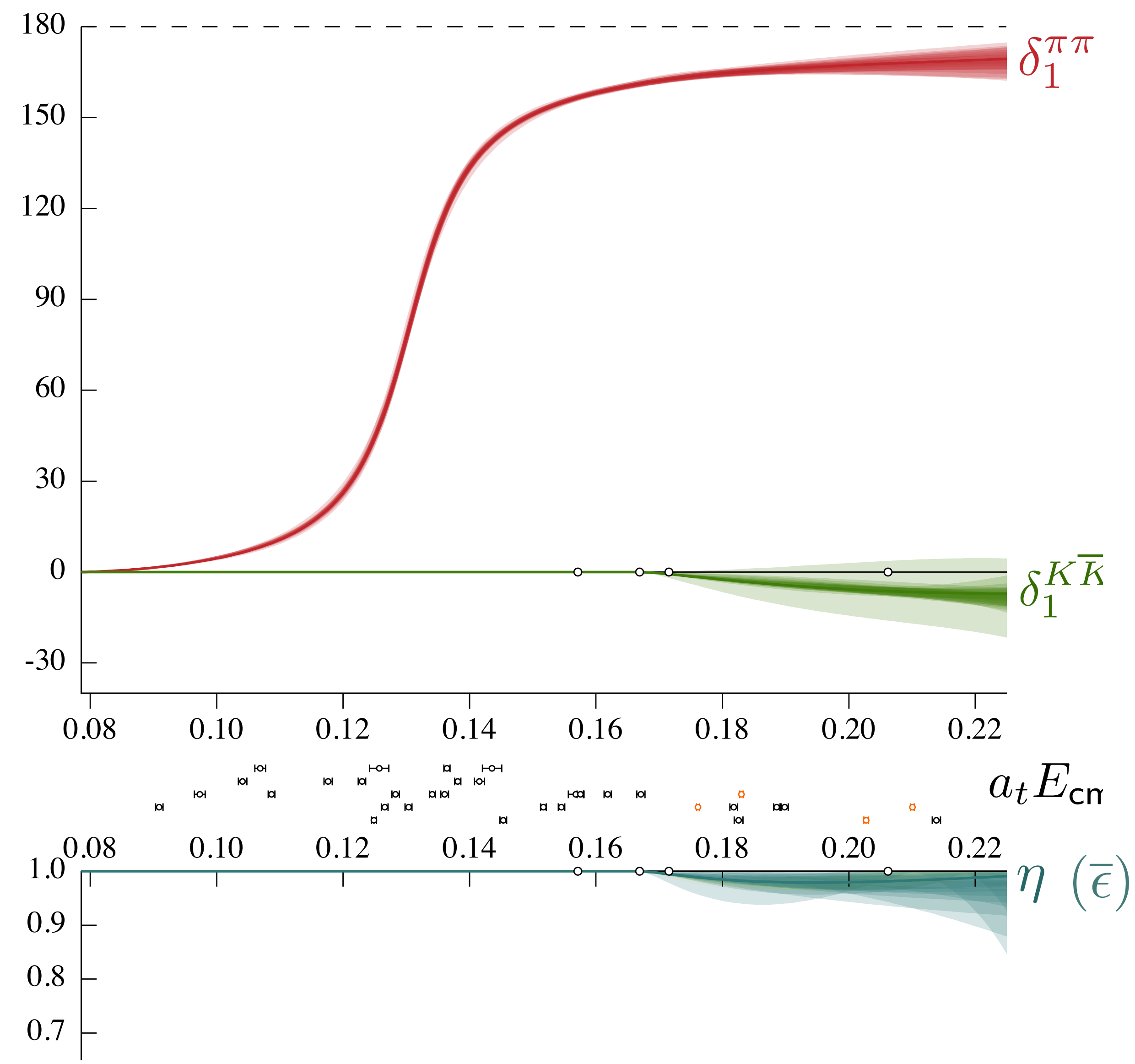
Wilson et al.(HadSpec), Phys.Rev. D92 (2015), 094502

Using a range of parametrizations:

Pole position:



All three scattering parameters:



$N_f = 2+1, m_\pi = 236\ \mathrm{MeV},\ V \approx (4\ \mathrm{fm})^3$

SUMMARY OF LECTURE I

Lattice QCD workflow

GENERATE A SAMPLE OF VACUUM CONFIGURATIONS → COMPUTE EUCLIDEAN CORRELATION FUNCTIONS → ANALYZE CORRELATION FUNCTIONS: NUMERICS AND ANALYTICAL WORK

GENERATE A SAMPLE OF VACUUM CONFIGURATIONS

— Hybrid Monte Carlo to sample gauge configurations
— Determinant of a high-dimensional matrix required

COMPUTE EUCLIDEAN CORRELATION FUNCTIONS

— Quark contractions
— Inverting a high-dimensional matrix required (to get the quark propagators)

ANALYZE CORRELATION FUNCTIONS: NUMERICS AND ANALYTICAL WORK

— Assess stat. and sys. uncertainties (take the continuum and infinite-volume limits)
— Connect to physical observables

LECTURE II: NUCLEON STRUCTURE FROM LATTICE QCD…

LECTURE II:
NUCLEON STRUCTURE FROM LATTICE QCD

Let's enumerate some of the methods that give access to structure quantities in general:

Three(four)-point functions

For e.g., form factors, moments of structure functions, Compton amplitude, transition amplitudes

Background-field methods

For e.g., EM moments and polarizabilities, charge radius, form factors and transition amplitudes.

Feynman-Hellmann inspired methods

Similar to background fields. For e.g., axial charge, form factors, EM moments, transition amplitudes

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Feynman-Hellmann inspired methods

Similar to background fields. For e.g., axial charge, form factors, EM moments, transition amplitudes

A three-point (3pt) function:

$$C_{\tilde{\chi}\mathcal{O}\chi}(x', y, x) \equiv \langle \underbrace{\chi(x')}_{\text{Annihilate the state}} \underbrace{\mathcal{O}(y)}_{\text{Insert the operator}} \underbrace{\tilde{\chi}(x)}_{\text{Create the state}} \rangle$$

Chambers, http://inspirehep.net/record/1744874/

A three-point (3pt) function:

$$C_{\widetilde{\chi}\mathcal{O}\chi}(x', y, x) \equiv \langle \chi(x')\mathcal{O}(y)\widetilde{\chi}(x)\rangle$$

Chambers, http://inspirehep.net/record/1744874/

Annihilate the state

Insert the operator

Create the state

Spectral decomposition of the 3pt function in Euclidean spacetime

$$G_{\chi\mathcal{O}\widetilde{\chi}}(\mathbf{p}', \mathbf{p}; t', \tau, t) = \sum_{\mathrm{X,Y}} \frac{e^{-E_{\mathrm{X}}(\mathbf{p}')(t'-\tau)}}{2E_{\mathrm{X}}(\mathbf{p}')} \frac{e^{-E_{\mathrm{Y}}(\mathbf{p})(\tau-t)}}{2E_{\mathrm{Y}}(\mathbf{p})}$$

$$\langle\Omega|\chi(0)|\mathrm{X}(\mathbf{p}')\rangle\ \langle\mathrm{X}(\mathbf{p}')|\mathcal{O}(0)|\mathrm{Y}(\mathbf{p})\rangle\ \langle\mathrm{Y}(\mathbf{p})|\widetilde{\chi}(0)|\Omega\rangle$$

A complete set of states

Another complete set of states

A three-point (3pt) function:

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Annihilate the state

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A complete set of states

Another complete set of states

Long-separation behavior dominated by ground states

$$G_{\chi\mathcal{O}\widetilde{\chi}}(\mathbf{p}', \mathbf{p}; t', \tau, t) \xrightarrow{\text{large } t'-\tau, \tau-t} \frac{e^{-E_{\mathrm{X}_0}(\mathbf{p}')(t'-\tau)}}{2E_{\mathrm{X}_0}(\mathbf{p}')} \frac{e^{-E_{\mathrm{X}_0}(\mathbf{p})(\tau-t)}}{2E_{\mathrm{X}_0}(\mathbf{p})} \sum_{r', r} \langle \Omega|\chi(0)|\mathrm{X}_0(\mathbf{p}', r')\rangle \, \langle \mathrm{X}_0(\mathbf{p}', r')|\mathcal{O}(0)|\mathrm{X}_0(\mathbf{p}, r)\rangle \, \langle \mathrm{X}_0(\mathbf{p}, r)|\widetilde{\chi}(0)|\Omega\rangle$$

If there are degenerate ground states

Desired ground state to ground state matrix element (unrenormalized and in a finite volume)

A three-point (3pt) function:

$$C_{\widetilde{\chi}\mathcal{O}\chi}(x', y, x) \equiv \langle \chi(x')\mathcal{O}(y)\widetilde{\chi}(x)\rangle$$

Annihilate the state

Insert the operator

Create the state

Spectral decomposition of the 3pt function in Euclidean spacetime

$$G_{\chi\mathcal{O}\widetilde{\chi}}(\mathbf{p}', \mathbf{p}; t', \tau, t) = \sum_{\mathrm{X},\mathrm{Y}} \frac{e^{-E_{\mathrm{X}}(\mathbf{p}')(t'-\tau)}}{2E_{\mathrm{X}}(\mathbf{p}')} \frac{e^{-E_{\mathrm{Y}}(\mathbf{p})(\tau-t)}}{2E_{\mathrm{Y}}(\mathbf{p})} \langle\Omega|\chi(0)|\mathrm{X}(\mathbf{p}')\rangle \langle\mathrm{X}(\mathbf{p}')|\mathcal{O}(0)|\mathrm{Y}(\mathbf{p})\rangle \langle\mathrm{Y}(\mathbf{p})|\widetilde{\chi}(0)|\Omega\rangle$$

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If there are degenerate ground states

Desired ground state to ground state matrix element (unrenormalized and in a finite volume)

Taking a proper ratio to 2pt functions

$$R_{\chi\mathcal{O}\widetilde{\chi}}(\mathbf{p}', \mathbf{p}; t', \tau, t) \overset{\text{large } t'-\tau, \tau-t}{\propto} \langle\mathrm{X}_0(\mathbf{p}', r')|\mathcal{O}(0)|\mathrm{X}_0(\mathbf{p}, r)\rangle$$

EXERCISE 4

If the computational resources do not allow large source, operator and sink time separations to be achieved, one should worry about the effect of excited states. One way to have more confidence over the extracted ground state to ground state matrix element is to perform a multi-exponential fits to the ratio of 3pt to 2pt functions as a function of both the source-sink and the source-operator separations. Assume that both the ground state and the first excited states contribute significantly to such a ratio. Write down a generic form for such a multi-exponential function.

BONUS EXERCISE 3

In the above exercise, sum over the time insertions of the operator and write down a new form for the ratio of 3pt to 2pt functions, which now is only a function of the source-sink time separation. This is referred to as the summation method in literature.

Example: The application of 3pt function method to obtain the axial charge/form factors of the nucleon

Constantinou, arXiv:1411.0078 [hep-lat].

$$\langle N(p',s')|\bar{\psi}(x)\,\gamma_\mu\,\gamma_5\,\psi(x)|N(p,s)\rangle = i\left(\frac{m_N^2}{E_N(\mathbf{p}')E_N(\mathbf{p})}\right)^{1/2}\bar{u}_N(p',s')\left[G_A(q^2)\gamma_\mu\gamma_5+\frac{q_\mu\gamma_5}{2m_N}G_p(q^2)\right]u_N(p,s)$$

Axial-vector current

Nucleon spinor

Axial and pseudo scalar form factors

$G_A(0) = g_A$

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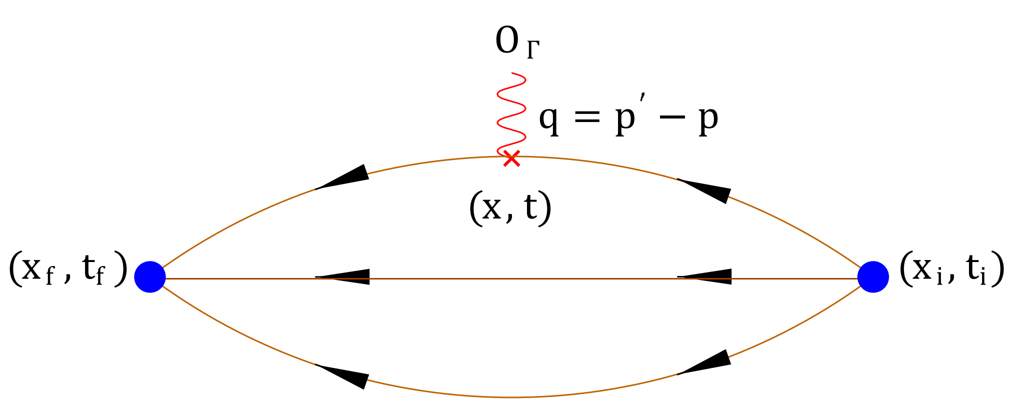
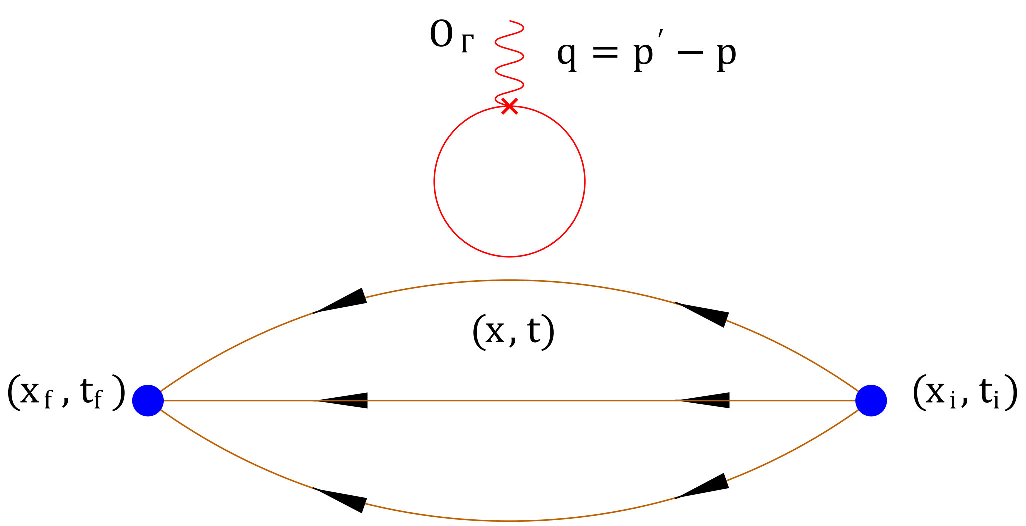
Axial and pseudo scalar form factors

$G_A(0) = g_A$



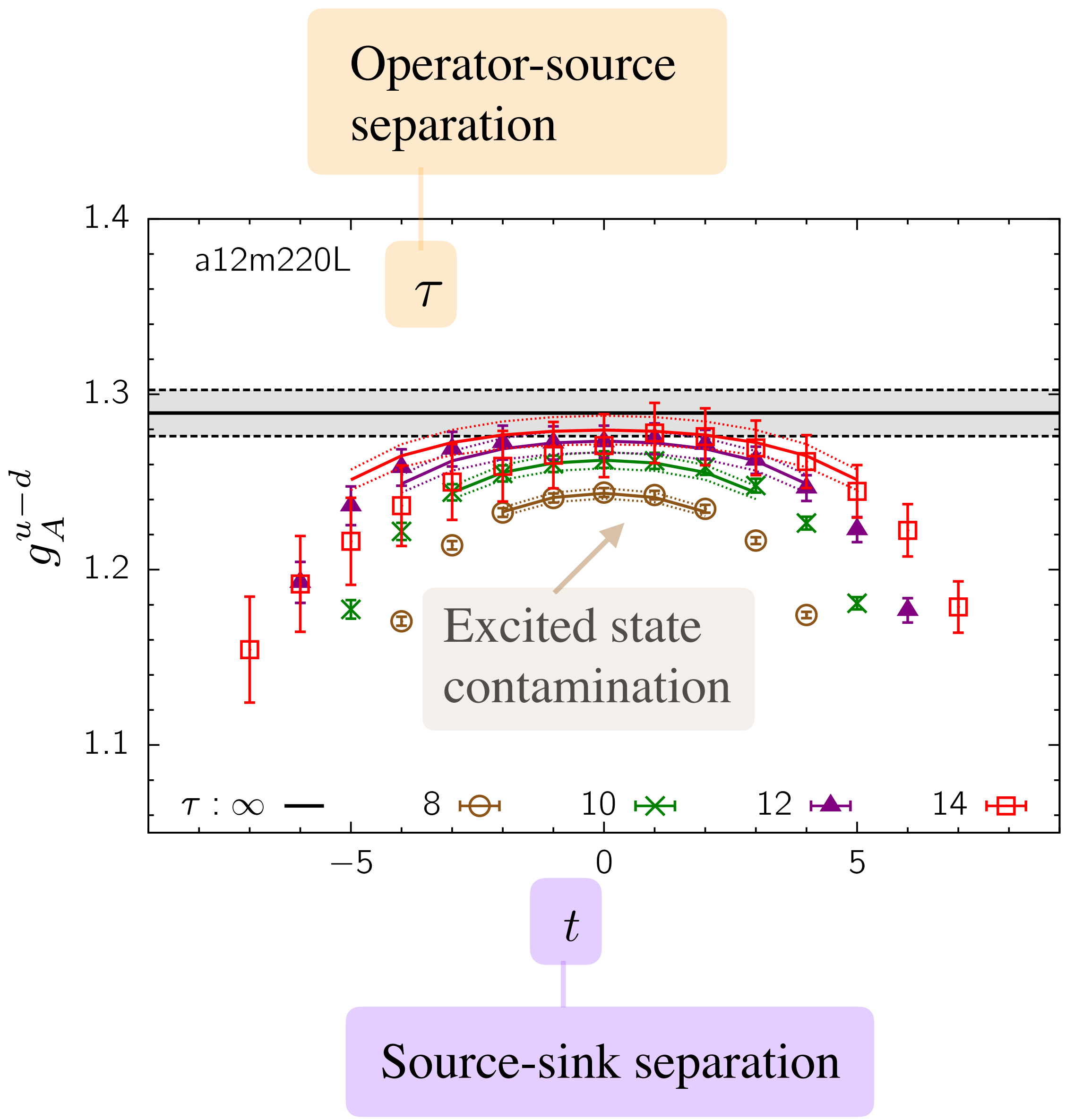
Connected contribution



Disconnected contribution
(vanishes at isospin limit for isovector quantities)

Example: The application of 3pt function method to obtain the axial charge/form factors of the nucleon

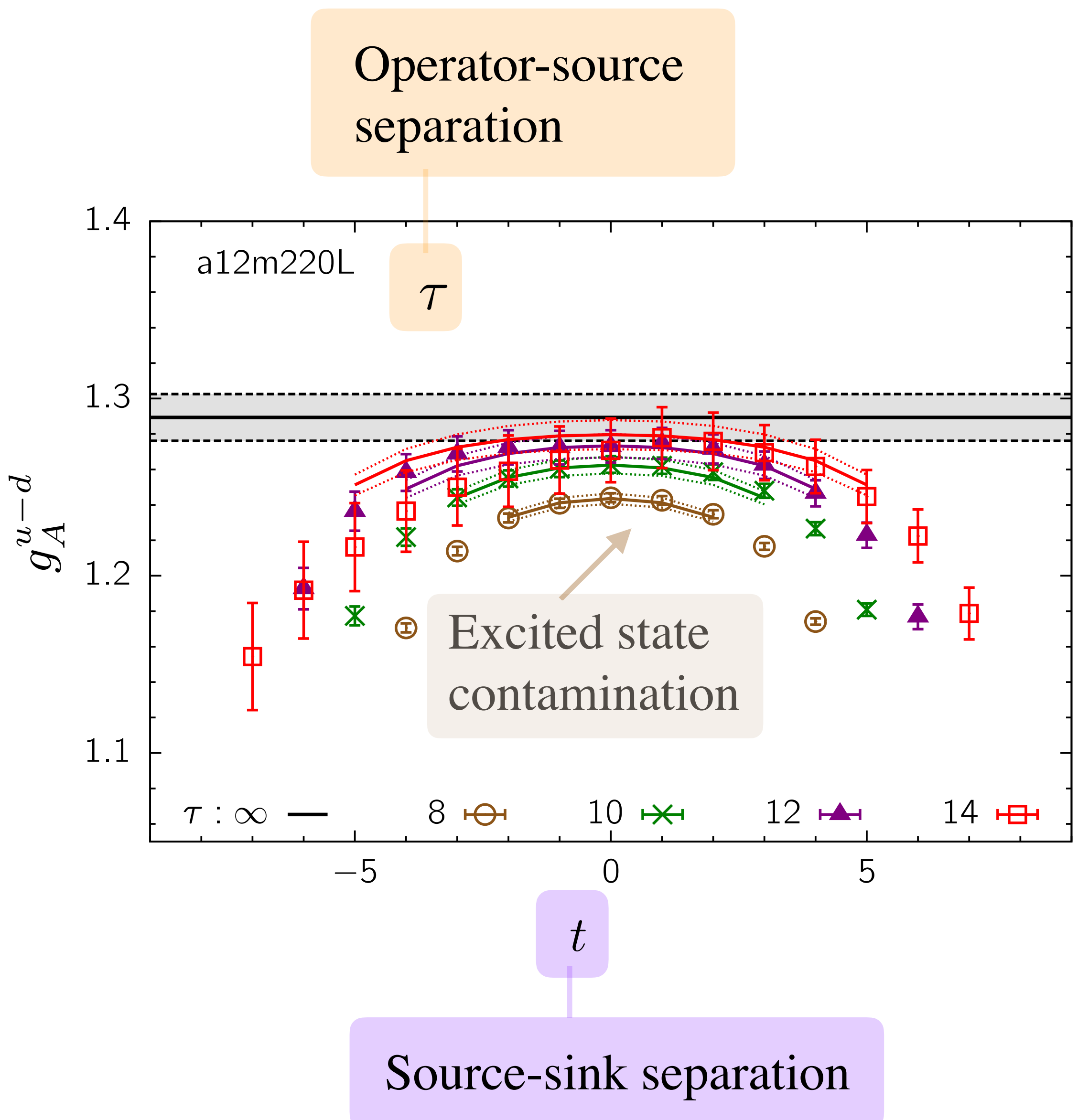
Gupta et al (PNDME), Phys. Rev. D 98, 034503 (2018)



3pt function for a single lattice spacing, volume and quark masses

Example: The application of 3pt function method to obtain the axial charge/form factors of the nucleon

Gupta et al (PNDME), Phys. Rev. D 98, 034503 (2018)



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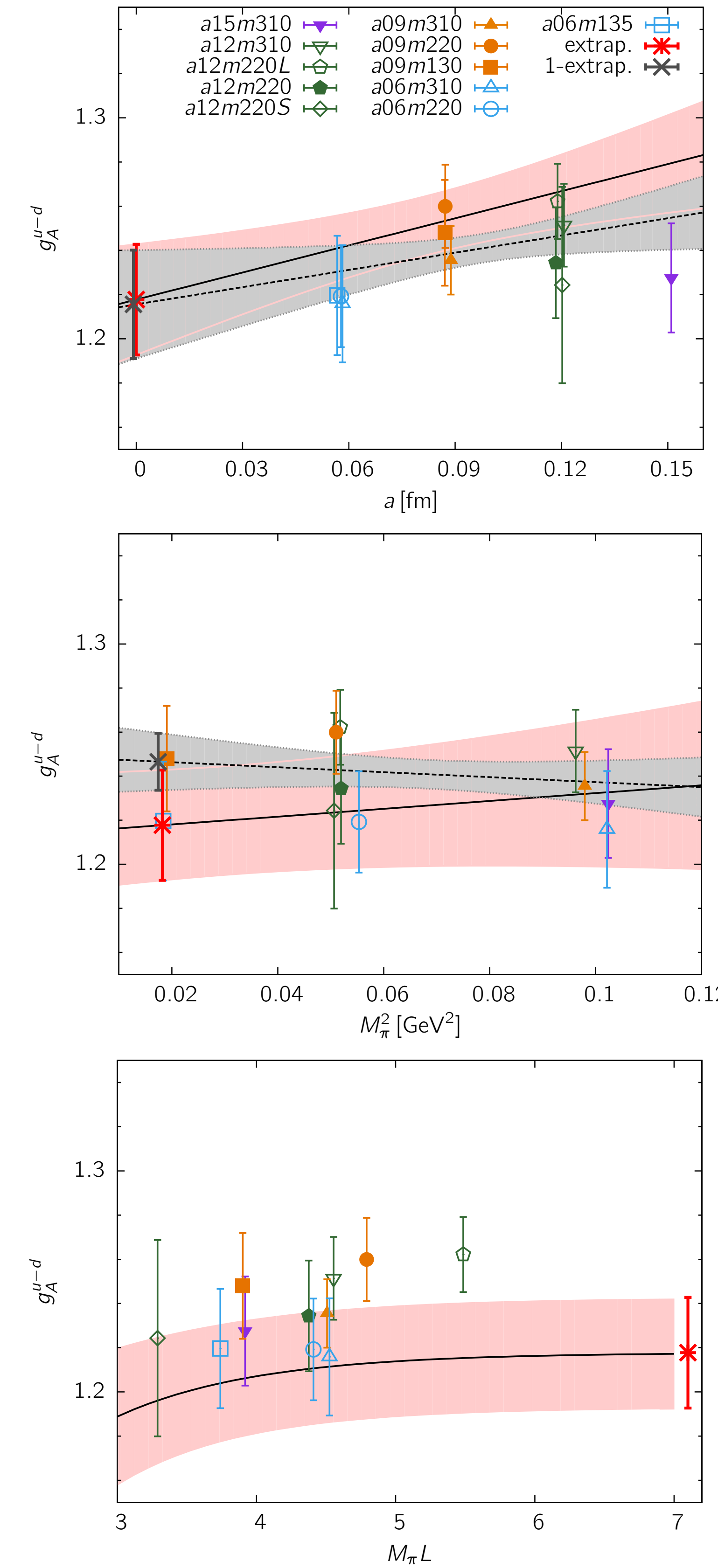
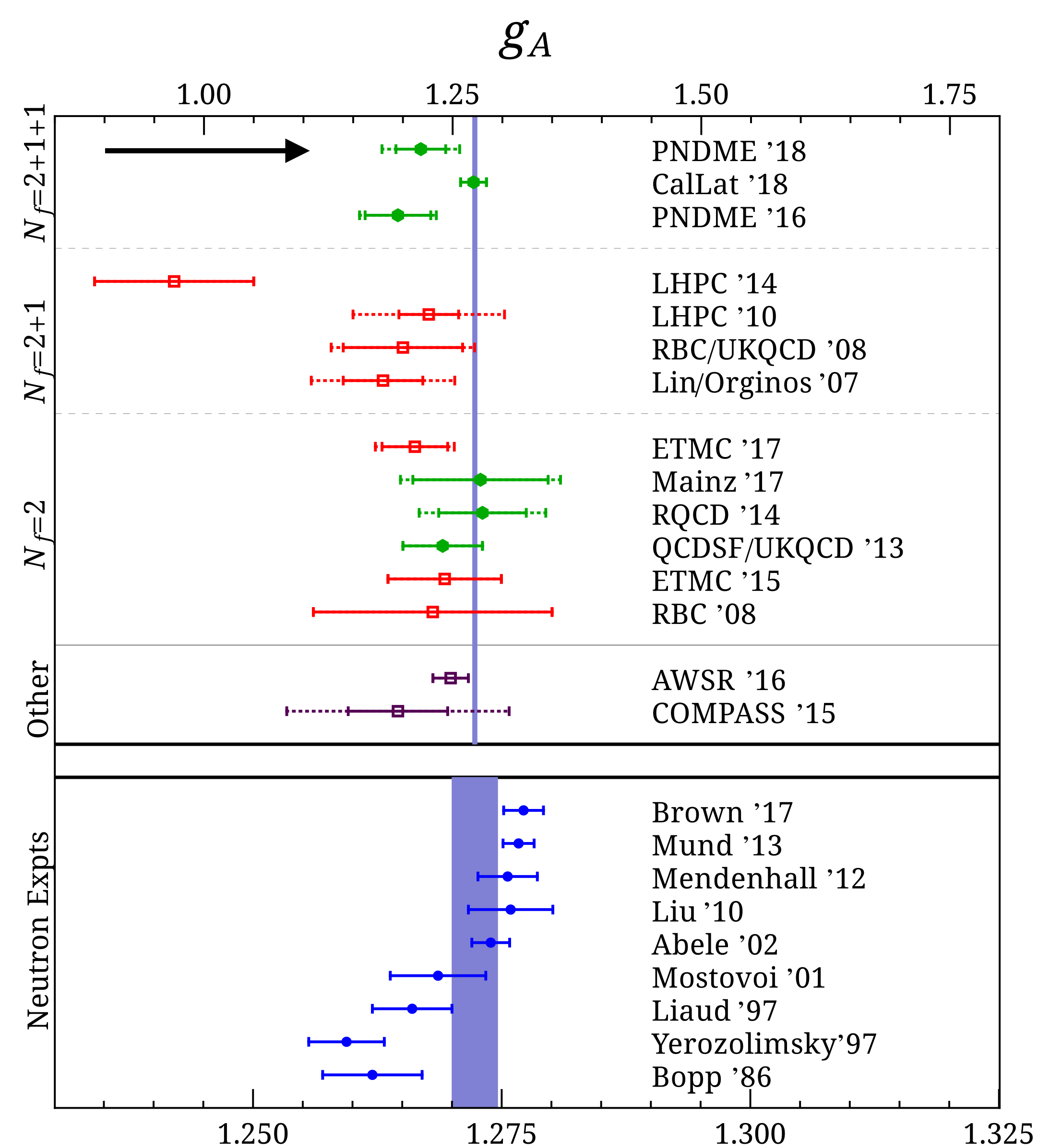


Extrapolation to continuum, infinite volume and physical quark masses

Example: The application of 3pt function method to obtain the axial charge/form factors of the nucleon

Gupta et al (PNDME), Phys. Rev. D 98, 034503 (2018)

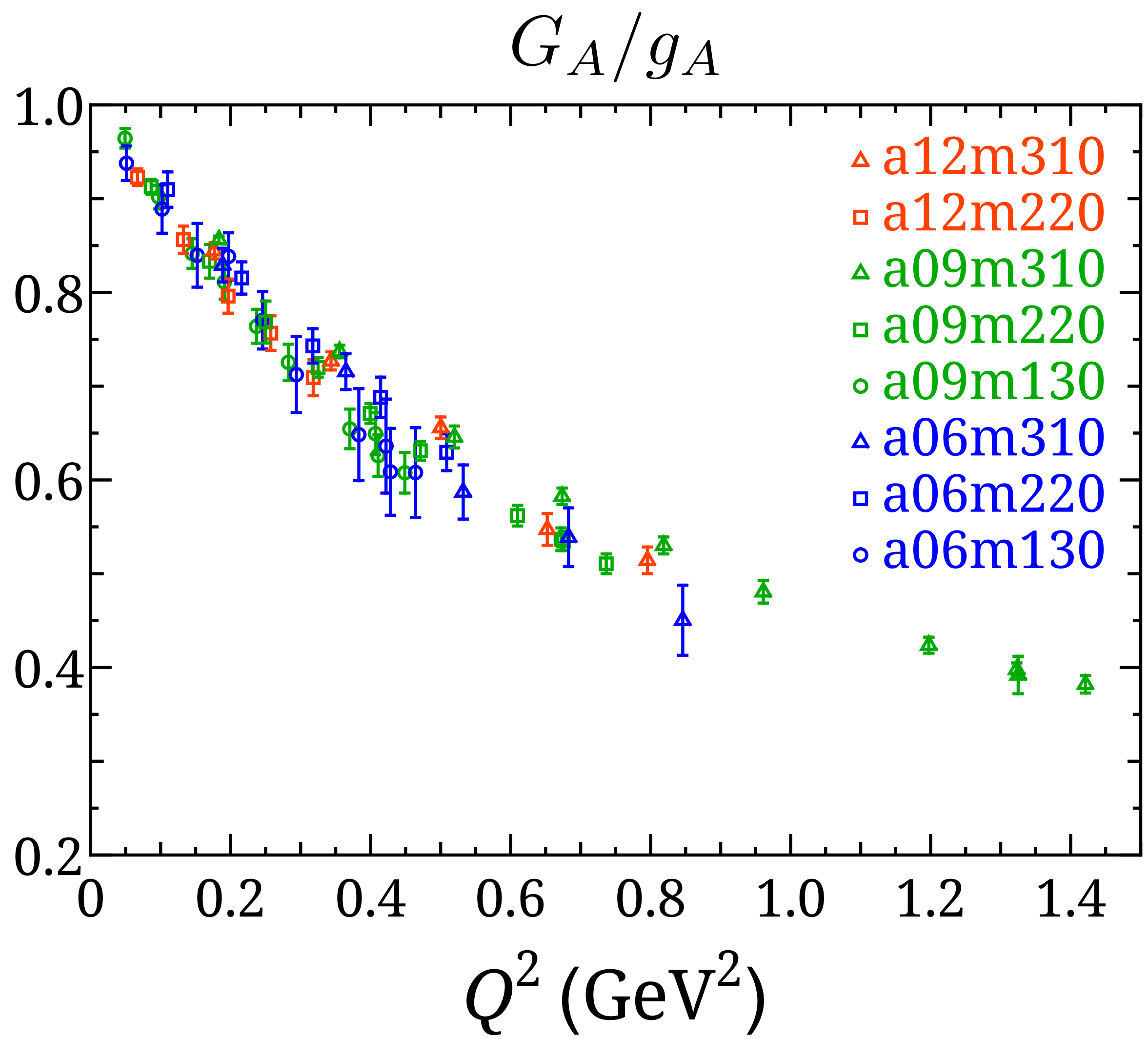


Compilation of results

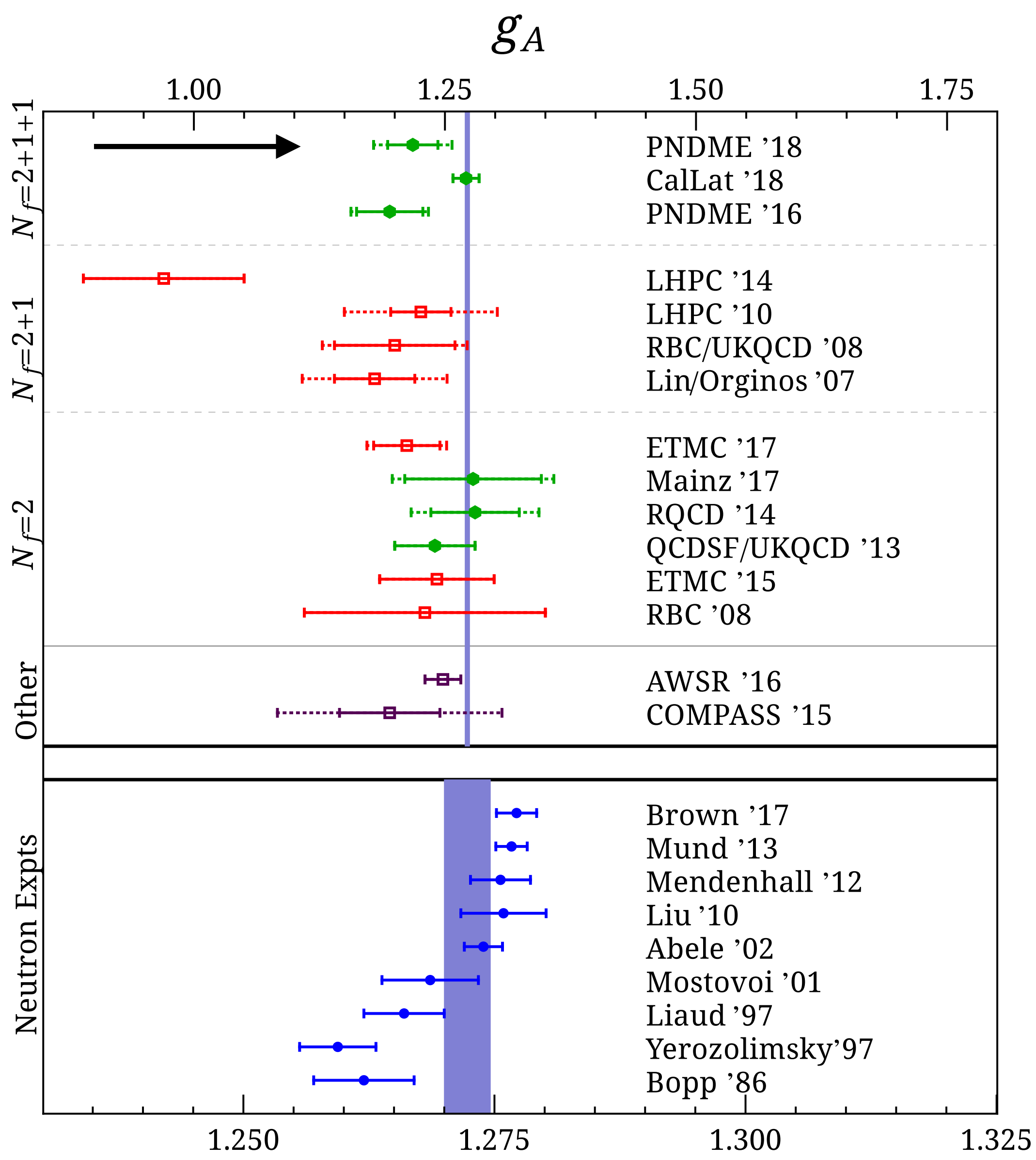
Example: The application of 3pt function method to obtain the axial charge/form factors of the nucleon

Gupta et al (PNDME), Phys. Rev. D 98, 034503 (2018)

Jang et al, EPJ Web Conf. 175, 06033 (2018)



Axial form factor results



Compilation of results

Example: The spin decomposition of the nucleon

Alexandru, Phys. Rev. Lett. 119, 142002 (2017).

$$J_N = \sum_{q=u,d,s,c\cdots} \left(\frac{1}{2}\Delta\Sigma_q + L_q \right) + J_g$$

Quark spin

Quark orbital angular momentum

Total gluon angular momentum

Ji, Phys. Rev. Lett. 78, 610 (1997).

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Quark orbital angular momentum

Total gluon angular momentum

Ji, Phys. Rev. Lett. 78, 610 (1997).

Matrix elements needed

$$\langle N(p,s')|\mathcal{O}_A^{\mu}|N(p,s)\rangle = \bar{u}_N(p,s')\left[g_A^q \gamma^\mu \gamma_5\right] u_N(p,s)$$

$$\langle N(p',s')|\mathcal{O}_V^{\mu\nu}|N(p,s)\rangle = \bar{u}_N(p',s')\Lambda^q_{\mu\nu}(Q^2) u_N(p,s)$$

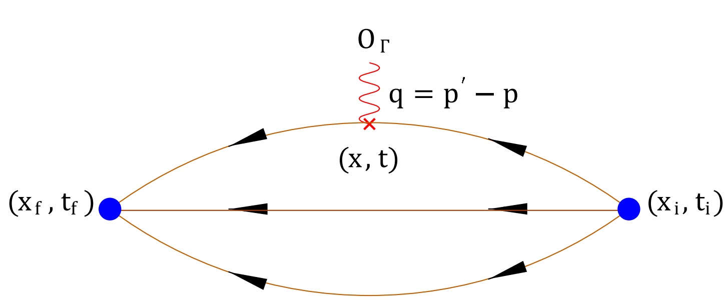
$$\langle N(p',s')|\mathcal{O}_g^{\mu\nu}|N(p,s)\rangle = \bar{u}_N(p',s')\Lambda^g_{\mu\nu}(Q^2) u_N(p,s)$$

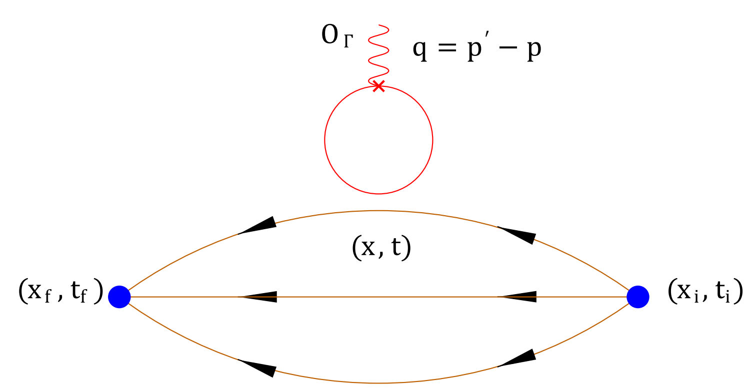
With operators

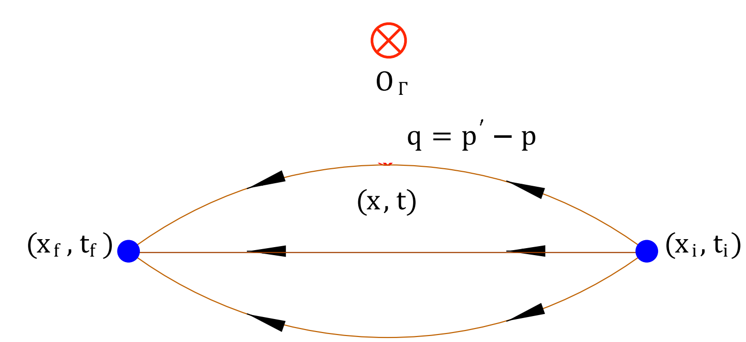
$$\mathcal{O}_A^{\mu} = \bar{q}\gamma_\mu\gamma_5 q$$

$$\mathcal{O}_V^{\mu\nu} = \bar{q}\gamma^{\{\mu}\overleftrightarrow{D}^{\nu\}} q$$

$$\mathcal{O}_g^{\mu\nu} = 2\mathrm{Tr}[G_{\mu\sigma}G_{\nu\sigma}]$$





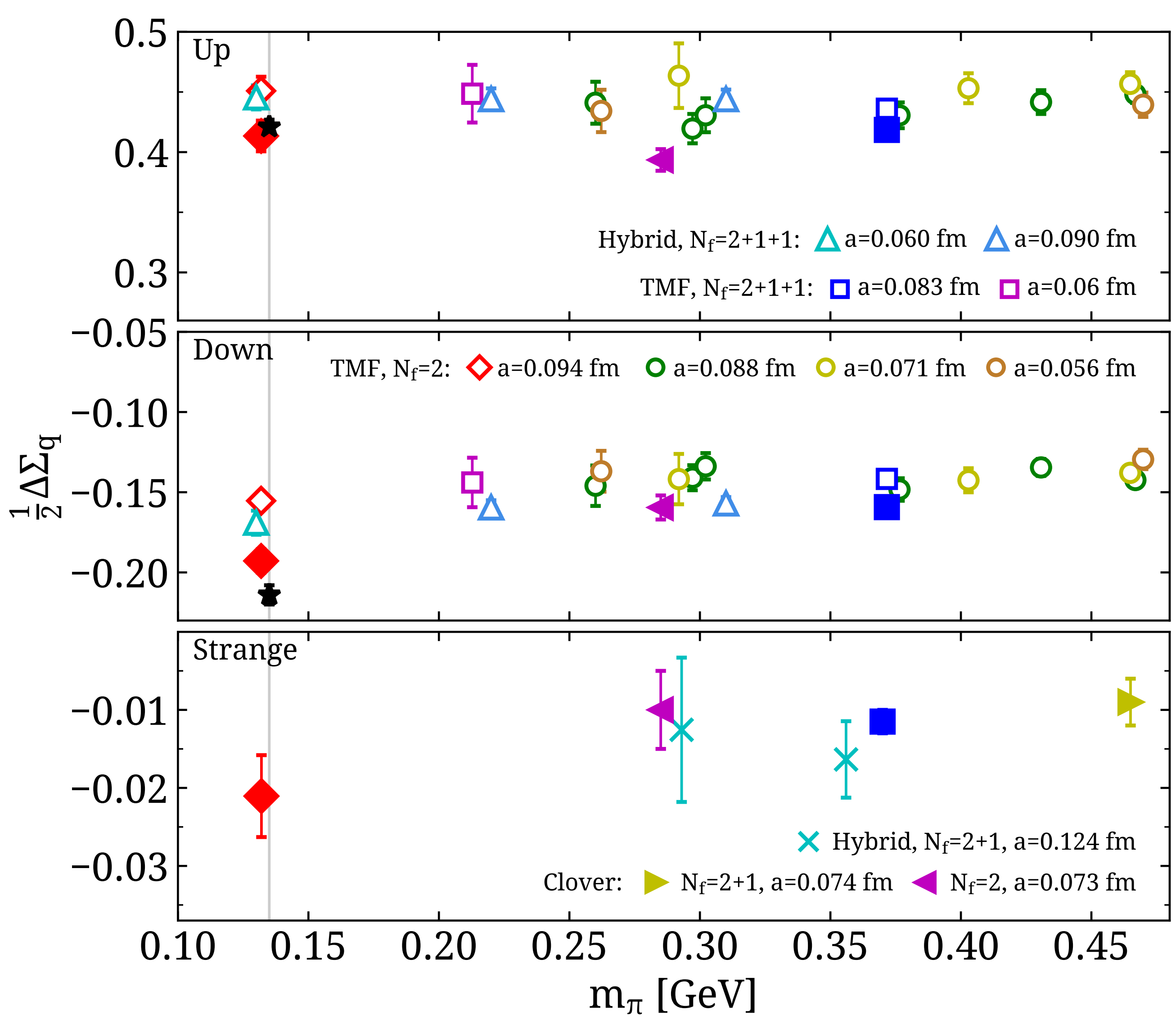


Quark contributions

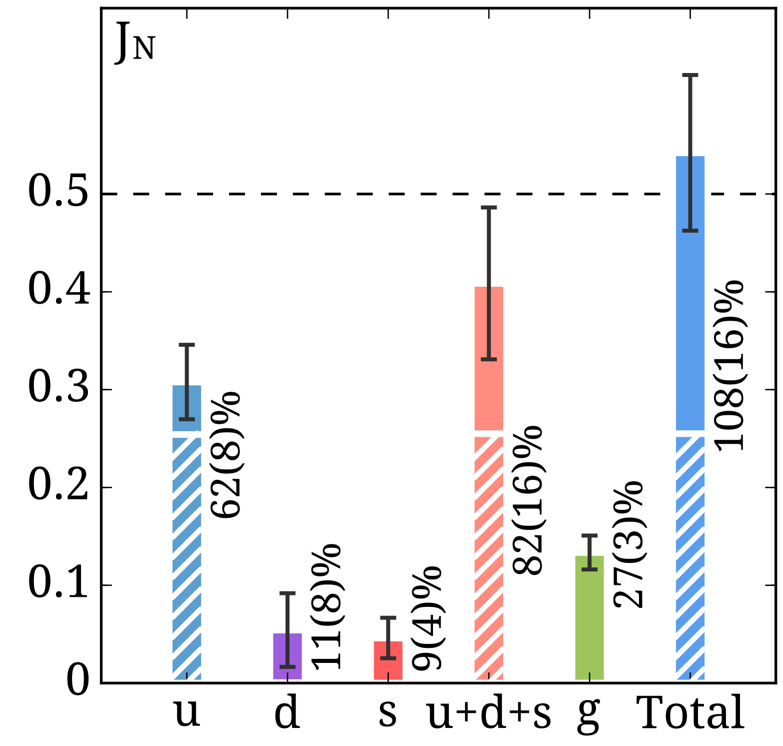
Qluonic contribution

Example: The spin decomposition of the nucleon

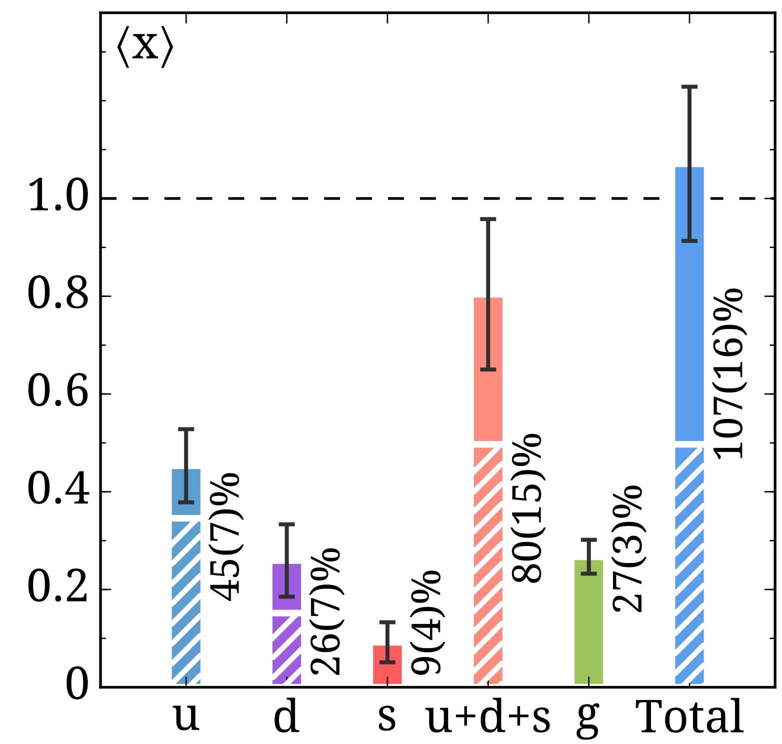
Alexandru, Phys. Rev. Lett. 119, 142002 (2017).



Quark spin contributions



Nucleon spin decomposition



Longitudinal momentum decomposition

[STILL CONTINUING ON] LECTURE II: NUCLEON STRUCTURE FROM LATTICE QCD

Let’s enumerate a some of the methods that give access to structure quantities in general:

Three(four)-point functions

For e.g., form factors, moments of structure functions, Compton amplitude, transition amplitudes

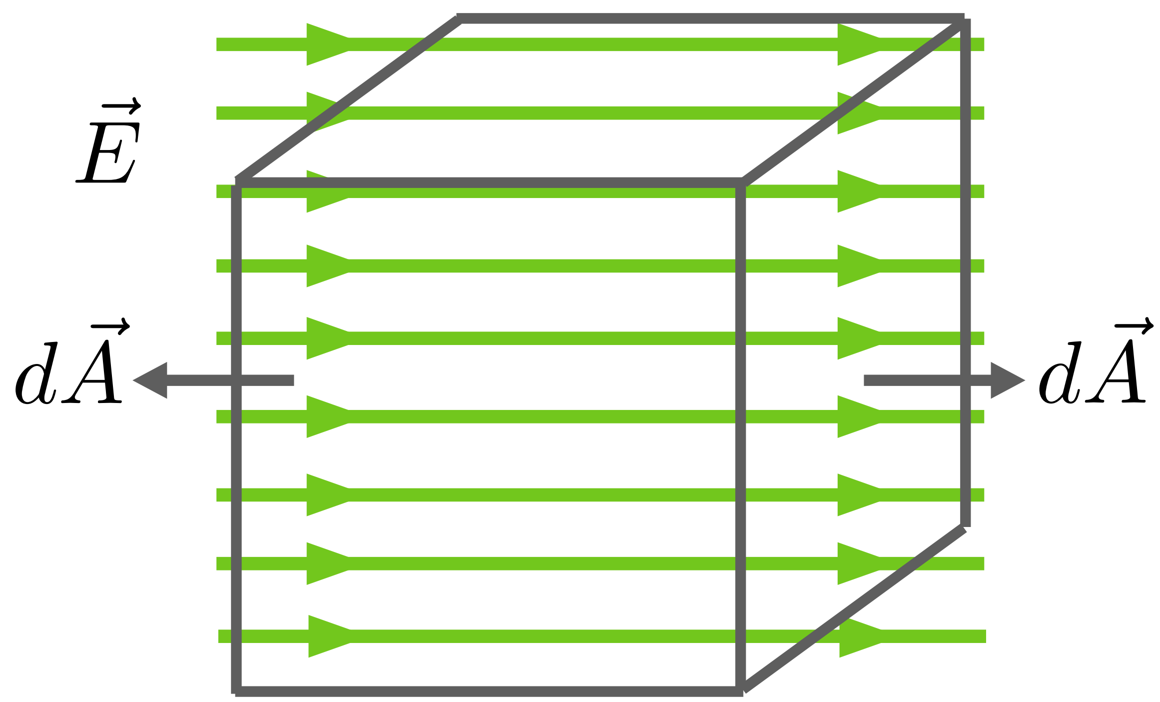
Background-field methods

For e.g., EM moments and polarizabilities, charge radius, form factors and transition amplitudes.

Feynman-Hellmann inspired methods

Similar to background fields. For e.g., axial charge, form factors, EM moments, transition amplitudes

Background fields are non-dynamical, i.e., there will be no pair creation and annihilation in vacuum with a classical EM background field. This mean the photon zero mode is no problem: it is absent in the calculation!



$$U^{(\mathrm{QCD})} \to U^{(\mathrm{QCD})} \times U^{(\mathrm{QED})}$$

Modify the links when forming the quark propagators (quench approx).

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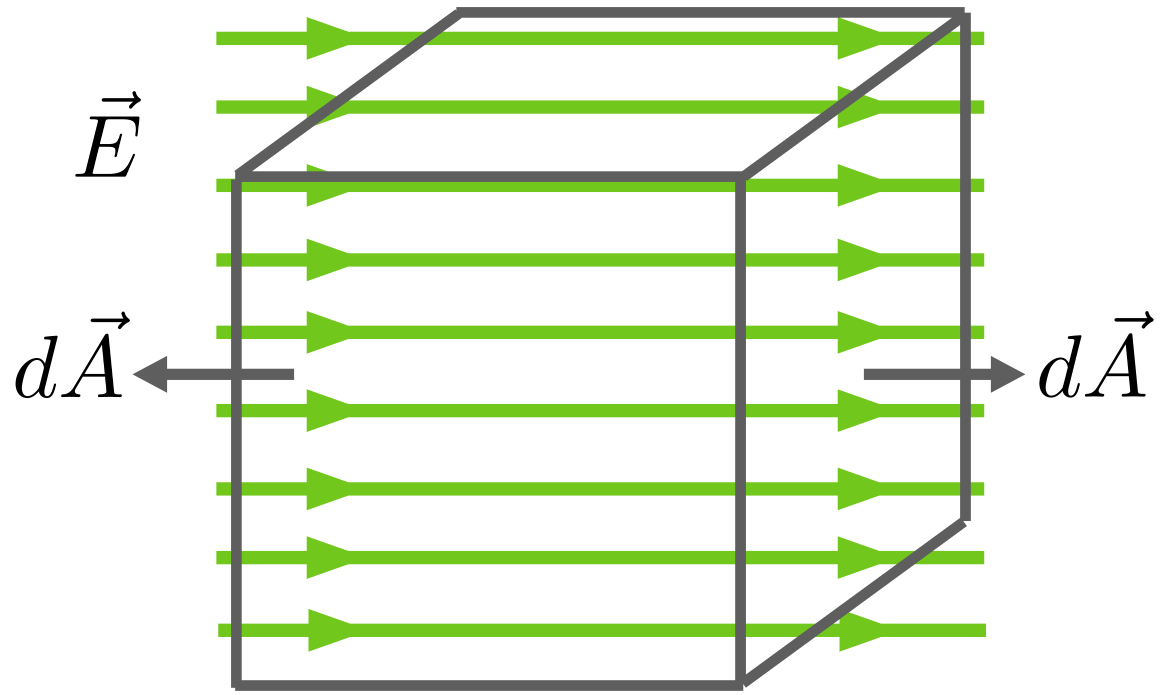
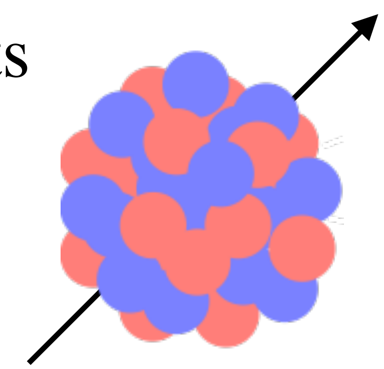


$$U^{(\mathrm{QCD})} \to U^{(\mathrm{QCD})} \times U^{(\mathrm{QED})}$$

Modify the links when forming the quark propagators (quench approx).

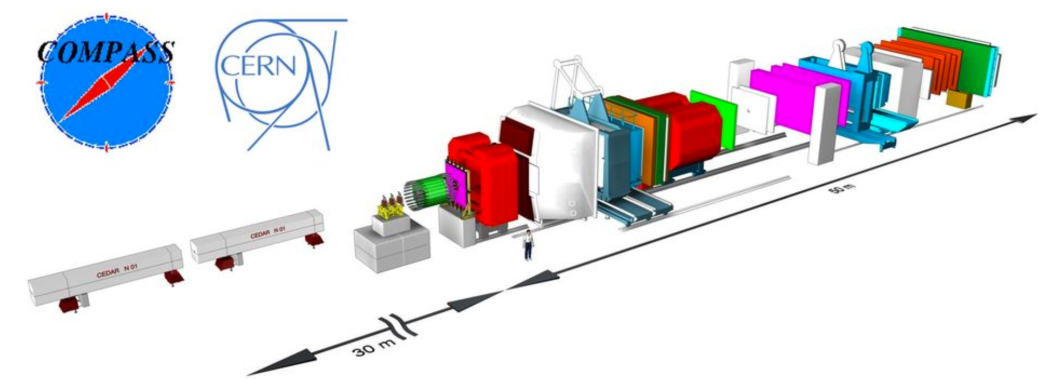
Traditionally they are used for constraining the response of hadrons/nuclei to external probes:

Magnetic moments



Electric and magnetic polarizabilities

COMPASS CERN



See e.g., BEANE et al (NPLQCD), Phys.Rev.Lett. 113 (2014) 25, 252001 and Phys.Rev. D92 (2015) 11, 114502. for nuclear-physics calculations.

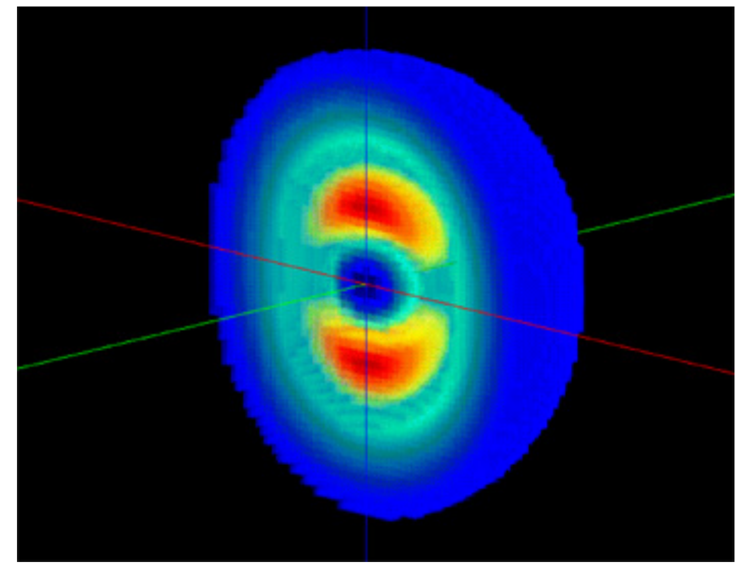
Various other structure properties of hadrons and nuclei, as well as their transitions, can be studied using more complex background fields:

1) EM charge radius

ZD and Detmold, Phys. Rev. D 93, 014509 (2016).

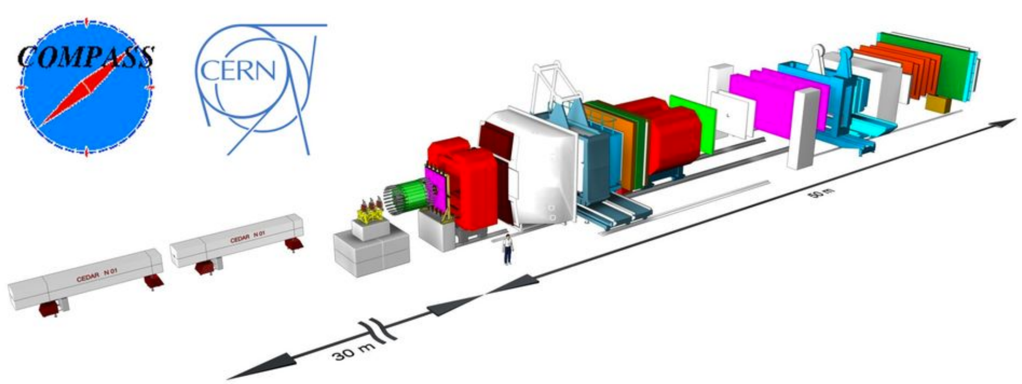
2) Electric quadrupole moment

ZD and Detmold, Phys. Rev. D 93, 014509 (2016).



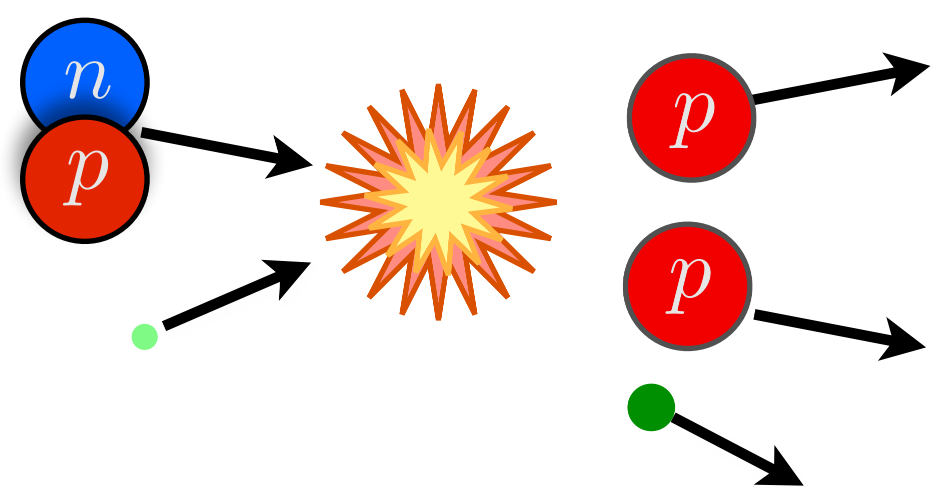
3) Form factors

Detmold, Phys.Rev. D71, 054506 (2005).



4) Axial background fields

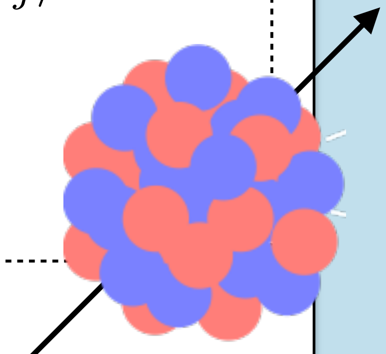
Beane at al, Phys.Rev. Lett, 115 132001 (2015).



Here's an application of the background-field technique to obtain magnetic moment and polarizabilities of the nucleon:

$$E_{h;j_z}(\mathbf{B}) = \sqrt{M_h^2 + P_\parallel^2 + \underbrace{(2n_L+1)|Q_h e\mathbf{B}|}_{\text{Landau levels for charged particles}}} - \underbrace{\boldsymbol{\mu}_h}_{\text{Magnetic moment}} \cdot \mathbf{B} - 2\pi \beta_h^{(M0)} |\mathbf{B}|^2 - 2\pi \beta_h^{(M2)} \langle \hat{T}_{ij} B_i B_j \rangle + \ldots$$

Magnetic polarizabilities



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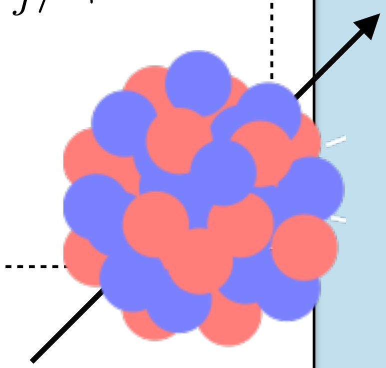
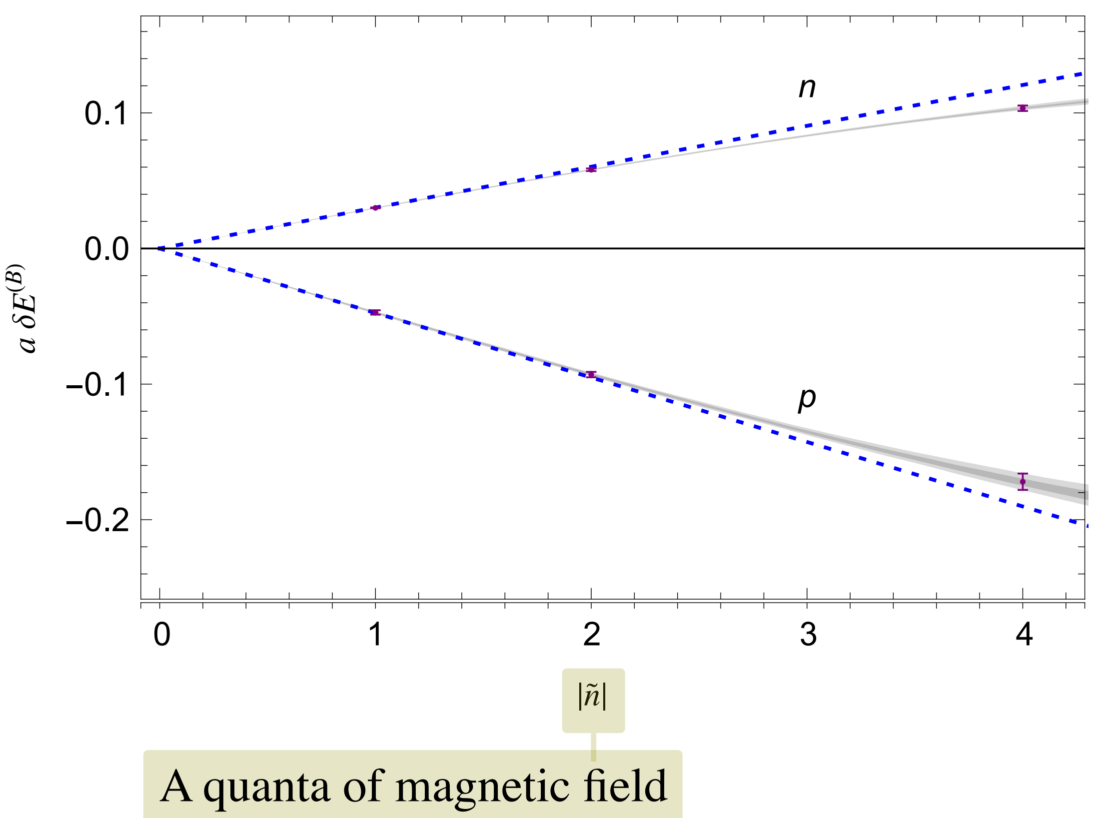
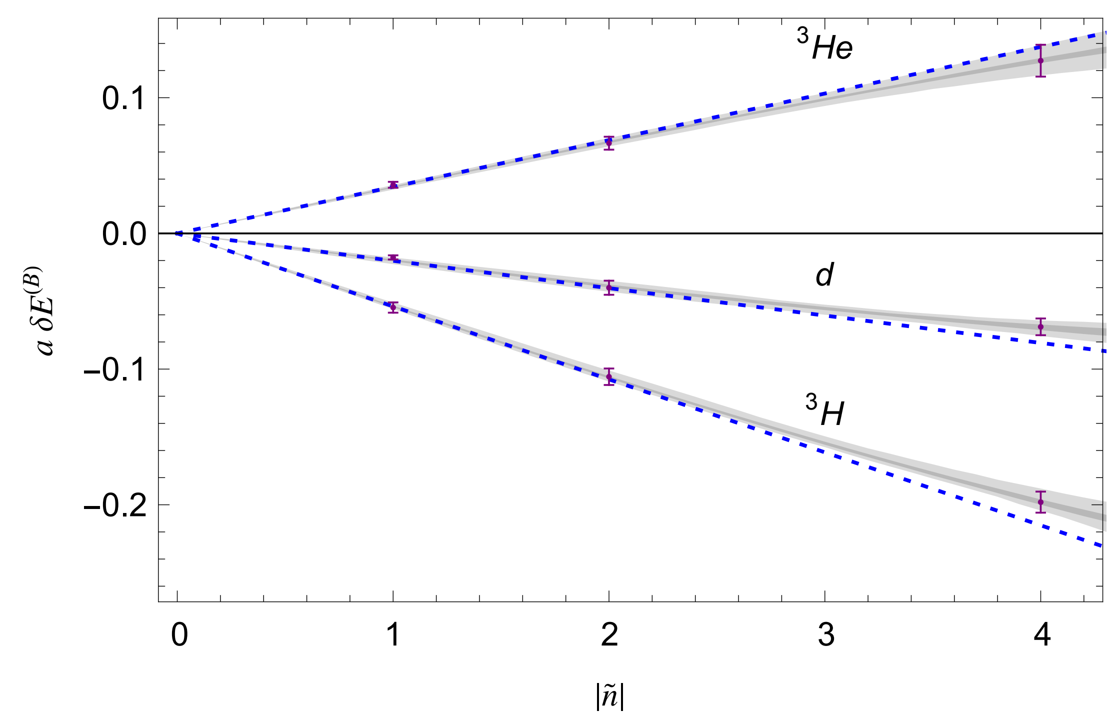


Nucleon



Light nuclei



$N_f = 3,\;\; m_\pi = 0.806\ \text{GeV},\;\; a = 0.145(2)\ \text{fm}$

Beane et al.(NPLQCD), phys.rev.lett.113 (2014) 25, 252001.
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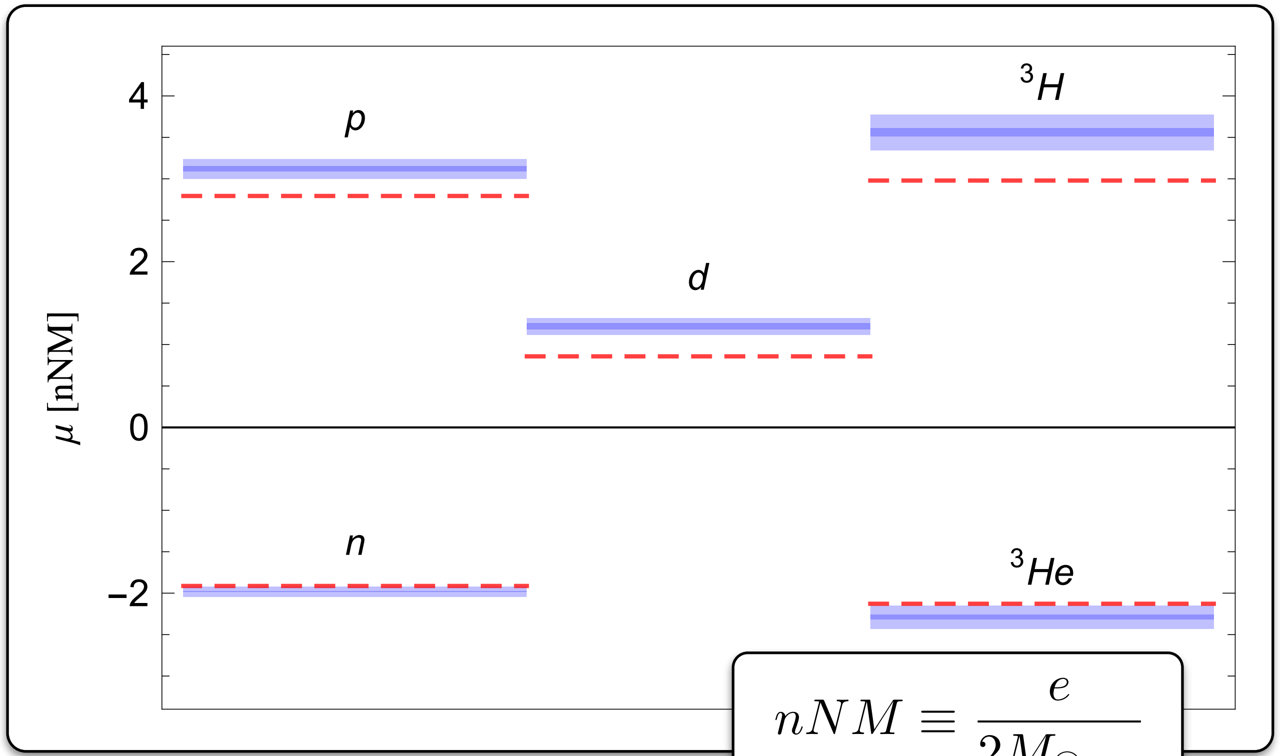
Magnetic polarizabilities

Magnetic moment



$$nNM \equiv \frac{e}{2M_{@m_q}}$$

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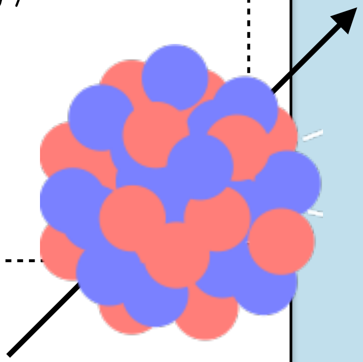
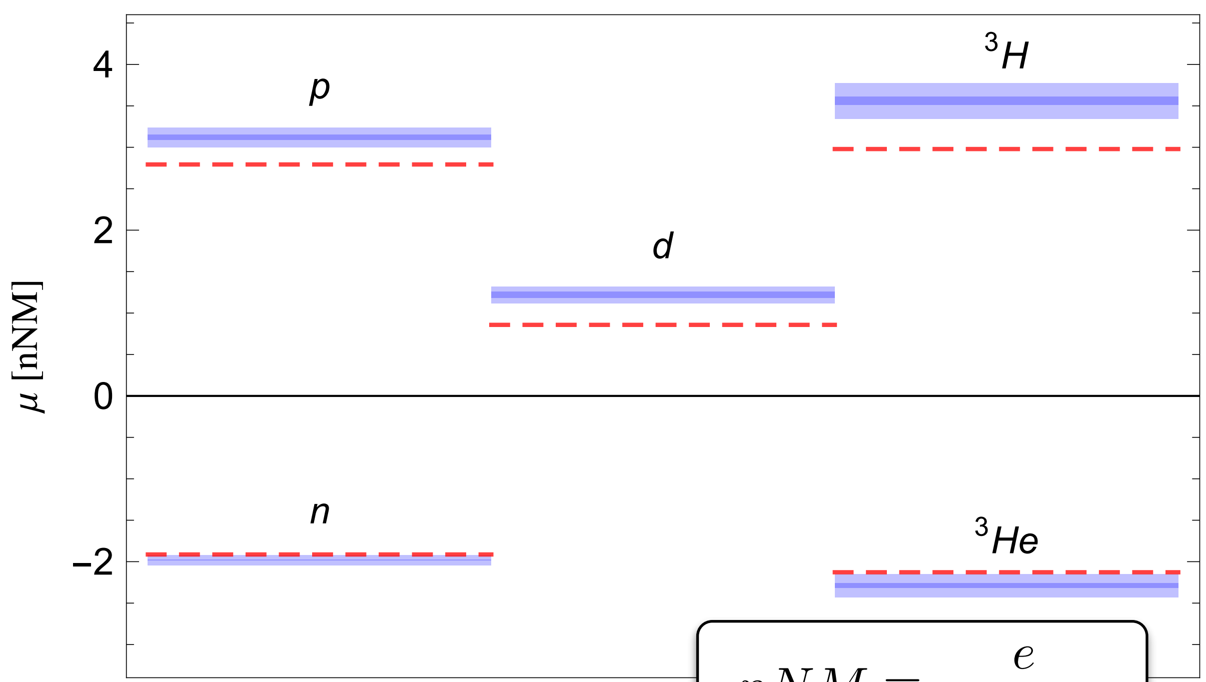
Magnetic polarizabilities



Magnetic moment



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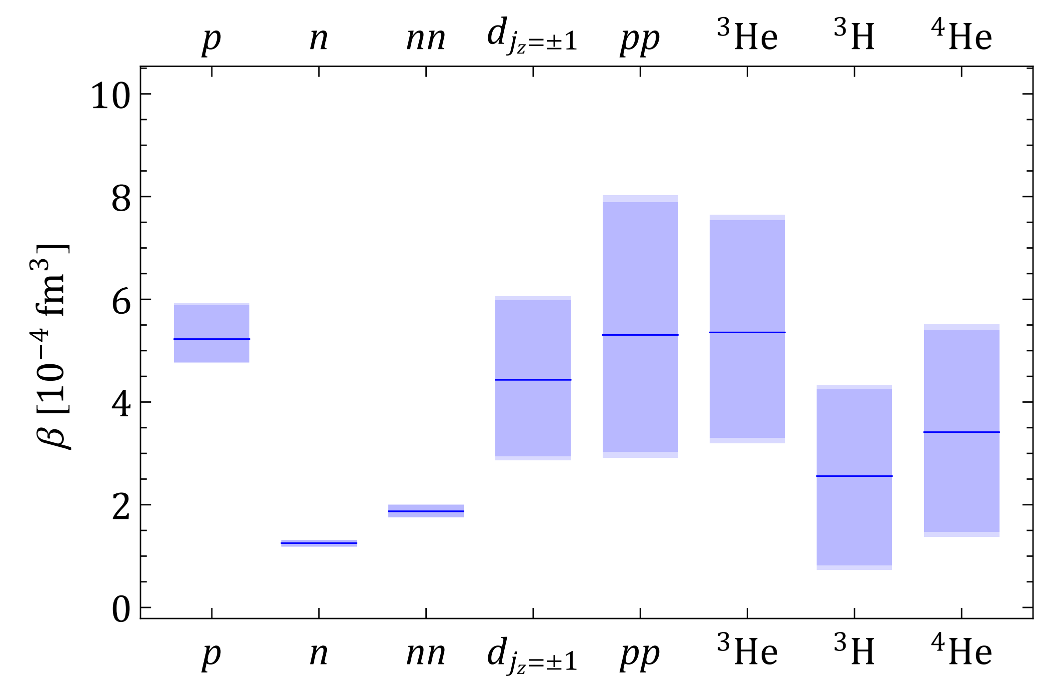
Magnetic polarizability



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Hamiltonian as a function of a variable parameter

$$\hat{H}(\lambda) = \hat{H} + \lambda \hat{V}$$

Energy eigenvalue

$$\frac{\mathrm{d}E_n}{\mathrm{d}\lambda} = \frac{\langle \psi_n | \frac{\mathrm{d}\hat{H}}{\mathrm{d}\lambda} | \psi_n \rangle}{\langle \psi_n | \psi_n \rangle}$$

Energy eigenstate

Example: sigma term

$$m_q \frac{\partial m_N}{\partial m_q}\bigg|_{m_q = m_q^{\mathrm{phy}}} = \langle \mathcal{N} | m_q \bar{q} q | \mathcal{N} \rangle$$

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Generalization to correlation functions

$$C_\lambda(t) = \langle \lambda | \mathcal{O}(t) \mathcal{O}^\dagger(0) | \lambda \rangle = \frac{1}{\mathcal{Z}_\lambda} \int D\Phi e^{-S-S_\lambda} \mathcal{O}(t) \mathcal{O}^\dagger(0)$$

Just a 2pt function

$$S_\lambda = \lambda \int d^4x j(x)$$

Integrated matrix element

$$-\frac{\partial C_\lambda(t)}{\partial \lambda}\bigg|_{\lambda=0} = -C(t) \int dt' \langle \Omega | \mathcal{J}(t') | \Omega \rangle + \int dt' \langle \Omega | T\{\mathcal{O}(t) \mathcal{J}(t') \mathcal{O}^\dagger(0)\} | \Omega \rangle$$

$$\mathcal{J}(t) = \int d^3x j(t, \vec{x}).$$

Buochard et al (CALLATT), Phys.Rev.D96,014504(2017).

Example: axial charge of the nucleon and triton!

Since the operator here is a quark bilinear, a clever to implement this is by modifying the quark propagator.

$$S^{(q)}_{\lambda_q;\Gamma}(x,y) = S^{(q)}(x,y) + \lambda_q \int dz\; S^{(q)}(x,z)\Gamma S^{(q)}(z,y)$$

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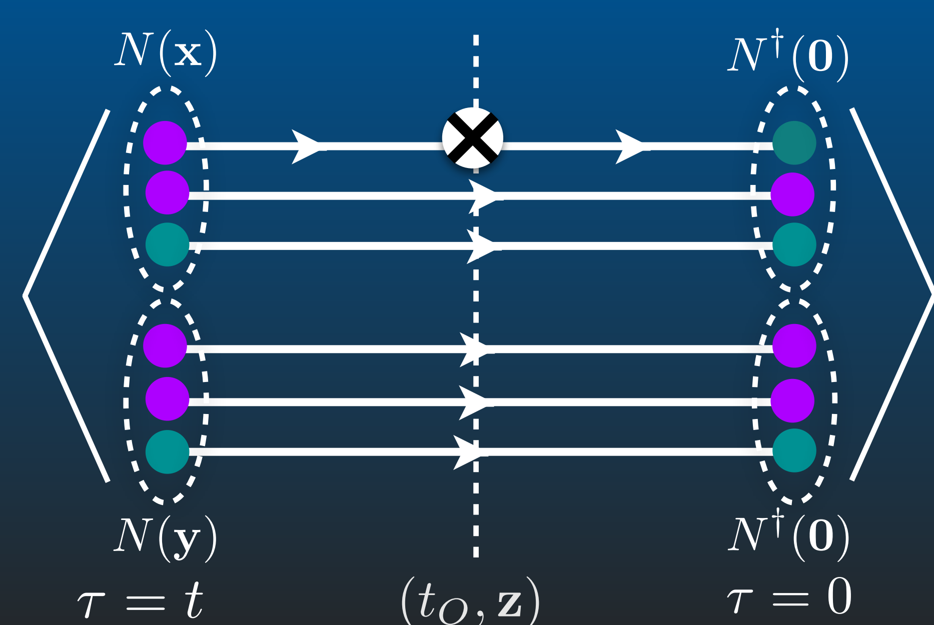
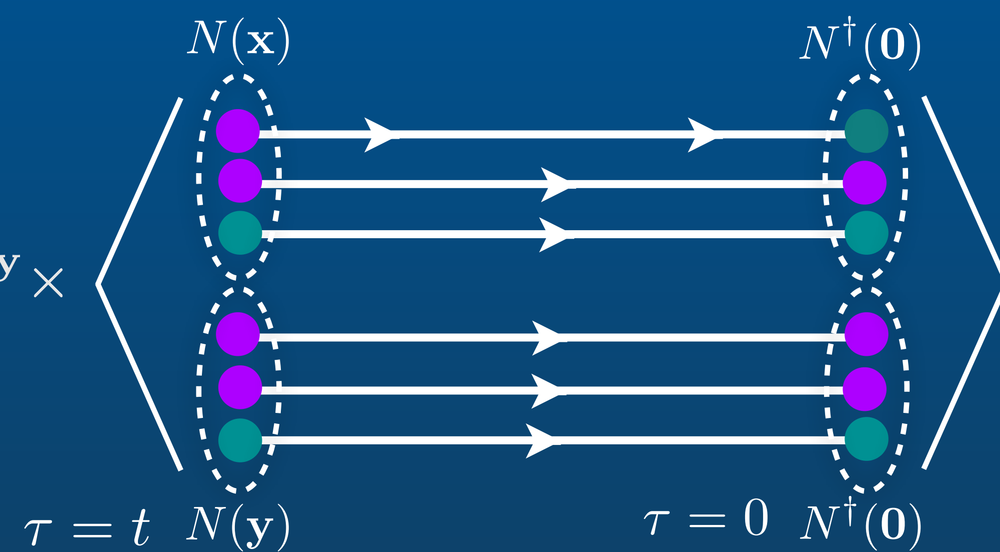
e.g.,

$$C(\mathbf{P};t,t_O) = \sum_{\mathbf{p}_1+\mathbf{p}_2=\mathbf{P}} \sum_{\mathbf{x},\mathbf{y},\mathbf{z}} e^{i\mathbf{p}_1\cdot\mathbf{x}+i\mathbf{p}_2\cdot\mathbf{y}} \times$$

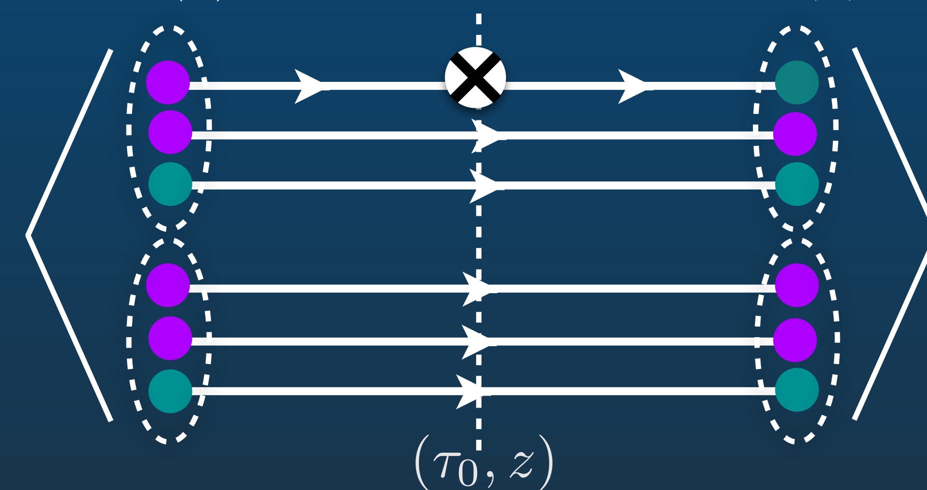


This gives more generally:

$$C_\lambda(\mathbf{P}; t, t_O) = \sum_{\mathbf{p}_1+\mathbf{p}_2=\mathbf{P}} \sum_{\mathbf{x},\mathbf{y},\mathbf{z}} e^{i\mathbf{p}_1\cdot\mathbf{x}+i\mathbf{p}_2\cdot\mathbf{y}} \times$$



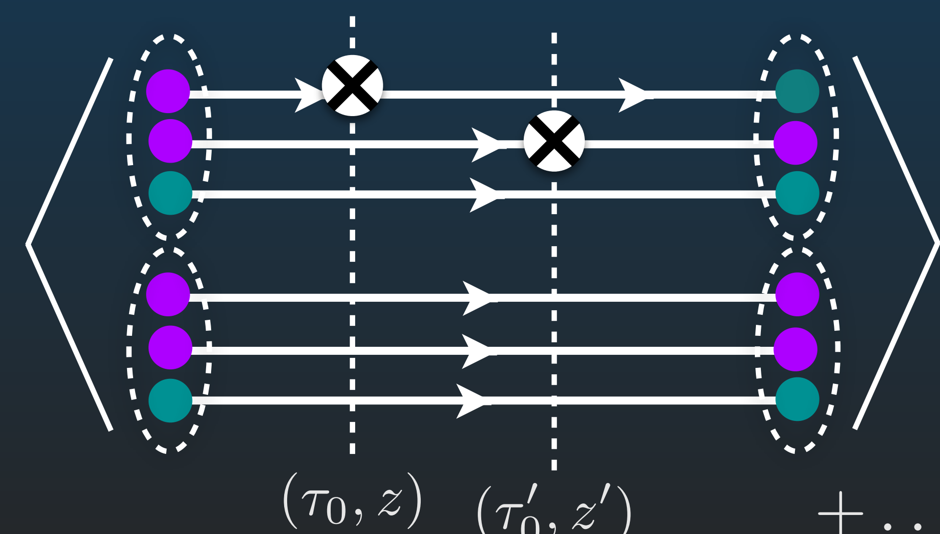
All possibilities $\longrightarrow$ $+\lambda \sum_{\tau_0=0}^{T} \sum_{z}$



time-ordered producT

All possibilities

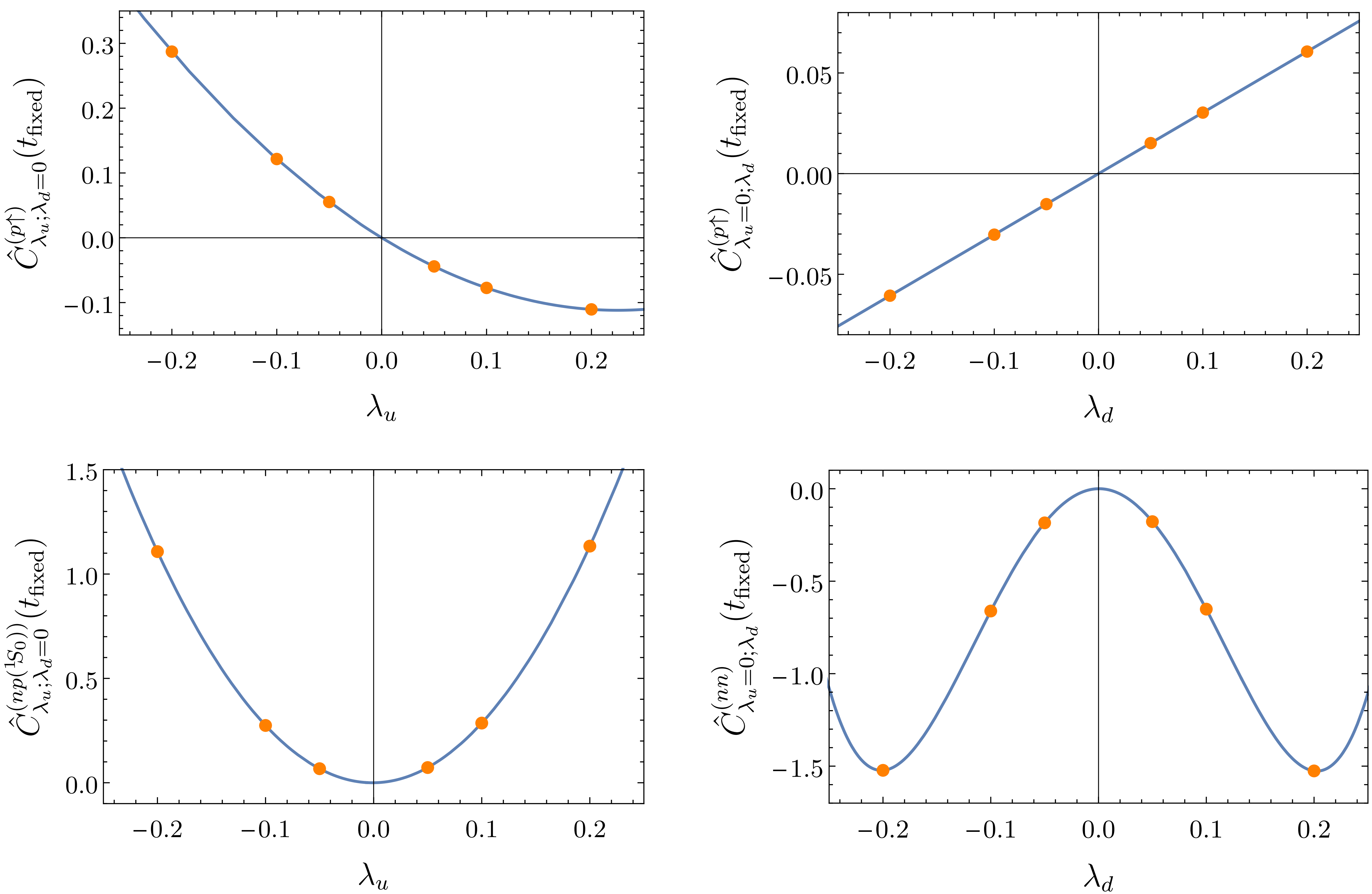
$\longrightarrow$ $+\lambda^2 \sum_{\tau_0=0}^{T} \sum_{\tau_0'=0}^{T} \sum_{z} \sum_{z'}$



$+\ldots$

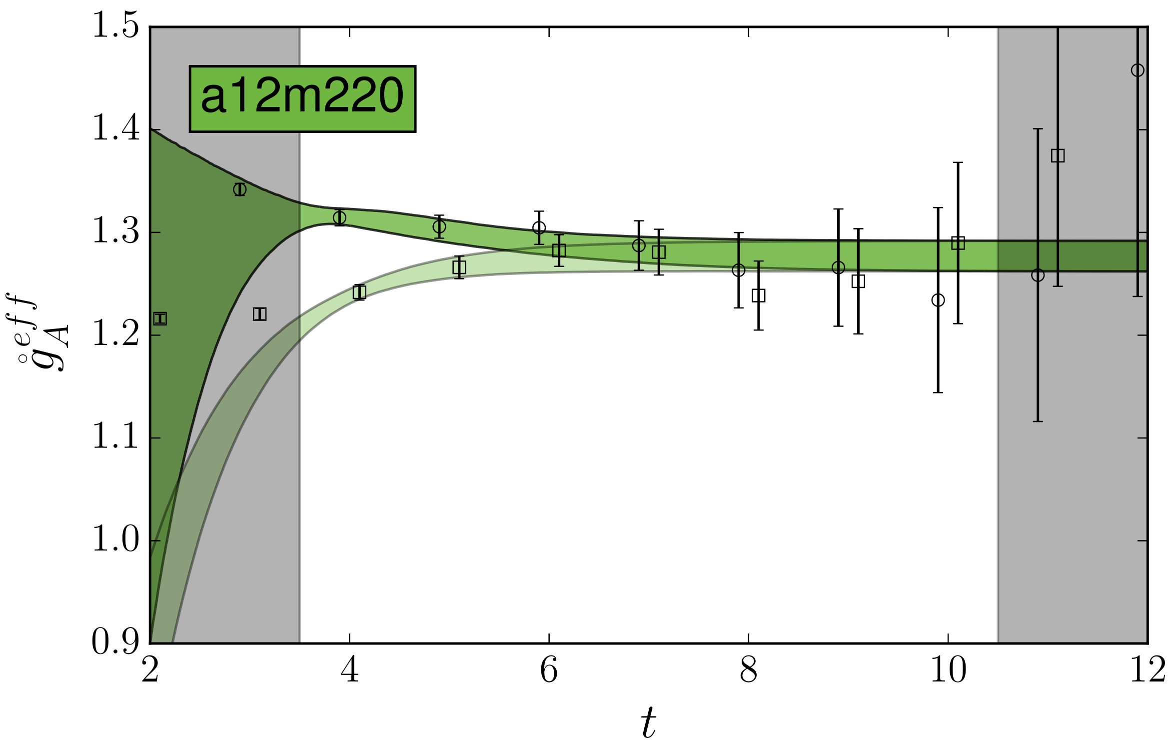
Double-current MEs are exact for isotensor quantities.

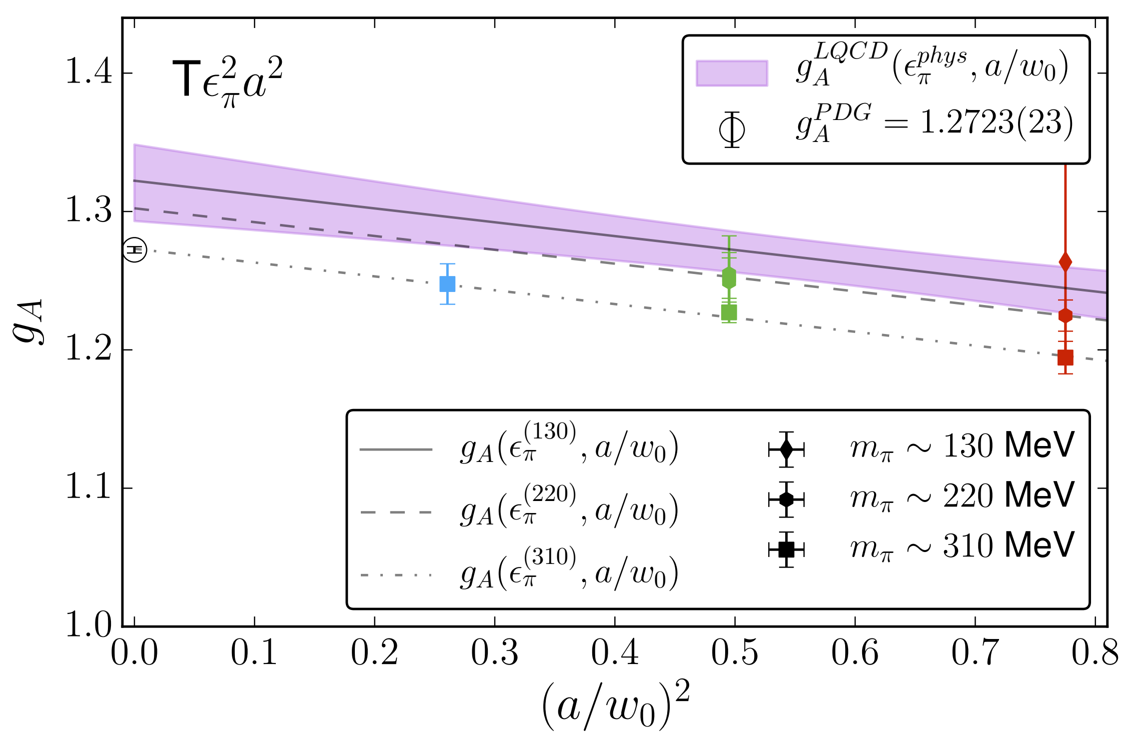
Matrix elements from a compound propagator/background field



Tiburzi et al (NPLQCD), Phys. Rev. D 96, 054505 (2017).

Example of a work using the method:
Axial charge of the nucleon





Chang at al (CALLATT), Nature volume 558, 91–94 (2018).

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We did not discuss many other interesting directions in the field, e.g.,

- Moments of structure functions
- Quasi-PDFs and pseudo-PDFs
- Hadron tensor through inverse transform methods
- GPDs, TMDs, gluonic observables, etc.

LECTURE III: NUCLEAR STRUCTURE, CHALLENGES AND PROGRESS

LECTURE III:
TOWARDS NUCLEAR STRUCTURE FROM LATTICE QCD

Three features make lattice QCD calculations of nuclei hard:

i) The complexity of systems grows rapidly with the number of quarks.

Detmold and Orginos, Phys. Rev. D 87, 114512 (2013).

See also: Detmold and Savage, Phys.Rev.D82 014511 (2010).
Doi and Endres, Comput. Phys. Commun. 184 (2013) 117.

ii) Excitation energies of nuclei are much smaller than the QCD scale.

Beane at al (NPLQCD), Phys.Rev.D79 114502 (2009).
Beane, Detmold, Orginos, Savage, Prog. Part. Nucl. Phys. 66 (2011).
Junnakar and Walker-Loud, Phys.Rev. D87 (2013) 114510.
Briceno, Dudek and Young, Rev. Mod. Phys. 90 025001.

iii) There is a severe signal-to-noise degradation.

Paris (1984) and Lepage (1989).

Wagman and Savage, Phys. Rev. D 96, 114508 (2017).
Wagman and Savage, arXiv:1704.07356 [hep-lat].

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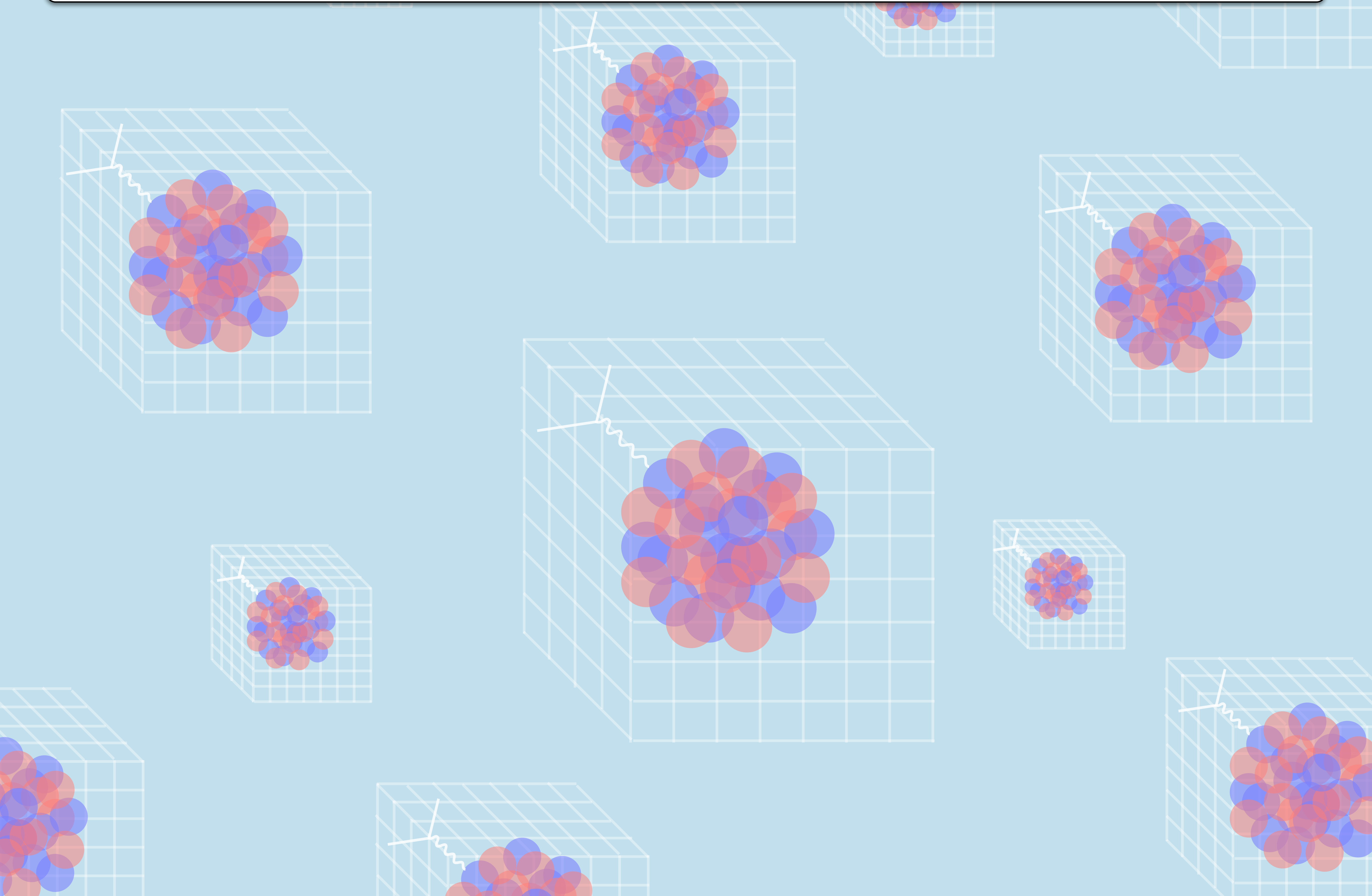

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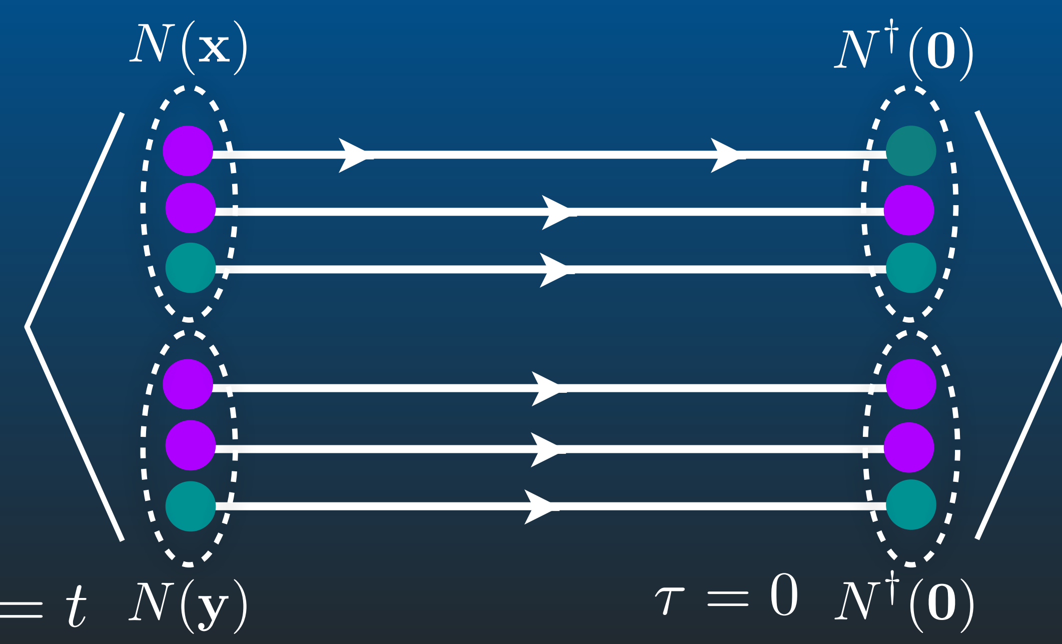

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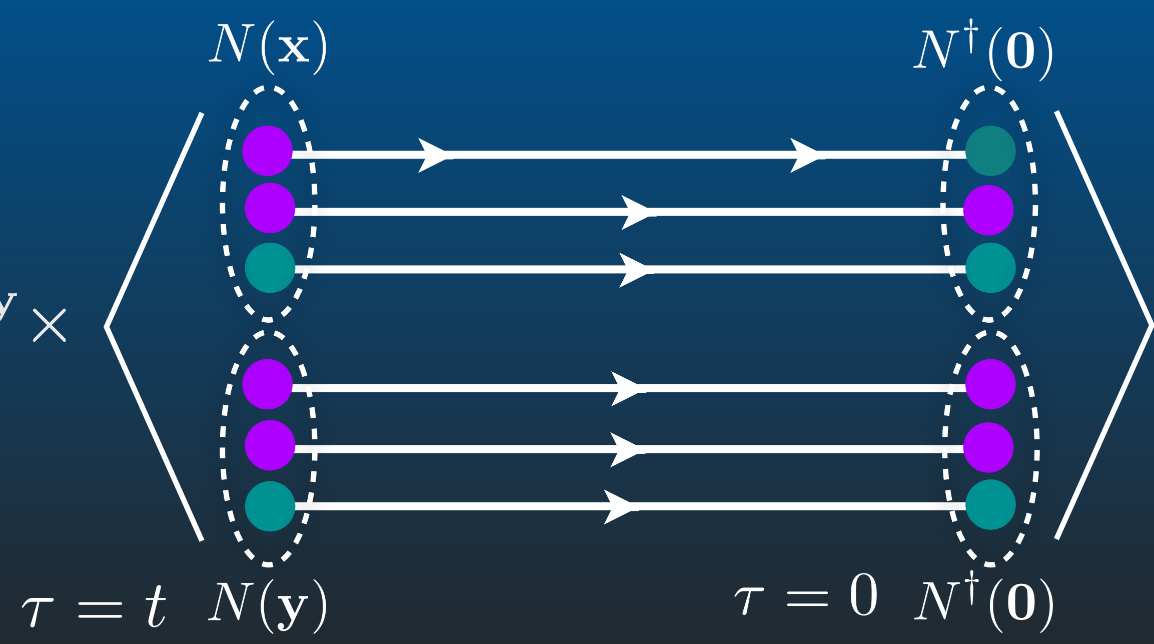

COMPLEXITIES OF QUARK-LEVEL INTERPOLATING FIELDS

COMPLEXITIES OF QUARK CONTRACTIONS

Detmold and Orginos (2013).

Naively the number of quark contractions for a nucleus goes as:

$$(2N_p + N_n)!\,(N_p + 2N_n)!$$

How bad is this?
Example: Consider radium-226 isotope.
the number of contractions required is ~ 10^{1425}

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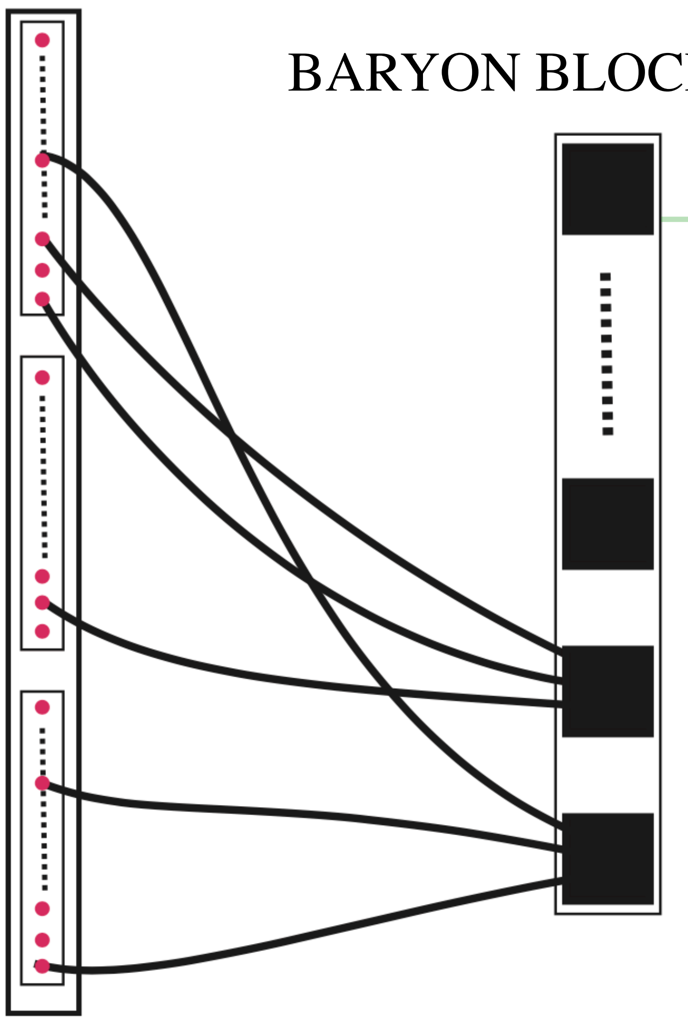
An example of a more efficient algorithm:



BARYON BLOCKS

$$\mathcal{B}_b^{a_1,a_2,a_3}(\mathbf{p},t;x_0) = \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \sum_{k=1}^{N_{B(b)}} \tilde{w}_b^{(c_1,c_2,c_3),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,i_3} S(c_{i_1},x;a_1,x_0) S(c_{i_2},x;a_2,x_0) S(c_{i_3},x;a_3,x_0)$$

Can also start propagators at different locations.

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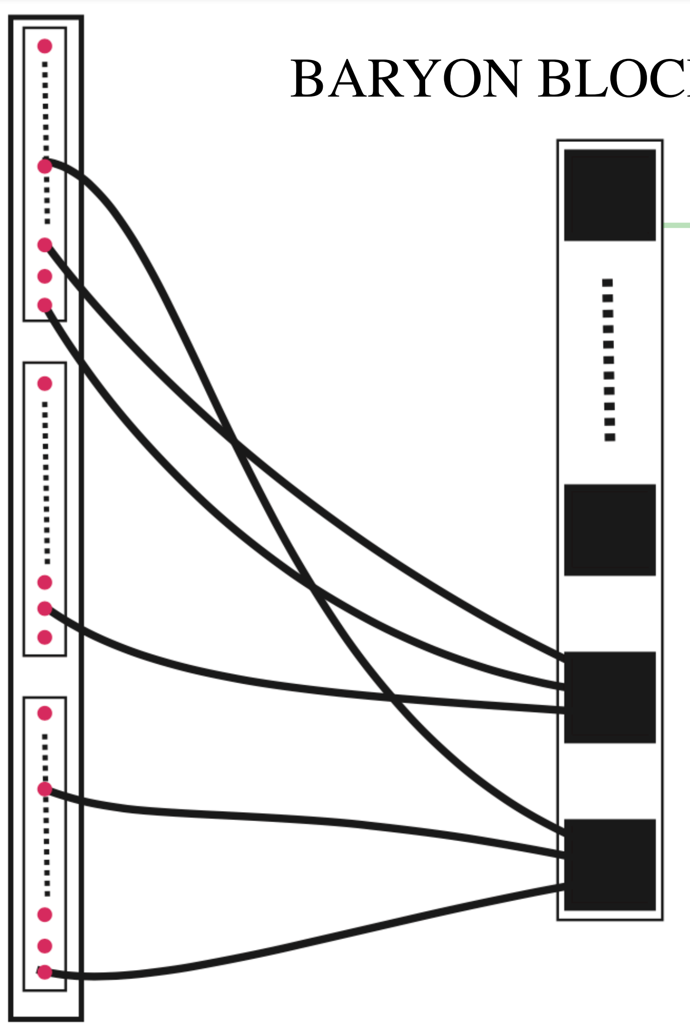

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Can also start propagators at different locations.

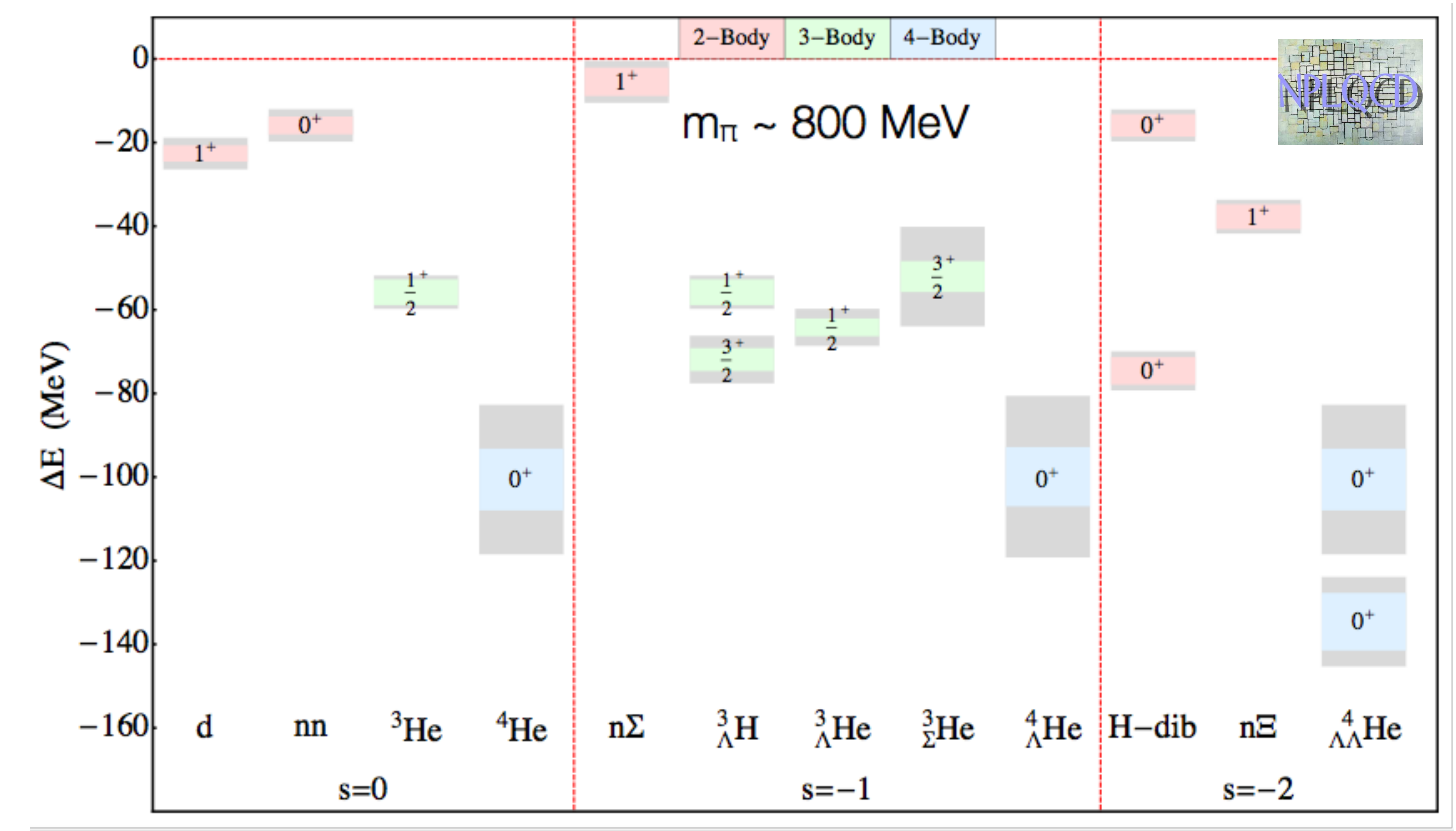
The new scaling is: $M_w \cdot N_w \cdot \dfrac{(3A)!}{(3!)^A}$

Number of terms in the sink

Number of terms in the source

Nuclei obtained from such an approach (at a heavier quark masses)

$N_f = 3,\ m_\pi = 0.806\ \mathrm{GeV},\ a = 0.145(2)\ \mathrm{fm}$

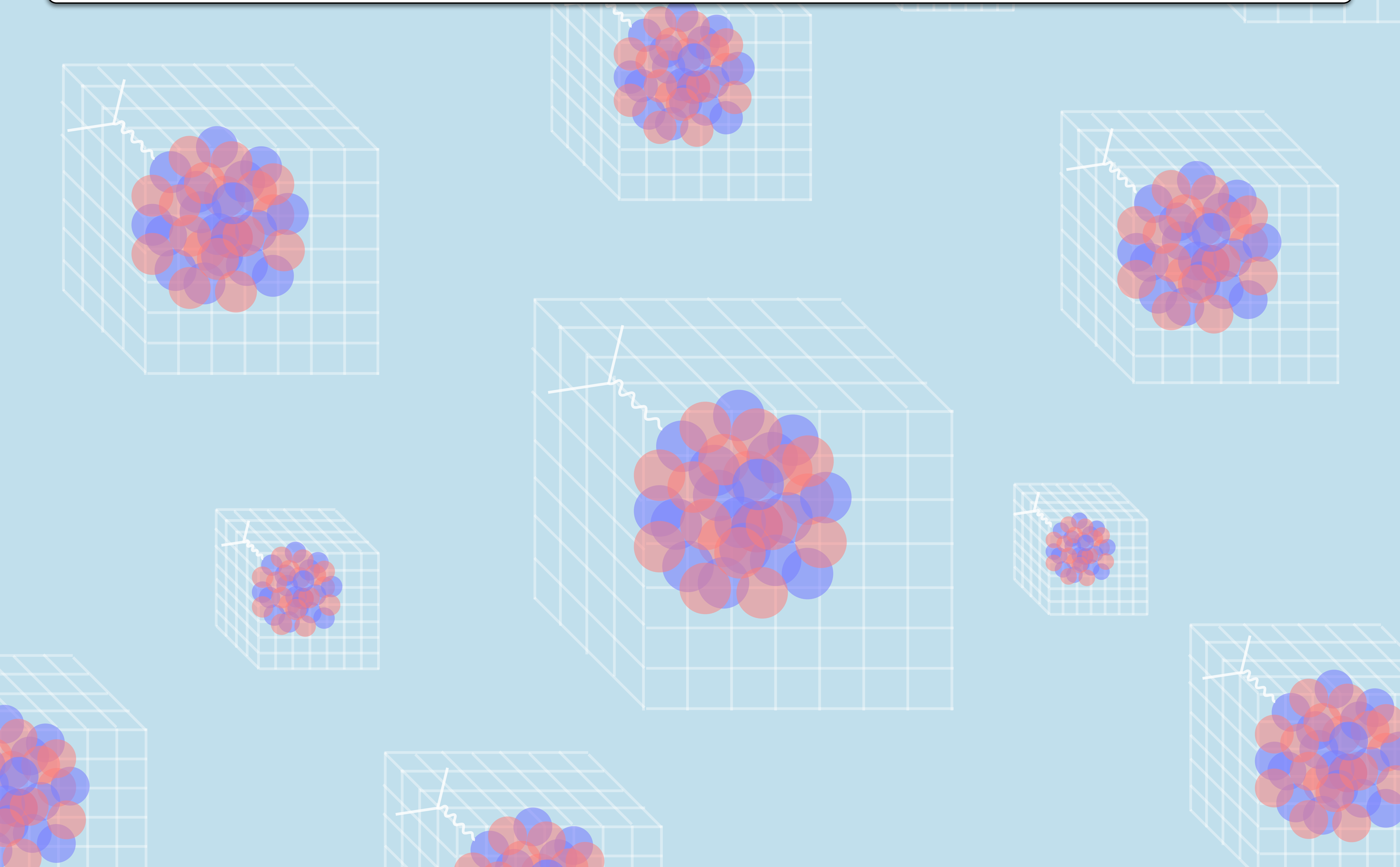


Beane, et al. (NPLQCD), Phys.Rev. D87 (2013) , Phys.Rev. C88 (2013)

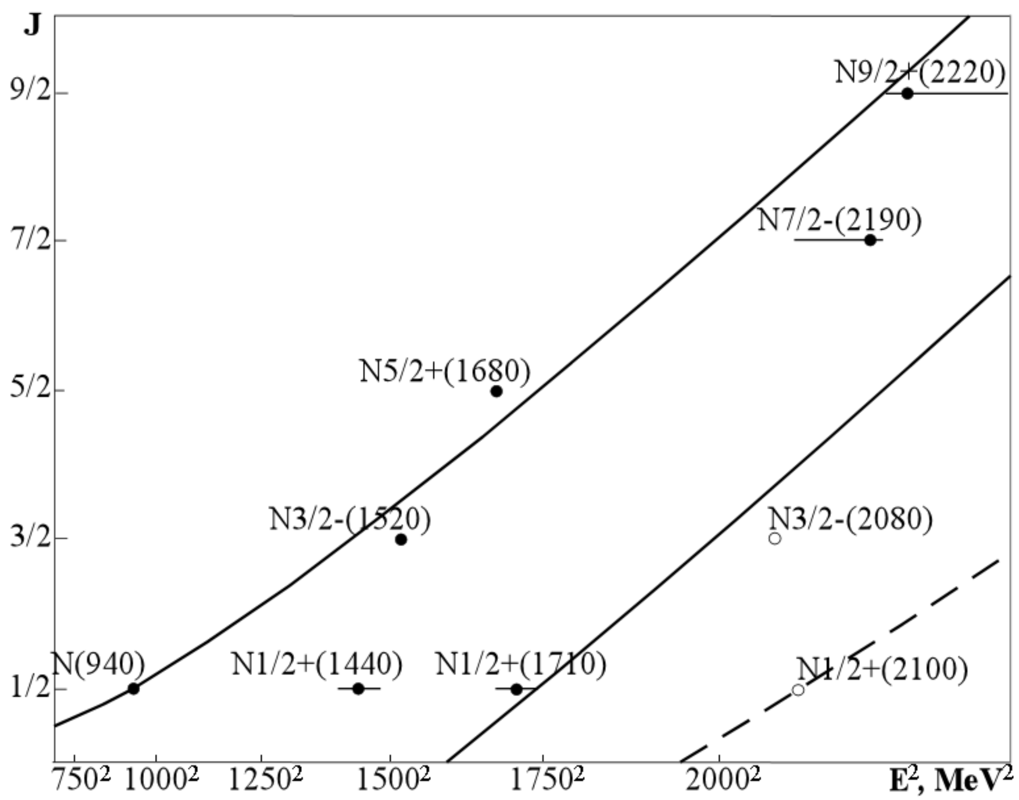
EXERCISE 6

According to the naive counting, how many contractions are required for a nucleus at the source and sink with atomic numbers A = 4, 8, 12, 16? How many contractions are there with the use of the efficient algorithm described?

ii) Excitation energies of nuclei are much smaller than the QCD scale.

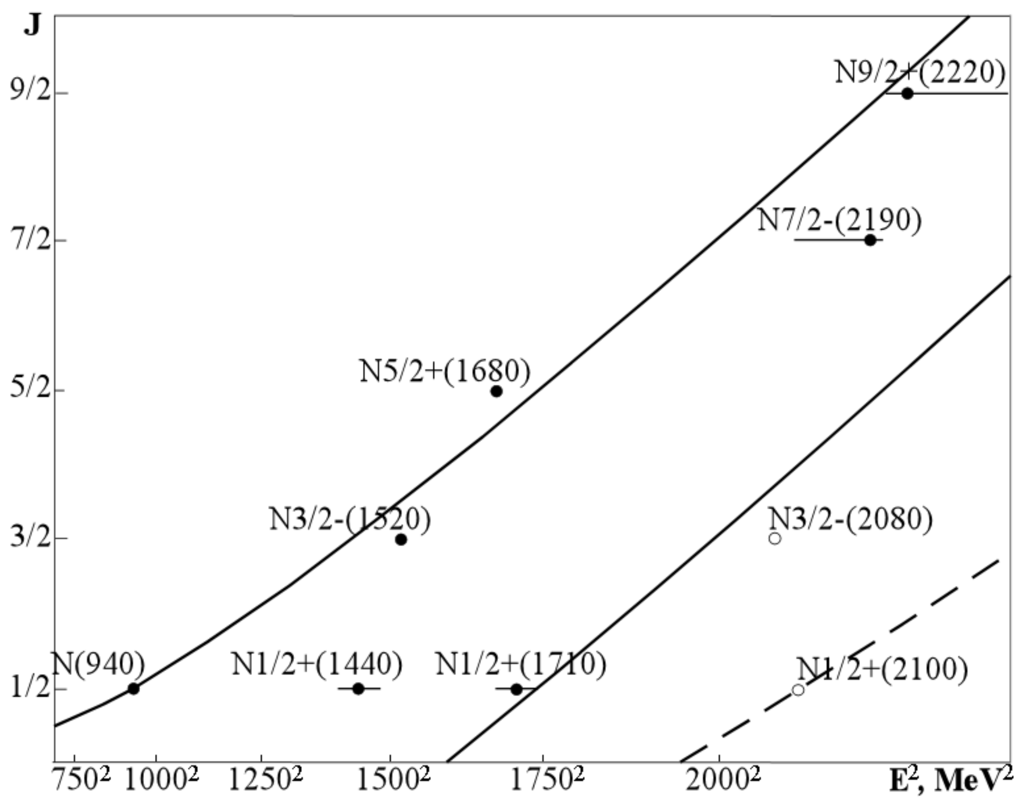


Nucleon excitations



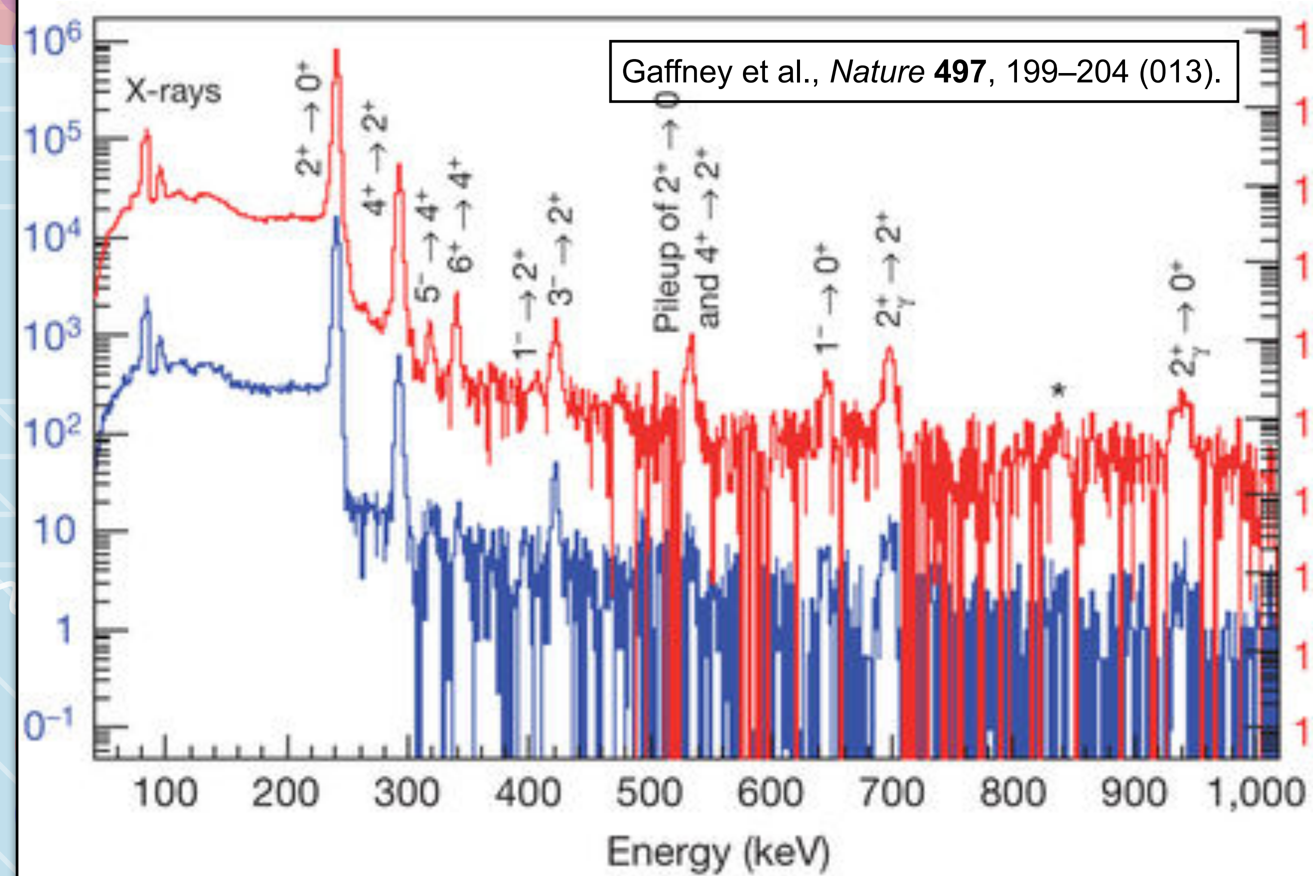
Kulikov, Dmitry A. et al., Central Eur.J.Phys. 11 (2013) .

Nucleon excitations



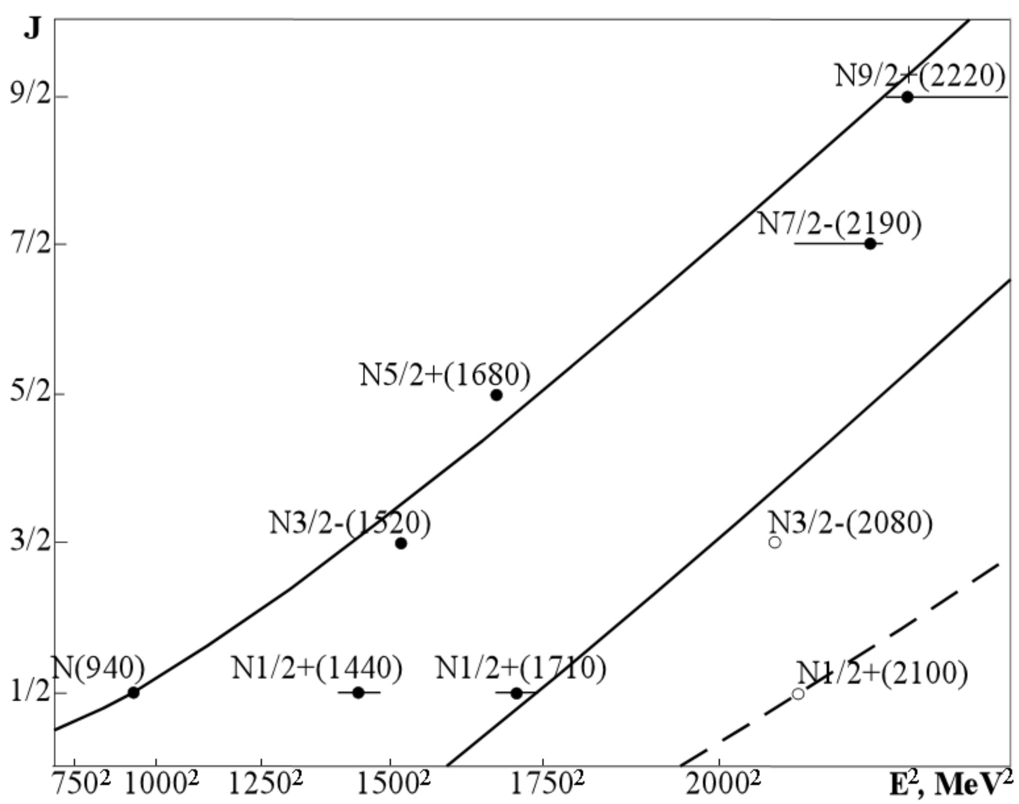
Kulikov, Dmitry A. et al., Central Eur.J.Phys. 11 (2013) .

Nuclear excitations of two pear-shaped nuclei (radium and radon)



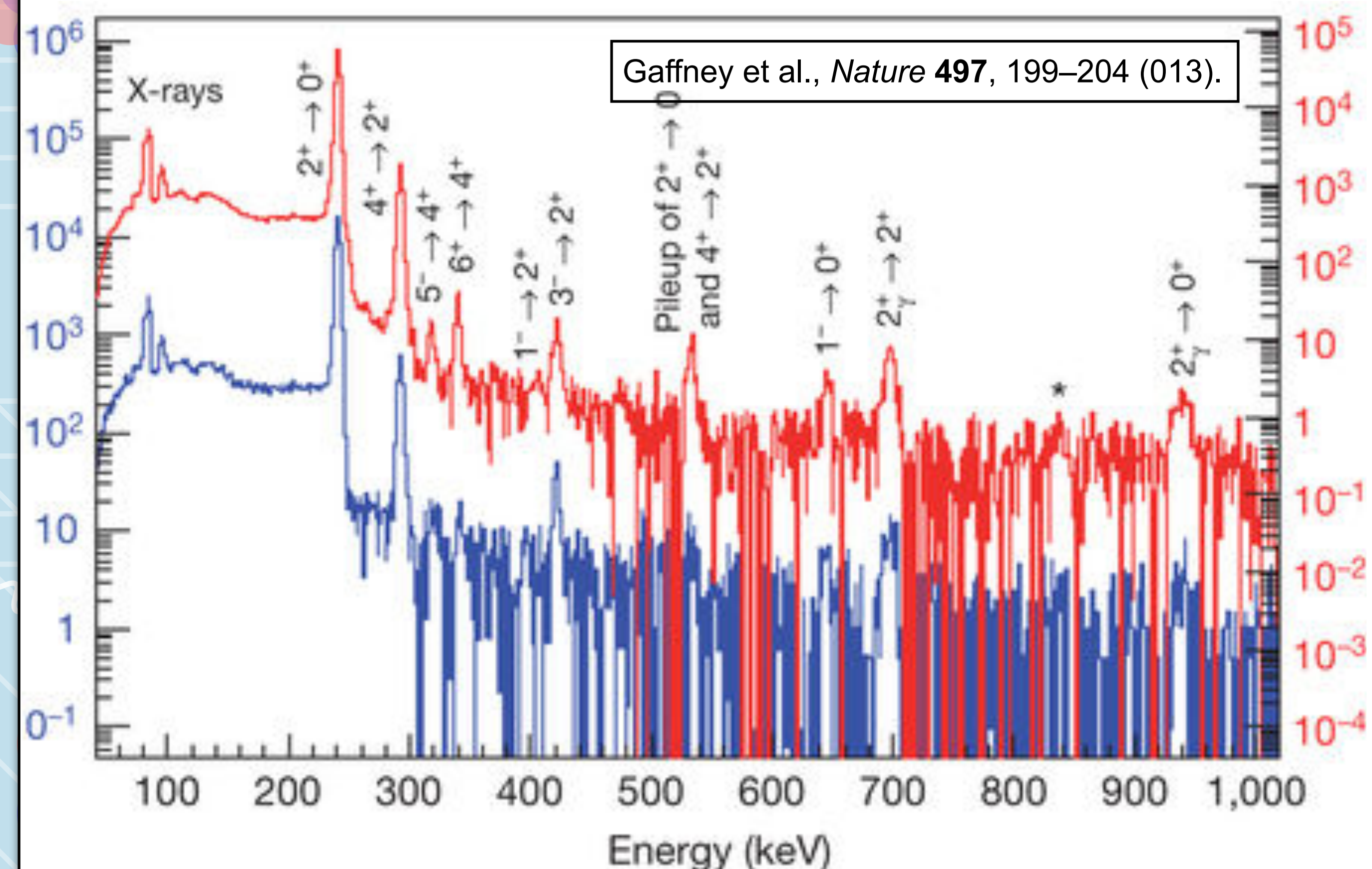
Gaffney et al., *Nature* **497**, 199–204 (013).

Nucleon excitations



Kulikov, Dmitry A. et al., Central Eur.J.Phys. 11 (2013) .

Nuclear excitations of two pear-shaped nuclei (radium and radon)



Gaffney et al., *Nature* **497**, 199–204 (013).

Getting radium directly from QCD will remain challenging for a long time! One should first compute A = 2, 3, 4 systems well. This is till not that easy: *B_d* = 2 MeV!

EXERCISE 7

With a given amount of computational resources, you have achieved a 1% statistical uncertainty on the extracted mass of the nucleon from your lattice QCD calculation. By what factor should you increase your computing resources (your statistics) to also achieve a 1% statistical uncertainty on the binding energy of the deuteron?

So what to do?

- With the most naive operators with similar overlaps to all states, unreasonably large times are needed to resolve nuclear energy gaps.

- The key to success of this program is in the use of good interpolating operators for nuclei. Since nuclei are bound states, interpolating operators with good overlap to compact states in a volume are desired.

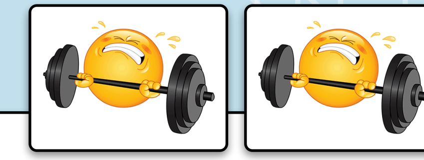
- Ideally need to use a large set of operators for a variational analysis, but this has remained too costly in nuclear calculations, and only recently possible.

Applications in mesonic sector: Briceno, Dudek, and Young, Rev. Mod. Phys. 90 025001.

- Methods such as matrix Prony that eliminate the excited states in linear combinations of interpolators or correlations functions have shown to be useful.

A good review: Beane, Detmold, Orginos, Savage, Prog. Part. Nucl. Phys. 66 (2011).

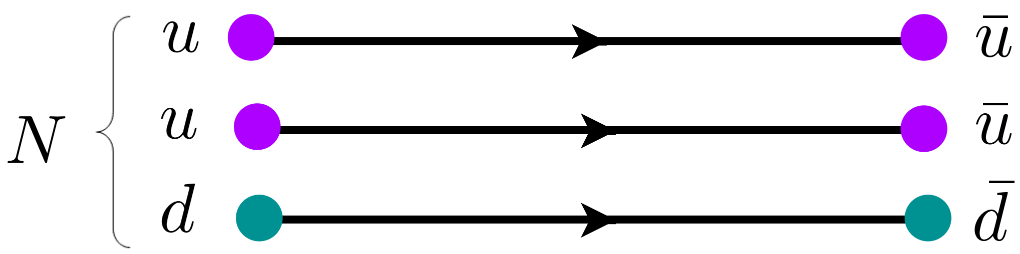
EXERCISE 8



Consider a simple two-state model in the spectral decomposition of a Euclidean two-point function. Demonstrate that the time scale to reach the ground state of the model with a finite statistical precision can depend highly on the corresponding overlap factor for the state. It is sufficient to show this numerically and for a set of chosen energies and overlap factors.

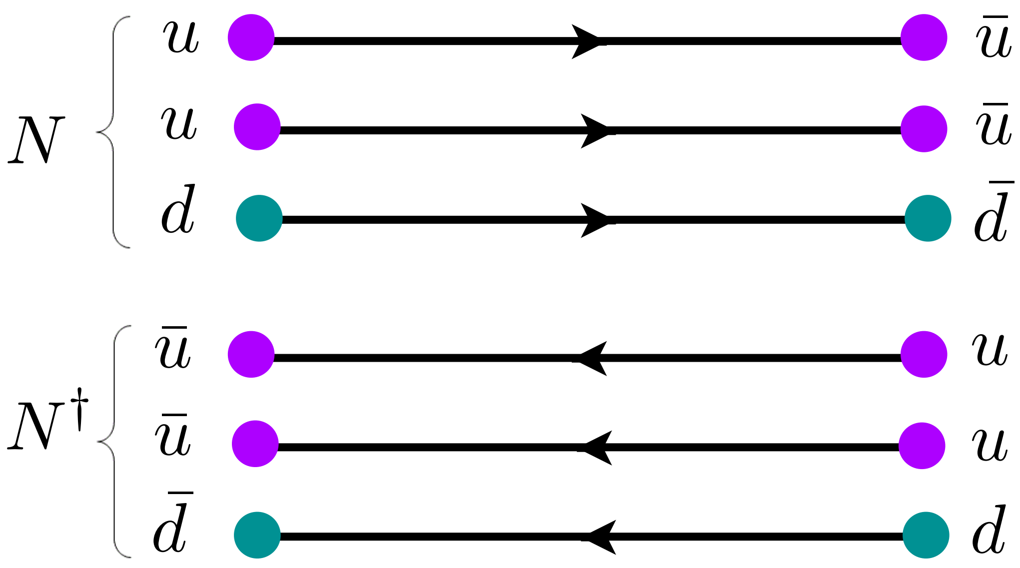
iii) There is a severe signal-to-noise degradation.

The origin of noise



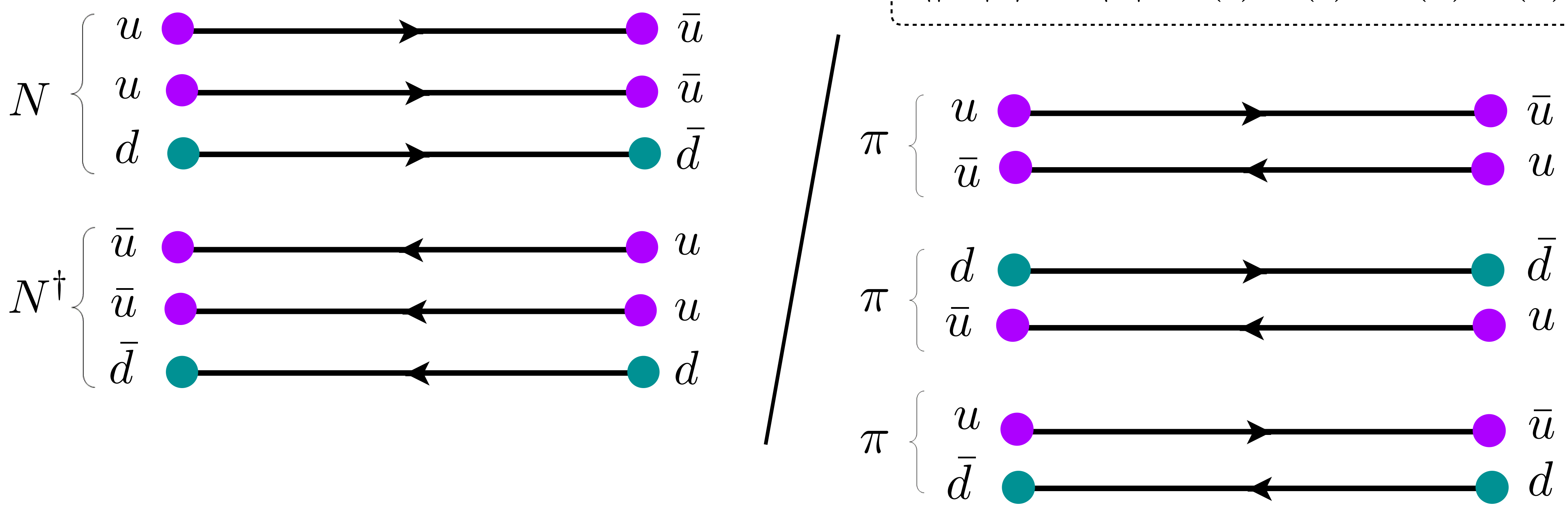
The origin of noise

$$\langle |C|^2 \rangle = \langle 0 | N^\dagger(t) N(t) N^\dagger(0) N(0) | 0 \rangle$$



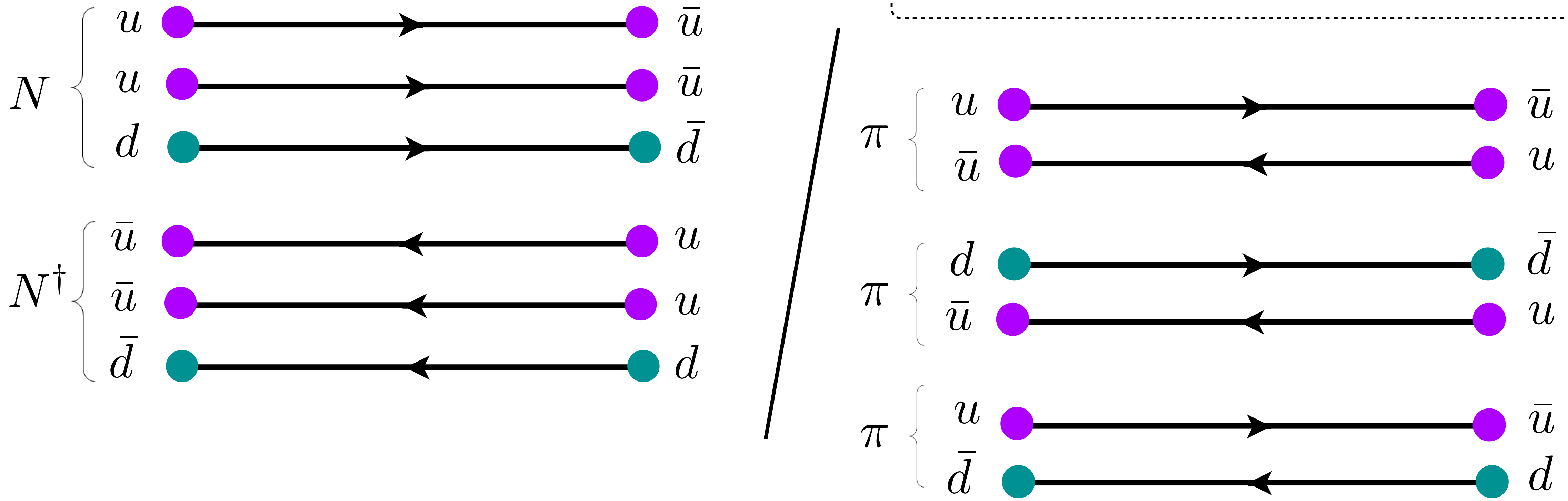
The origin of noise

$$\langle |C|^2 \rangle = \langle 0 | N^\dagger(t) N(t) N^\dagger(0) N(0) | 0 \rangle$$



The origin of noise

$$\langle |C|^2 \rangle = \langle 0 | N^\dagger(t) N(t) N^\dagger(0) N(0) | 0 \rangle$$

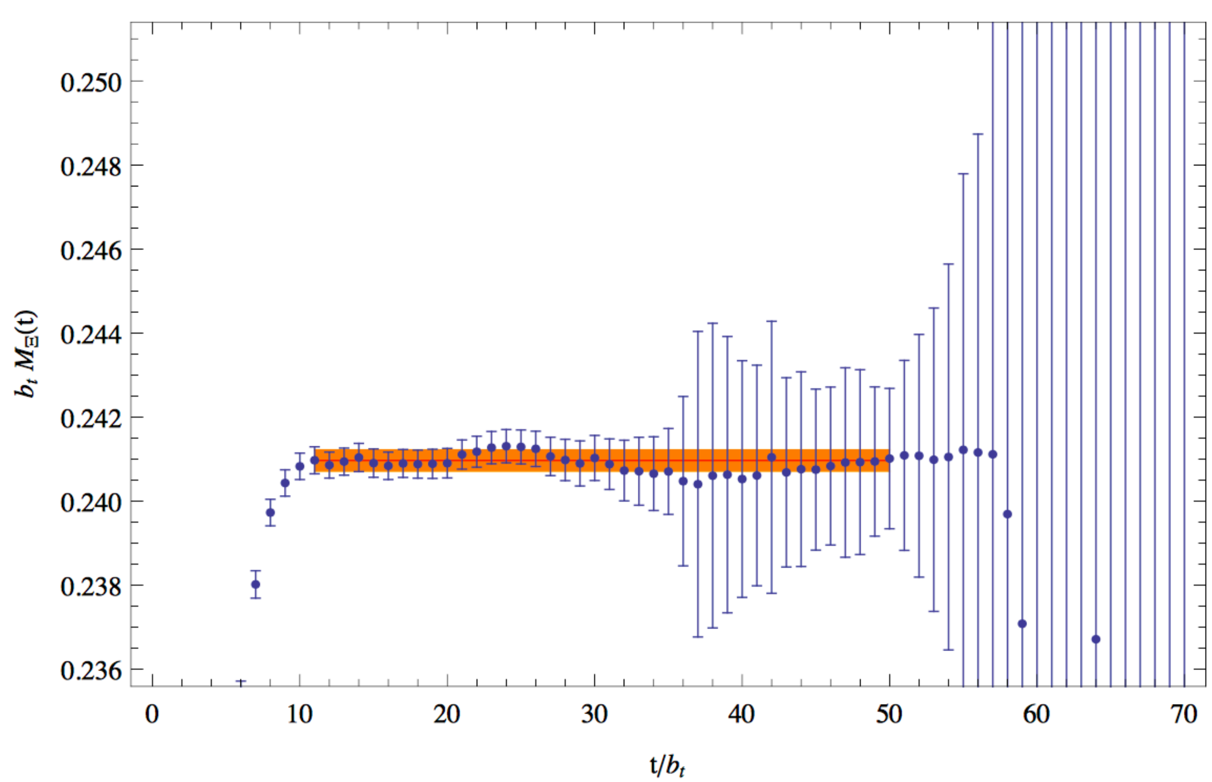


The ground-state of the variance correlator is three pions and not two nucleons:

$$\mathrm{StN}(C_i) \sim \frac{\langle C_i \rangle}{\sqrt{\langle |C_i|^2 \rangle}} \sim e^{-(M_N - \frac{3}{2} m_\pi)t}.$$

Parisi (1984) and Lepage (1989).

Wagman and Savage (2016,2017).

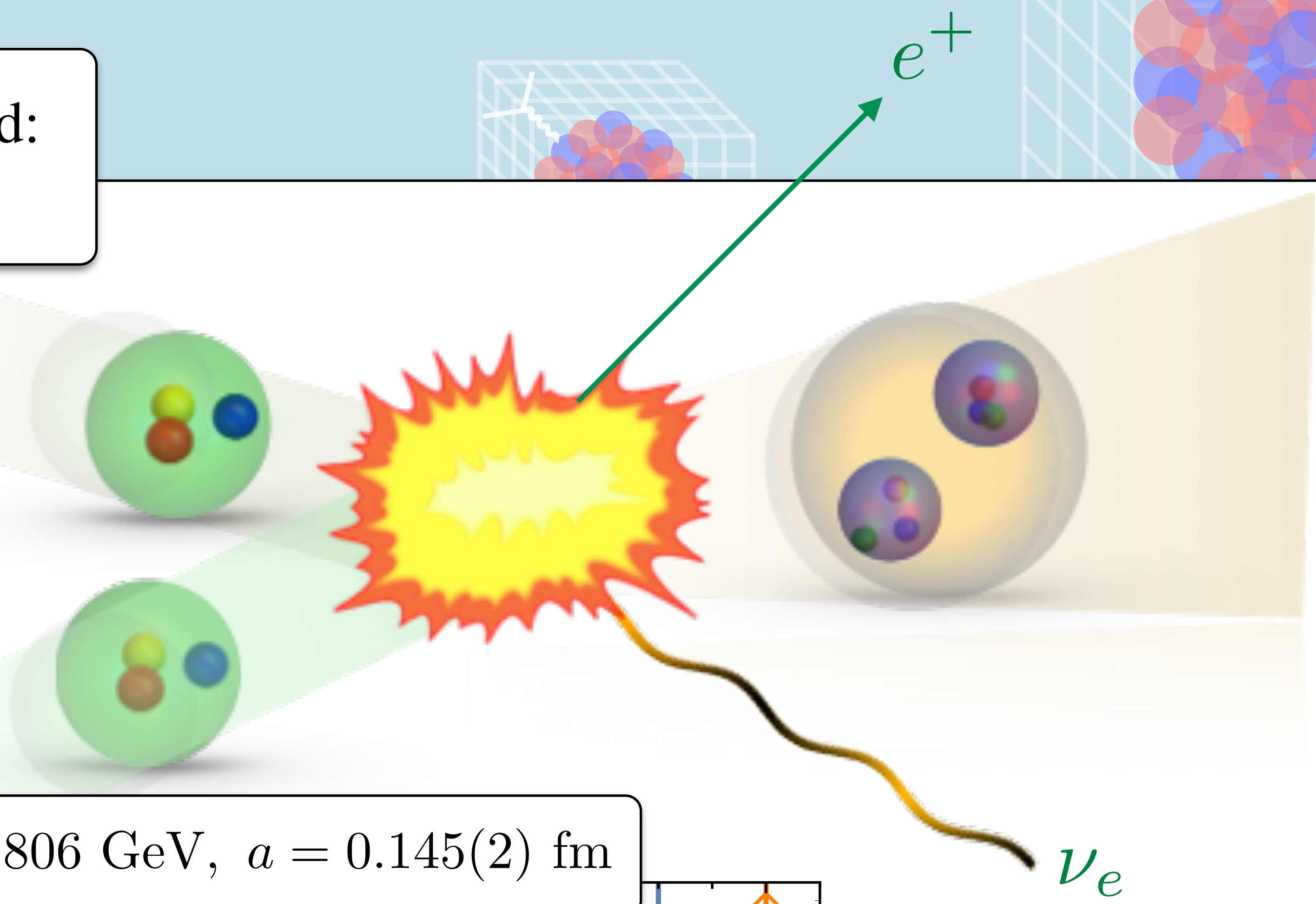


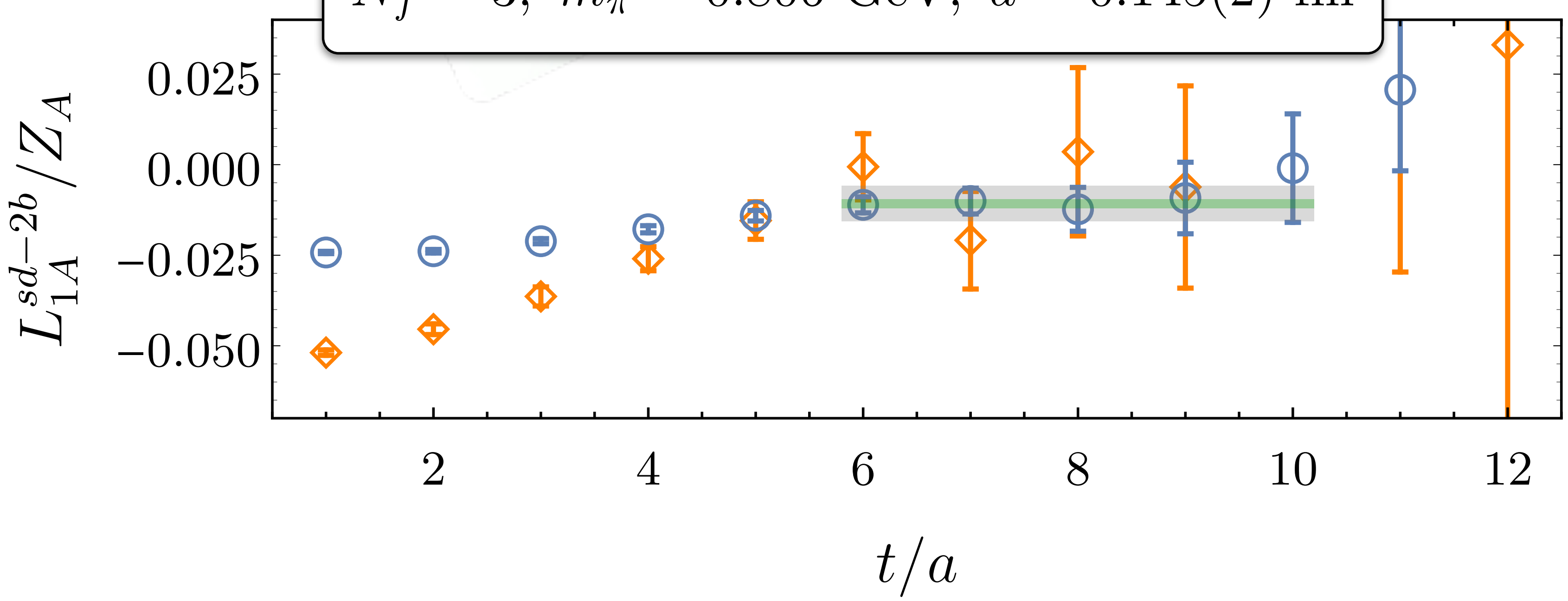
Despite these challenges, efficient algorithms and new computational and analysis strategies have allowed studies of small nuclei from lattice QCD, albeit yet at unphysical quark masses, but the progress continues…

Let us go through several example of the success of lattice in nuclear structure studies…

Application of Feynman-Hellmann method:
pp fusion $p + p \to d + e^+ + \nu_e$

Savage et al (NPLQCD), Phys. Rev. Lett. 119, 062002 (2017).

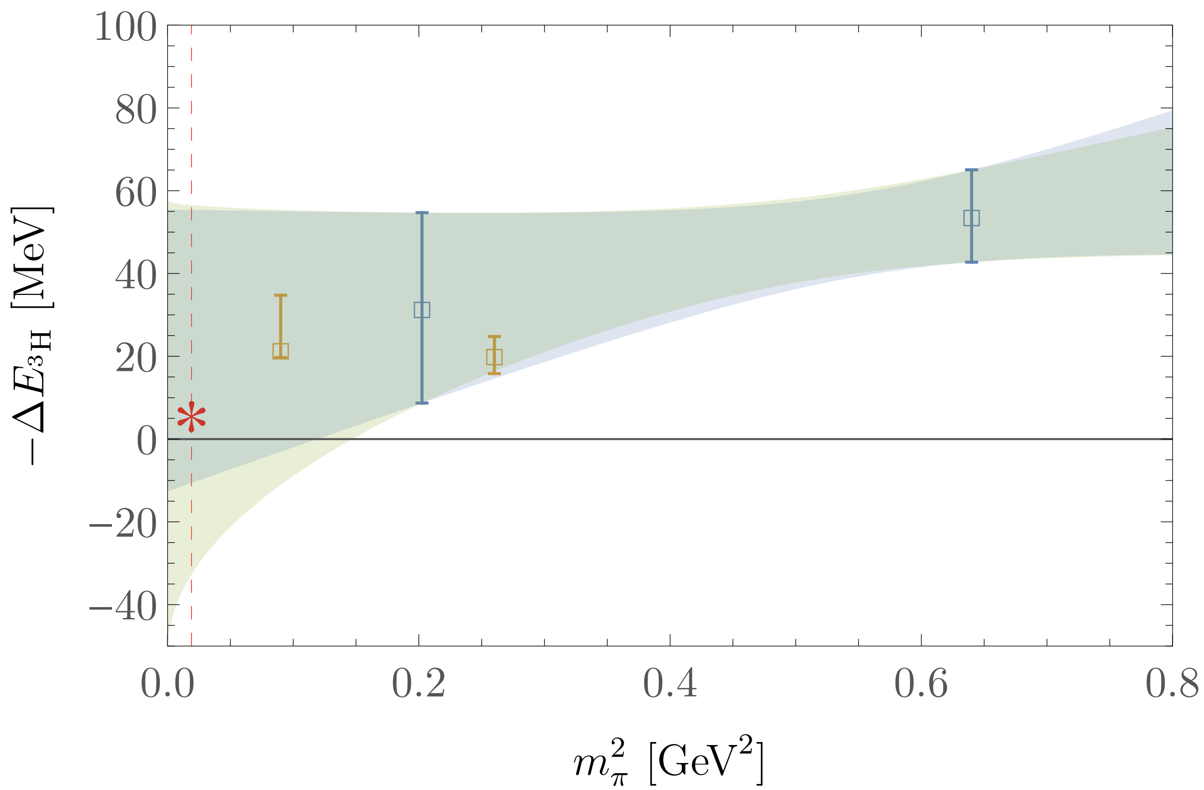


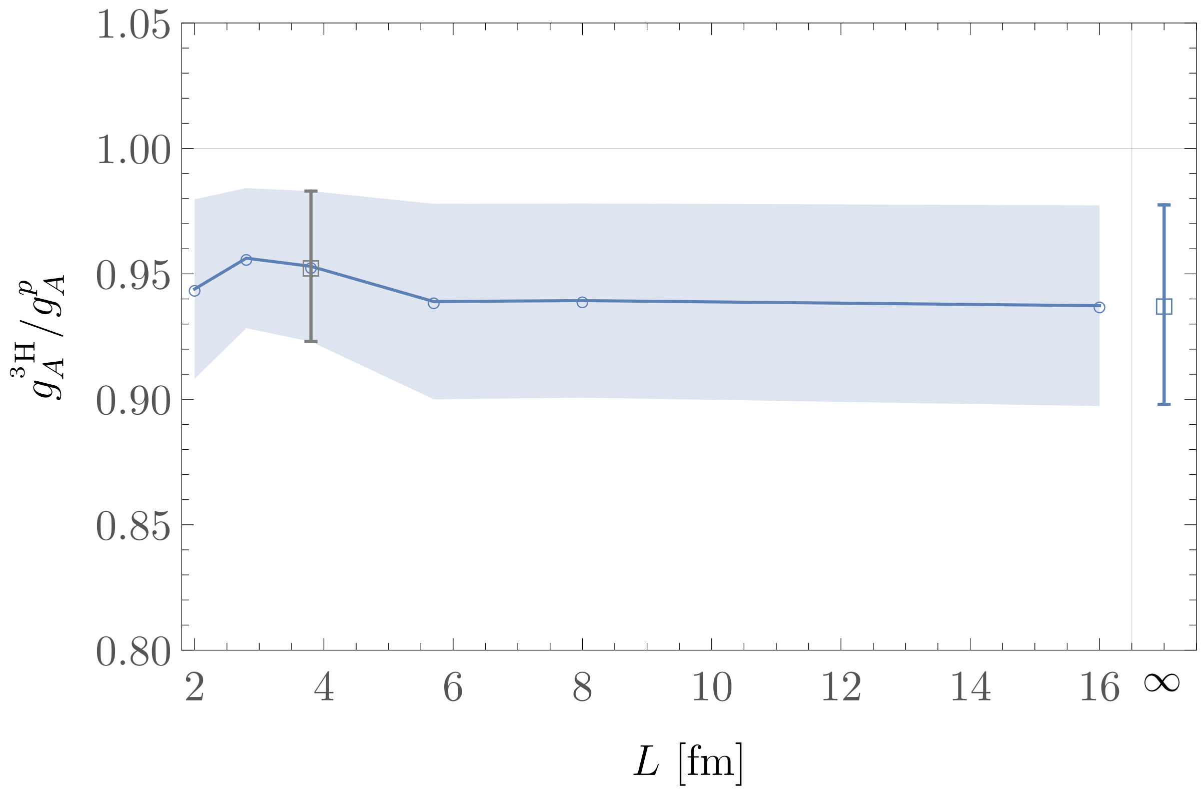


$L_{1,A} \approx 3.9(0.2)(1.0)(0.4)(0.9)\ \text{fm}^3$ @ $\mu = m_\pi^{\text{phys.}} = 140$ MeV

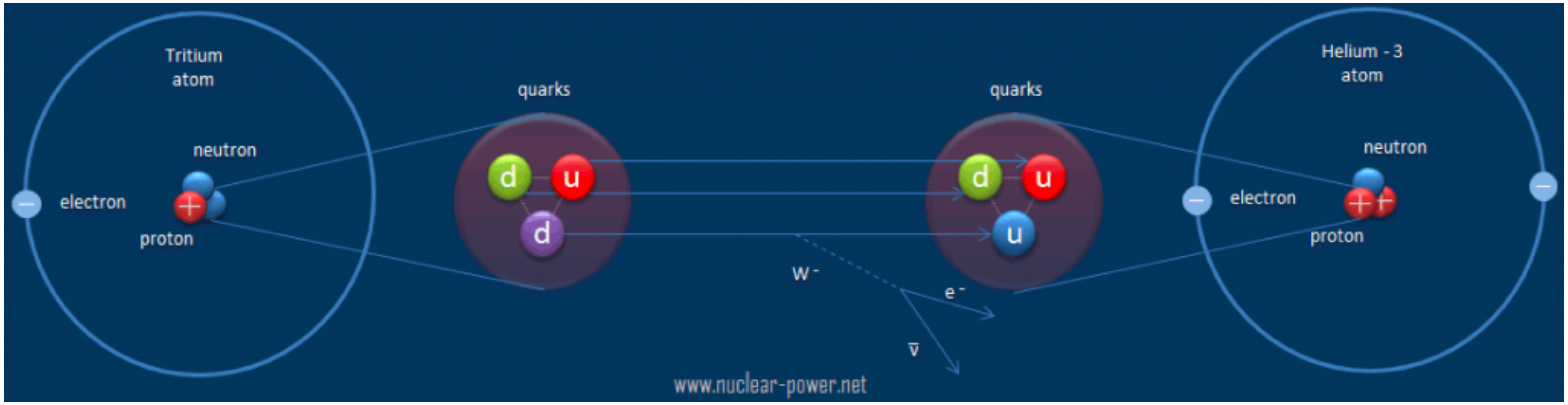
Application of Feynman-Hellmann method: Tritium beta decay!

$N_f = 3,\ m_\pi = 0.806\ \text{GeV},\ a = 0.145(2)\ \text{fm}$

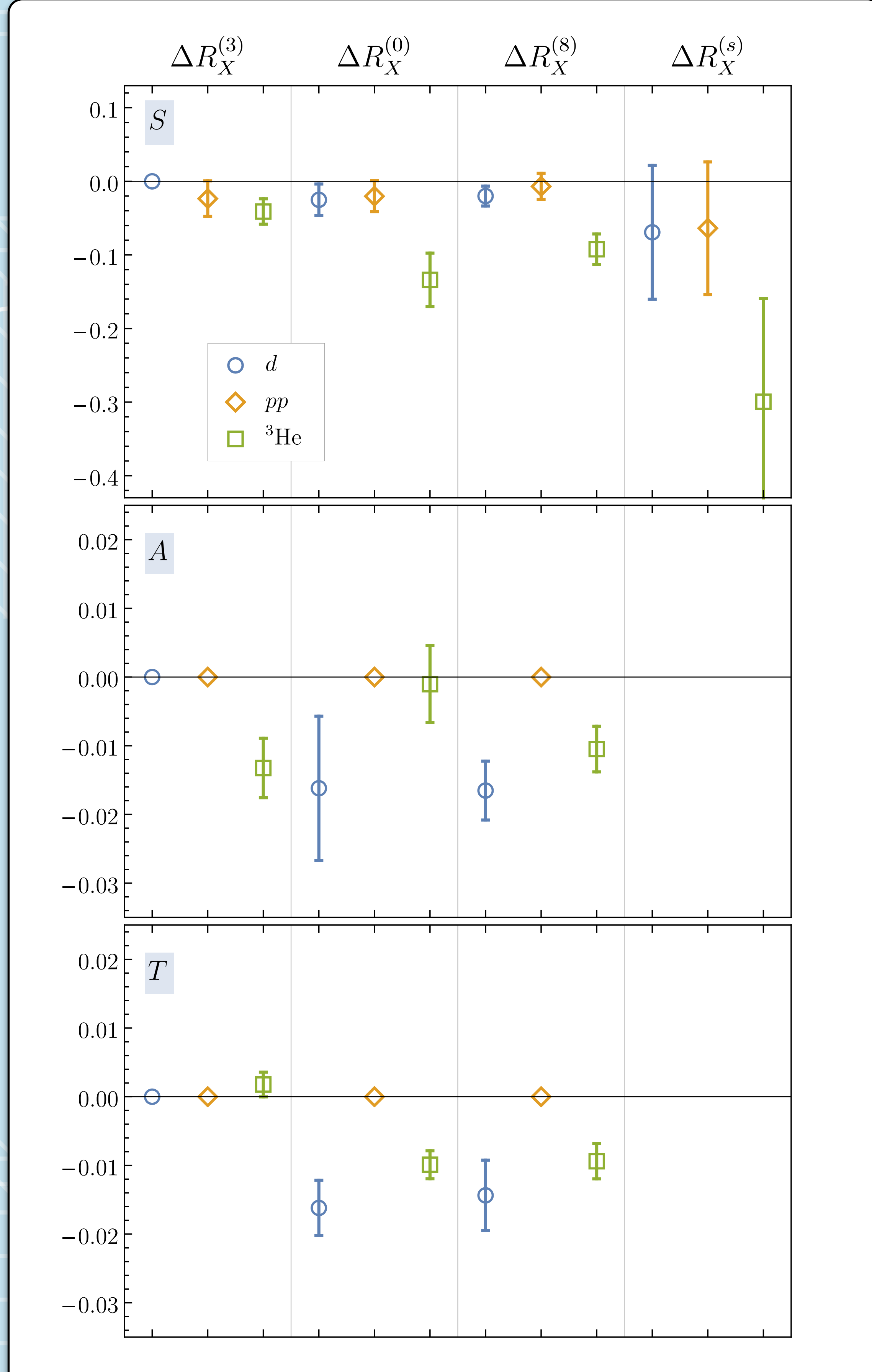




Parreno et al (NPLQCD), Phys. Rev. D 103, 074511 (2021),
Savage et al (NPLQCD), Phys. Rev. Lett. 119,062002(2017).



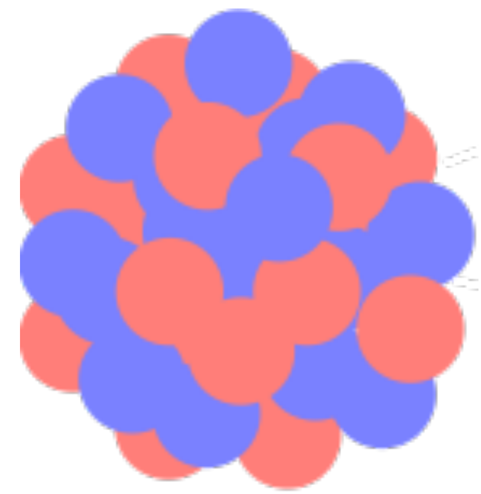
$N_f = 3,\ m_\pi = 0.806\ \text{GeV},\ a = 0.145(2)\ \text{fm}$

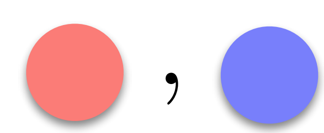


EMC effect from QCD?

How does the distributions of quarks in a nucleon change if bound to a nucleus?

CHANG et al.(NPLQCD), Phys.Rev.Lett. 120 (2018) 15, 152002.

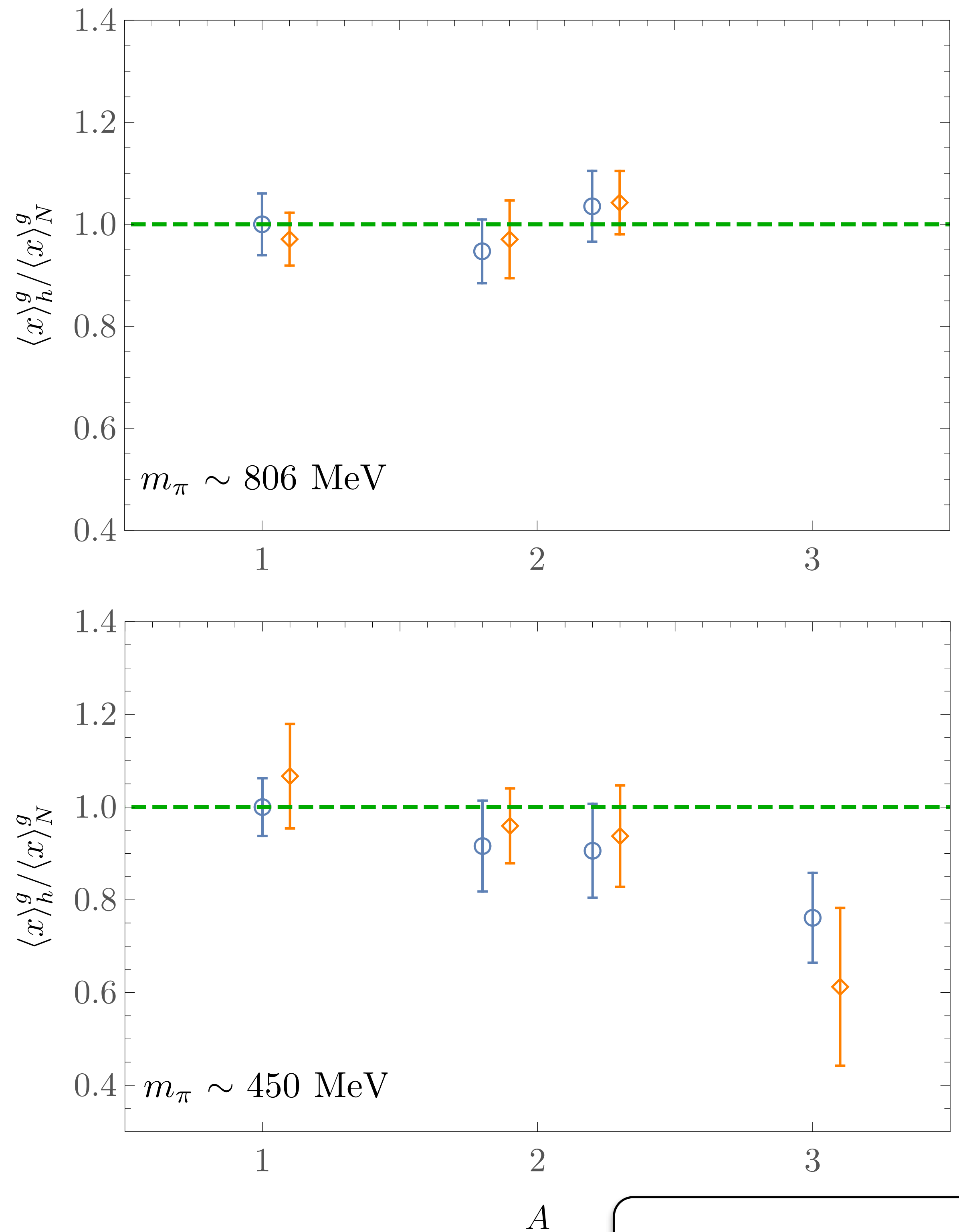


$= \sum$  ?

$$g_X^{(f)}(A) = \langle A|\bar{q}_f \Gamma_X q_f|A\rangle$$

$$R_X^{(f)}(A) = g_X^{(f)}(A)/g_X^{(f)}(p)$$

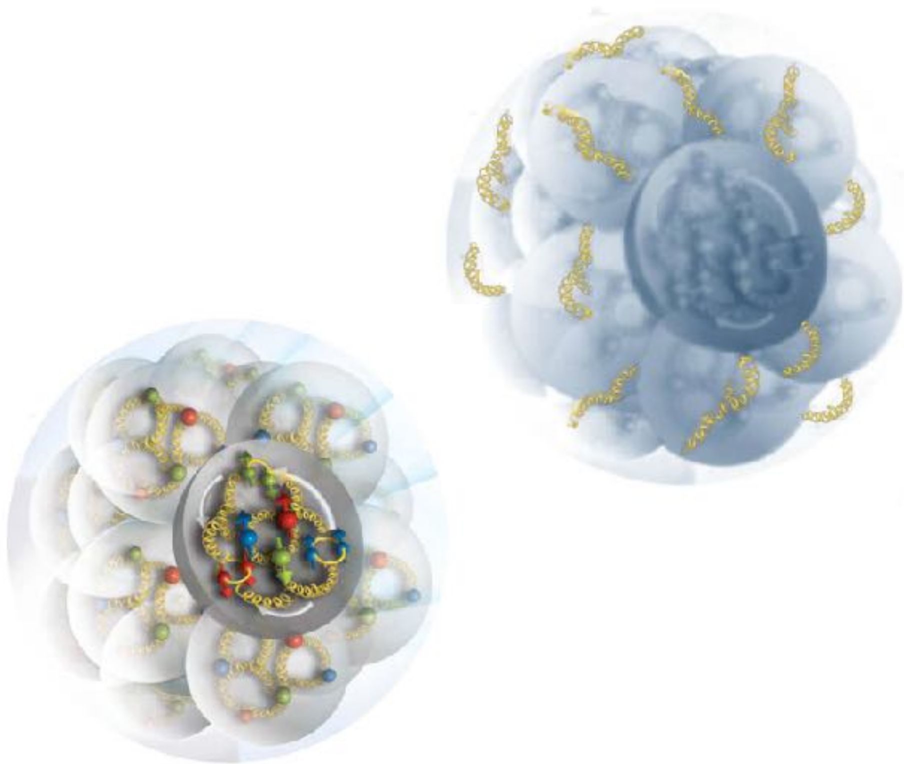
$N_f = 2+1\ , m_\pi \approx 450\ \mathrm{MeV}, a \approx 0.12\ \mathrm{fm}$



A gluonic EMC effect?

How does the distributions of gluons in a nucleon change if bound to a nucleus?

Winter et al.(NPLQCD), Phys.Rev. D96 (2017) 9, 094512



Graphic: EIC white paper (left), P. Shanahan (right)

$$\overline{\mathcal{O}}_{\mu_1\ldots\mu_n}(\mu) = S\left[G_{\mu_1\alpha} i\overleftrightarrow{D}_{\mu_3}\ldots i\overleftrightarrow{D}_{\mu_n} G_{\mu_2}^{\ \alpha}\right]$$

ROADMAP FOR NUCLEAR PHYSICS FROM LATTICE QCD

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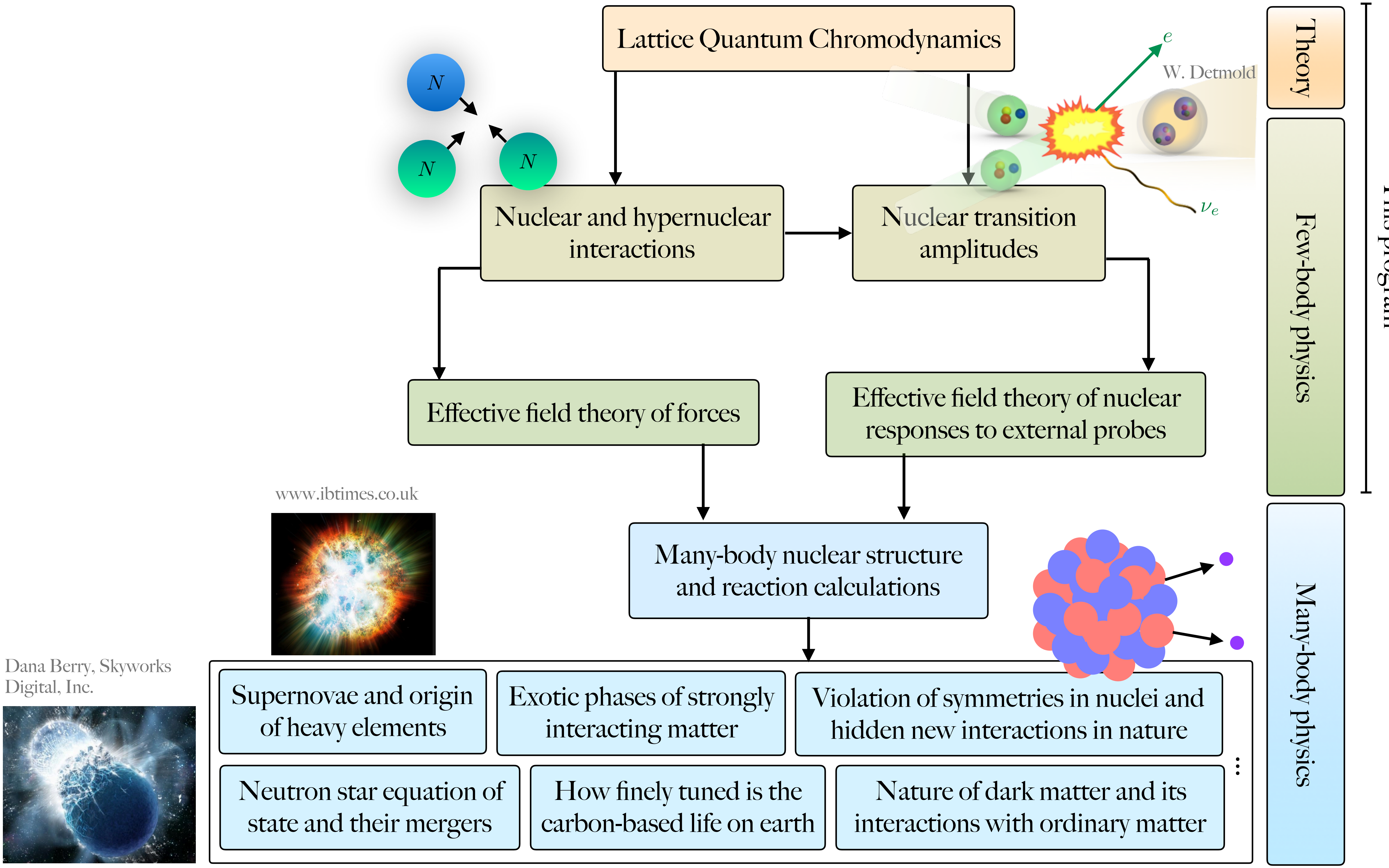
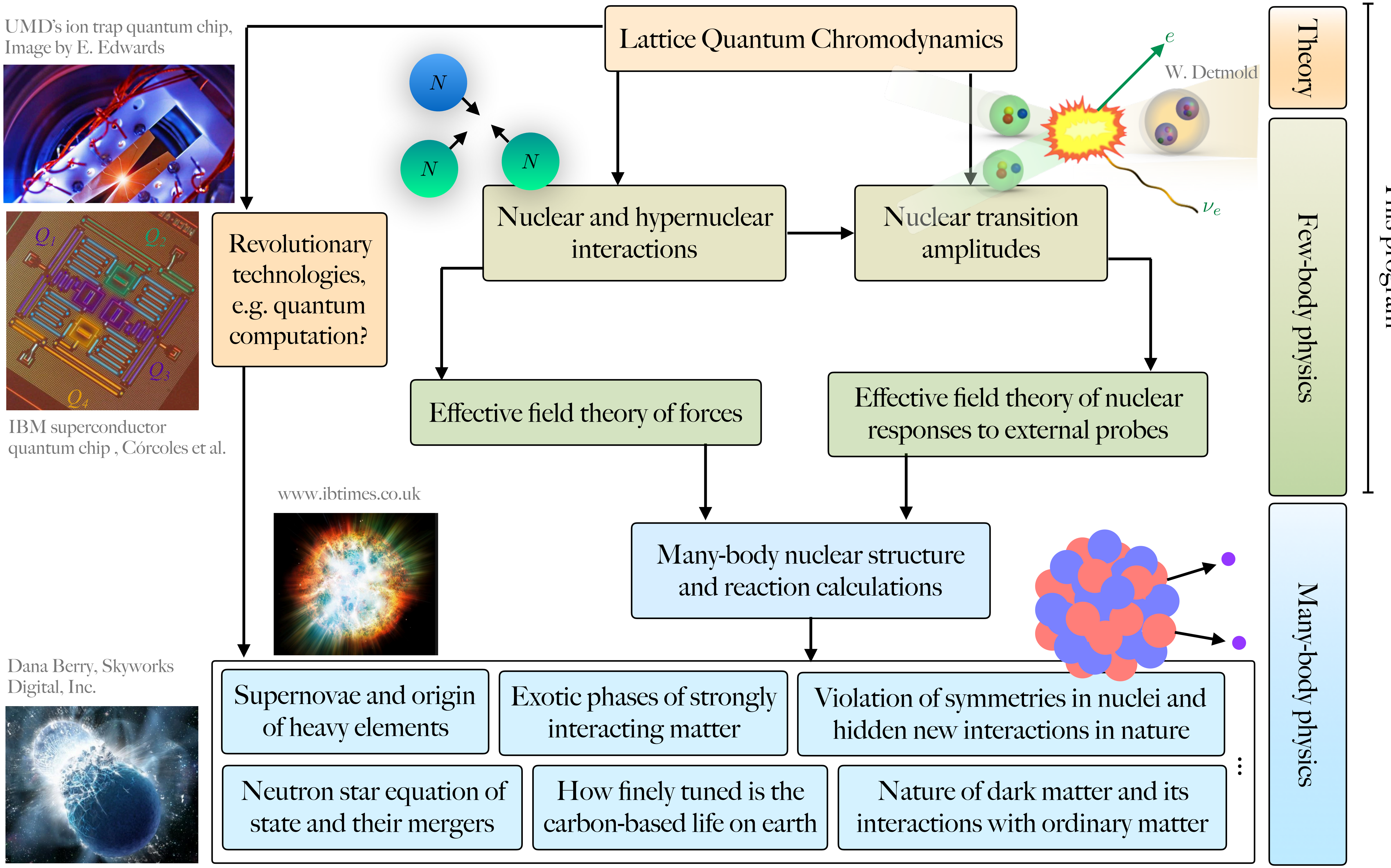


ROADMAP FOR NUCLEAR PHYSICS FROM LATTICE QCD



DESPITE CHALLENGES, GREAT PROGRESS HAS BEEN MADE. LQCD IS ON TRACK TO DELIVER RESULTS ON IMPORTANT QUANTITIES FOR THE EIC PHYSICS.

QUESTIONS?