



THE 2021 NATIONAL NUCLEAR PHYSICS SUMMER SCHOOL

LATTICE QCD
AND
NUCLEON(US) STRUCTURE

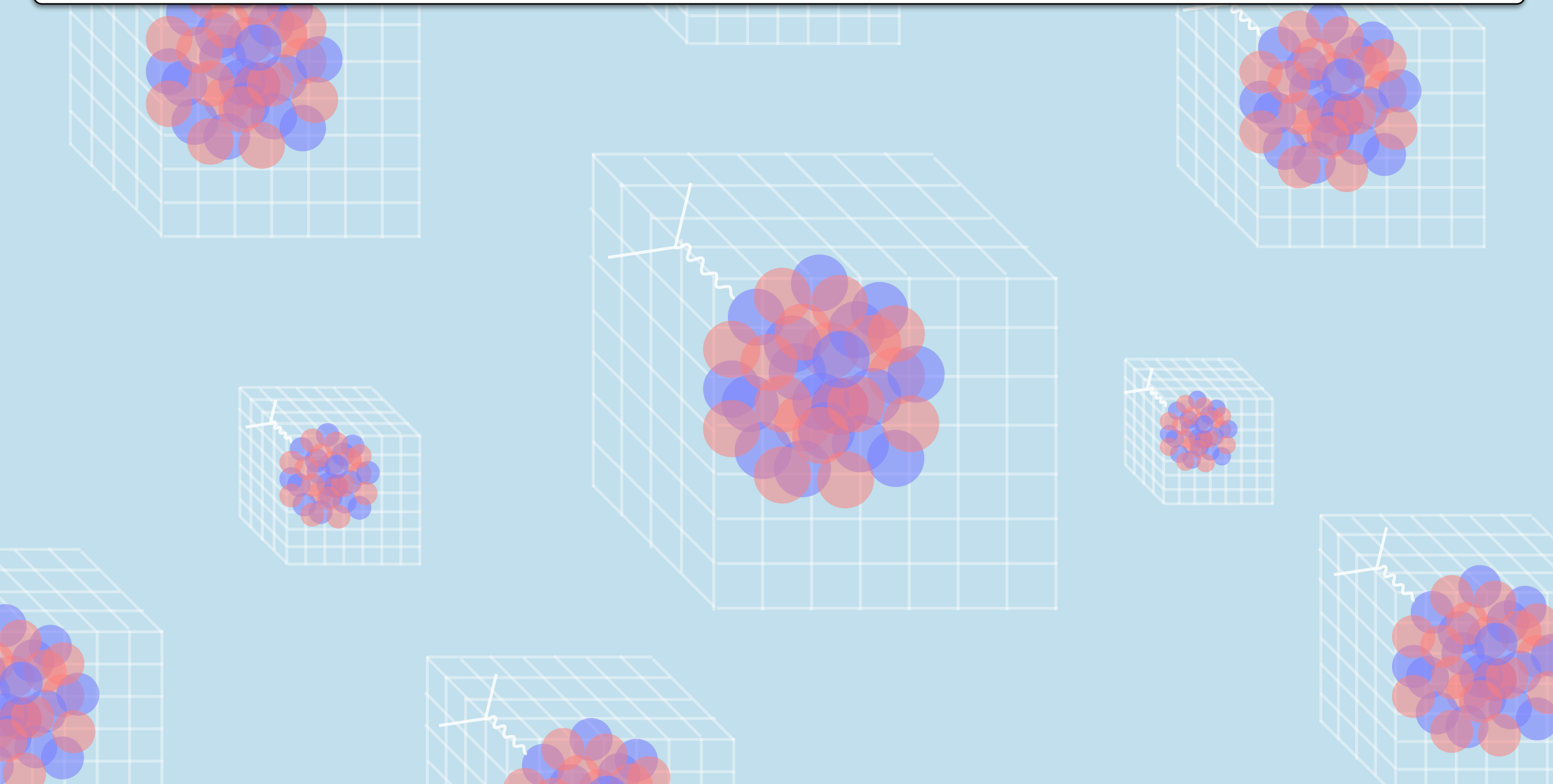
ZOHREH DAVOUDI
UNIVERSITY OF MARYLAND AND RIKEN FELLOW

**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

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

$$-\frac{1}{4} F_{\mu\nu}^i F^{i\mu\nu} + \frac{g}{2} f_{ijk} F_{\mu\nu}^i A^{j\mu} A^{k\nu} - \frac{g^2}{4} f_{ijk} f_{klm} A_\mu^j A_\nu^k A^{l\mu} A^{m\nu}$$

Gluons kinetic and interaction terms

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Quark kinetic and mass term Quark/gluon interactions

Gluons kinetic and interaction terms

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: $\alpha_s(\mu') = \frac{1}{2b_0 \log \frac{\mu'}{\Lambda_{QCD}}}$

Positive constant for $N_f \leq 16$

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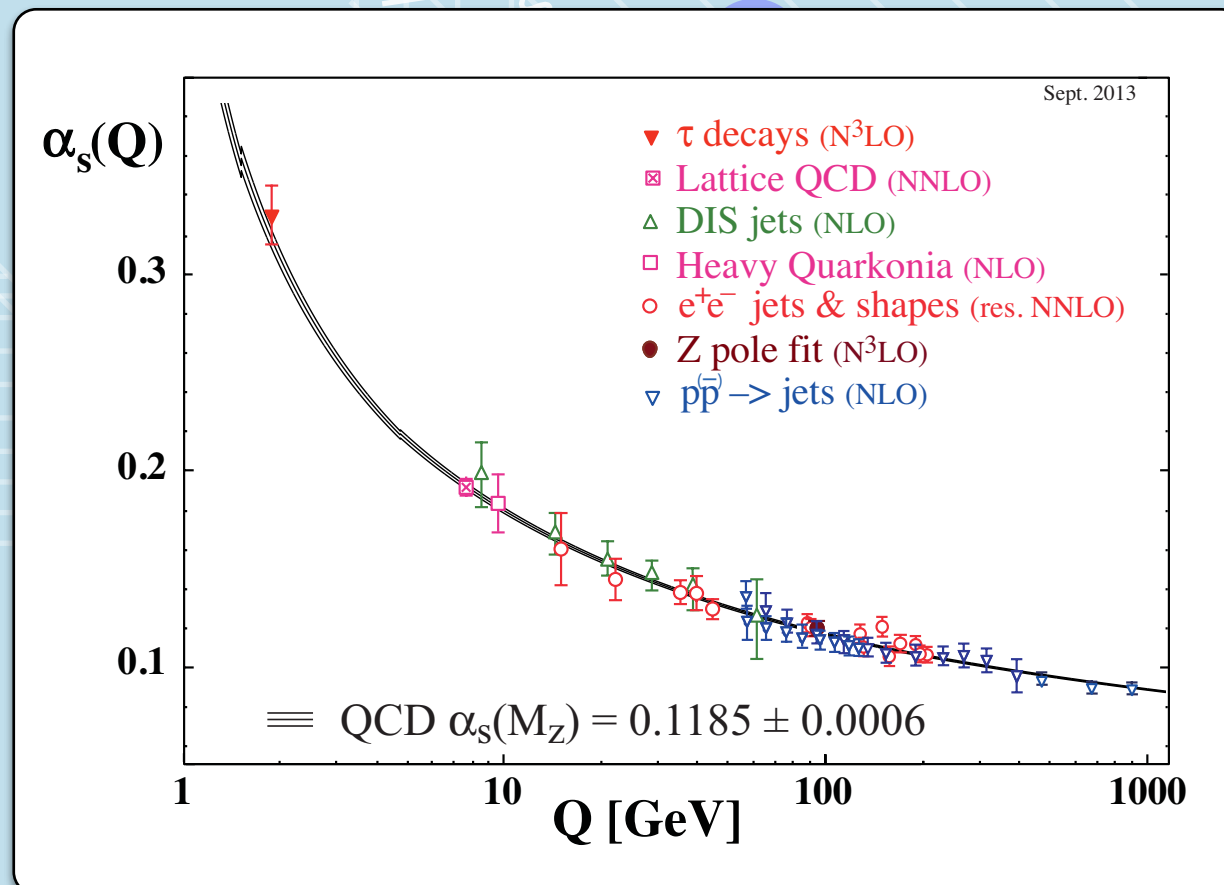
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Gluons kinetic and interaction terms



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.

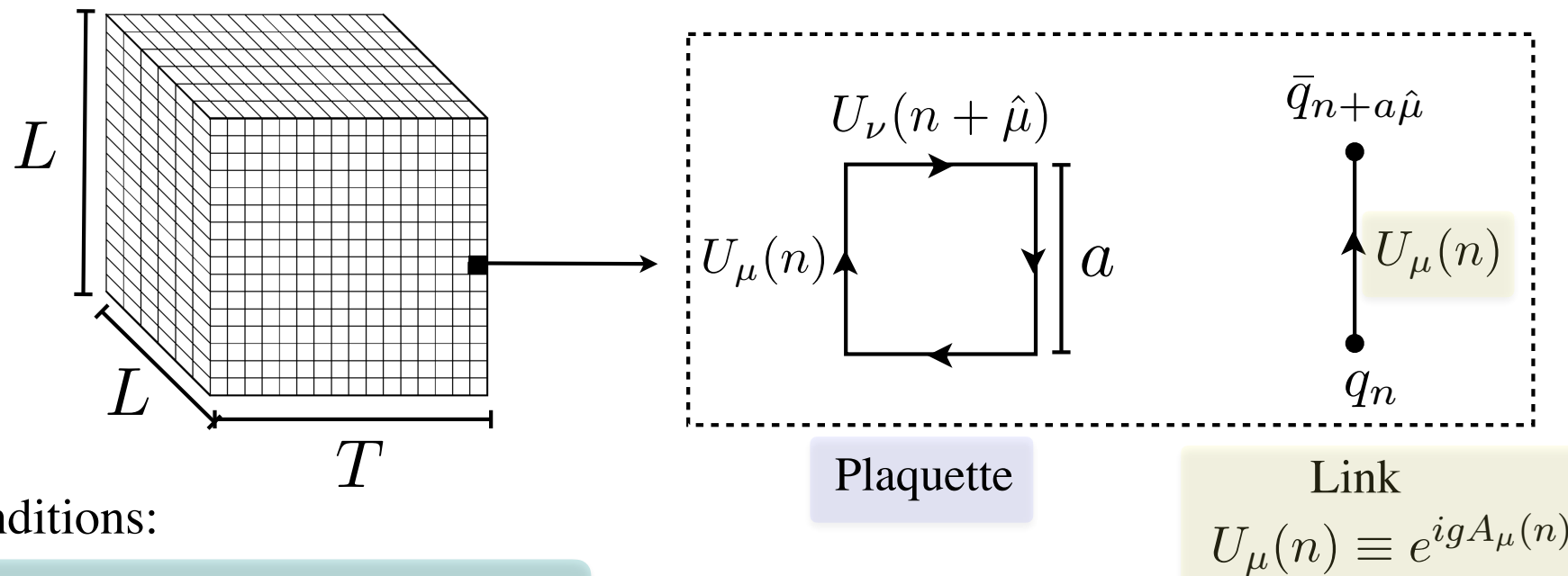
Step III: Form the correlation functions by contracting the quark fields. Need to specify the interpolating operators for the state under study.

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

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

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

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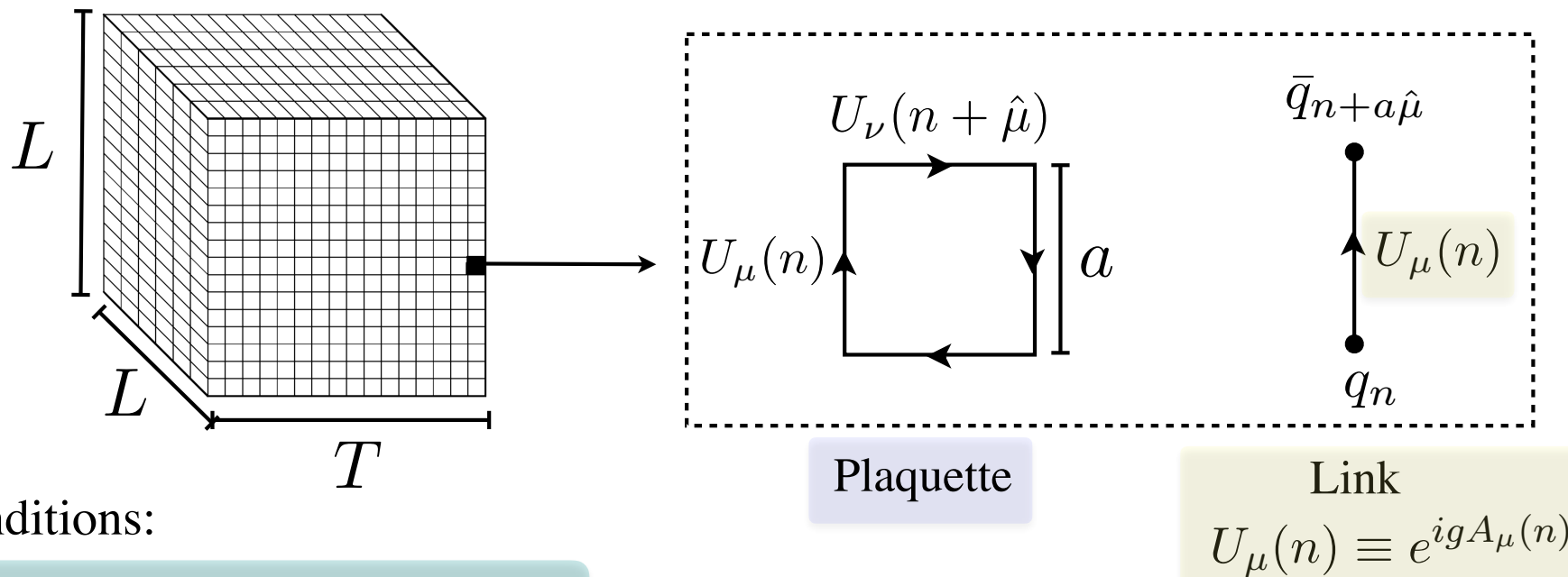


Two conditions:

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

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

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An example of a discretized action by K. Wilson:

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

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

For discussions of actions consistent with chiral symmetry of continuum see: Kaplan, arXiv:0912.2560 [hep-lat].

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

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

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Quark part of expectation values

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Quark part of expectation values

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$$\mathcal{Z}_F = \int \mathcal{D}q \mathcal{D}\bar{q} e^{-S_{\text{lattice}}^{(F)}[U, q, \bar{q}]} = \prod_f \det D_f \quad \text{Dirac matrix}$$

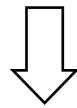
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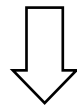
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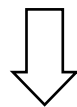
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$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{N} \sum_i^N \langle \hat{\mathcal{O}} \rangle_F [U^{(i)}]$$

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

Steps II is computationally costly...

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

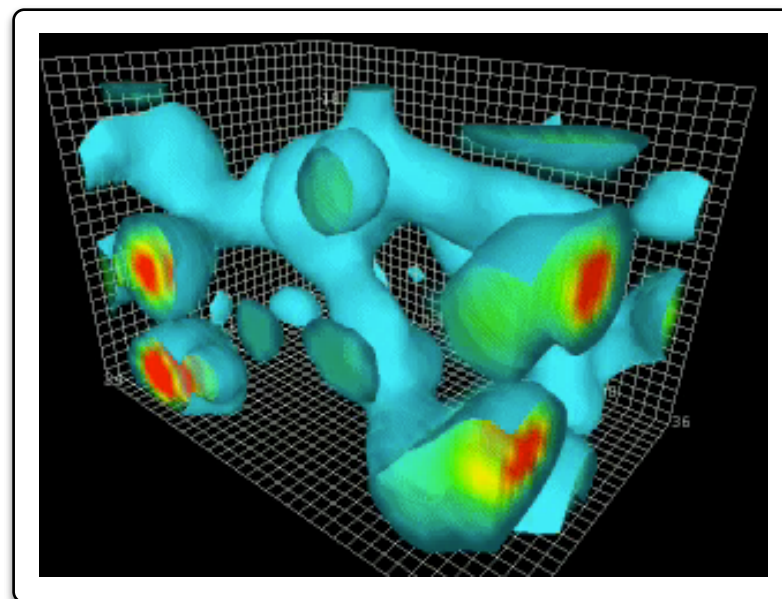
Sampling SU(3) matrices. Already for one sample requires storing

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

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.

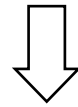


Step III: Form the correlation functions by contracting the quarks. Need to specify the interpolating operators for the state under study.

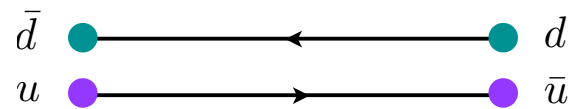
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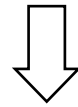


e.g., $\hat{\mathcal{O}} = \bar{u} \gamma_5 d$

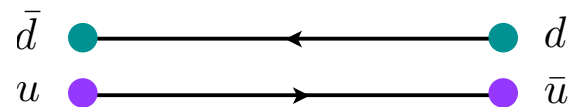


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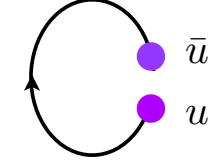
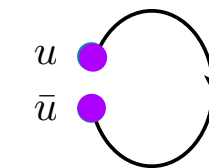
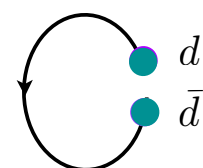
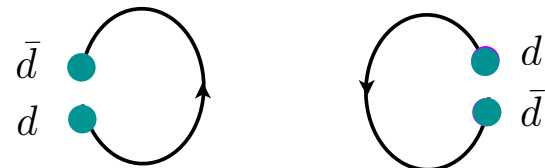
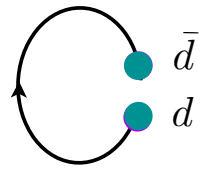
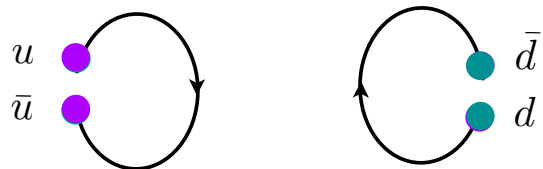
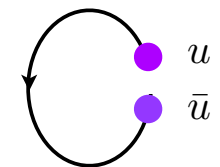
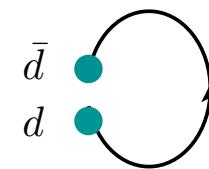
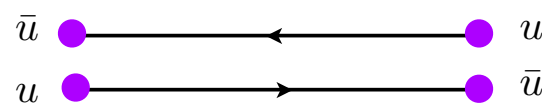
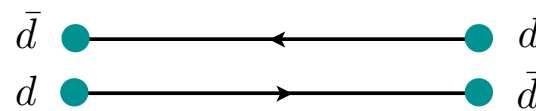
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e.g., $\hat{\mathcal{O}} = \bar{u}\gamma_5 d$



e.g., $\hat{\mathcal{O}} = \frac{1}{\sqrt{2}} (\bar{u}\gamma_5 u - \bar{d}\gamma_5 d)$



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

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

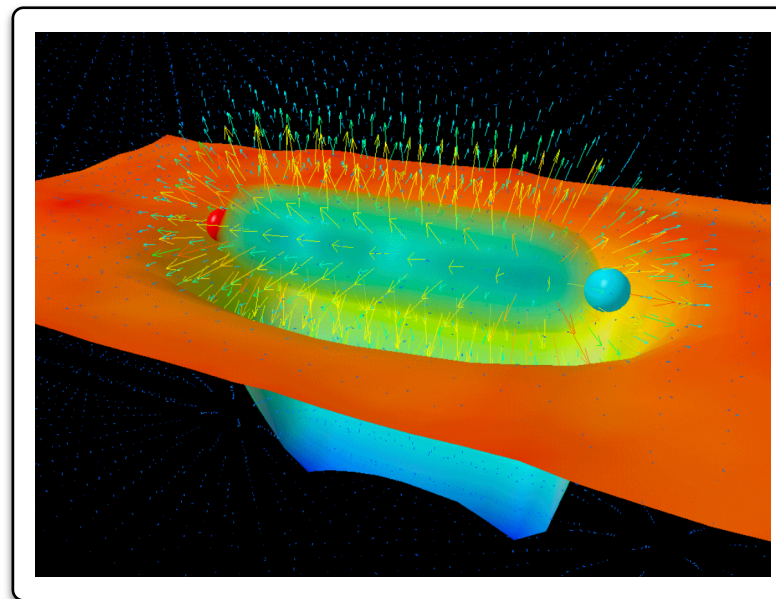
Dirac
matrix

Quark
propagator

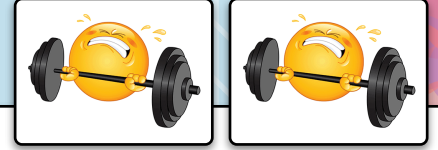
Source

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

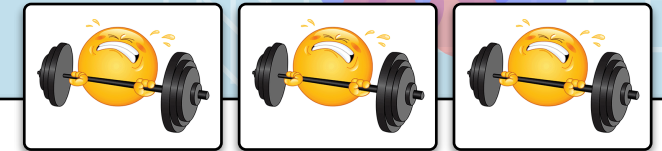


Show that for the correlation function of the charged pion:

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

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:

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

Step IV: Extract energies and matrix elements from correlation functions

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

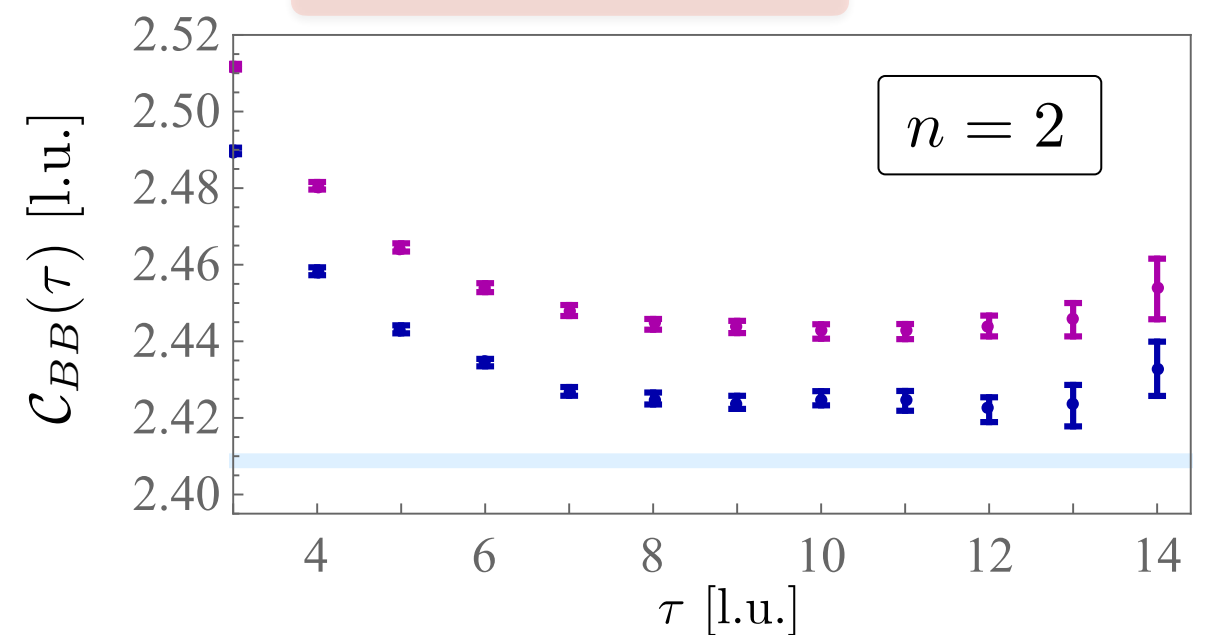
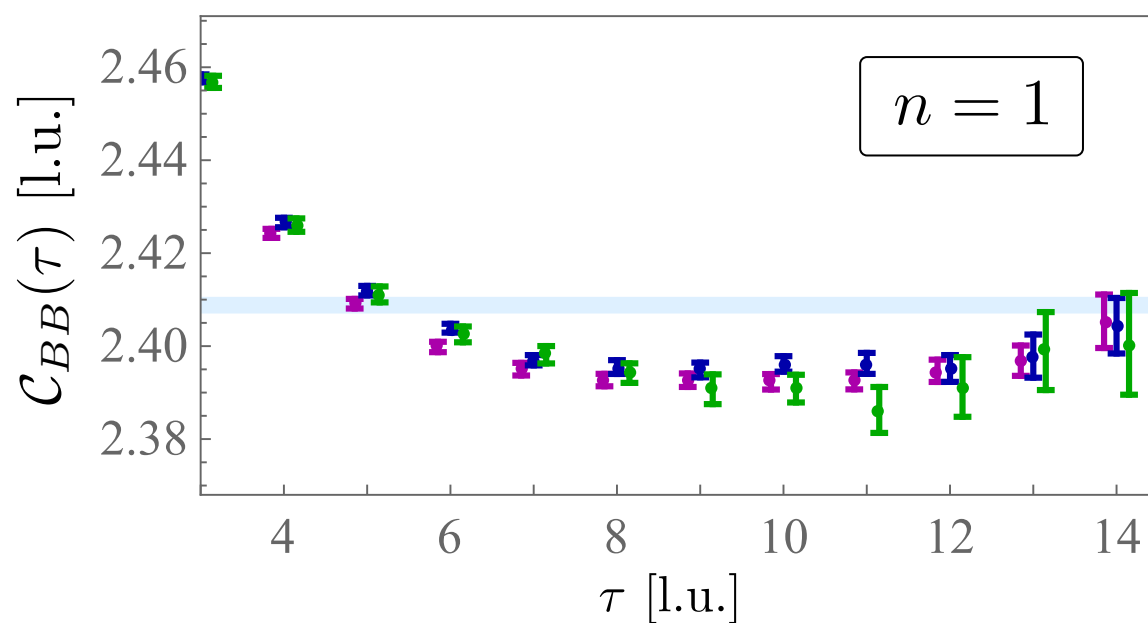
Ground state and a tower of excited states are, in principle, accessible!

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

Example: $NN (^1S_0)$



What should we make of the volume dependence?

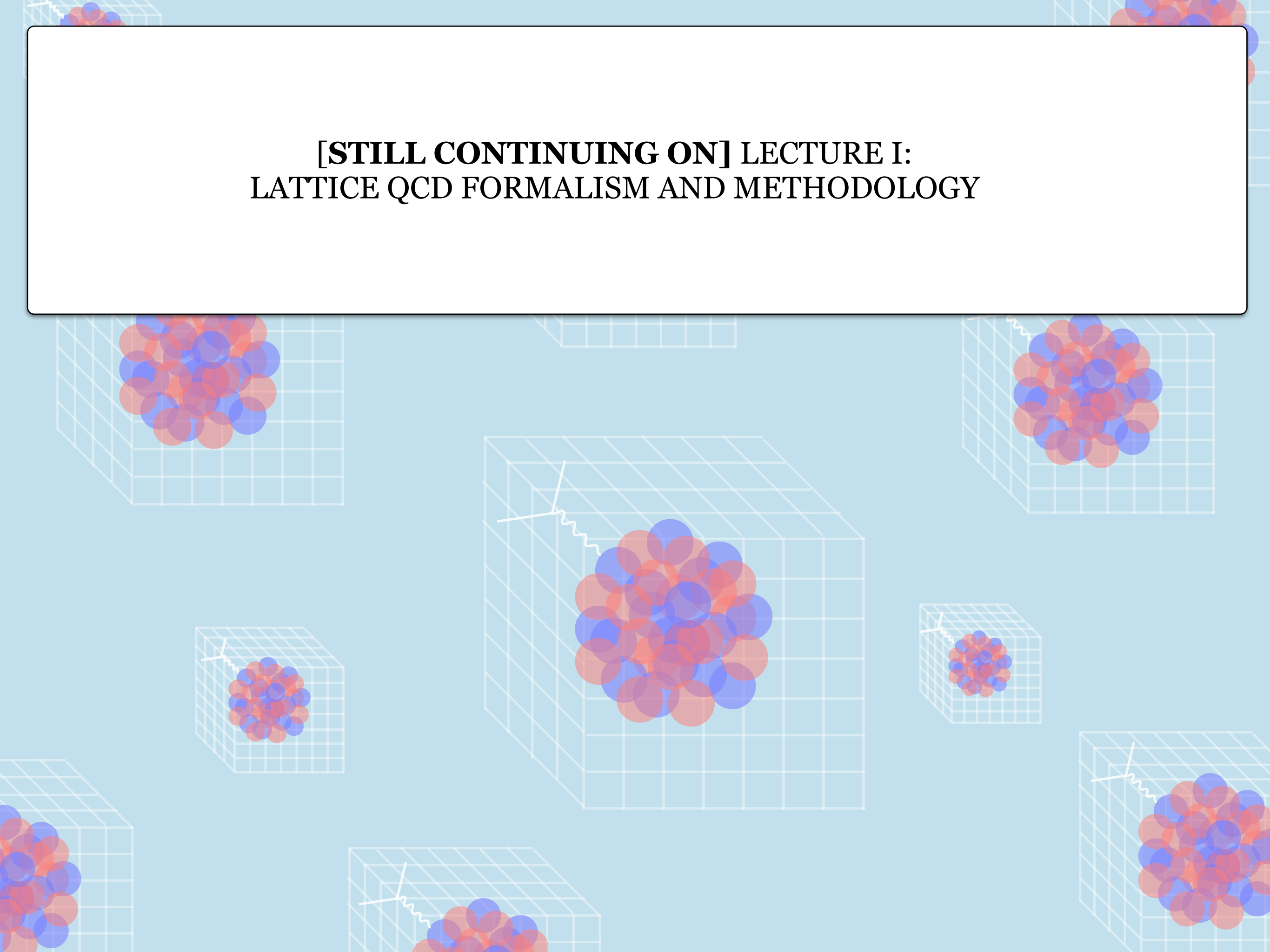
$\color{magenta}\Uparrow 24^3 \times 48$

$\color{blue}\Uparrow 32^3 \times 48$

$\color{green}\Uparrow 48^3 \times 64$

$\color{lightblue}\rule{1cm}{0.4pt} 2M_N$

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



[Recap] Steps involved in any lattice QCD calculation:

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

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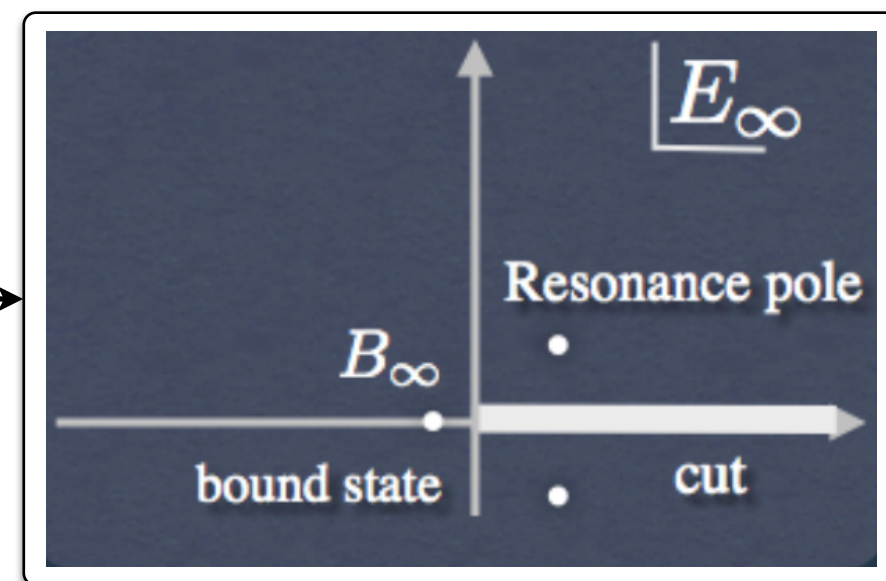
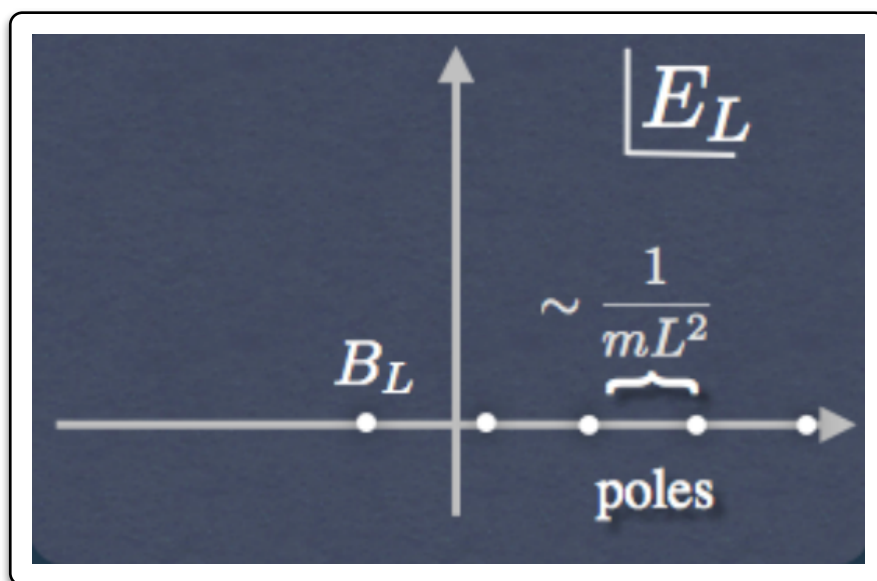
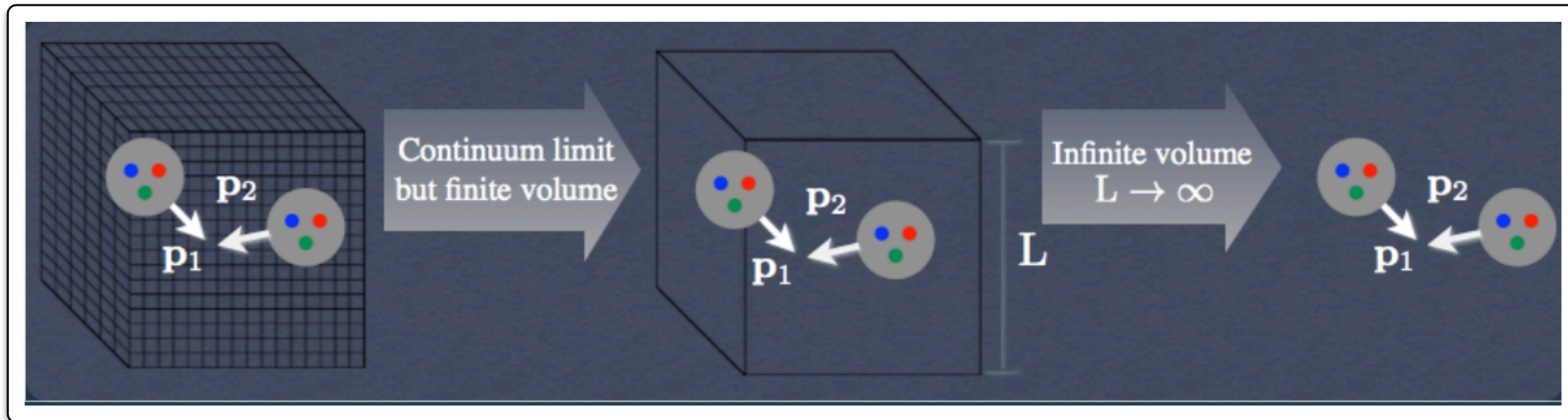
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See e.g., ZD, arXiv:1409.1966 [hep-lat]

Step V: Make the connection to physical observables, such as scattering amplitudes, decay rates, etc. Still not fully developed and presents challenge in multi-hadron systems.

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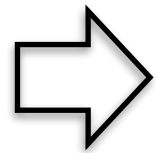
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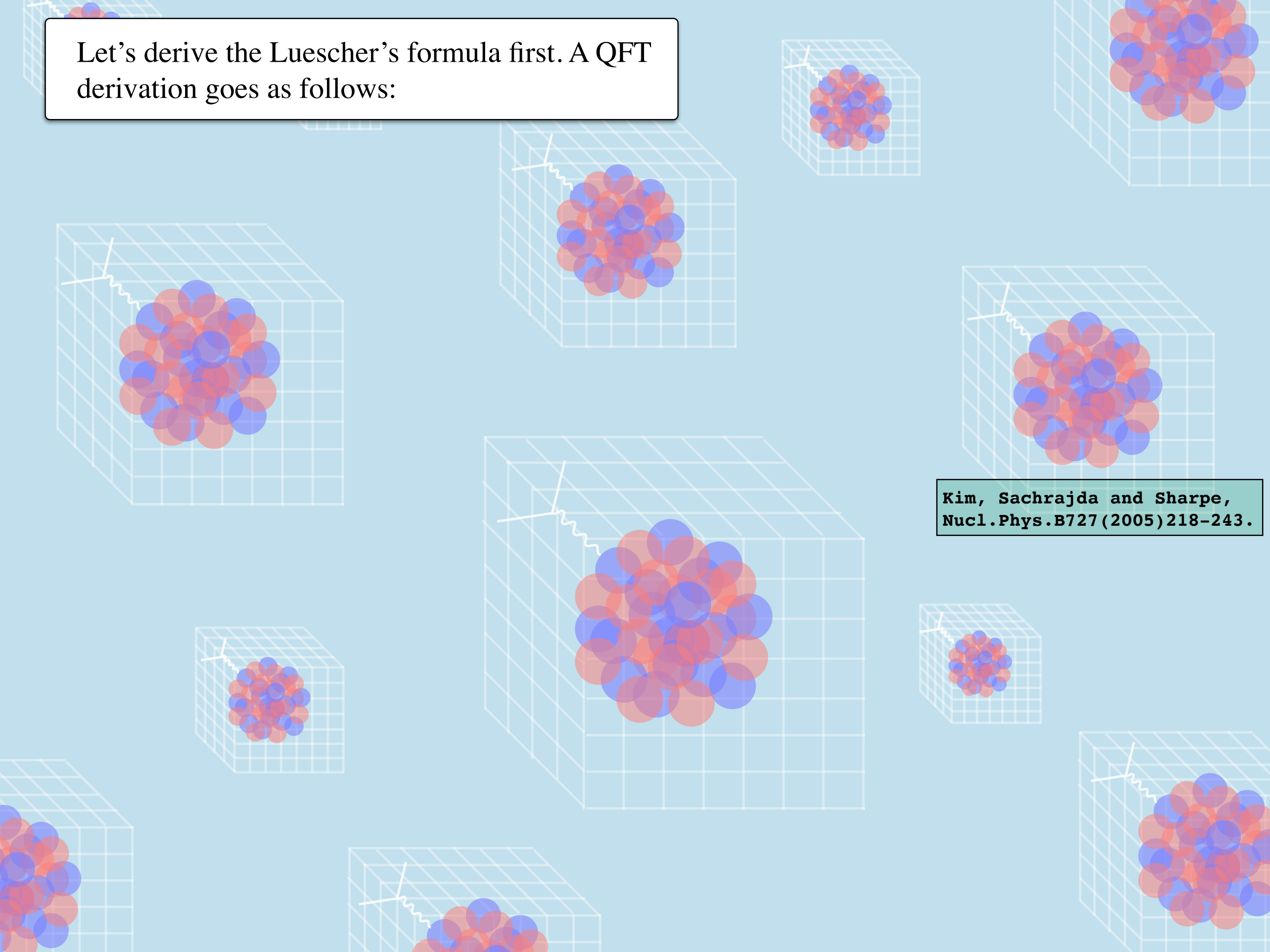
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See e.g., ZD, arXiv:1409.1966 [hep-lat, Briceno, Dudek and Young, Rev. Mod. Phys. 90.025001, Ann. Rev. Nucl. Part. Sci. 69 (2019).

Let's derive the Luescher's formula first. A QFT derivation goes as follows:



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

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$$C_V = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \dots$$

The diagram shows a series of Feynman diagrams representing the expansion of the vacuum expectation value of the operator V . Each diagram consists of a grey circle with four black dots at the top, bottom, left, and right. The left and right dots are connected to green circles labeled σ' and σ respectively. The top and bottom dots are connected to a central vertex labeled V . The first diagram is a single circle. The second diagram consists of two such circles connected at their right and left vertices, with a green circle labeled $-\kappa$ between them. The third diagram consists of three such circles connected in a chain, with green circles labeled $-\kappa$ between each adjacent circle. The series continues with an ellipsis.

$$T \rightarrow \infty, a \rightarrow 0$$

Kim, Sachrajda and Sharpe,
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The equation shows a series of Feynman diagrams for the correlator C_V . Each diagram consists of a grey circle with two black dots at the top and bottom. The first diagram has two green circles labeled σ' and σ on the left and right sides, with a V label inside. The second diagram has a green σ' on the left and a green σ on the right, with a V label in the first circle and a $-\kappa$ label in the second circle. The third diagram has a green σ' on the left and a green σ on the right, with V labels in all three circles and $-\kappa$ labels between the first and second, and between the second and third circles.

$$T \rightarrow \infty, a \rightarrow 0$$

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

$$(1) \text{ [diagram 1]} = \text{[diagram 2]} + \text{[diagram 3]}$$

The equation (1) shows a diagrammatic identity. The first diagram is a grey circle with two black dots at the top and bottom and a V label inside. The second diagram is a grey circle with two black dots at the top and bottom and an infinity symbol (∞) inside. The third diagram is a grey circle with two black dots at the top and bottom, a V label inside, and a dashed line passing through the circle from the top-right to the bottom-left.

Let's derive the Luescher's formula first. A QFT derivation goes as follows:

$$C_V = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \dots$$

The diagrams in the equation represent terms in a series expansion of the vacuum expectation value C_V . Each term consists of a chain of circles representing interaction vertices. The first term is a single circle with two external legs labeled σ' and σ , and a central vertex labeled V . The second term is a chain of two such circles, with the internal propagator labeled $-\kappa$. The third term is a chain of three such circles, with internal propagators labeled $-\kappa$. The circles are shaded gray, and the external legs are green.

$$T \rightarrow \infty, a \rightarrow 0$$

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

$$(1) \text{ [diagram 1]} = \text{[diagram 2]} + \text{[diagram 3]}$$

Diagram (1) shows a circle with two external legs and a central vertex labeled V . This is equal to the sum of two diagrams: a circle with two external legs and a central infinity symbol (∞), and a circle with two external legs and a central vertex labeled V connected to the rest of the diagram by a dashed line.

$$(2) \text{ [diagram 1]} = \text{[diagram 2]} + \text{[diagram 3]} + \text{[diagram 4]} + \dots$$

Diagram (2) shows a circle with four external legs and a central vertex labeled \mathcal{M}_∞ . This is equal to the sum of four diagrams: a circle with four external legs and a central vertex labeled $-\kappa$; a circle with four external legs, a central infinity symbol (∞), and two vertices labeled $-\kappa$ connected to the central infinity symbol; a circle with four external legs, two central infinity symbols (∞), and two vertices labeled $-\kappa$ connected to the central infinity symbols; and a circle with four external legs, two central infinity symbols (∞), and two vertices labeled $-\kappa$ connected to the central infinity symbols, with an additional vertex labeled $-\kappa$ connected to the central infinity symbols.

Let's derive the Luescher's formula first. A QFT derivation goes as follows:

$$\begin{aligned}
 C_V &= \text{diagram}_1 + \text{diagram}_2 + \text{diagram}_3 + \dots \\
 &= C_\infty + \text{diagram}_4 + \text{diagram}_5 + \text{diagram}_6 + \dots
 \end{aligned}$$

The diagrams are as follows:

- Diagram 1: A circle with two black dots at the top and bottom. Inside, a green circle labeled σ' is on the left and a green circle labeled σ is on the right. A vertical line labeled V connects the two dots.
- Diagram 2: Two circles as in Diagram 1, connected by a vertical line labeled $-\kappa$ between their inner green circles.
- Diagram 3: Three circles as in Diagram 1, connected by vertical lines labeled $-\kappa$ between their inner green circles.
- Diagram 4: A circle with two black dots. Inside, a teal circle labeled A' is on the left and a teal circle labeled A is on the right. A vertical line labeled V connects the two dots. A dashed line extends from the top of the circle.
- Diagram 5: Two circles as in Diagram 4, connected by a vertical line labeled M_∞ between their inner teal circles. Dashed lines extend from the top of each circle.
- Diagram 6: Three circles as in Diagram 4, connected by vertical lines labeled M_∞ between their inner teal circles. Dashed lines extend from the top of each circle.

$$T \rightarrow \infty, a \rightarrow 0$$

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

$$(1) \quad \text{diagram}_1 = \text{diagram}_2 + \text{diagram}_3$$

The diagrams are:

- Diagram 1: A circle with two black dots and a vertical line labeled V connecting them.
- Diagram 2: A circle with two black dots and an infinity symbol ∞ inside.
- Diagram 3: A circle with two black dots and a vertical line labeled V connecting them. A dashed line extends from the top of the circle.

$$(2) \quad \text{diagram}_4 = \text{diagram}_5 + \text{diagram}_6 + \dots$$

The diagrams are:

- Diagram 4: A teal circle labeled M_∞ with four black dots on its sides.
- Diagram 5: A green circle labeled $-\kappa$ with two black dots on its top and bottom.
- Diagram 6: A circle with two black dots and an infinity symbol ∞ inside. Two green circles labeled $-\kappa$ are attached to the left and right sides. A dashed line extends from the top of the circle.
- Diagram 7: Two circles as in Diagram 6, connected by a vertical line labeled ∞ between their inner infinity symbols.

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 $A(A')$?

Let's derive the Luescher's formula first. A QFT derivation goes as follows:

$$\begin{aligned}
 C_V &= \text{diagram}_1 + \text{diagram}_2 + \text{diagram}_3 + \dots \\
 &= C_\infty + \text{diagram}_4 + \text{diagram}_5 + \text{diagram}_6 + \dots
 \end{aligned}$$

The diagrams are as follows:

- Diagram 1: A circle with two black dots at the top and bottom. Inside, a green circle labeled σ' is on the left and a green circle labeled σ is on the right. A vertical line labeled V connects the two green circles.
- Diagram 2: Two circles as in Diagram 1, connected by a vertical line labeled $-\kappa$ between their green circles.
- Diagram 3: Three circles as in Diagram 1, connected by vertical lines labeled $-\kappa$ between their green circles.
- Diagram 4: A circle with two black dots at the top and bottom. Inside, a teal circle labeled A' is on the left and a teal circle labeled A is on the right. A vertical line labeled V connects the two teal circles. A dashed line extends from the top of the circle.
- Diagram 5: Two circles as in Diagram 4, connected by a vertical line labeled M_∞ between their teal circles. Dashed lines extend from the top of each circle.
- Diagram 6: Three circles as in Diagram 4, connected by vertical lines labeled M_∞ between their teal circles. Dashed lines extend from the top of each circle.

$$T \rightarrow \infty, a \rightarrow 0$$

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

$$(1) \quad \text{diagram}_V = \text{diagram}_\infty + \text{diagram}_V$$

The diagram on the left is a circle with two black dots at the top and bottom and a vertical line labeled V connecting them. The first diagram on the right is a circle with two black dots at the top and bottom and an infinity symbol ∞ inside. The second diagram on the right is a circle with two black dots at the top and bottom and a vertical line labeled V connecting them, with a dashed line extending from the top.

$$(2) \quad \text{diagram}_{M_\infty} = \text{diagram}_{-\kappa} + \text{diagram}_{-\kappa \infty -\kappa} + \text{diagram}_{-\kappa \infty \infty -\kappa} + \dots$$

The diagram on the left is a teal circle labeled M_∞ with four black dots on its sides. The first diagram on the right is a green circle labeled $-\kappa$ with four black dots on its sides. The second diagram on the right is a circle with two black dots at the top and bottom and an infinity symbol ∞ inside, with a green circle labeled $-\kappa$ on the left and another green circle labeled $-\kappa$ on the right. Dashed lines extend from the top of the circle. The third diagram on the right is a circle with two black dots at the top and bottom and an infinity symbol ∞ inside, with a green circle labeled $-\kappa$ on the left and another green circle labeled $-\kappa$ on the right, which is connected to a second circle with two black dots at the top and bottom and an infinity symbol ∞ inside. Dashed lines extend from the top of each circle.

Let's derive the Luescher's formula first. A QFT derivation goes as follows:

$$\begin{aligned}
 C_V &= \text{[diagram: circle with } \sigma', V, \sigma \text{]} + \text{[diagram: two circles with } \sigma', V, -\kappa, V, \sigma \text{]} + \text{[diagram: three circles with } \sigma', V, -\kappa, V, -\kappa, V, \sigma \text{]} + \dots \\
 &= C_\infty + \text{[diagram: circle with } A', V, A \text{]} + \text{[diagram: two circles with } A', V, \mathcal{M}_\infty, V, A \text{]} + \text{[diagram: three circles with } A', V, \mathcal{M}_\infty, V, \mathcal{M}_\infty, V, A \text{]} + \dots
 \end{aligned}$$

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

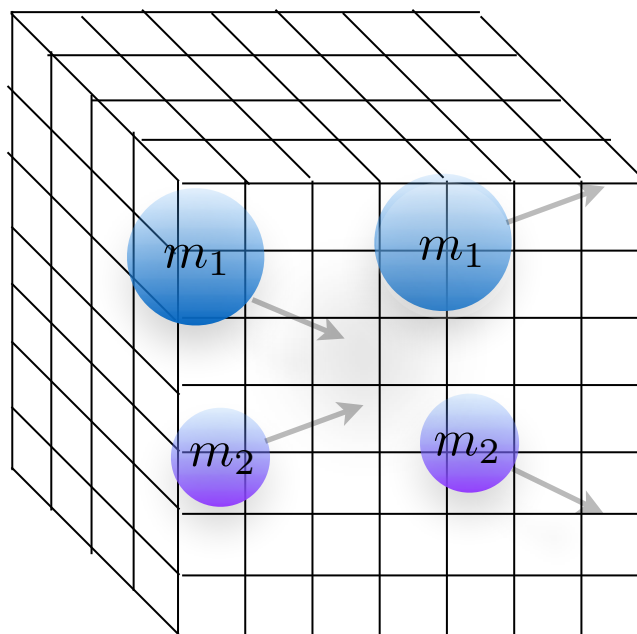
Kim, Sachrajda and Sharpe,
Nucl.Phys.B727(2005)218-243.

Finite-volume function Scattering amplitude

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

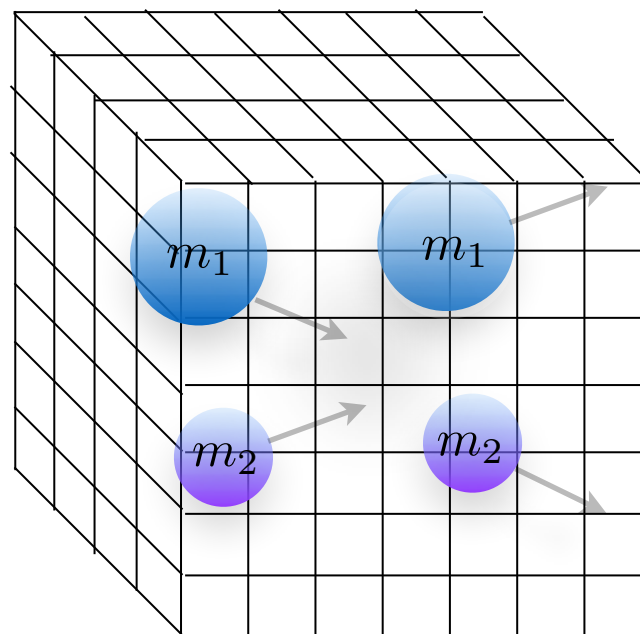
$$\det [\delta\mathcal{G}^V(E^*) + \mathcal{M}_\infty^{-1}(E^*)] = 0$$

Luescher (1986, 1991).



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

Luescher (1986, 1991).

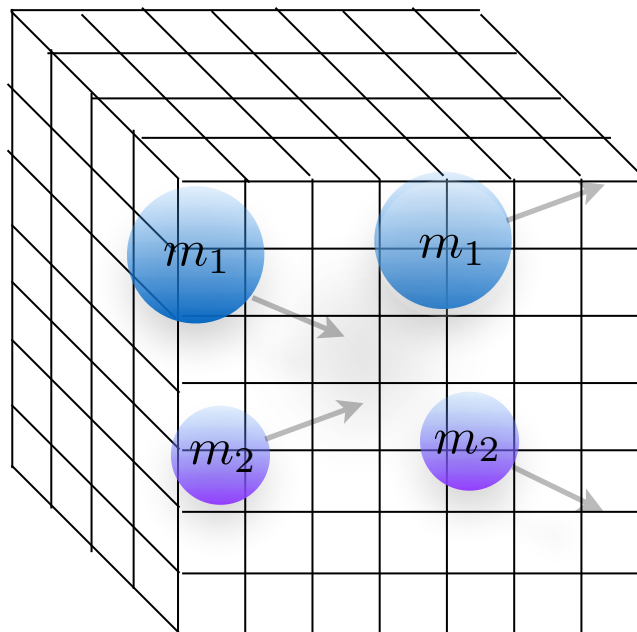


Elastic amplitude more closely...

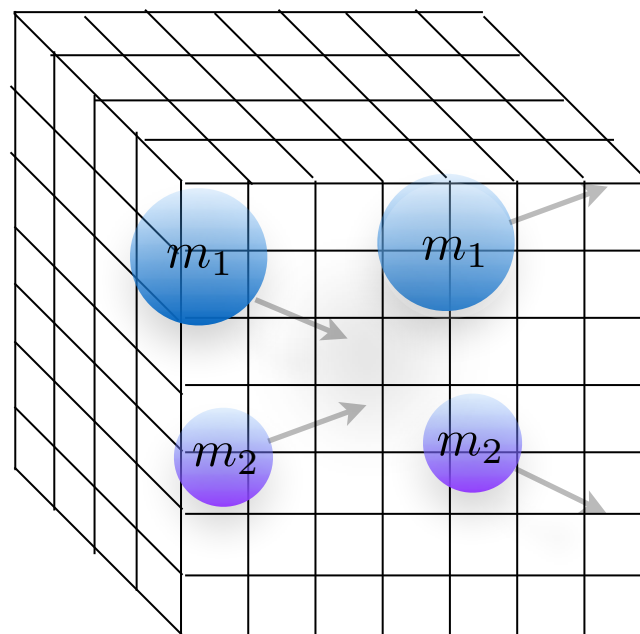
$$(\mathcal{M})_{l_1, m_1; l_2, m_2} = \delta_{l_1, l_2} \delta_{m_1, m_2} \frac{\overset{\text{CM energy}}{8\pi E^*}}{\underset{\text{Symmetry factor}}{nq^*}} \frac{\overset{\text{Phase shift}}{e^{2i\delta^{(l)}}(q^*)} - 1}{2i}$$

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

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



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



Finite-volume function more closely...

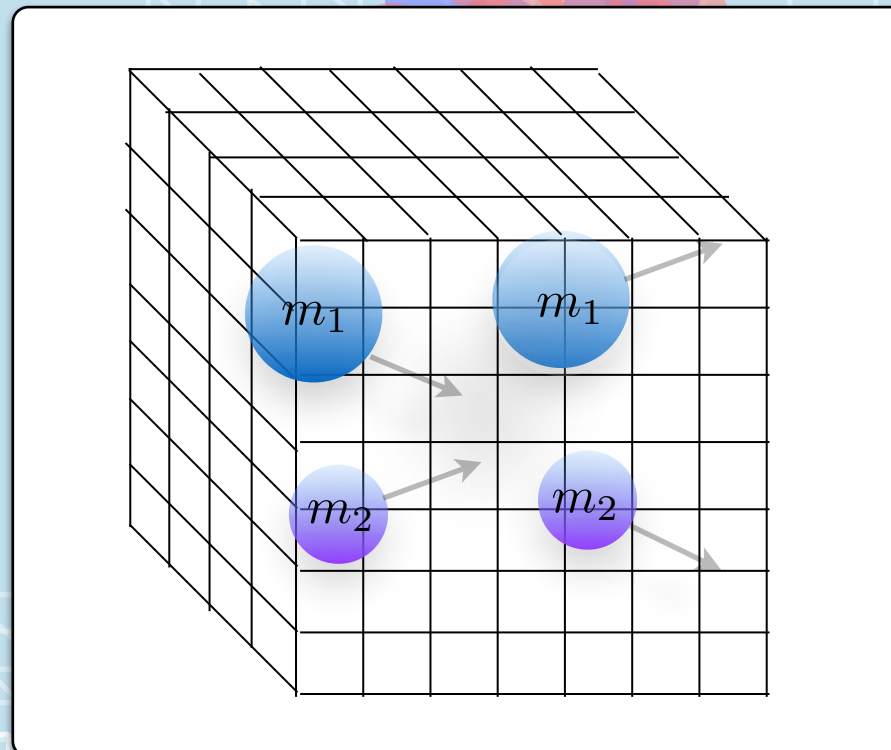
$$(\delta\mathcal{G}^V)_{l_1, m_1; l_2, m_2} = i \frac{q^* n}{8\pi E^*} \left(\delta_{l_1, l_2} \delta_{m_1, m_2} + i \frac{4\pi}{q^*} \sum_{l, m} \frac{\sqrt{4\pi}}{q^{*l}} c_{lm}^{\mathbf{P}}(q^{*2}) \int d\Omega^* Y_{l_1 m_1}^* Y_{lm}^* Y_{l_2 m_2} \right)$$

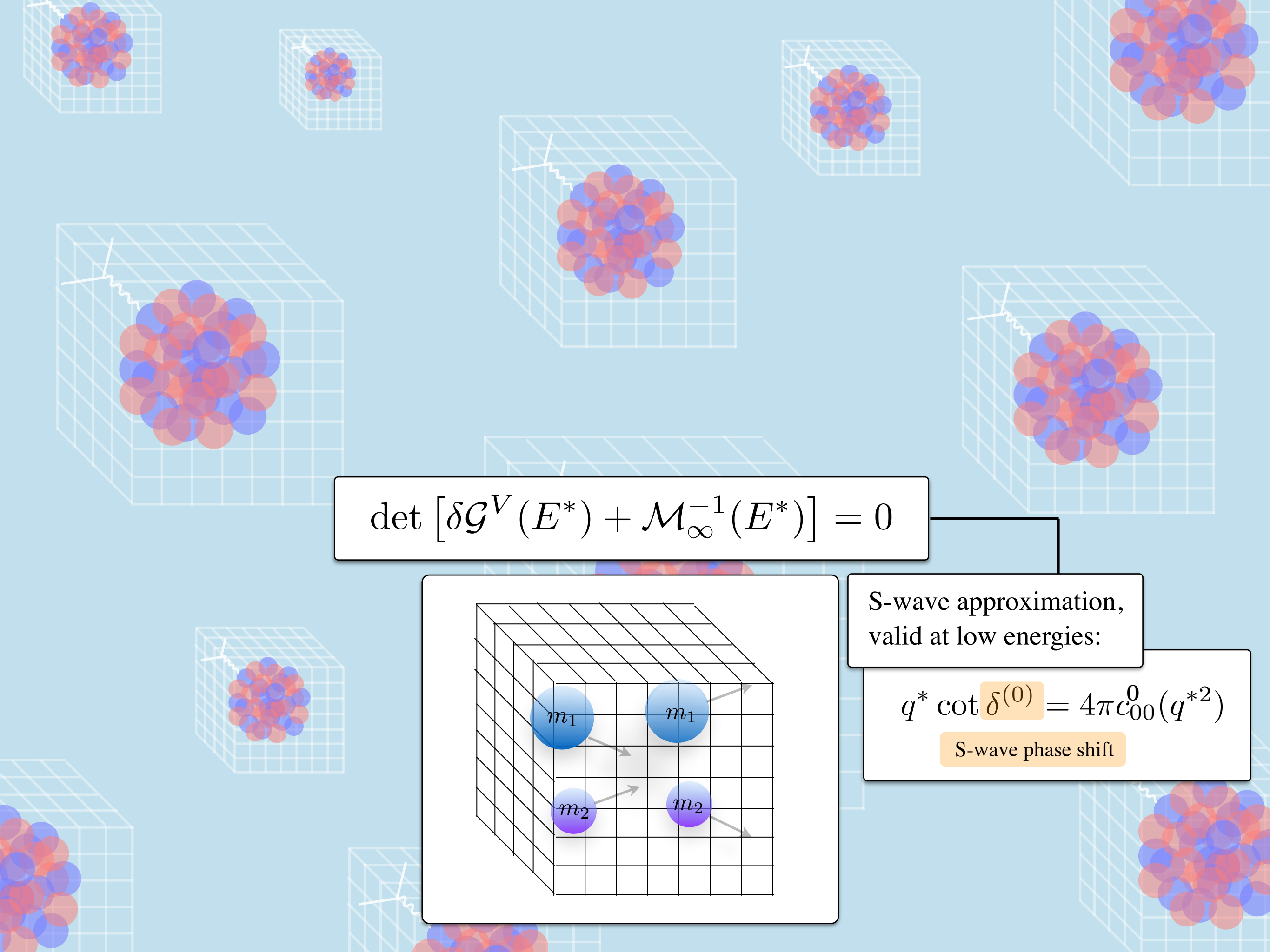
$$c_{lm}^{\mathbf{P}}(x) = \frac{1}{\gamma} \left[\frac{1}{L^3} \sum_{\mathbf{k}} -\mathcal{P} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\sqrt{4\pi} Y_{lm}(\hat{\mathbf{k}}^*) k^{*l}}{k^{*2} - x} \right]$$

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

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

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

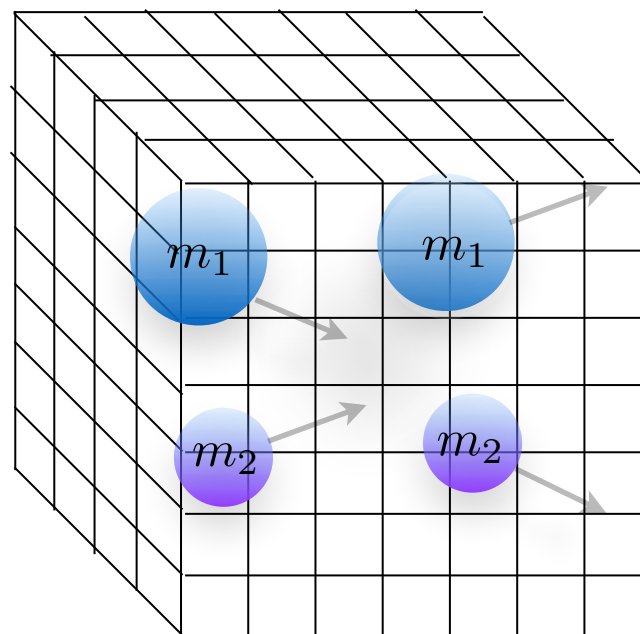



$$\det [\delta \mathcal{G}^V (E^*) + \mathcal{M}_\infty^{-1} (E^*)] = 0$$

S-wave approximation,
valid at low energies:

$$q^* \cot \delta^{(0)} = 4\pi c_{00}^0 (q^{*2})$$

S-wave phase shift

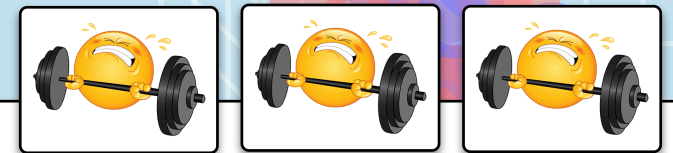


EXERCISE 3



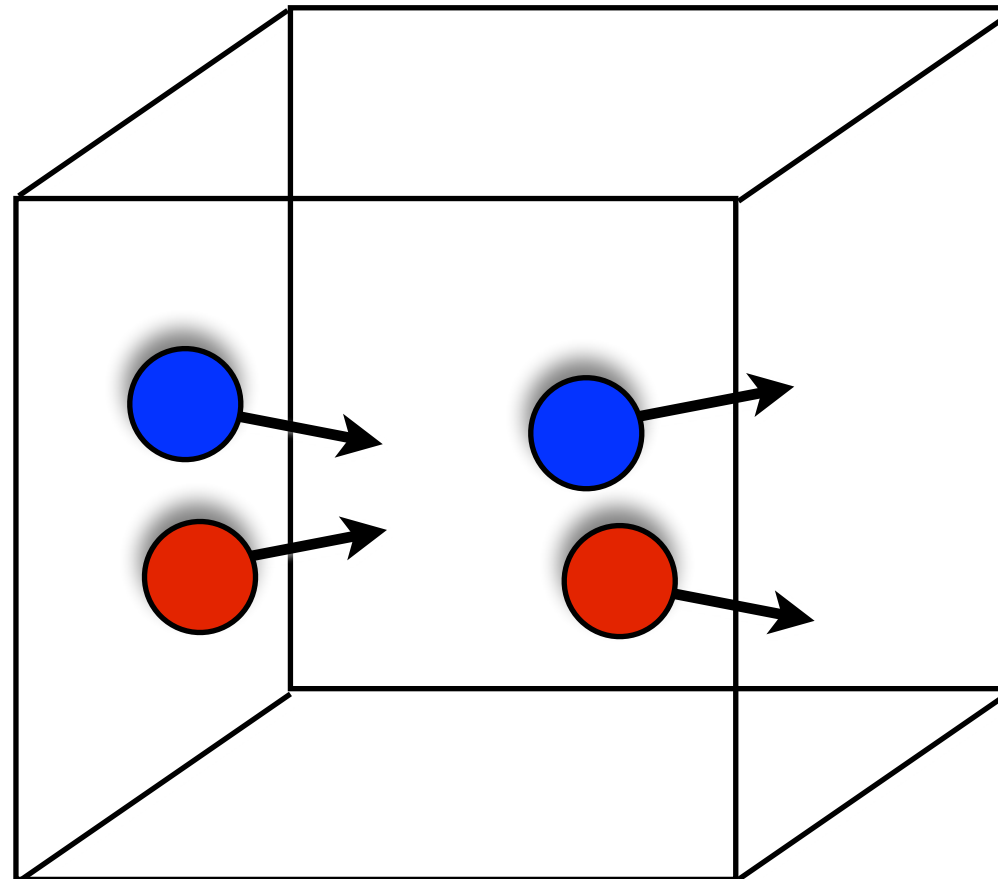
Derive the S-wave limit of Luescher's quantization condition from the master relation.

BONUS EXERCISE 2



Plot the S-wave finite-volume function c_{00}^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!):

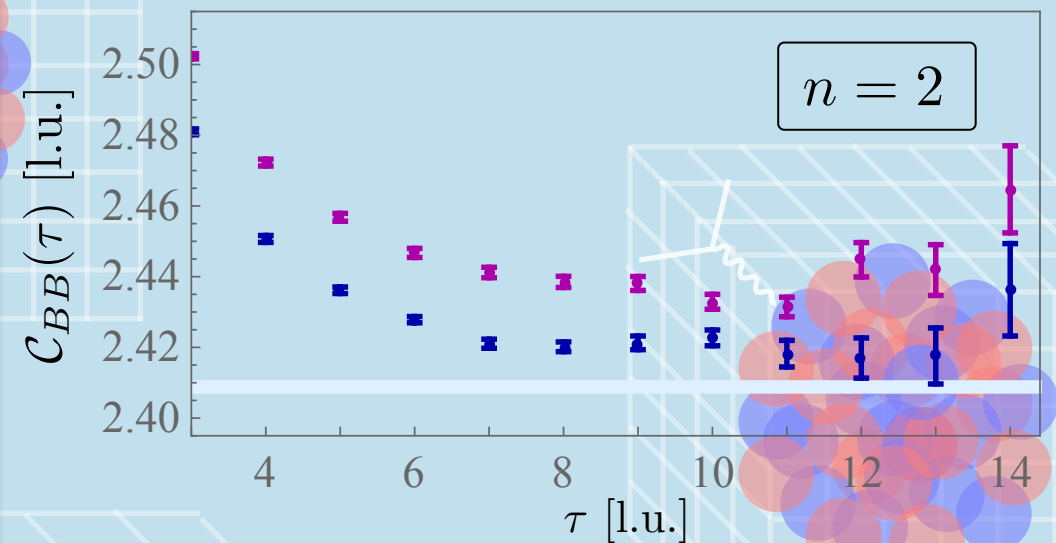
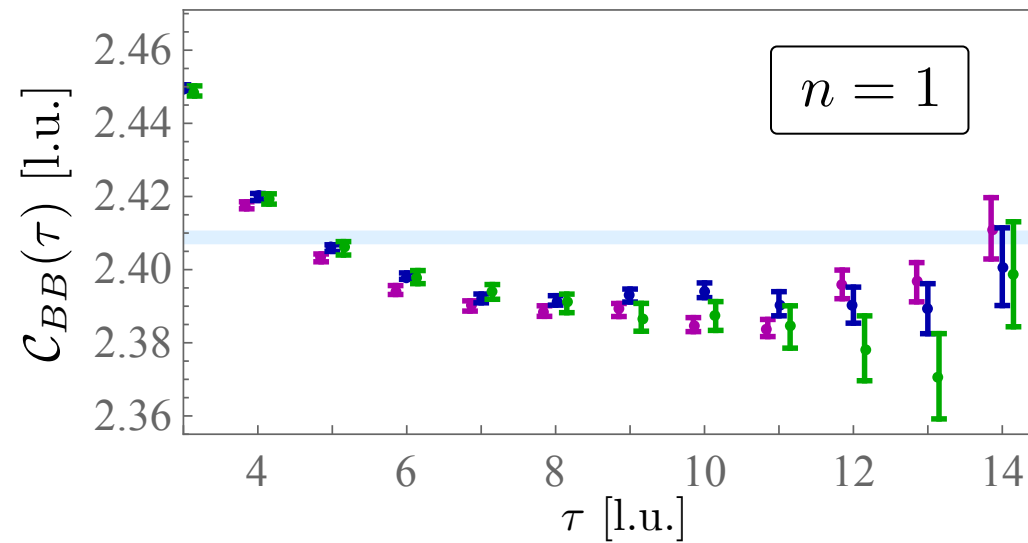


Wagman et al. (NPLQCD), Phys.Rev.D 96,114510(2017).

Step 1: Obtain the lowest-lying spectra

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

$NN (^3S_1)$



$24^3 \times 48$

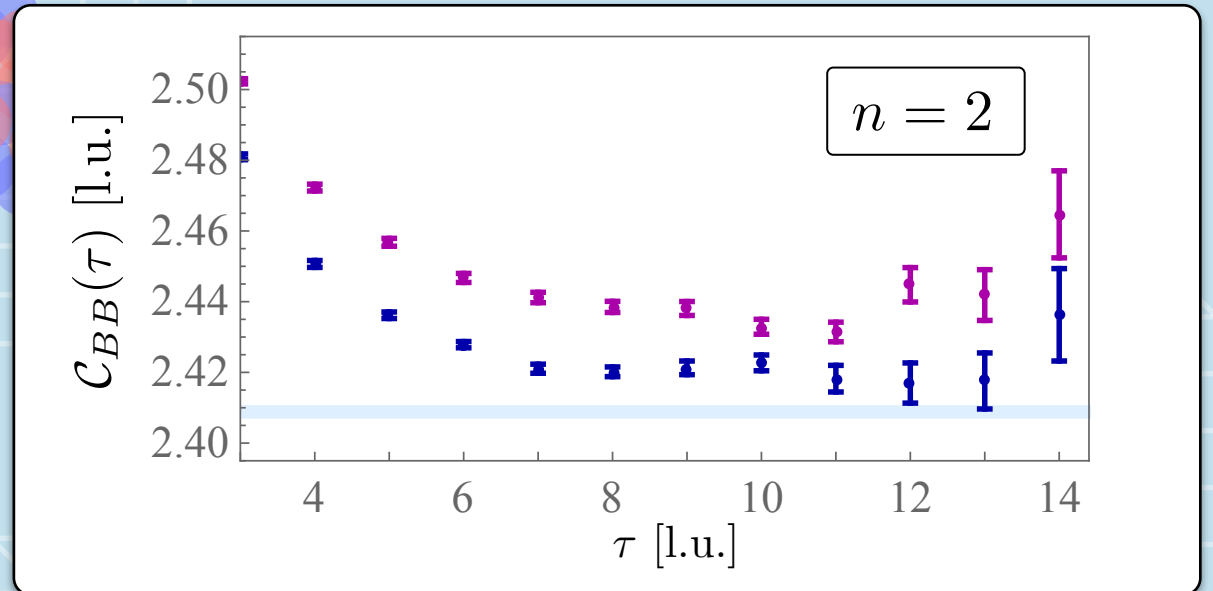
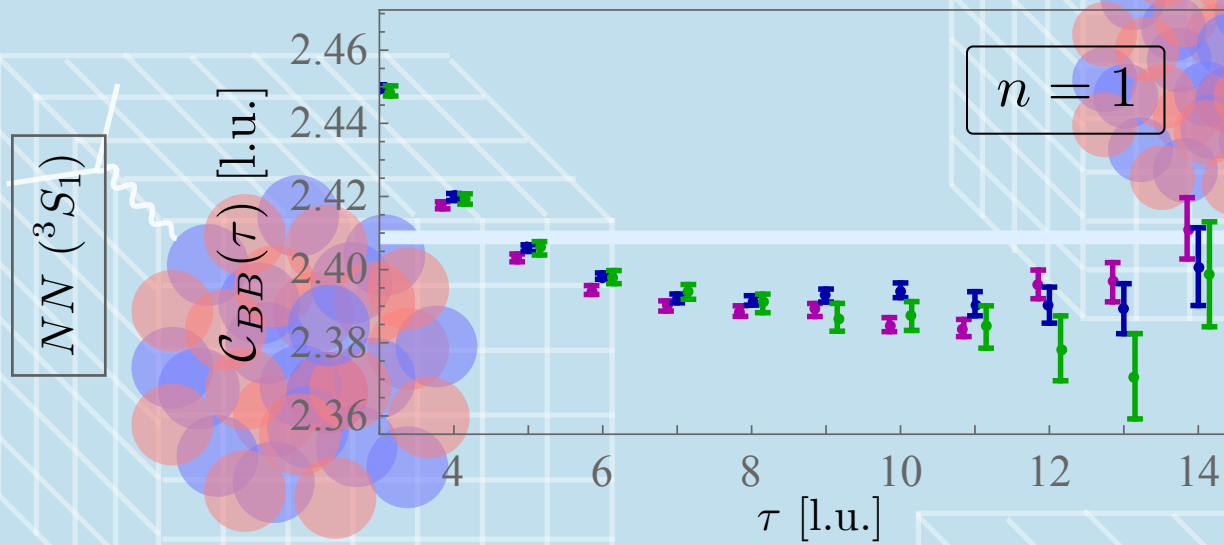
$32^3 \times 48$

$48^3 \times 64$

$2M_N$

Step 1: Obtain the lowest-lying spectra

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



$24^3 \times 48$

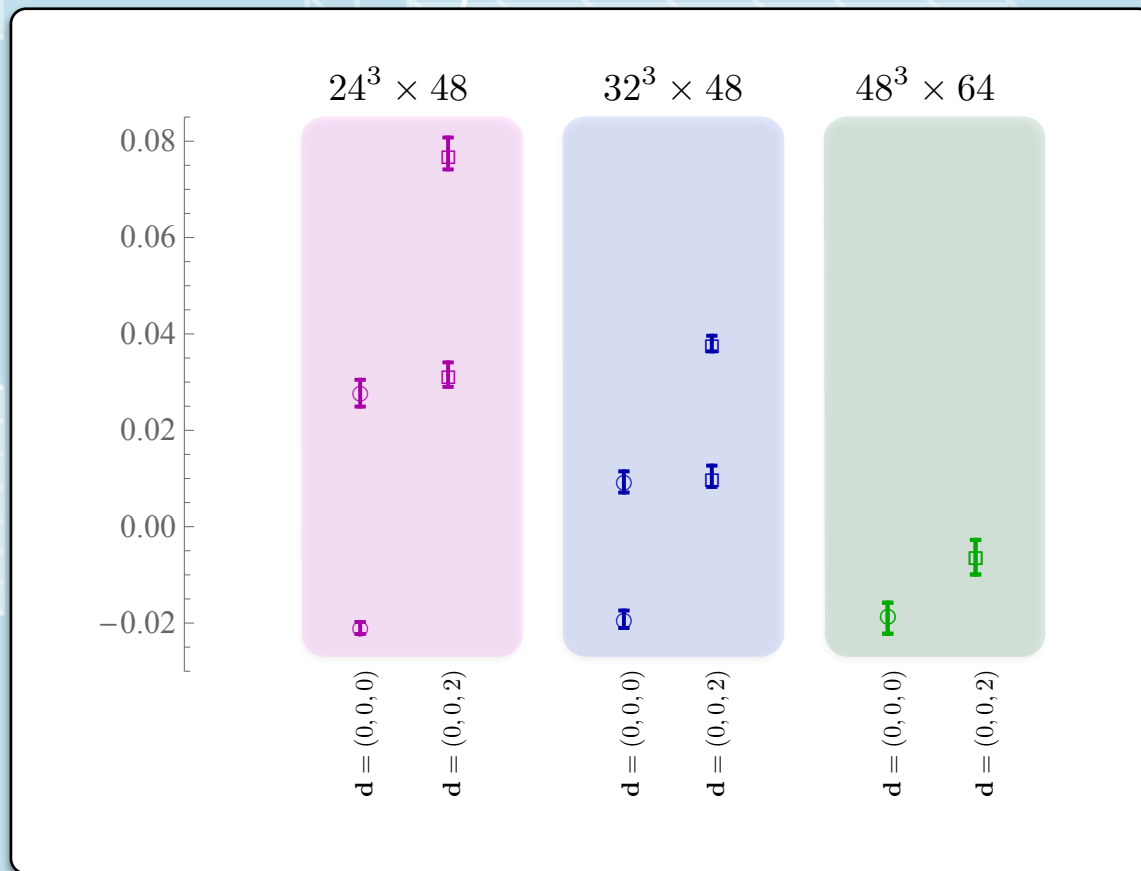
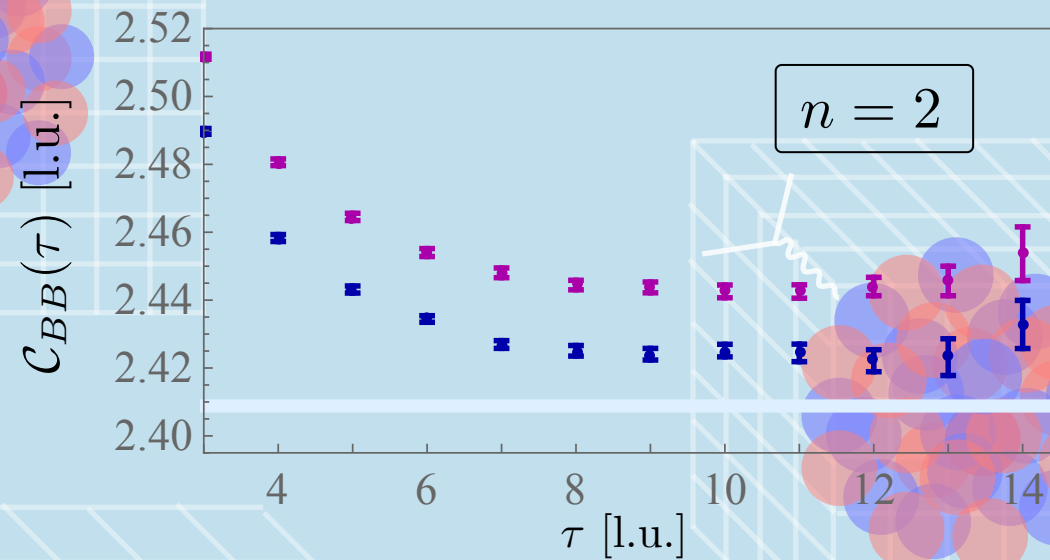
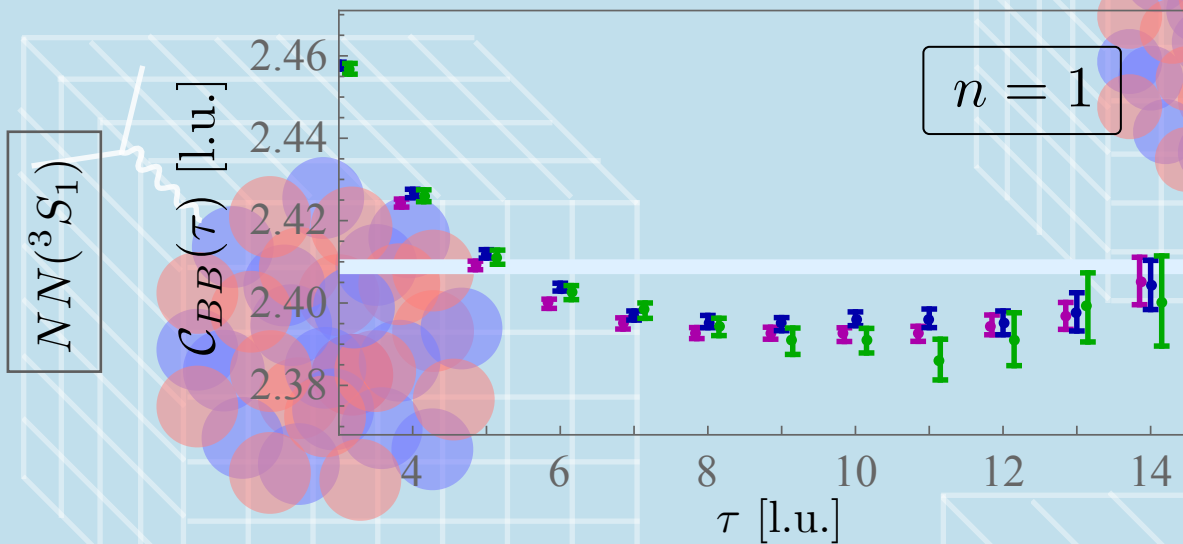
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Step 1: Obtain the lowest-lying spectra

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



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

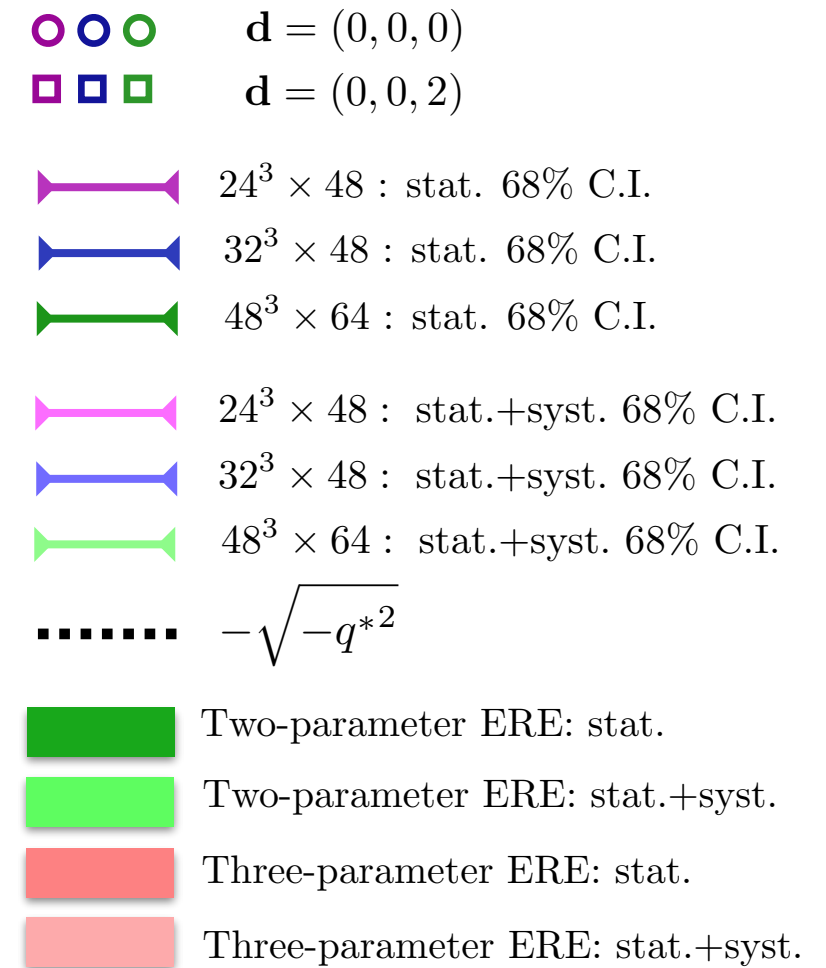
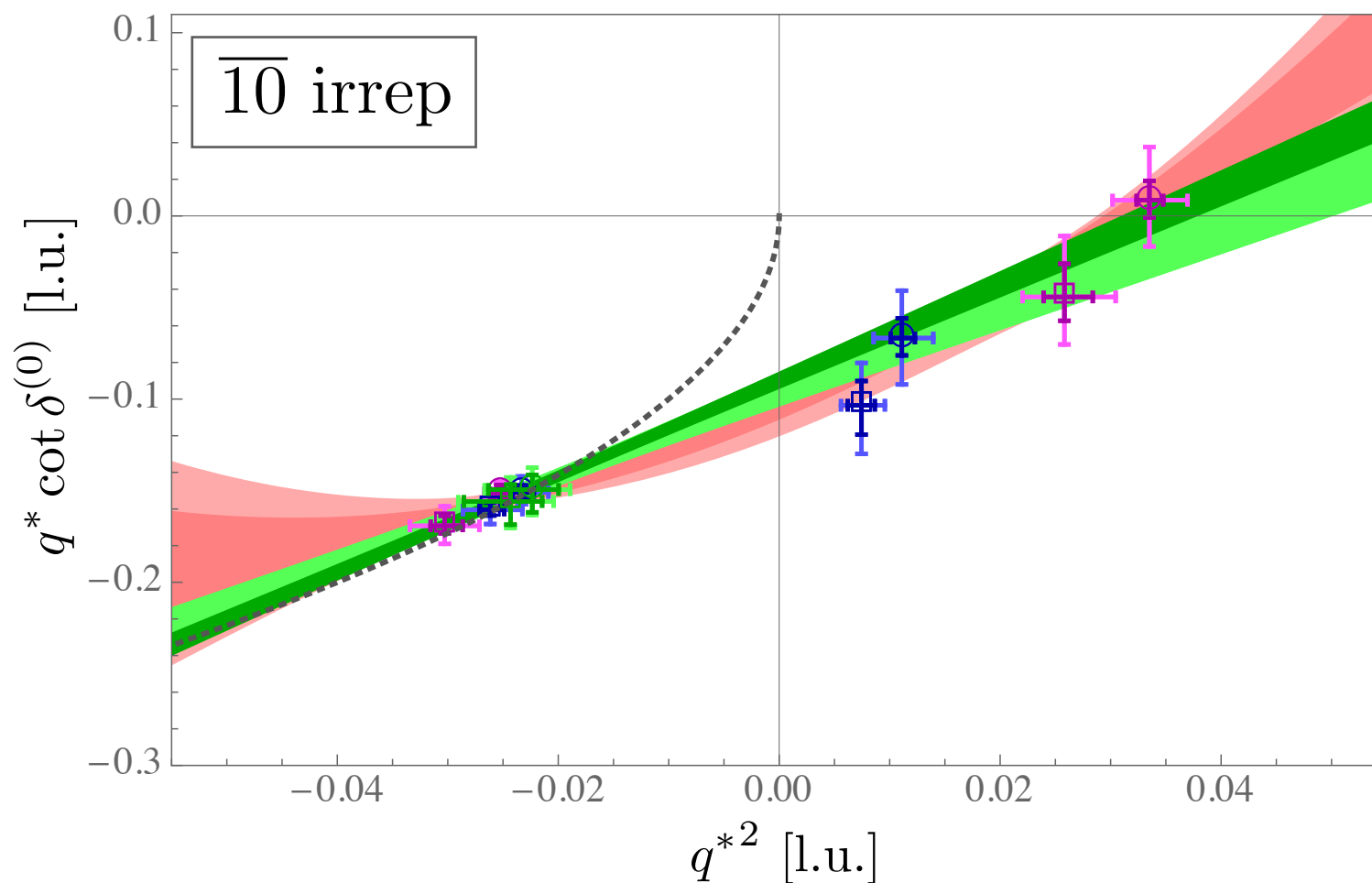
$$q^* \cot \delta^{(0)} = 4\pi c_{00}^0(q^{*2})$$

S-wave phase shift

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

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

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



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

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



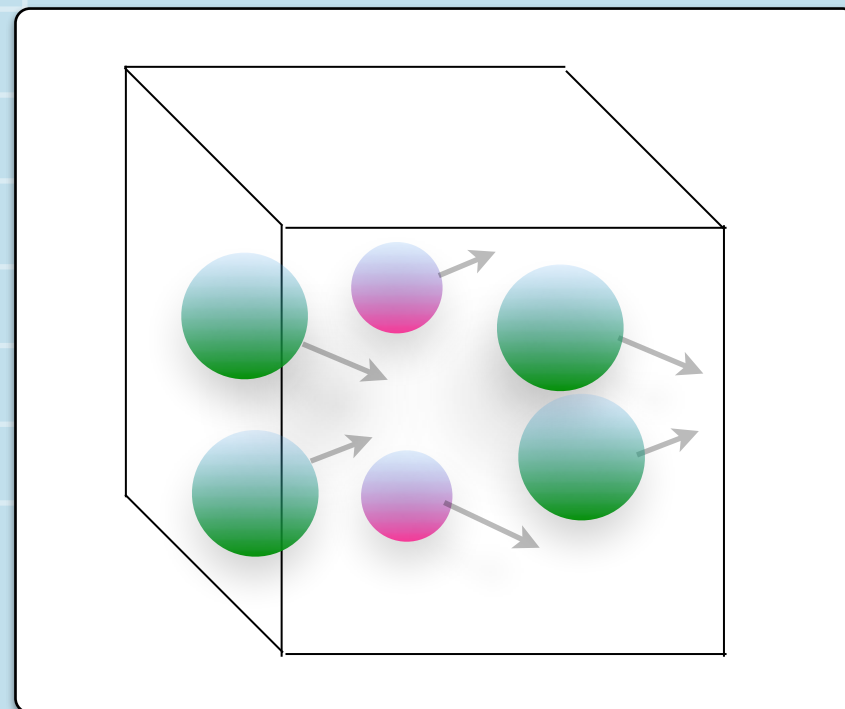
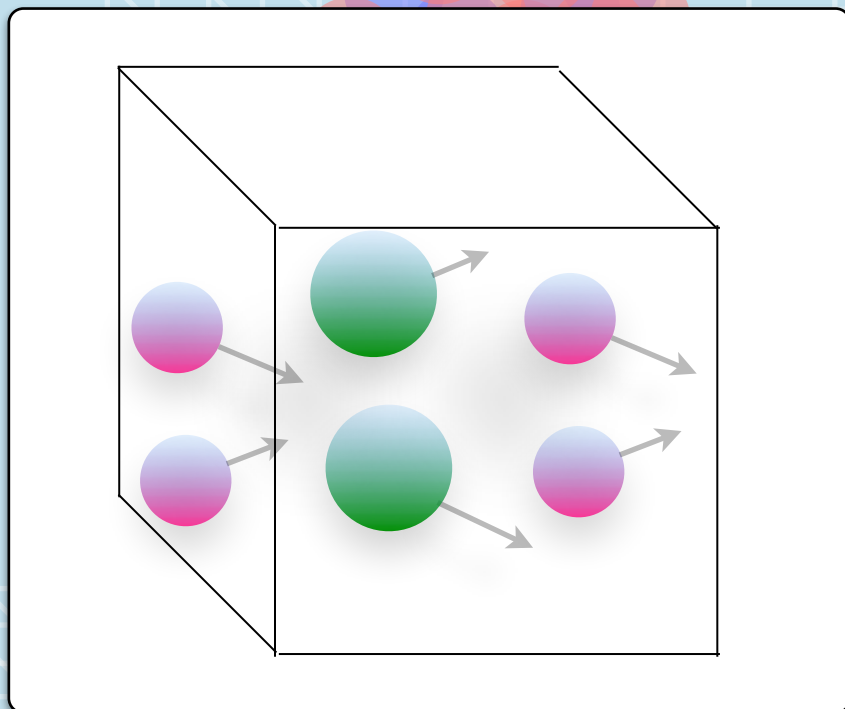
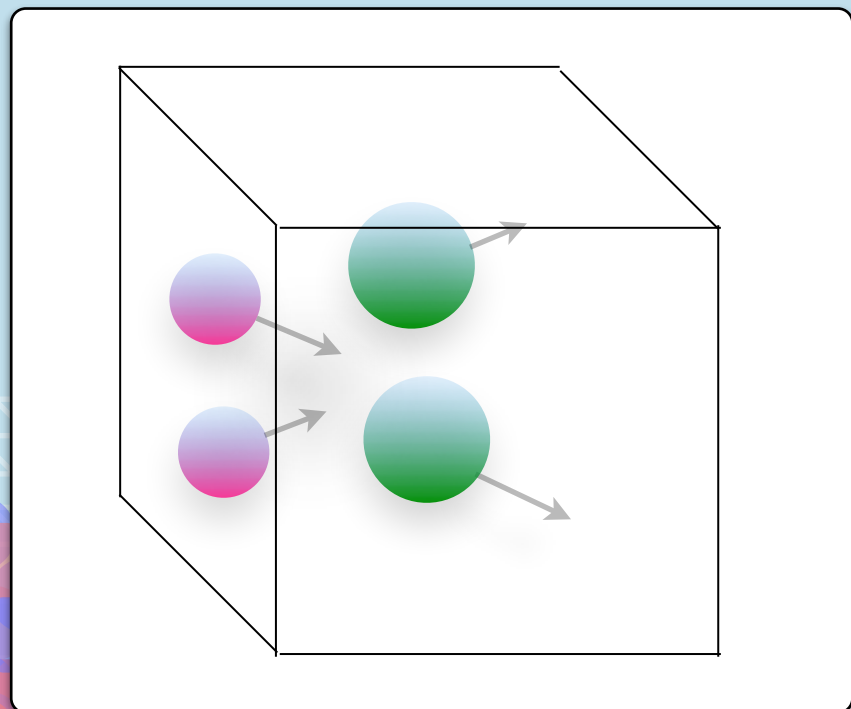
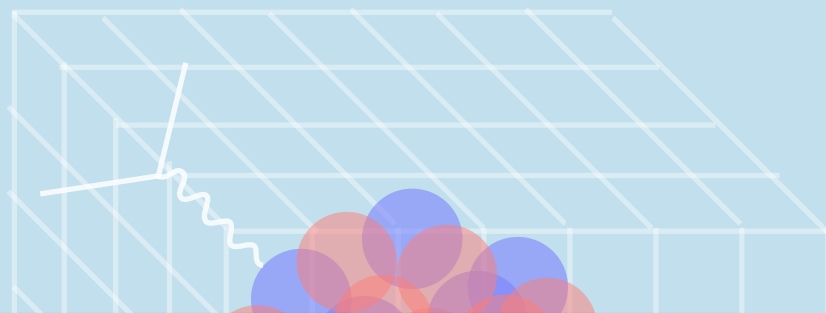
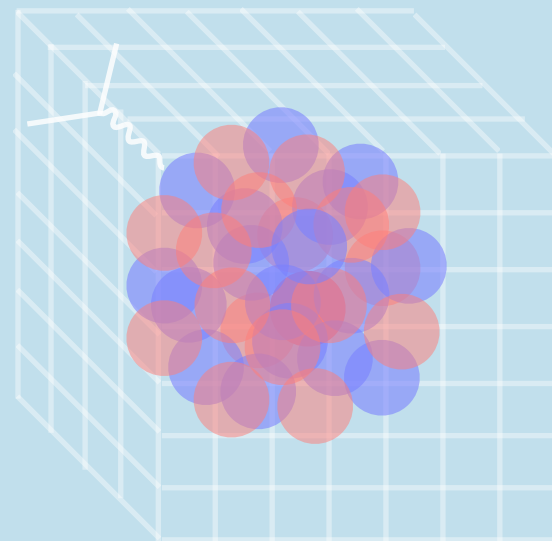
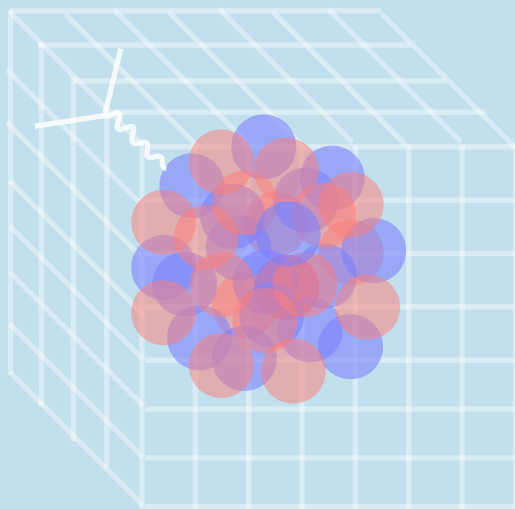
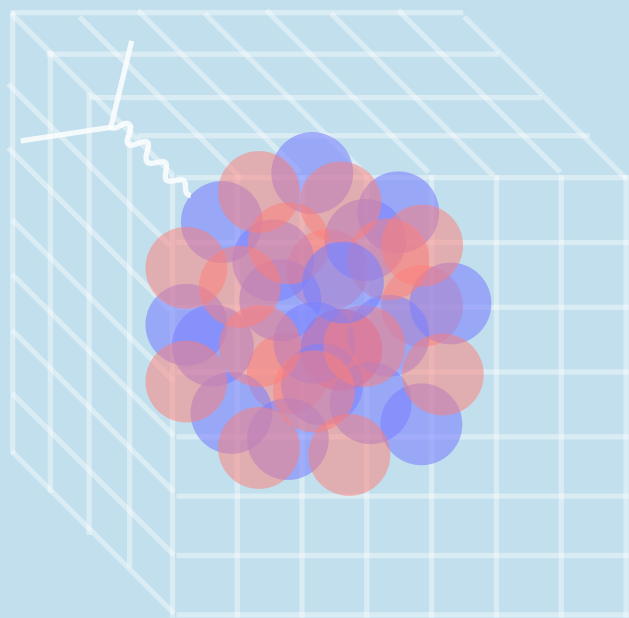
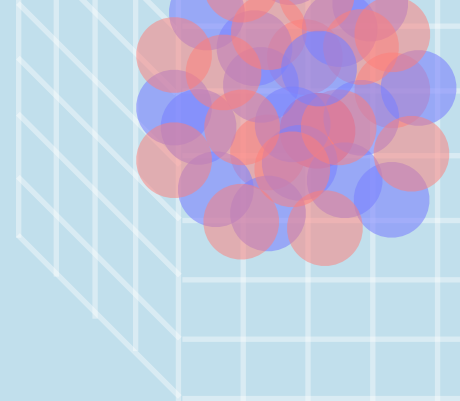
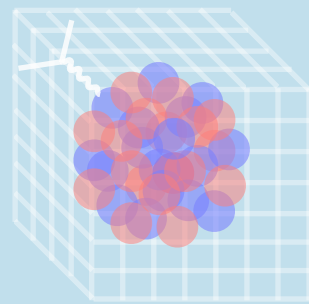
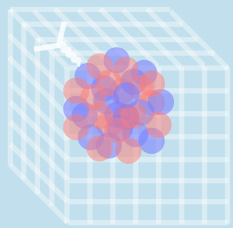
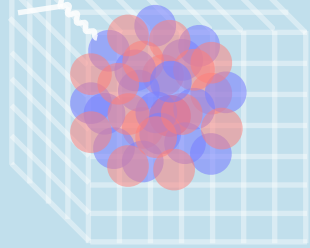
iii) Finite-volume formalism for coupled-channel two-hadron elastic scattering and resonances

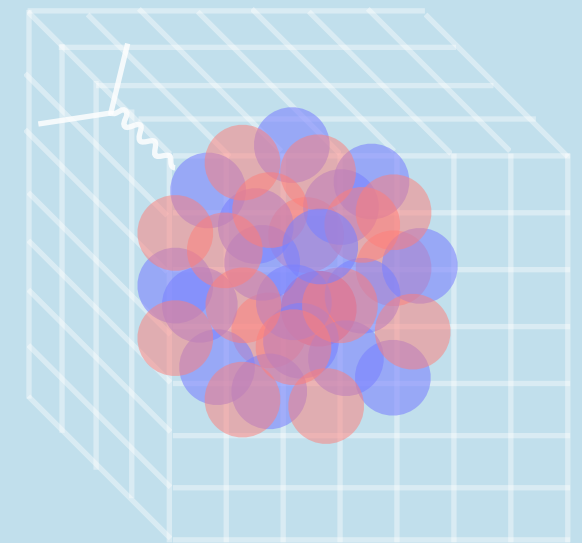
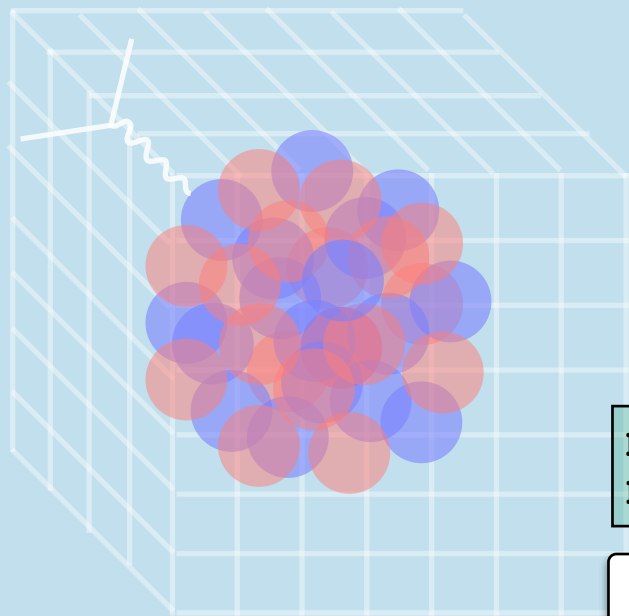
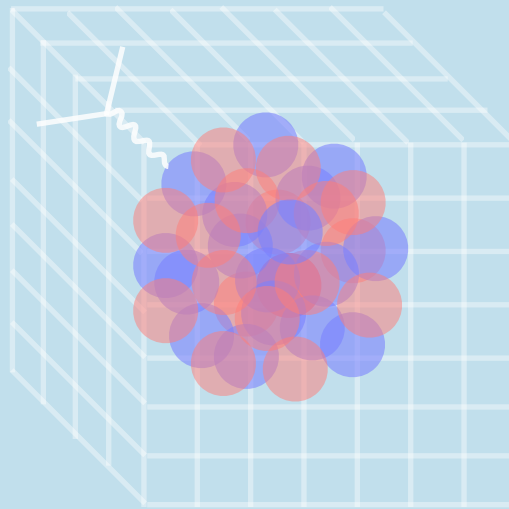
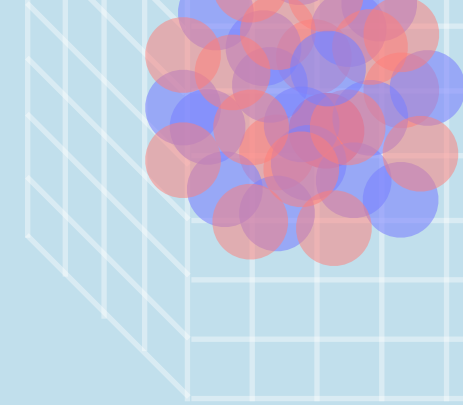
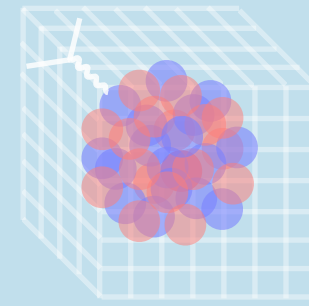
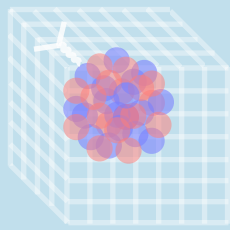
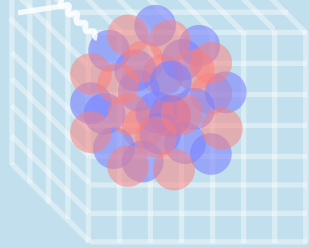
iv) Finite-volume formalism for transition amplitudes and resonance form factors

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).

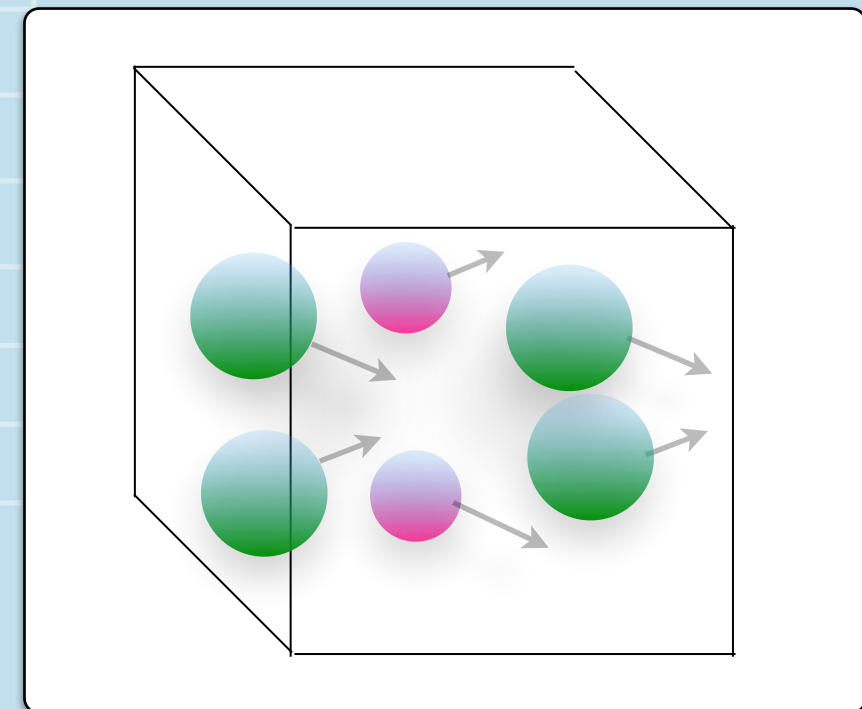
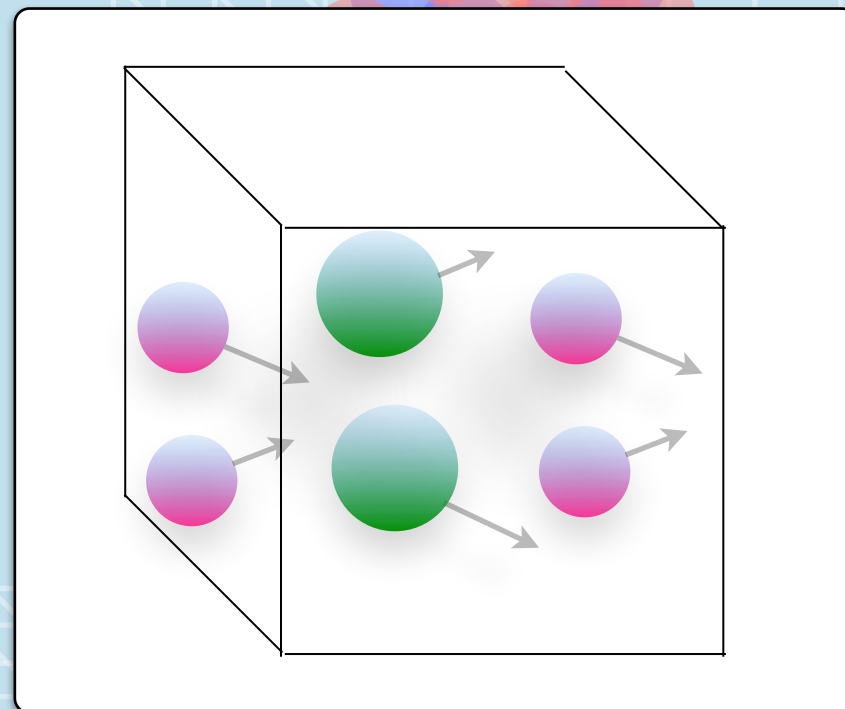
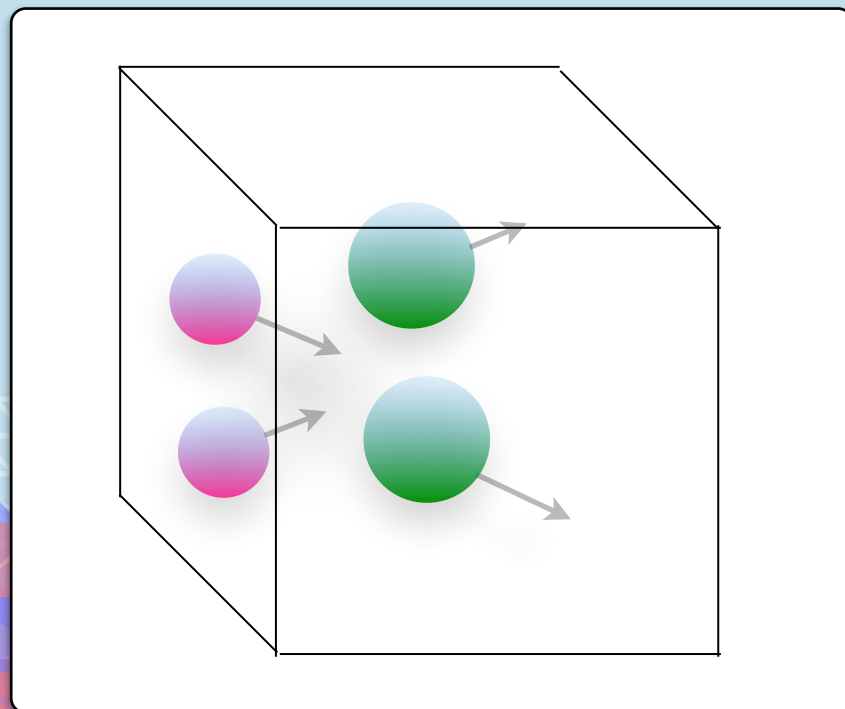




Briceno and ZD, Phys. Rev. D88, 094507 (2013).

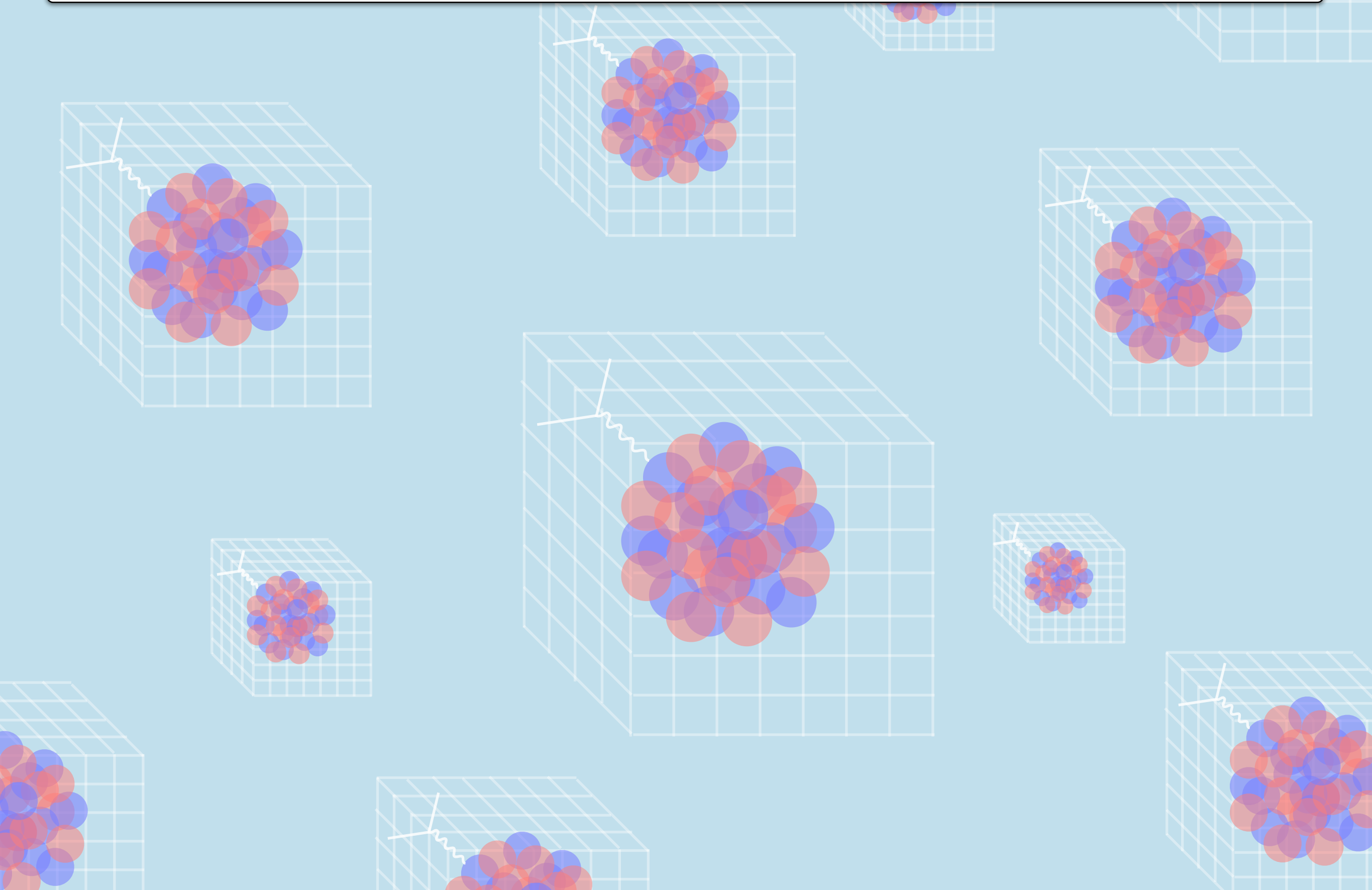
Hansen and Sharpe, Phys. Rev. D86, 016007 (2012).

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



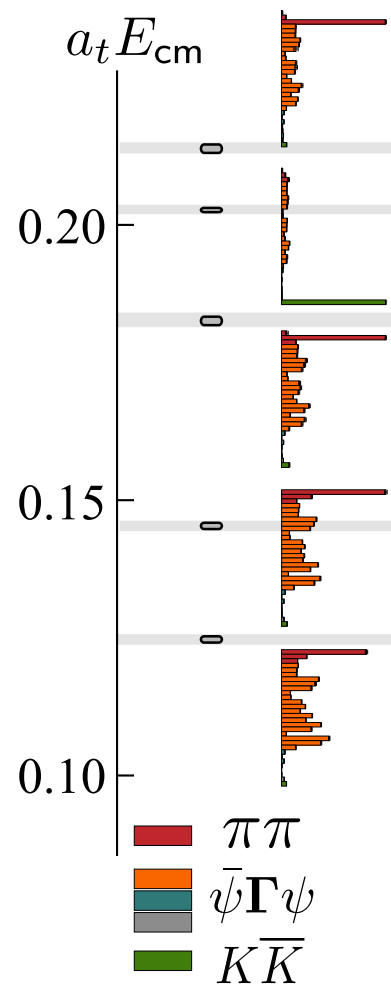
Now let's see an application of the coupled-channel formalism: Hunting resonances using lattice QCD in the P-wave coupled $\pi\pi - K\bar{K}$ channel

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



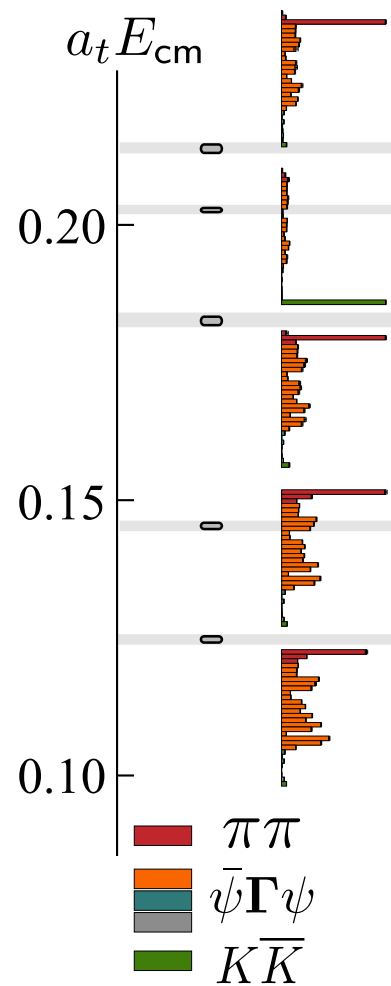
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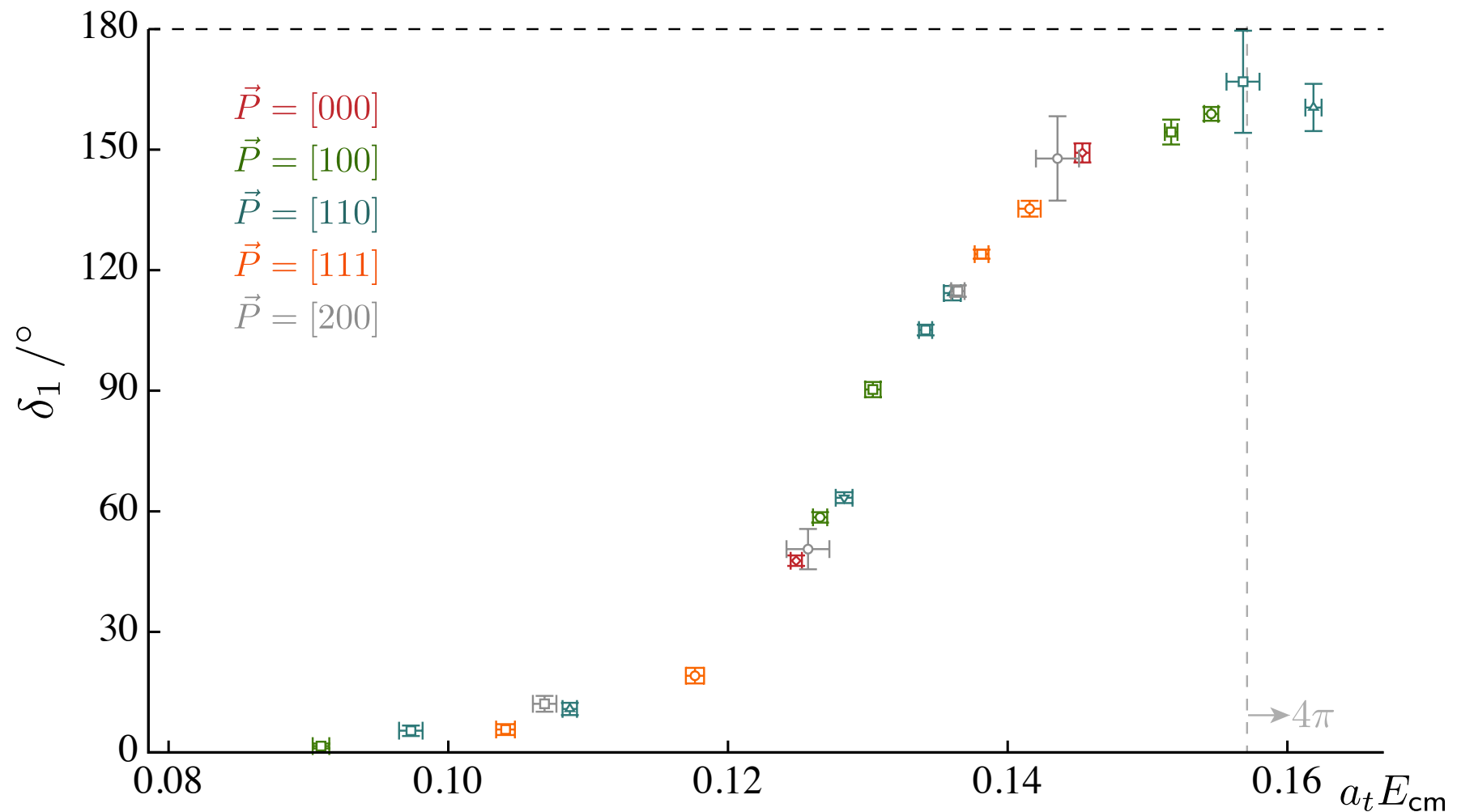


Example: T1 irrep
energies

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

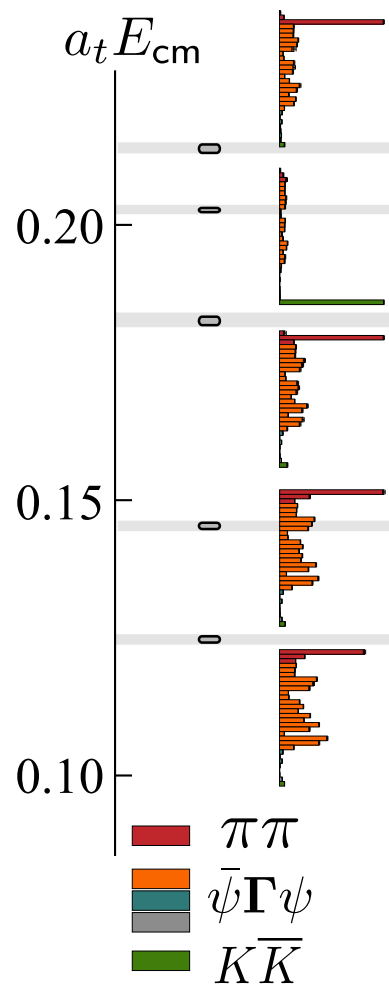


Example: T1 irrep
 energies

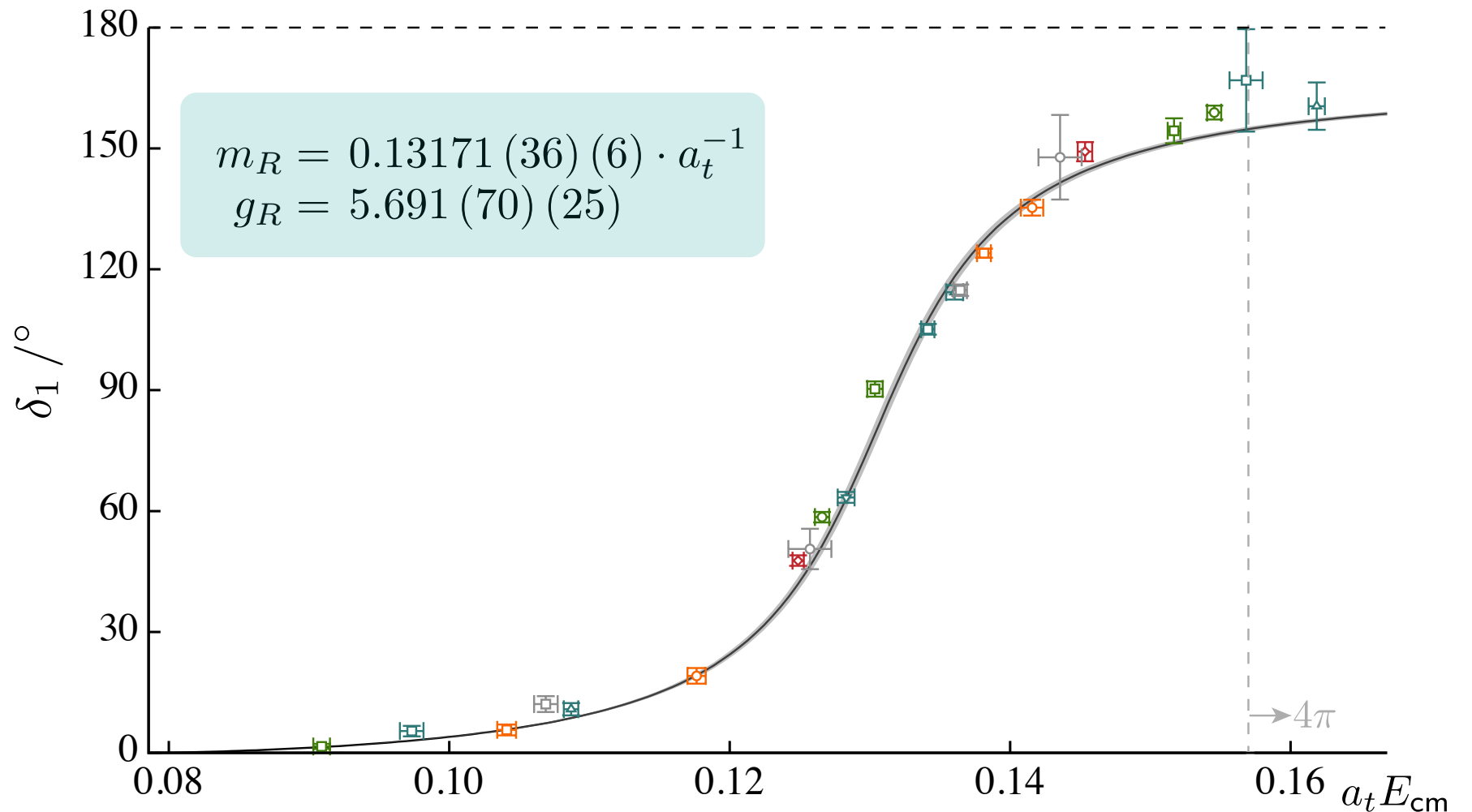


P-wave $\pi\pi$ phase shift as a function of energy

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



Example: T1 irrep energies



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

$$\rho_i(E_{\text{cm}}) = 2\bar{k}_i/E_{\text{cm}}$$

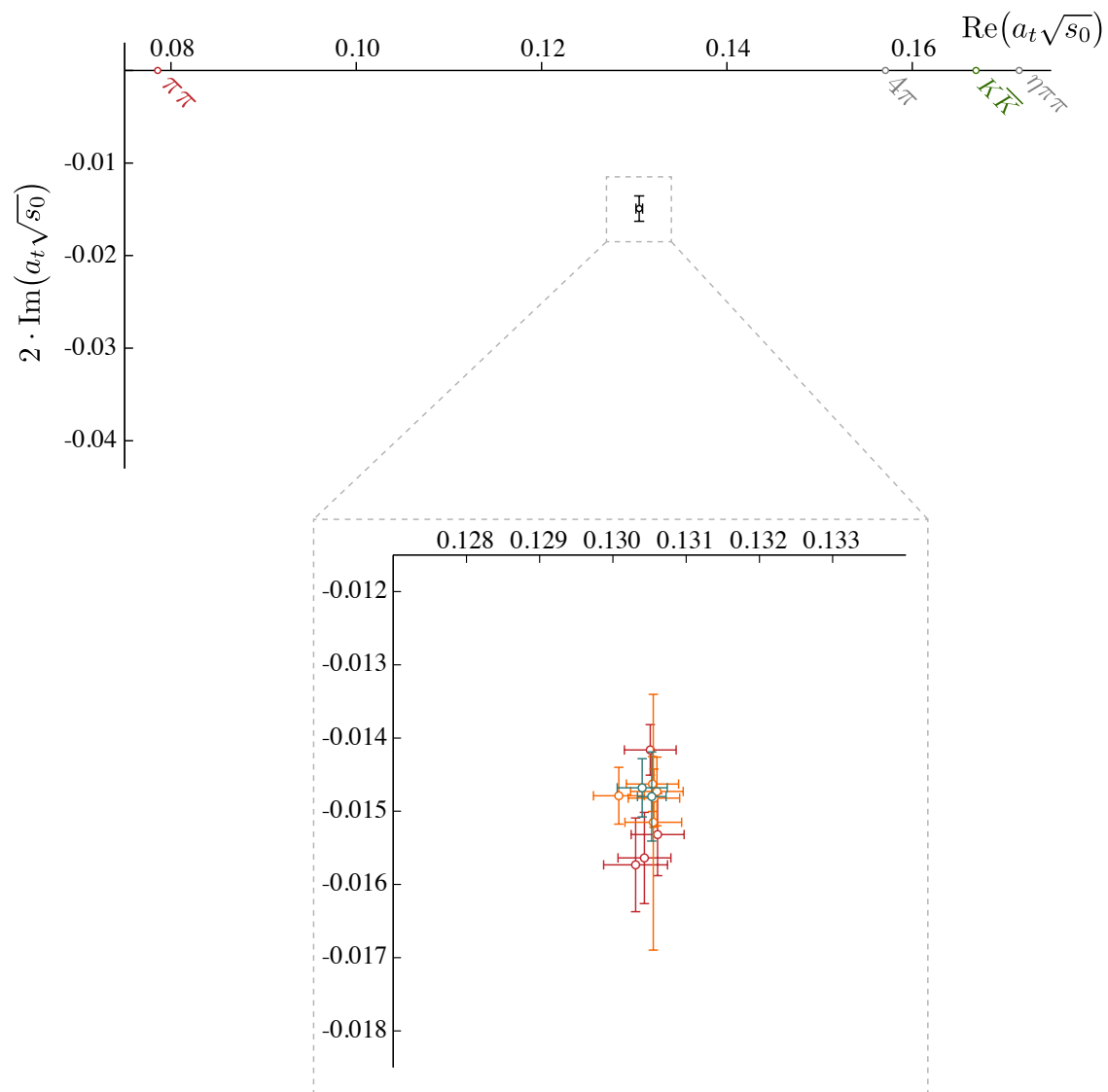
$$s = E_{\text{cm}}^2$$

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

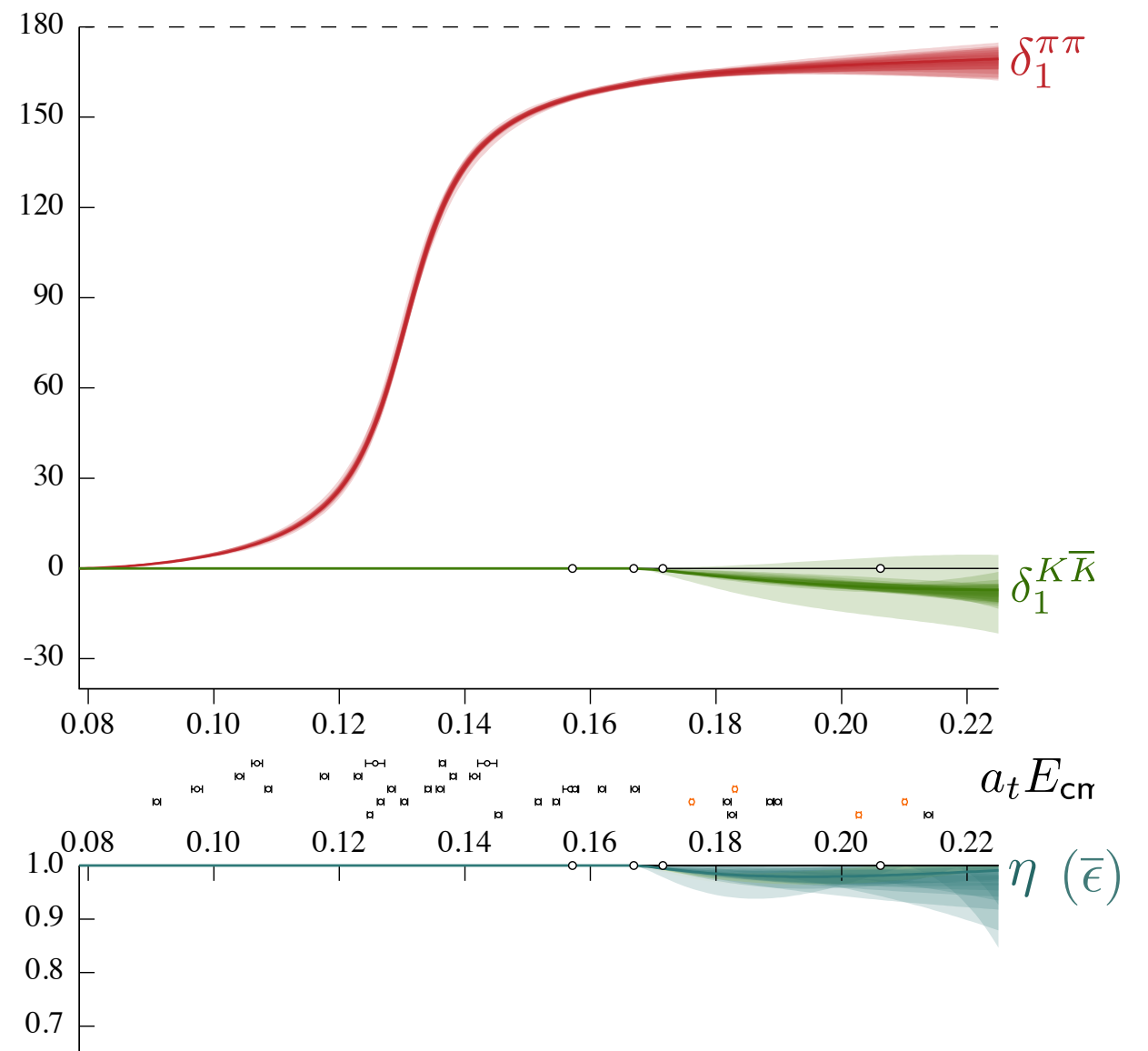
$$N_f = 2 + 1, m_\pi = 236 \text{ MeV}, V \approx (4 \text{ fm})^3$$

Using a range of parametrizations:

Pole position:



All three scattering parameters:



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

SUMMARY OF LECTURE I

Lattice QCD workflow

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...

The background of the slide features a repeating pattern of nucleon clusters. Each cluster is represented as a collection of overlapping red and blue spheres, resembling a nucleus, situated within a white 3D wireframe cube that represents a lattice. The clusters vary in size and orientation across the scene. A white zigzag line, representing a gluon field, is visible on the top surface of each cube.

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

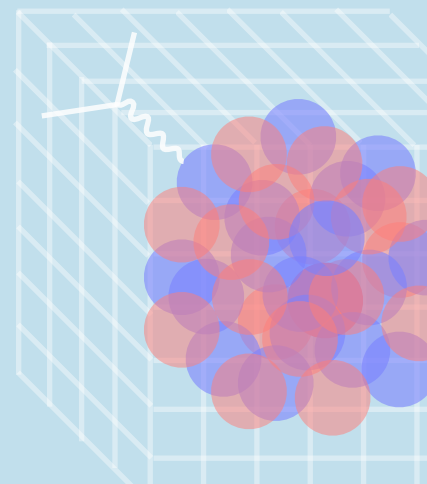
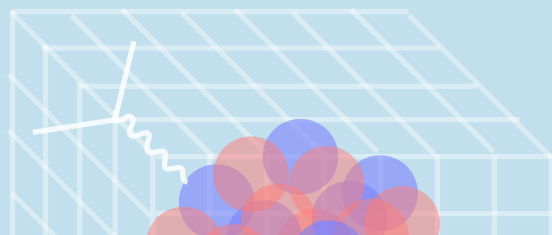
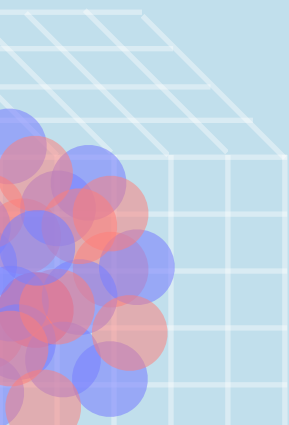
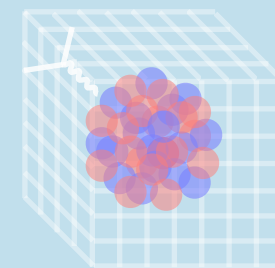
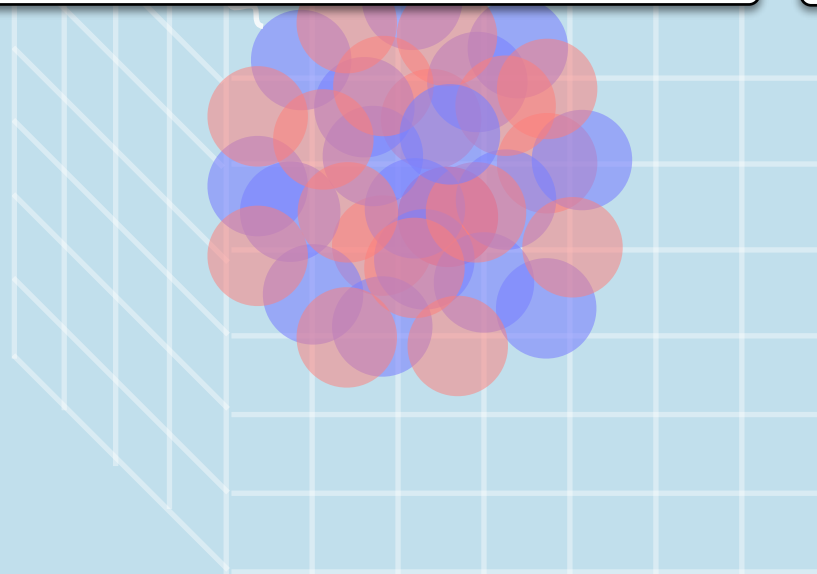
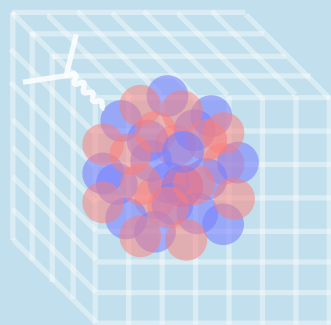
For e.g., form factors, moments of structure functions, Compton amplitude, transition amplitudes

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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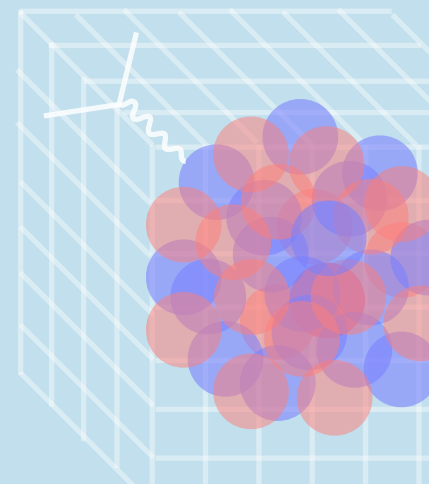
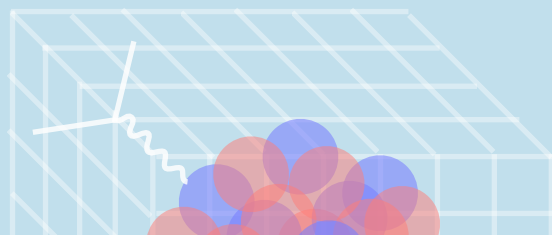
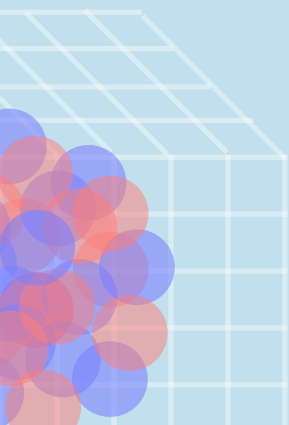
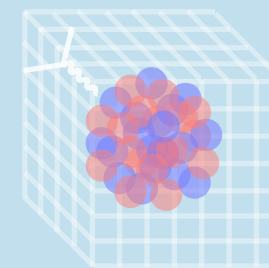
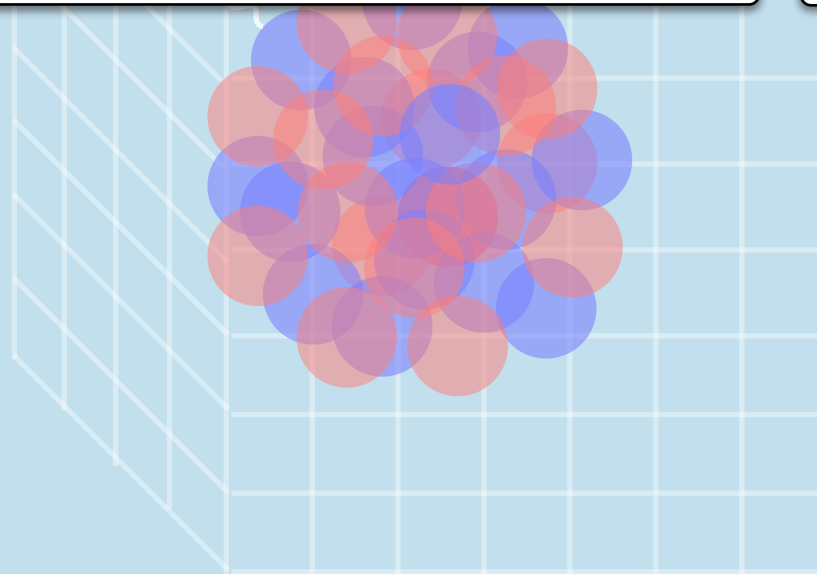
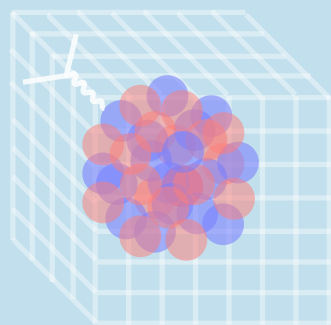
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A three-point (3pt)
function:

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

Chambers, [http://inspirehep.net/
record/1744874/](http://inspirehep.net/record/1744874/)

Annihilate the state

Insert the
operator

Create the state

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Spectral decomposition of the 3pt function in Euclidean spacetime

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

A complete set of states

Another complete set of states

A three-point (3pt) function:

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A complete set of states

Another complete set of states

Long-separation behavior dominated by ground states

$$G_{\chi\mathcal{O}\tilde{\chi}}(\mathbf{p}', \mathbf{p}; t', \tau, t) \xrightarrow{\text{large } t'-\tau, \tau-t} \frac{e^{-E_{X_0}(\mathbf{p}')(t'-\tau)}}{2E_{X_0}(\mathbf{p}')} \frac{e^{-E_{X_0}(\mathbf{p})(\tau-t)}}{2E_{X_0}(\mathbf{p})} \sum_{r', r} \langle \Omega | \chi(0) | X_0(\mathbf{p}', r') \rangle \langle X_0(\mathbf{p}', r') | \mathcal{O}(0) | X_0(\mathbf{p}, r) \rangle \langle X_0(\mathbf{p}, r) | \tilde{\chi}(0) | \Omega \rangle$$

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:

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Annihilate the state

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Spectral decomposition of the 3pt function in Euclidean spacetime

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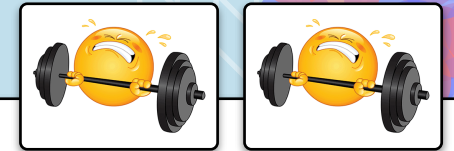
If there are degenerate ground states

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

Taking a proper ratio to 2pt functions

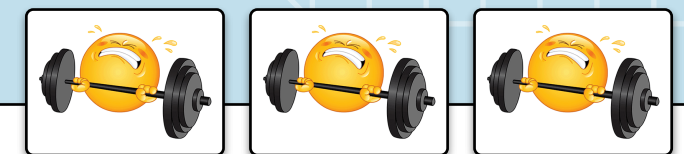
$$R_{\chi\mathcal{O}\tilde{\chi}}(\mathbf{p}', \mathbf{p}; t', \tau, t) \xrightarrow{\text{large } t'-\tau, \tau-t} \propto \langle X_0(\mathbf{p}', r') | \mathcal{O}(0) | X_0(\mathbf{p}, r) \rangle$$

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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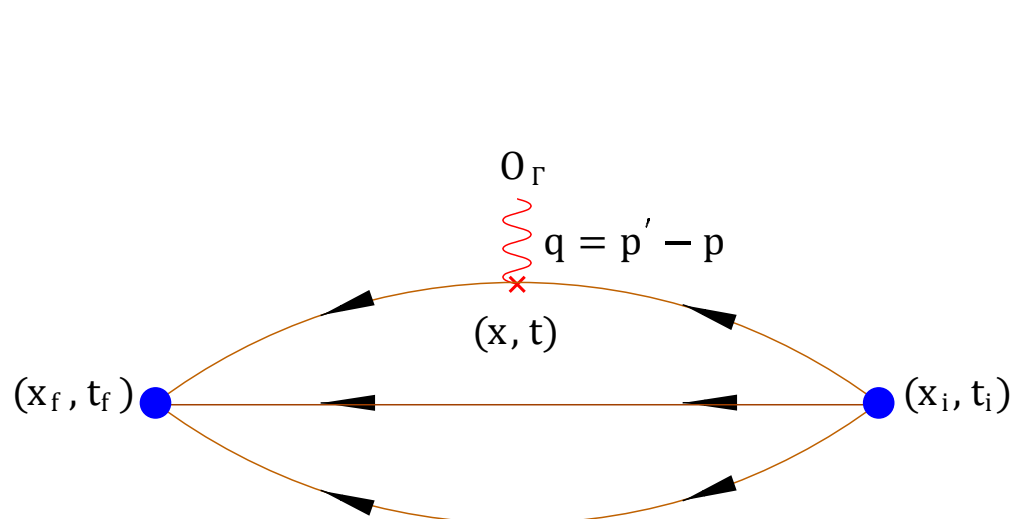
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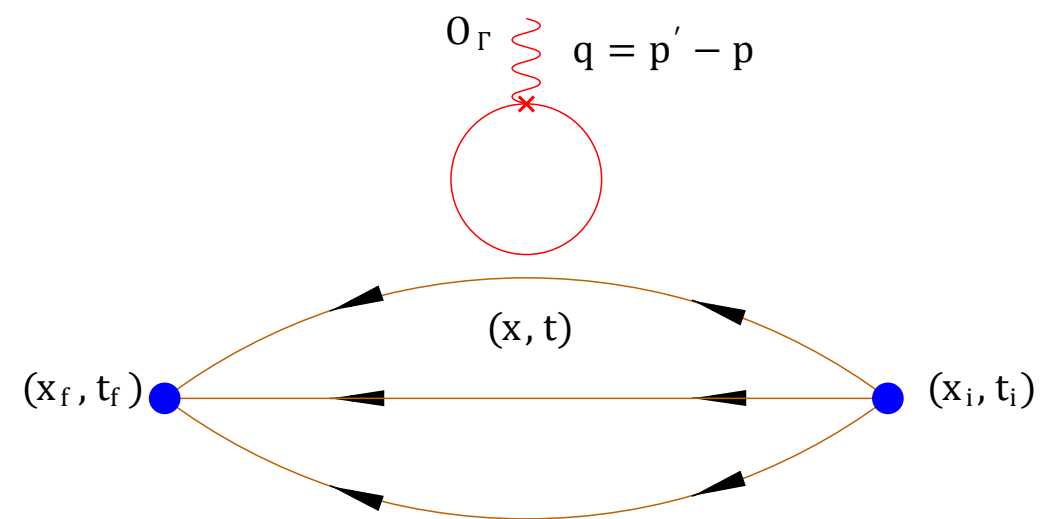
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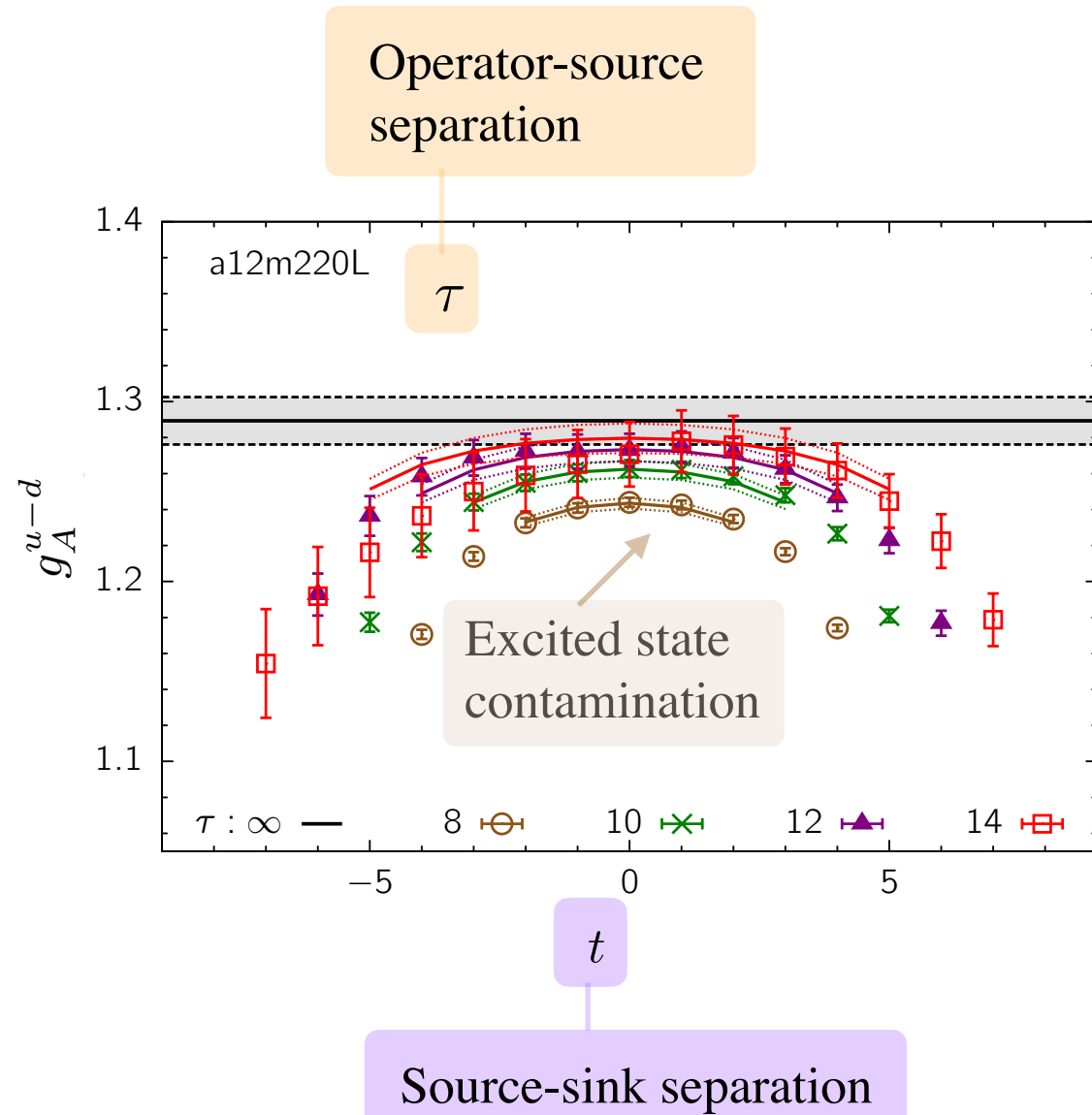
Connected contribution



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

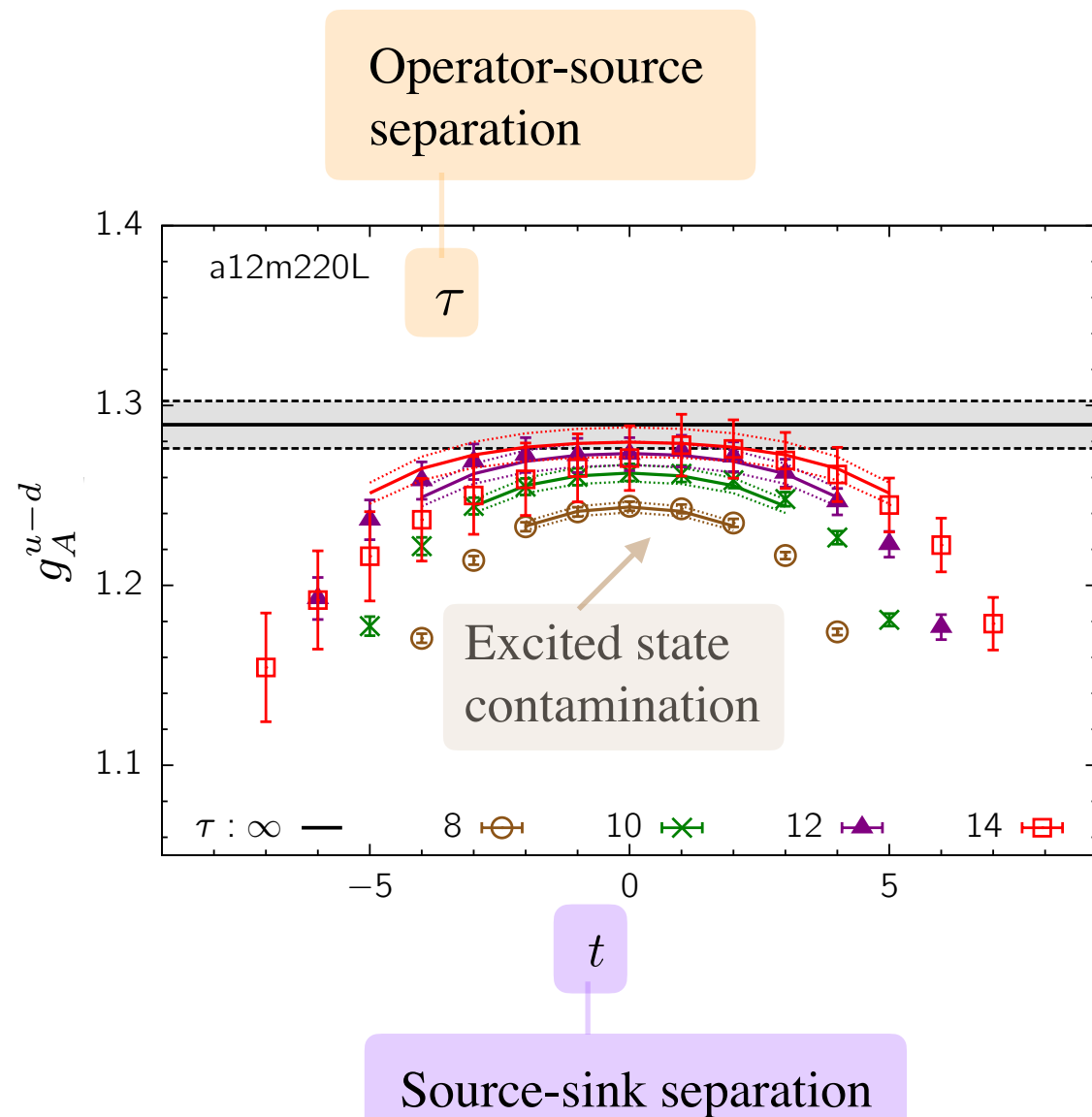
Gupta et al (PNDME), Phys. Rev. D 98, 034503 (2018)



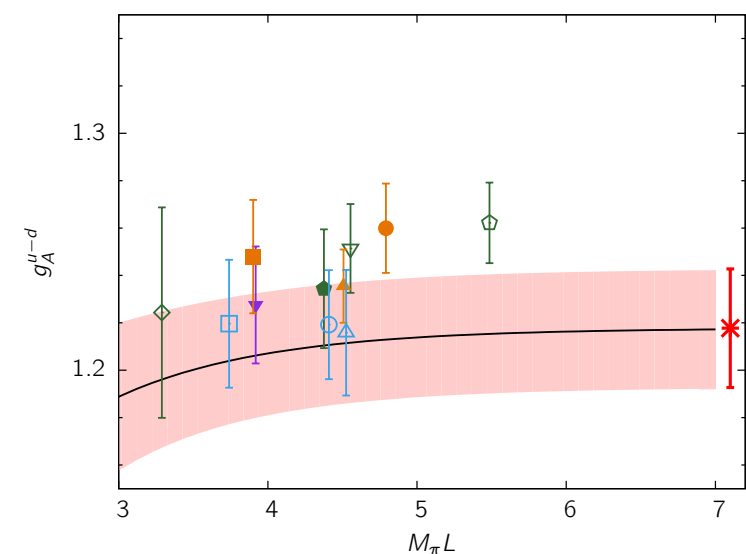
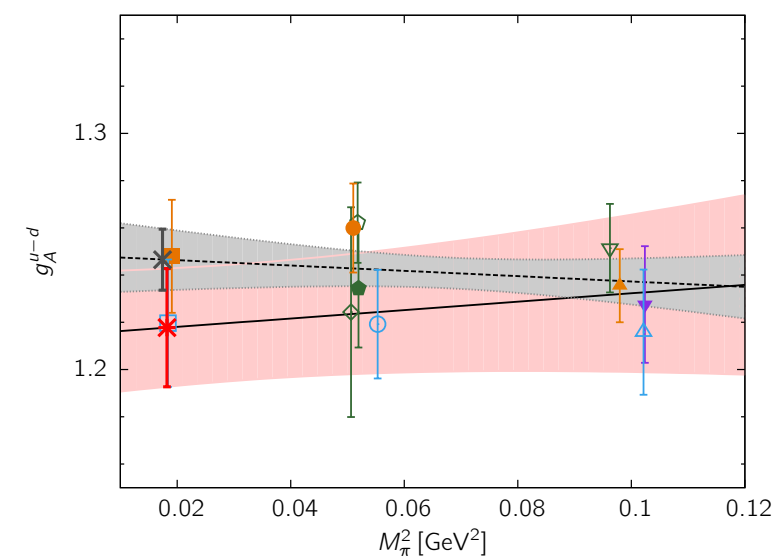
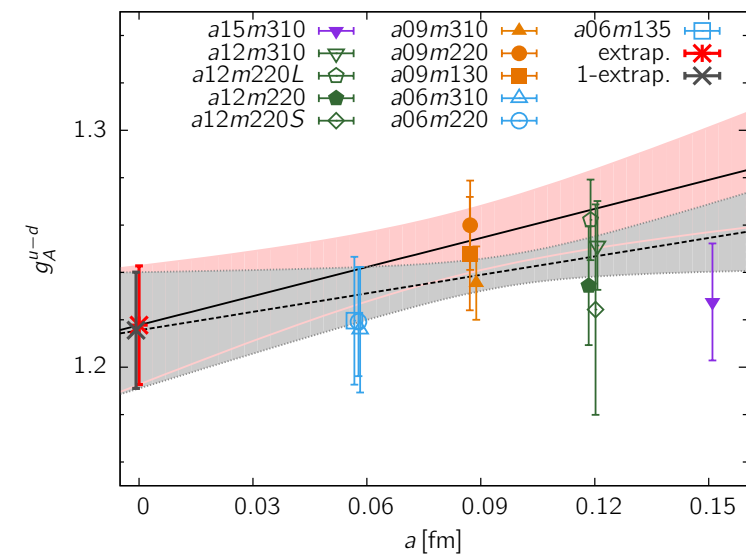
3pt function for a single lattice spacing, volume and quark masses

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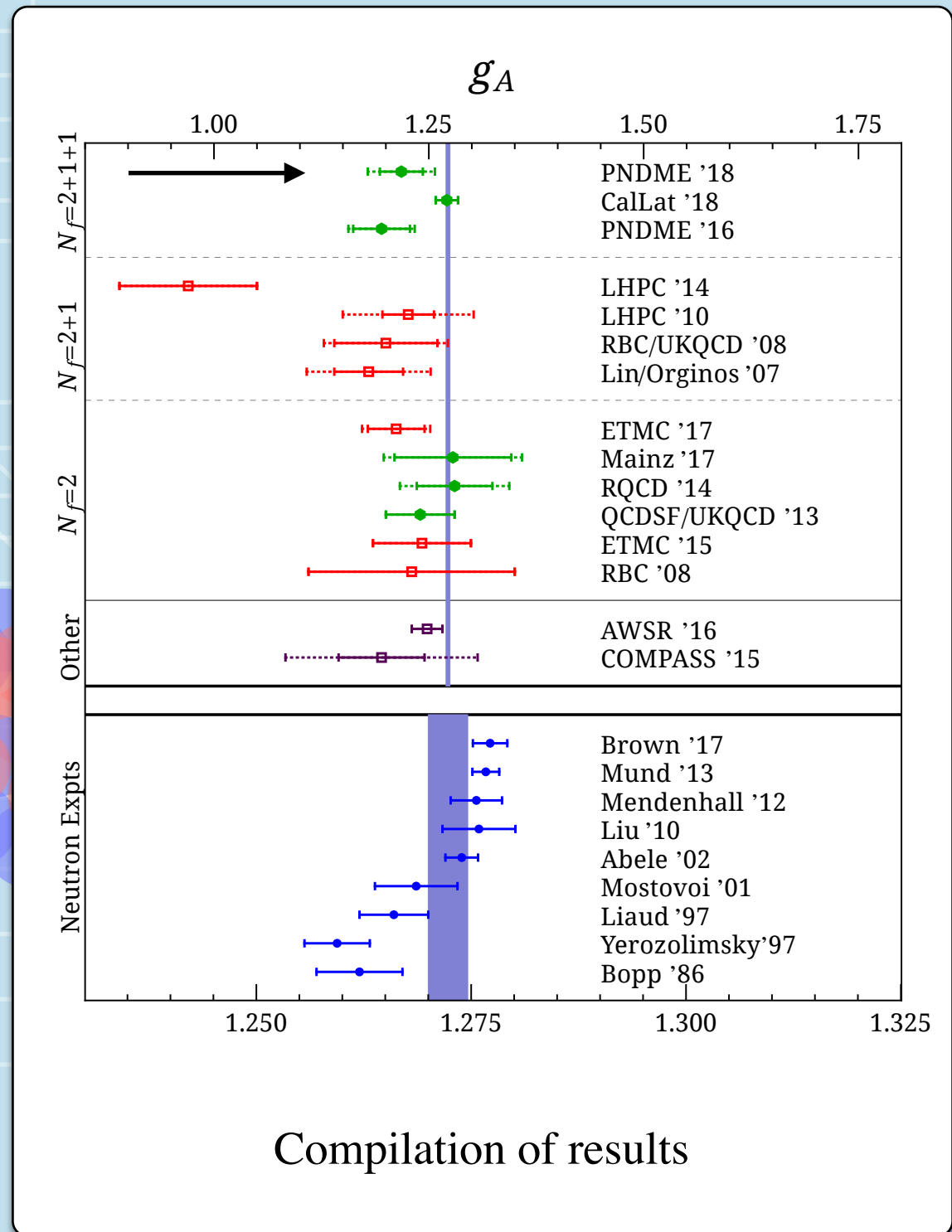
3pt function for a single lattice spacing, volume and quark masses



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

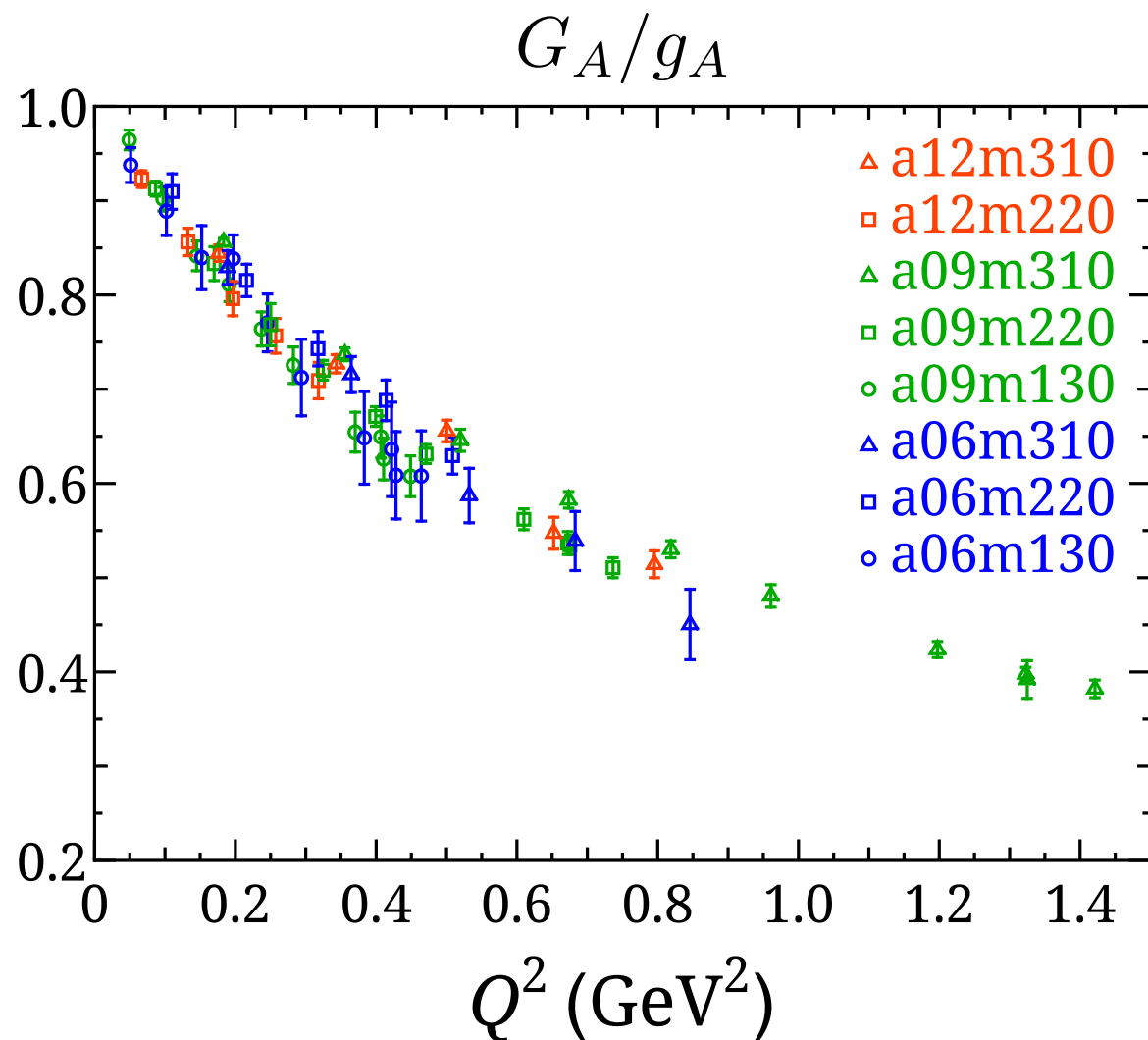
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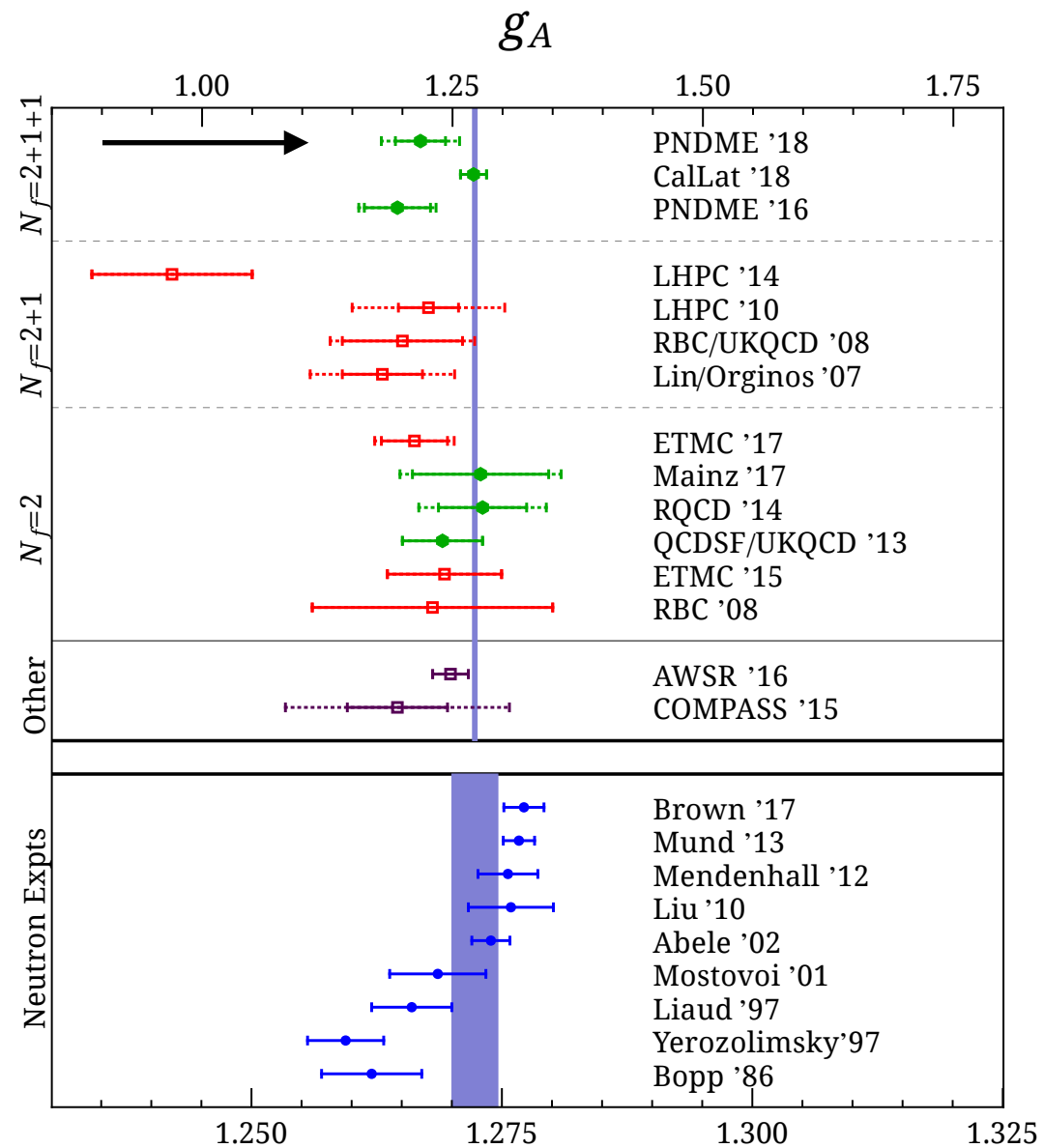
Example: The application of 3pt function method to obtain the axial charge/form factors of the nucleon

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).

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

Quark spin

Quark orbital
angular
momentum

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

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Matrix elements needed

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

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

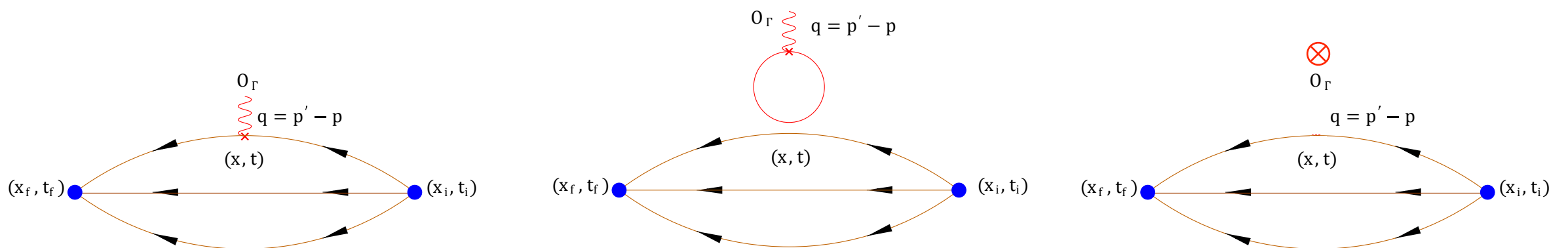
$$\langle N(p', s') | \mathcal{O}_g^{\mu\nu} | N(p, s) \rangle = \bar{u}_N(p', s') \Lambda_{\mu\nu}^g(Q^2) u_N(p, s)$$

With operators

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

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

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

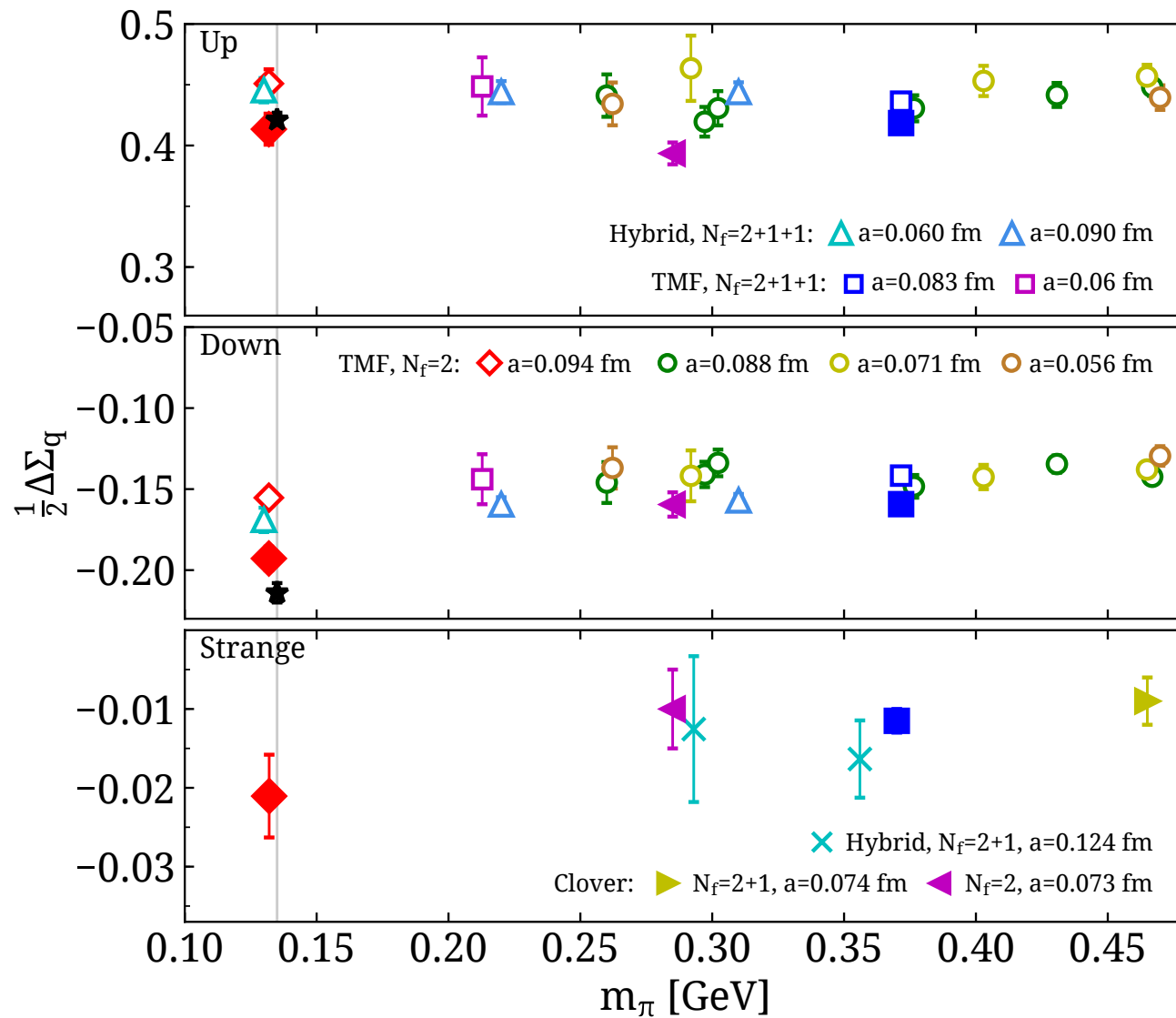


Quark contributions

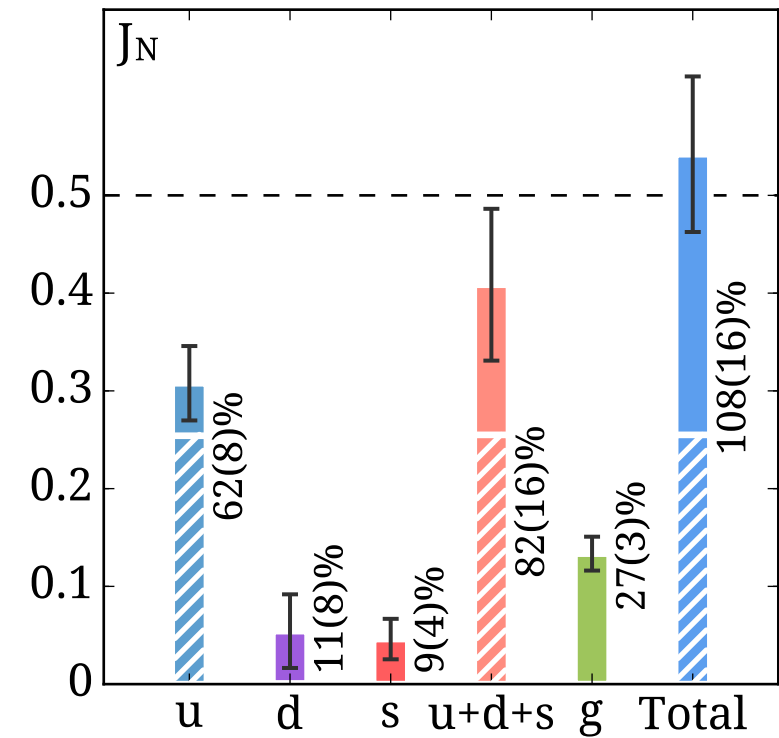
Quonic contribution

Example: The spin decomposition of the nucleon

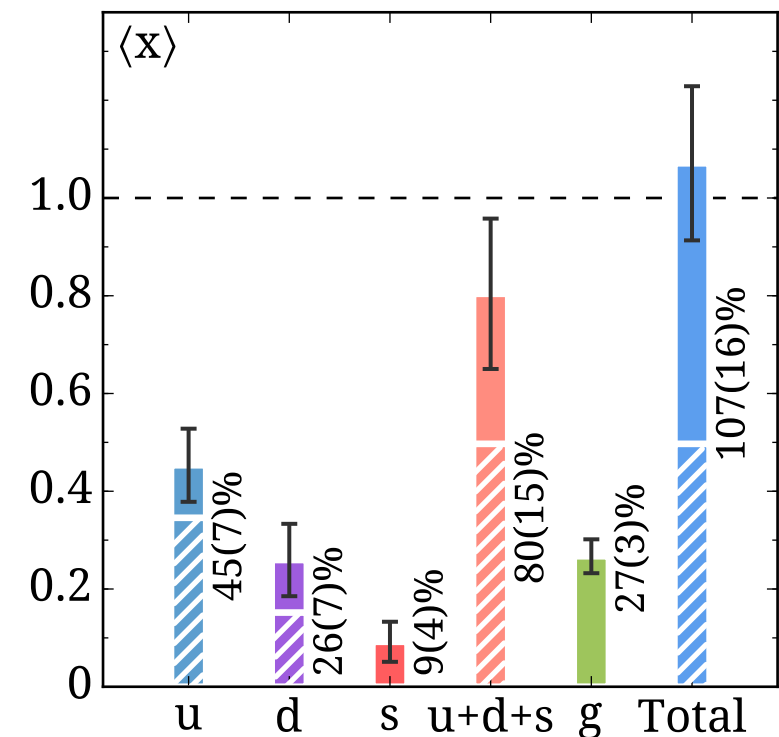
Alexandru, Phys. Rev. Lett. 119, 142002 (2017).



Quark spin contributions



Nucleon spin decomposition



Longitudinal momentum decomposition

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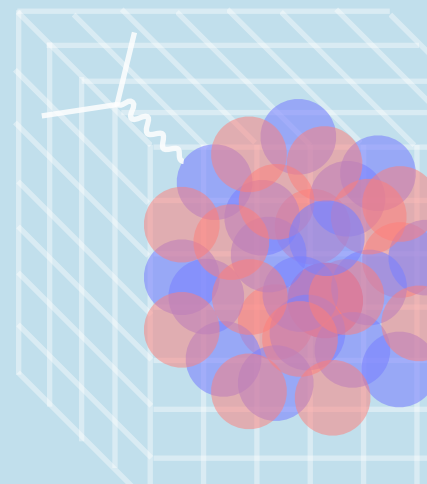
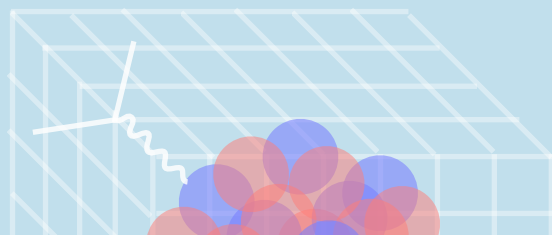
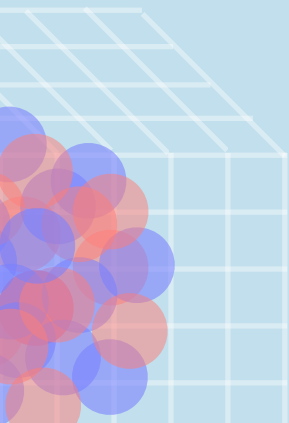
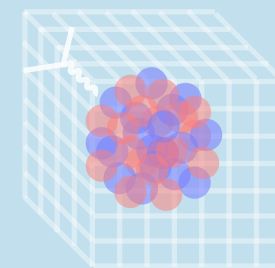
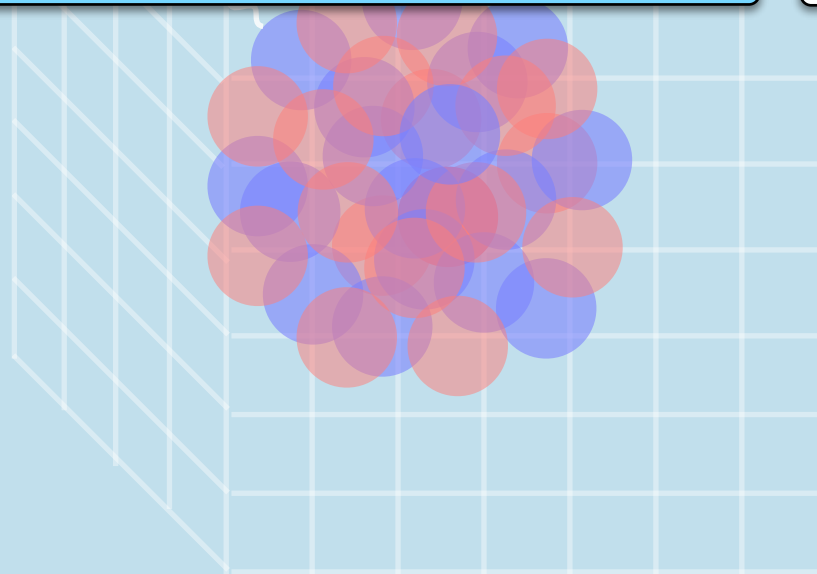
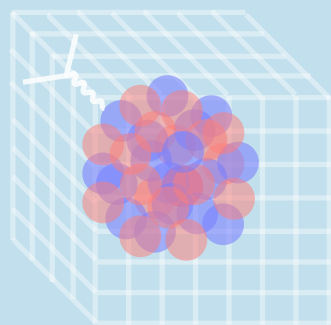
For e.g., form factors, moments of structure functions, Compton amplitude, transition amplitudes

Background-field methods

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

Feynman-Hellmann inspired methods

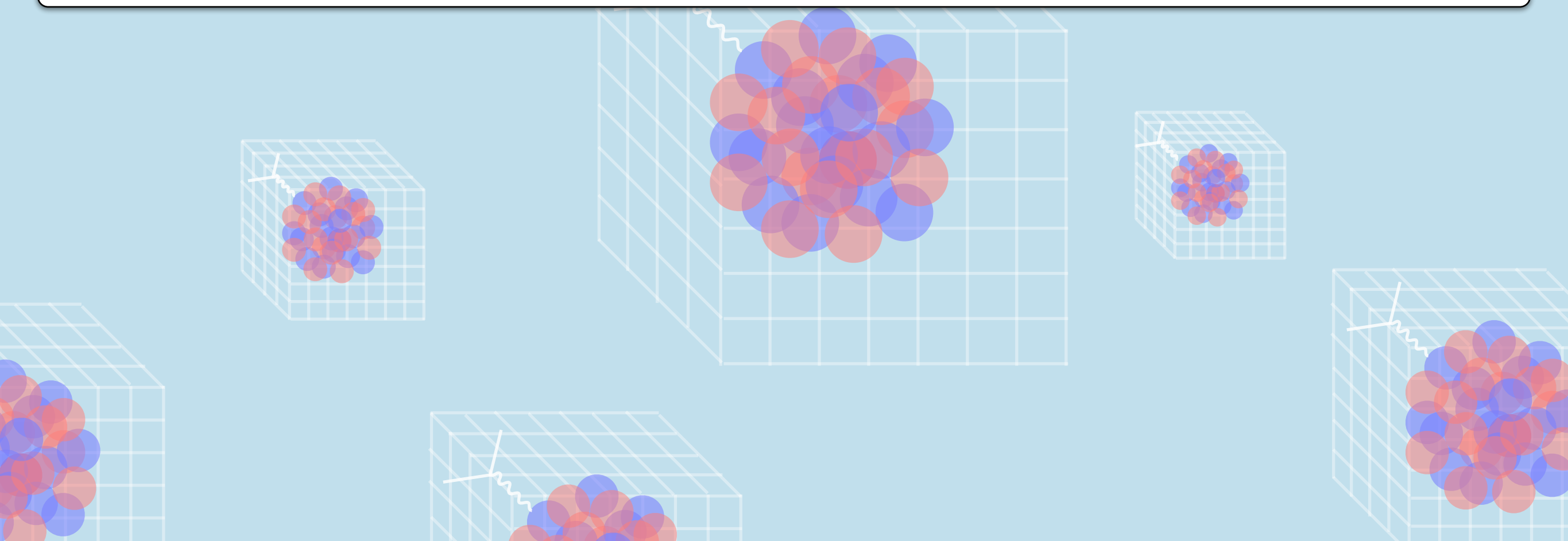
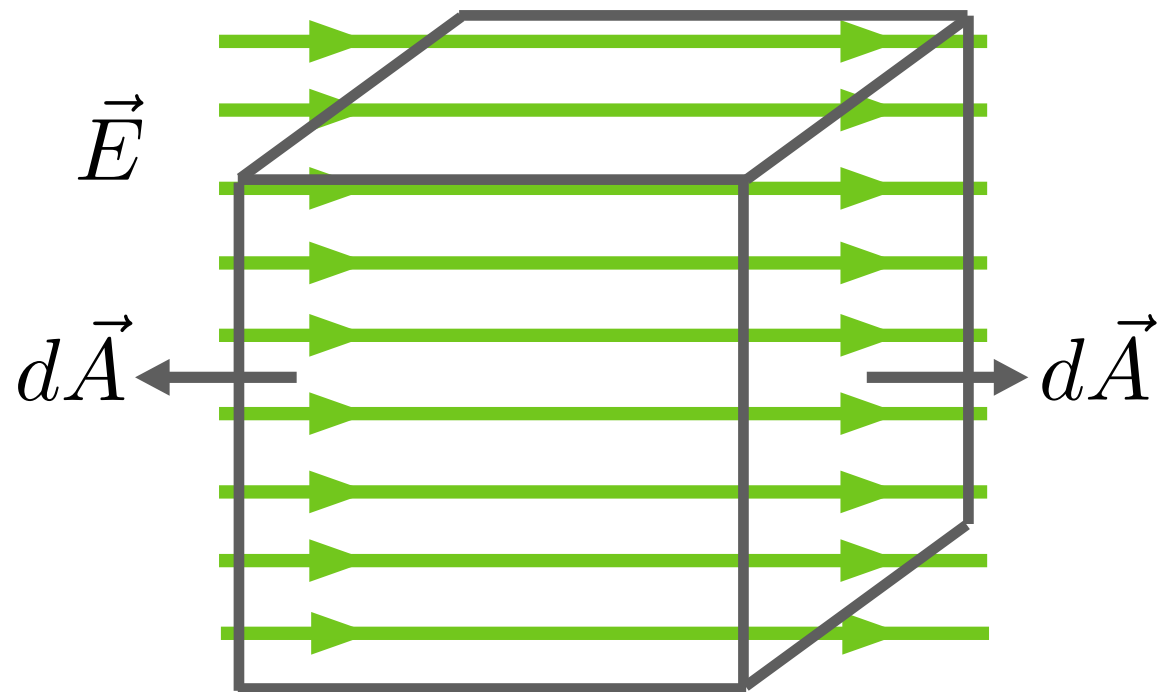
Similar to background fields. For e.g., axial charge, form factors, EM moments, transition amplitudes



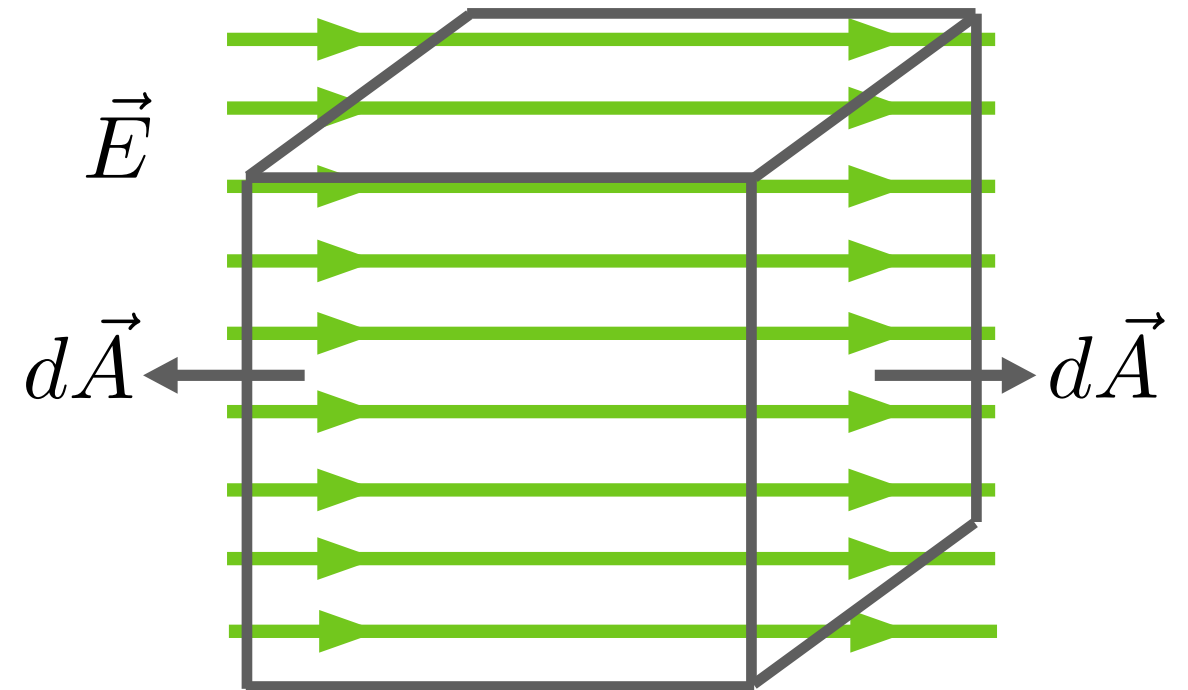
Background fields are non-dynamical, i.e., there will be no pair creation and annihilation in vacuum with a classical EM background field. This means the photon zero mode is no problem: it is absent in the calculation!

$$U(\text{QCD}) \rightarrow U(\text{QCD}) \times U(\text{QED})$$

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



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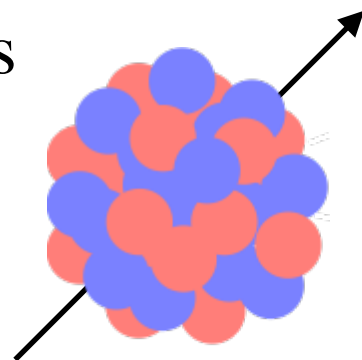


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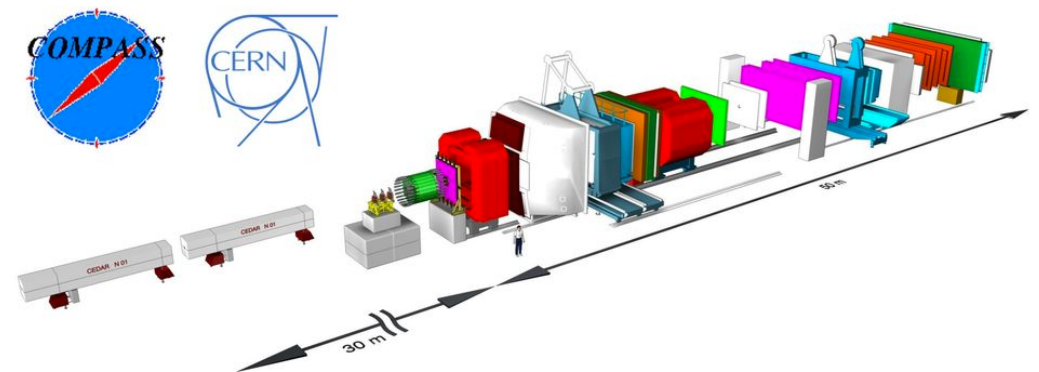
Modify the links when forming the quark propagators (quench approx).

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

Magnetic moments



Electric and magnetic polarizabilities



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:

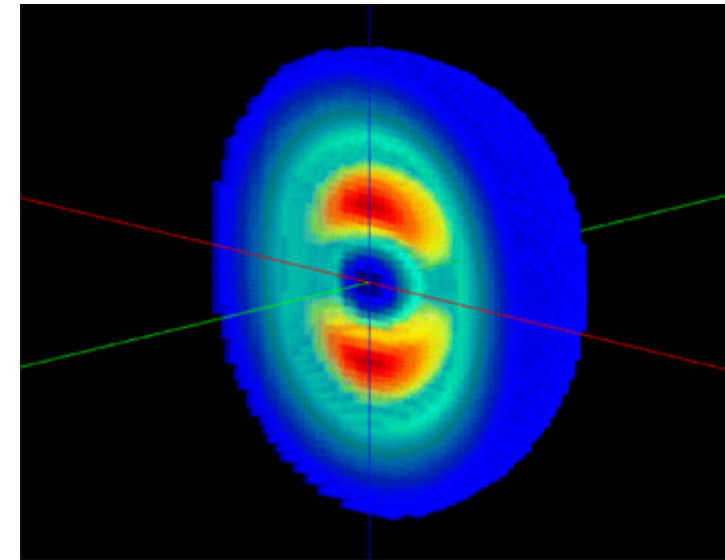
1) EM charge radius

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



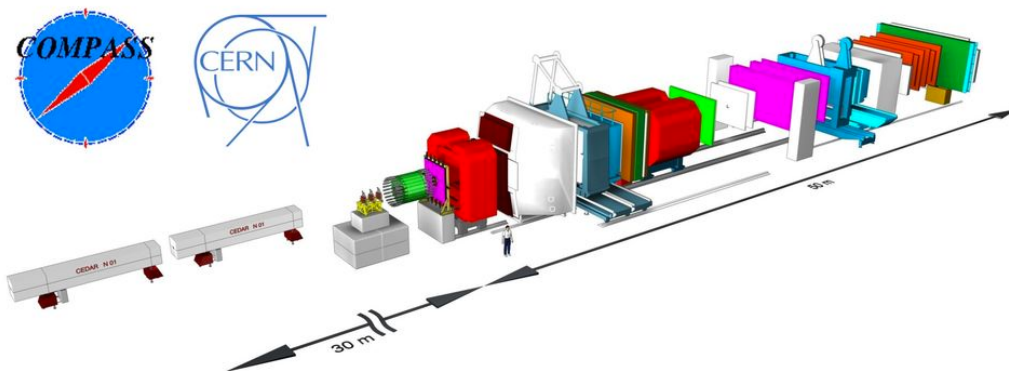
2) Electric quadrupole moment

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



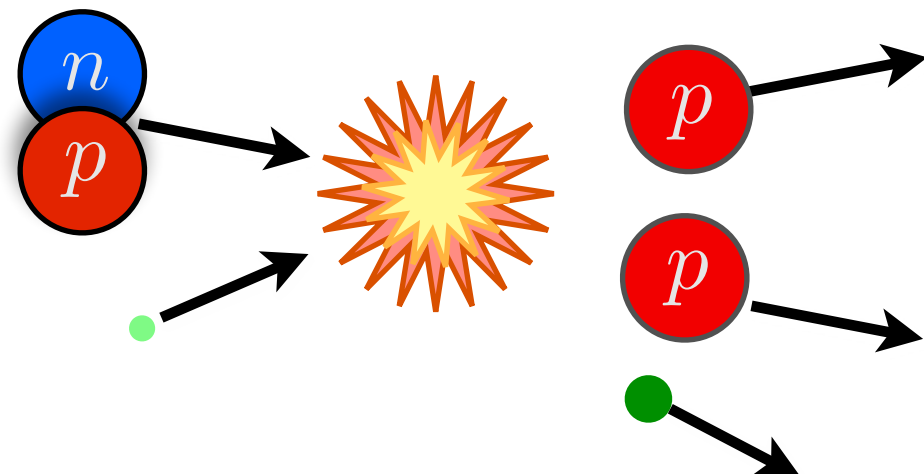
3) Form factors

Detmold, Phys. Rev. D 71, 054506 (2005).



4) Axial background fields

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



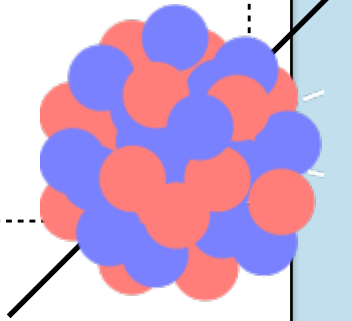
Here's an application of the background-field technique to obtain magnetic moment and polarizabilities of the nucleon:

$$E_{h;j_z}(\mathbf{B}) = \sqrt{M_h^2 + P_{\parallel}^2} + (2n_L + 1)|Q_h e \mathbf{B}| - \boldsymbol{\mu}_h \cdot \mathbf{B} - 2\pi\beta_h^{(M0)}|\mathbf{B}|^2 - 2\pi\beta_h^{(M2)}\langle\hat{T}_{ij}B_iB_j\rangle + \dots$$

Landau levels for
charged particles

Magnetic
moment

Magnetic polarizabilities



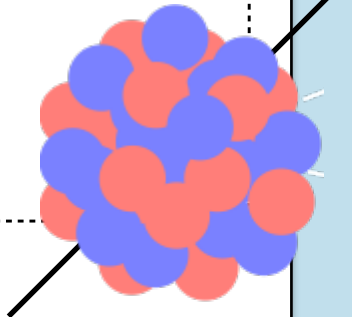
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$$E_{h;j_z}(\mathbf{B}) = \sqrt{M_h^2 + P_{\parallel}^2} + (2n_L + 1)|Q_h e \mathbf{B}| - \boldsymbol{\mu}_h \cdot \mathbf{B} - 2\pi\beta_h^{(M0)}|\mathbf{B}|^2 - 2\pi\beta_h^{(M2)}\langle \hat{T}_{ij} B_i B_j \rangle + \dots$$

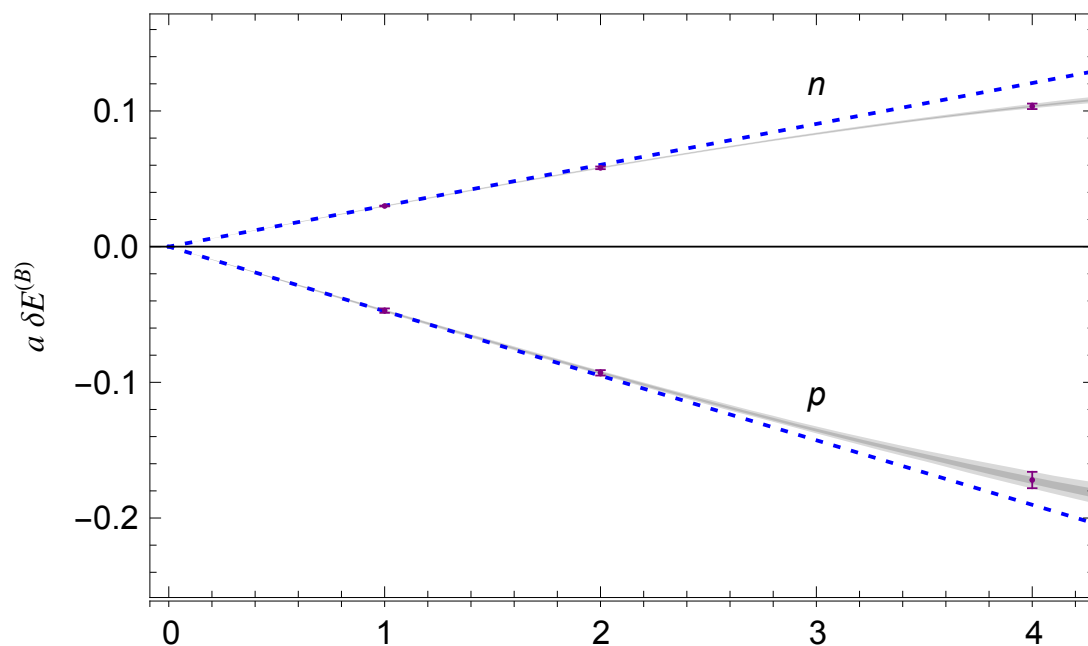
Landau levels for charged particles

Magnetic moment

Magnetic polarizabilities



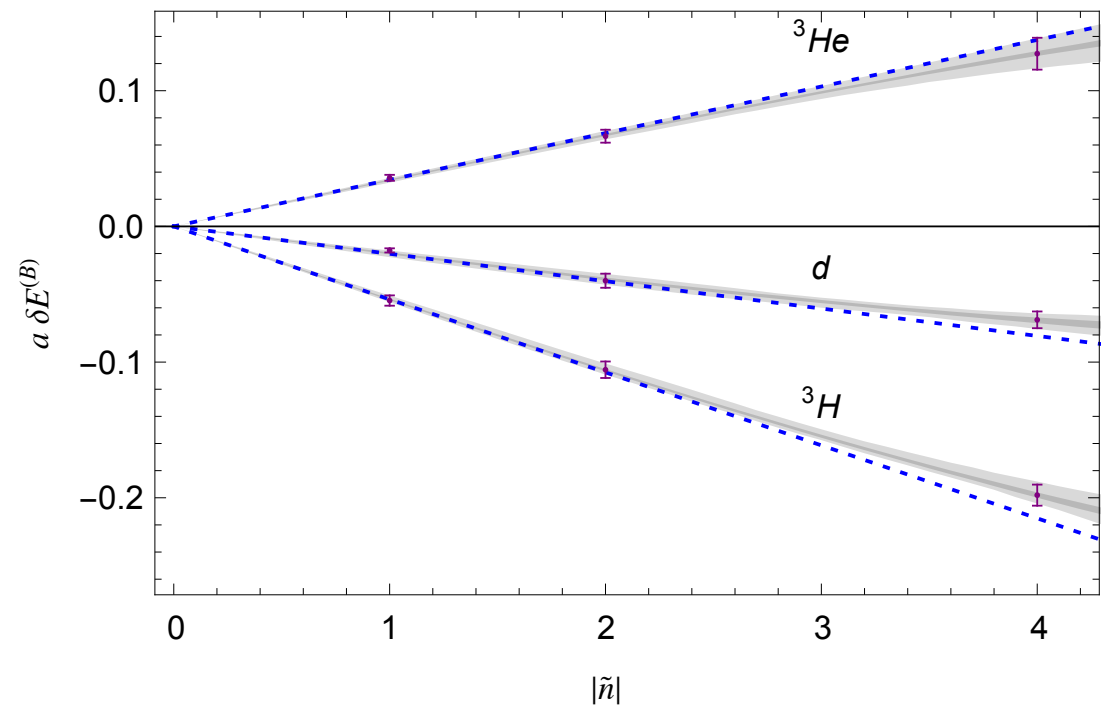
Nucleon



$|\tilde{n}|$

A quanta of magnetic field

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.
 Beane et al. (NPLQCD), *phys.rev.* D92 (2015) 11, 114502.

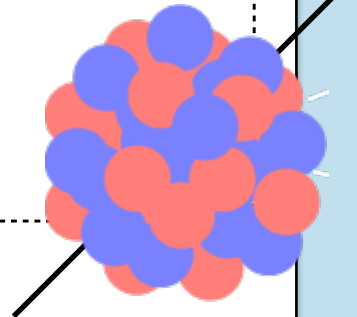
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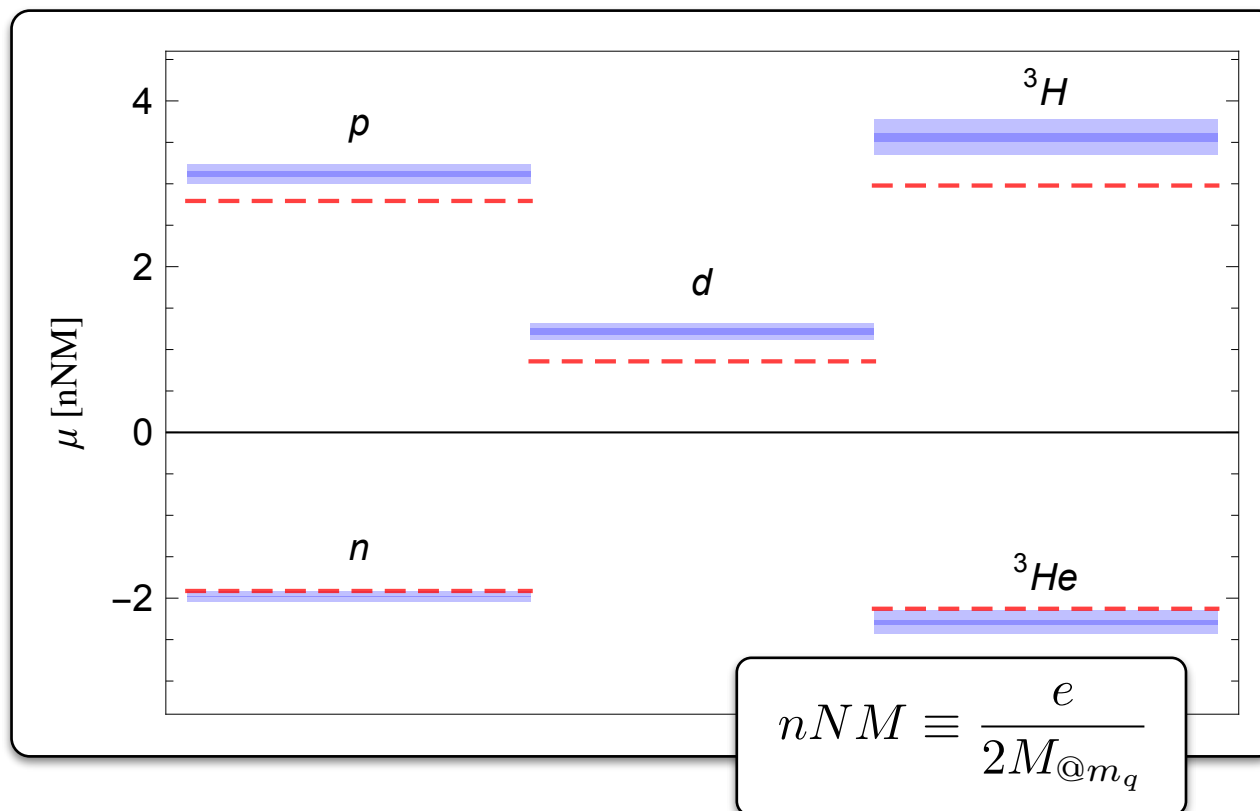
Landau levels for charged particles

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Magnetic moment



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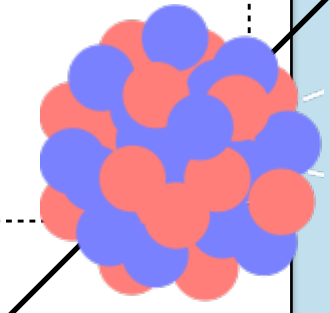
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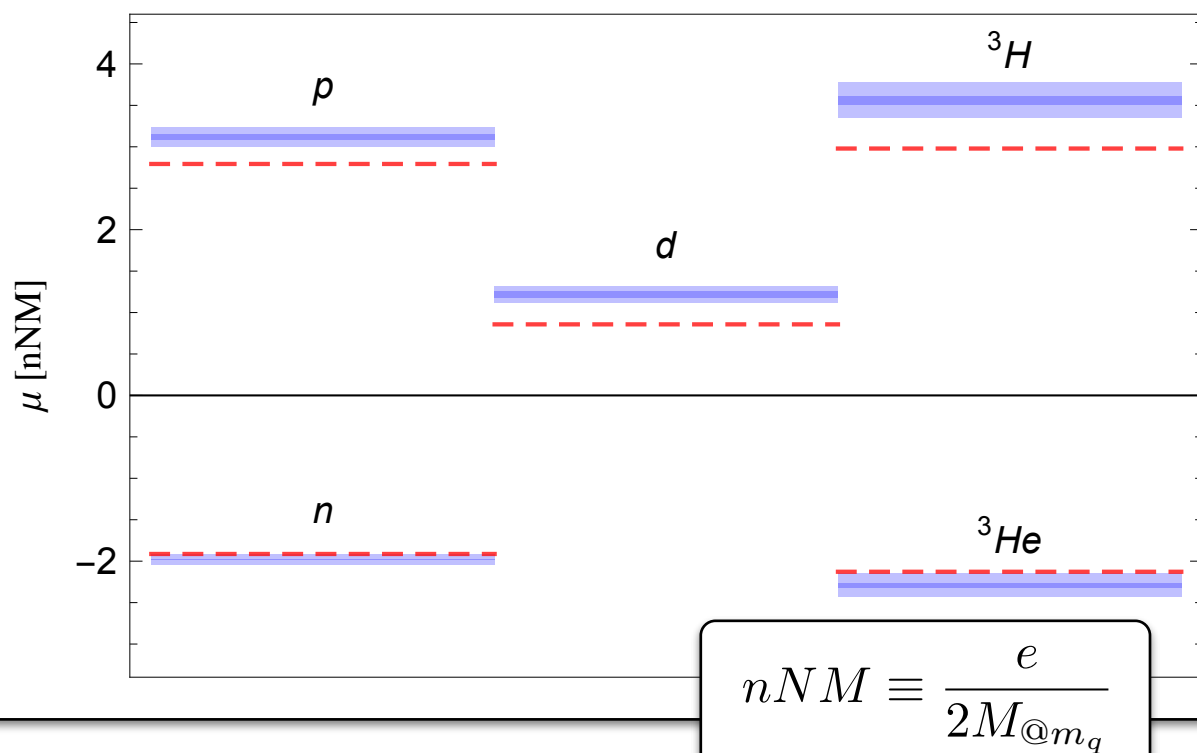
Landau levels for charged particles

Magnetic moment

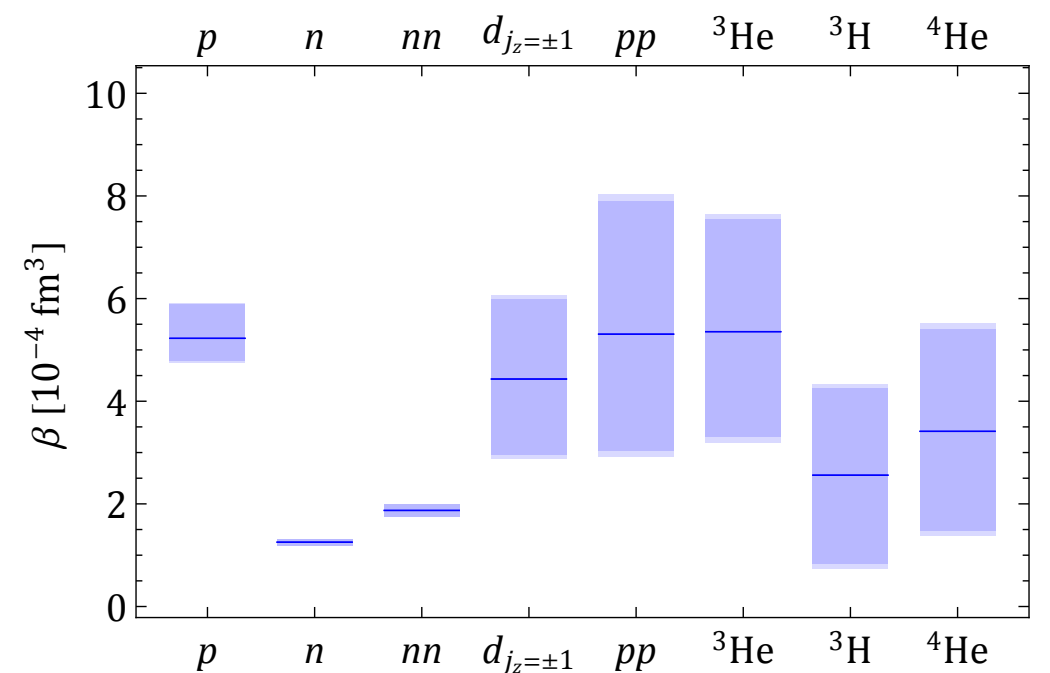
Magnetic polarizabilities



Magnetic moment



Magnetic polarizability



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

Beane et al. (NPLQCD), *phys.rev.lett.* 113 (2014) 25, 252001.
 Beane et al. (NPLQCD), *phys.rev.* D92 (2015) 11, 114502.

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

