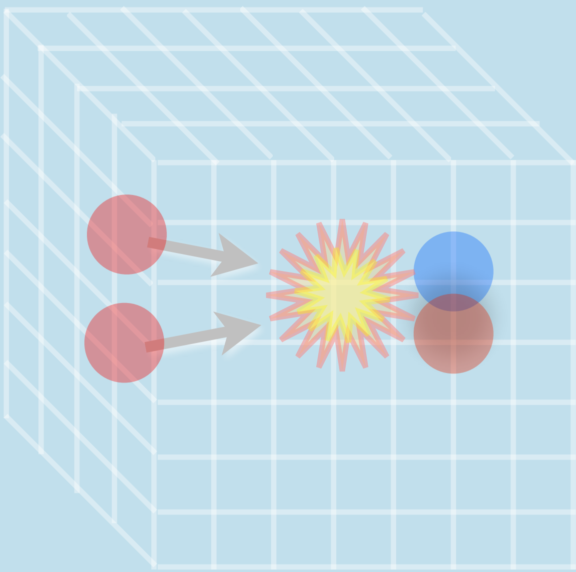
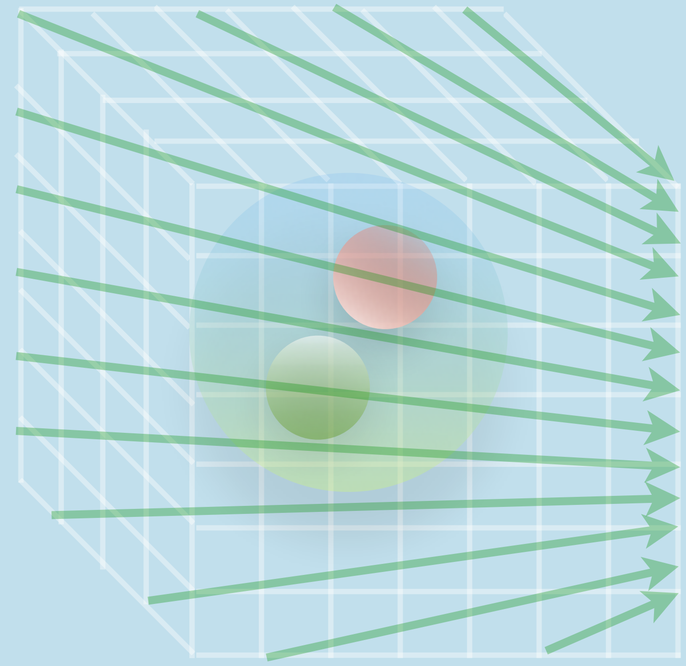
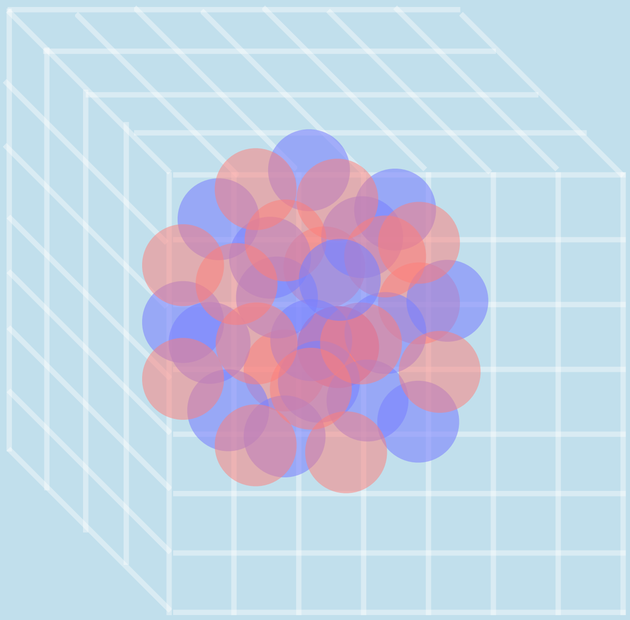
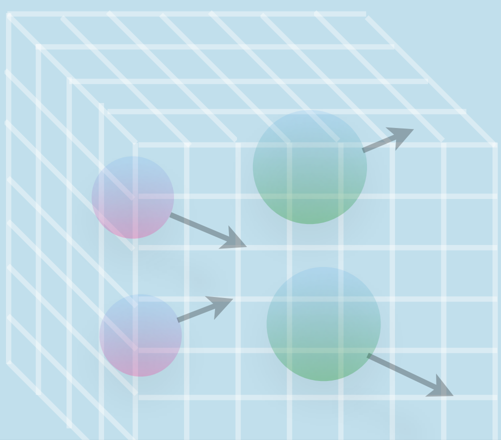
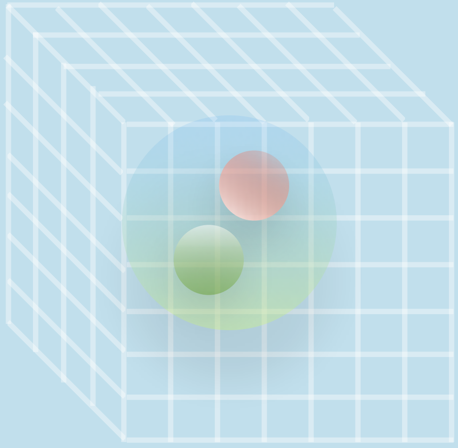






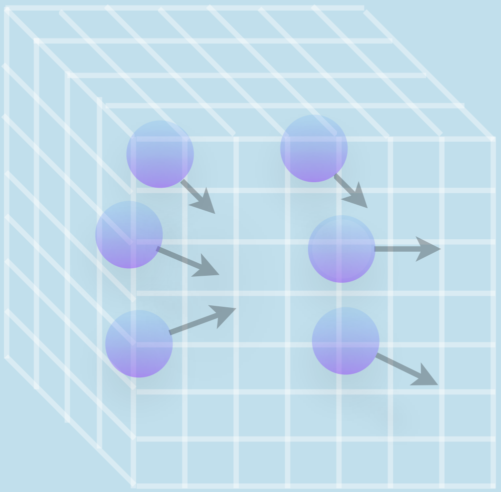




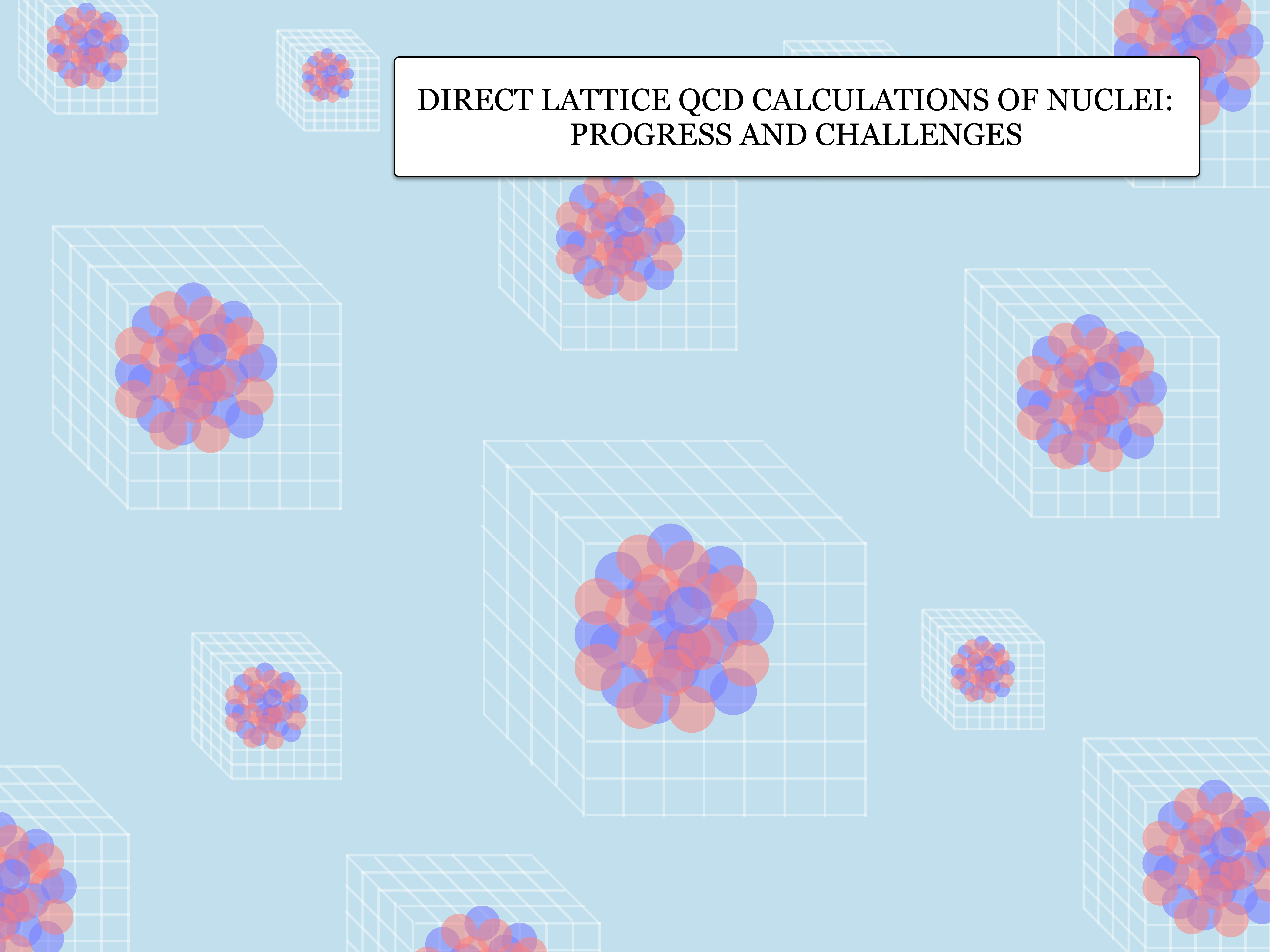
TALENT COURSE ON
FROM QUARKS AND GLUONS TO NUCLEAR FORCES AND STRUCTURE

LATTICE QCD
AND
MULTI-HADRON PHYSICS

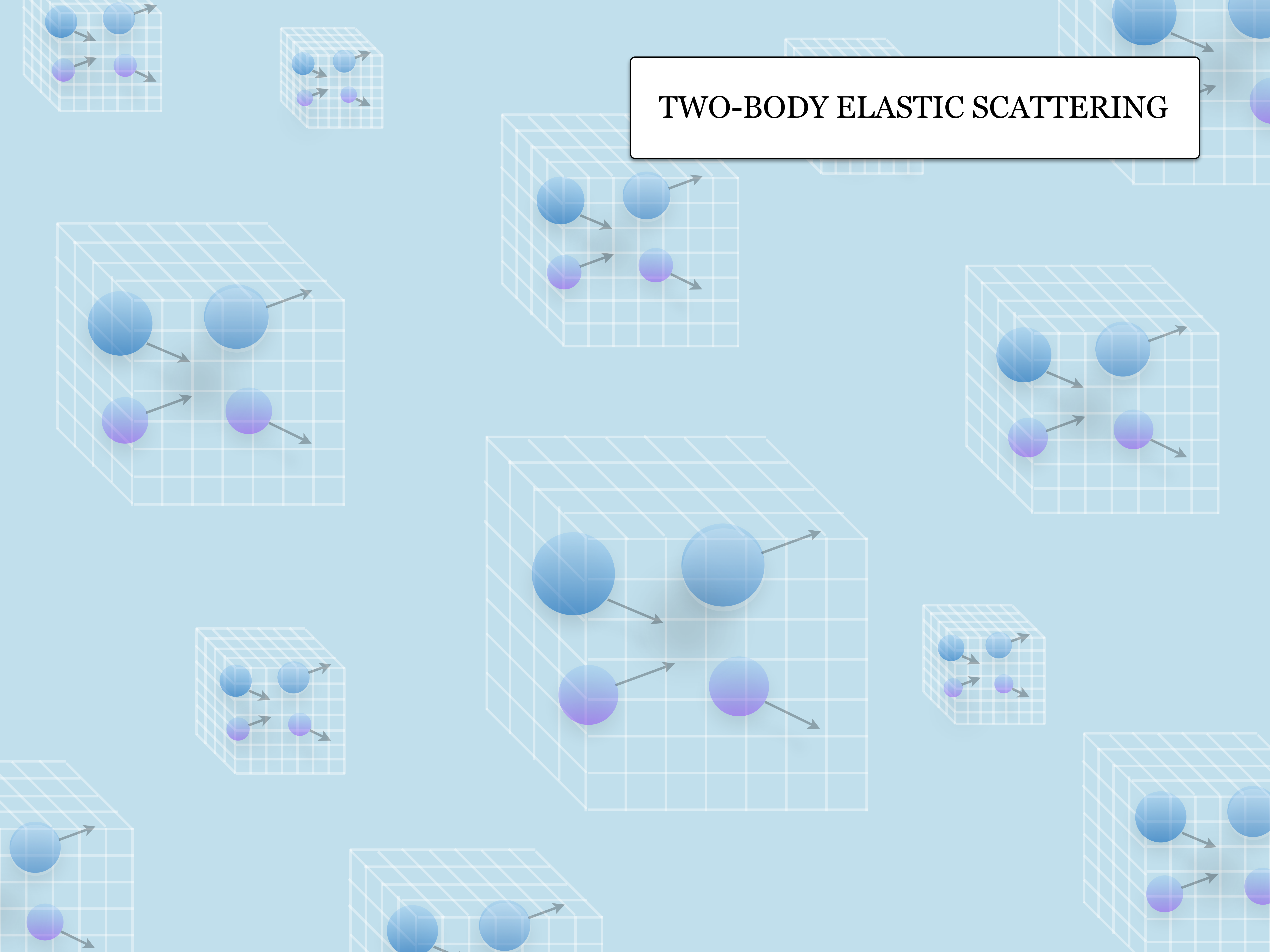
ZOHREH DAVOUDI
UNIVERSITY OF MARYLAND



DIRECT LATTICE QCD CALCULATIONS OF NUCLEI: PROGRESS AND CHALLENGES

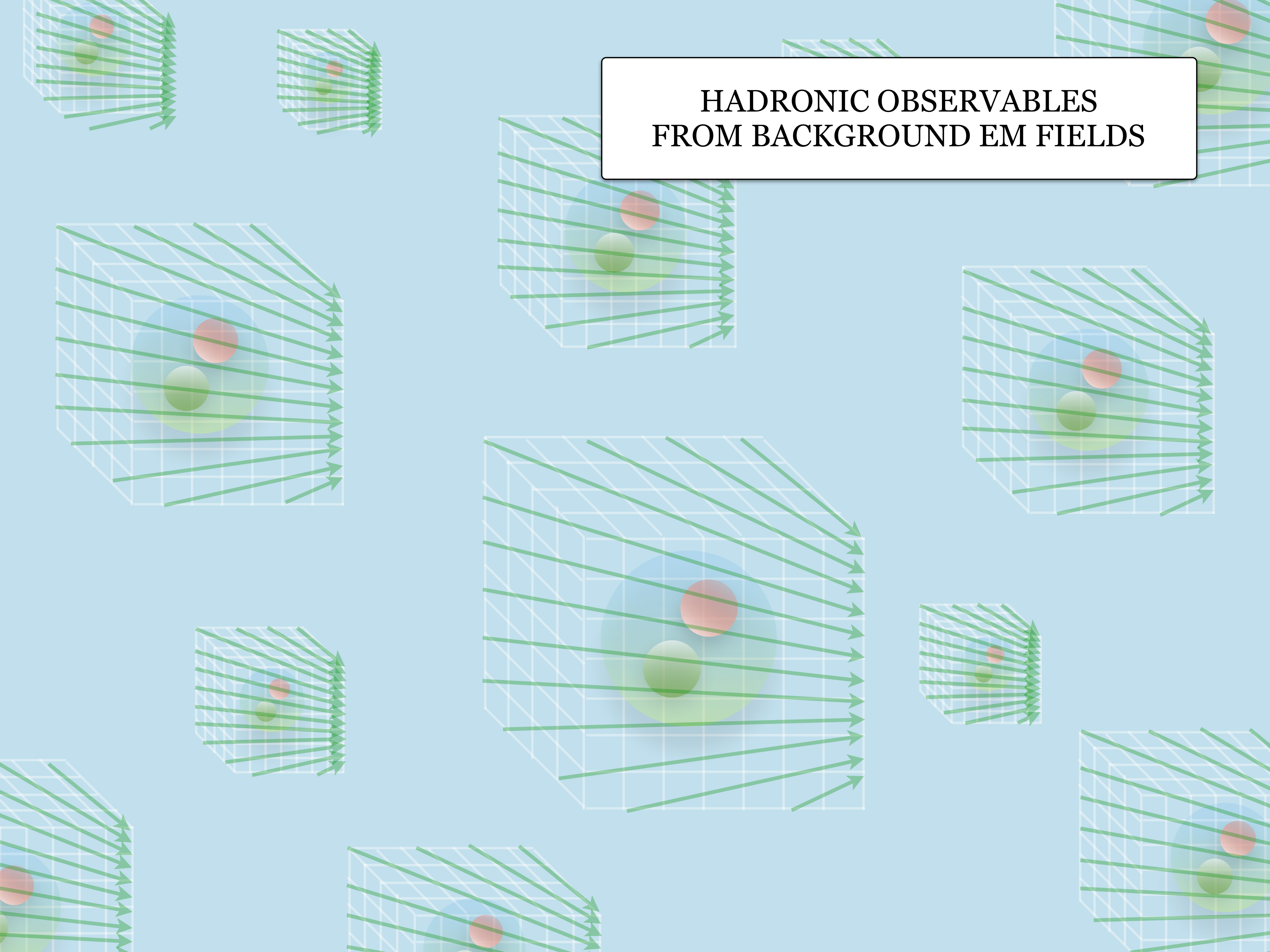


TWO-BODY ELASTIC SCATTERING



TWO-BODY INELASTIC SCATTERING

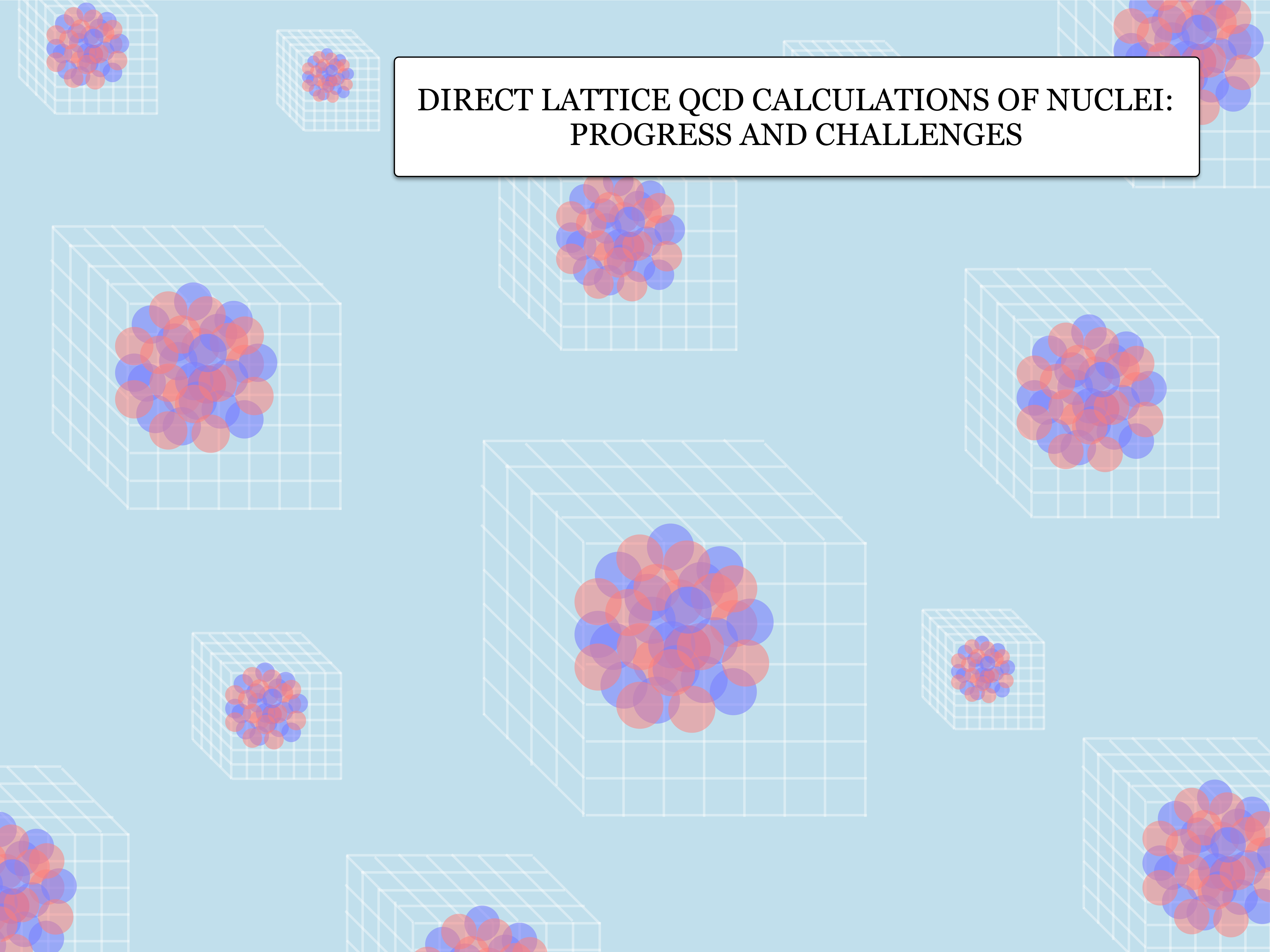
TWO-NUCLEON OBSERVABLES



HADRONIC OBSERVABLES FROM BACKGROUND EM FIELDS

HADRONIC OBSERVABLES FROM THREE-POINT FUNCTIONS

DIRECT LATTICE QCD CALCULATIONS OF NUCLEI: PROGRESS AND CHALLENGES



THREE FEATURES MAKE LQCD 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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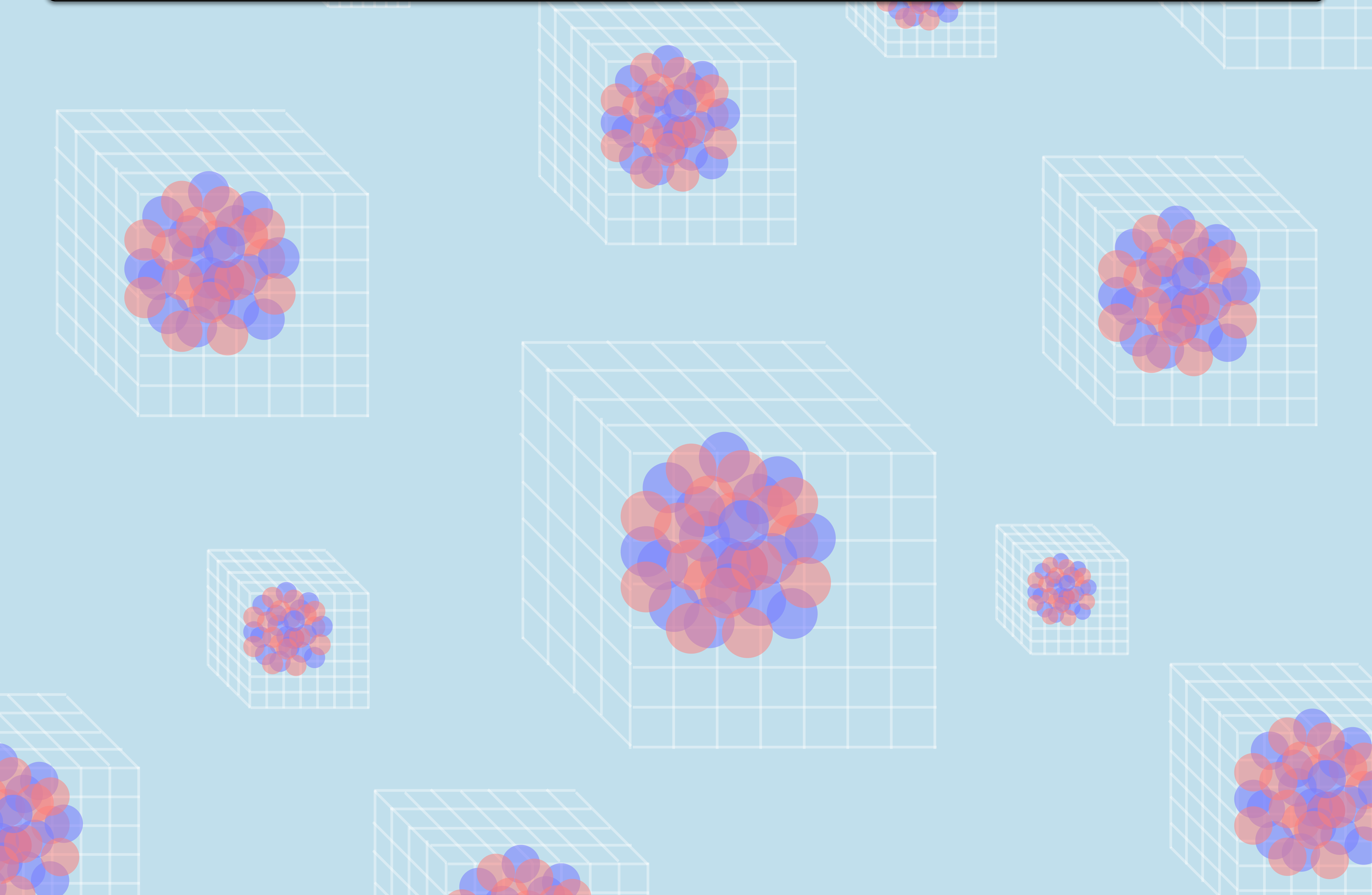
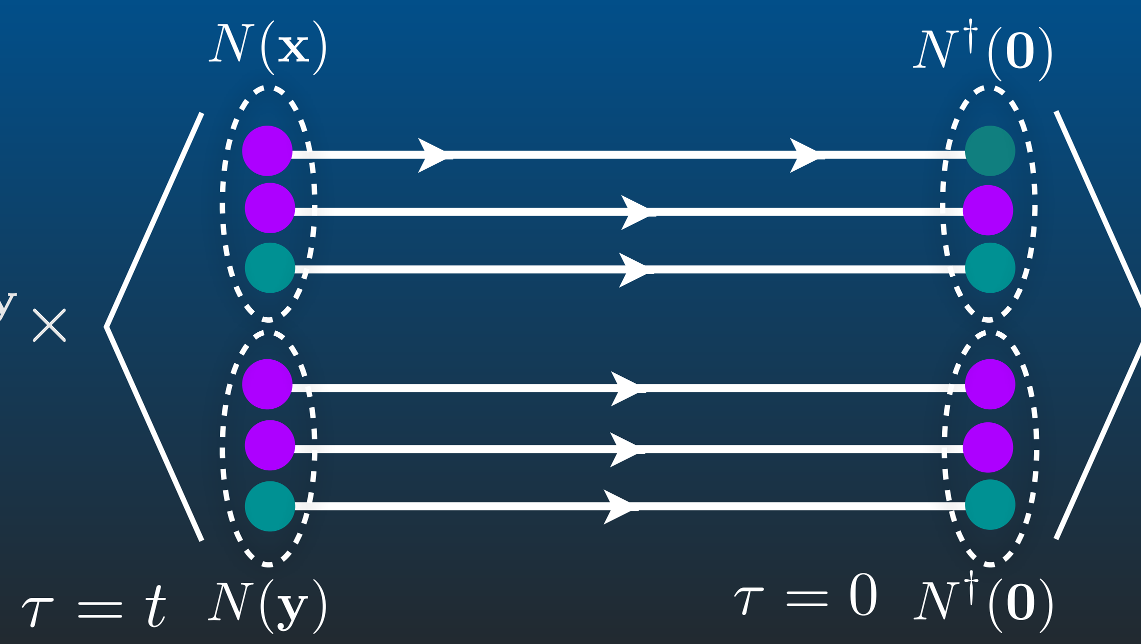


$$C(\mathbf{P}; t, t_O) = \sum_{\mathbf{p}_1+\mathbf{p}_2=\mathbf{P}} \sum_{\mathbf{x},\mathbf{y},\mathbf{z}} e^{i\mathbf{p}_1\cdot\mathbf{x}+i\mathbf{p}_2\cdot\mathbf{y}} \times$$



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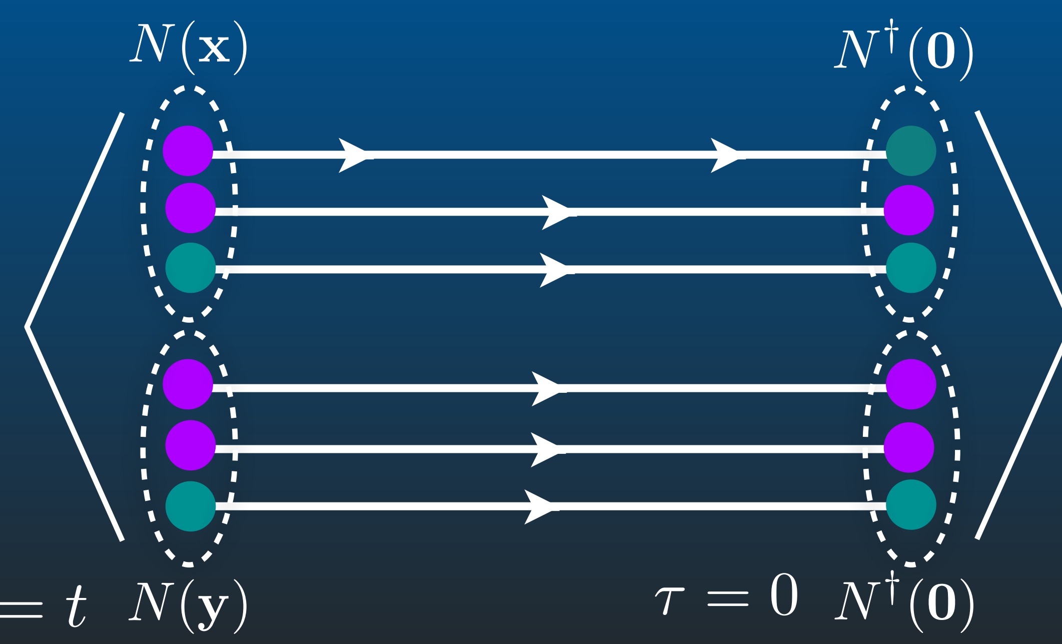
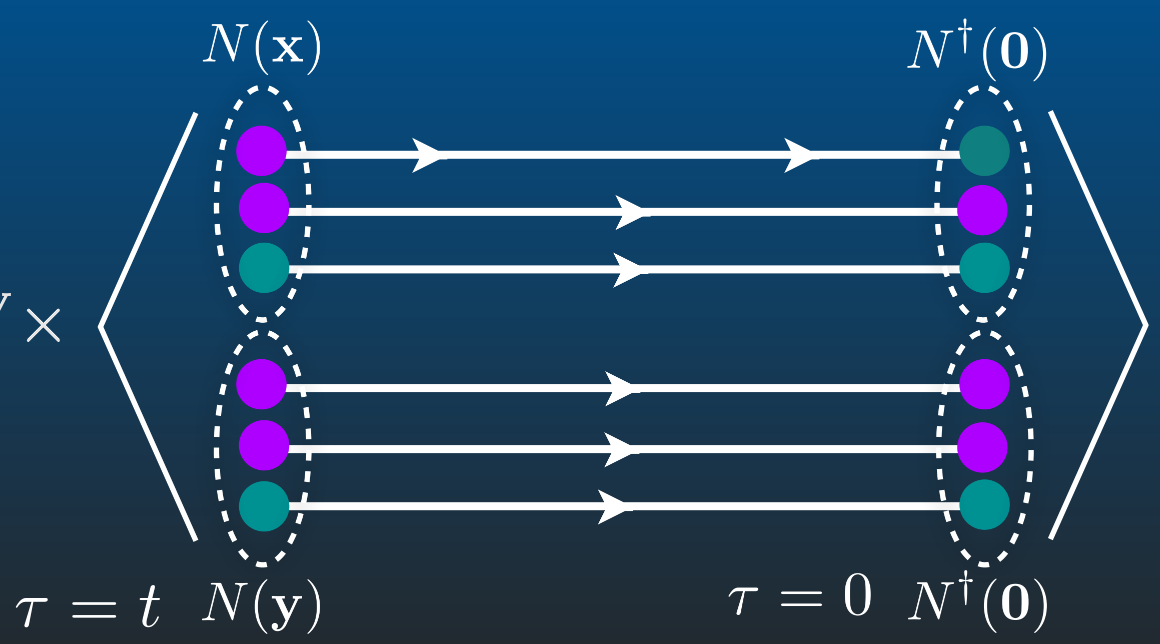


COMPLEXITIES OF QUARK-LEVEL INTERPOLATING FIELDS

COMPLEXITIES OF QUARK CONTRACTIONS

Detmold and Orginos (2013).

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



COMPLEXITIES OF QUARK-LEVEL INTERPOLATING FIELDS

Detmold and Orginos (2013).

Number of terms in the interpolating operators of a nucleus?

$$\bar{\mathcal{N}}^h = \sum_{\mathbf{a}} w_h^{a_1,a_2\cdots a_{n_q}} \bar{q}(a_1)\bar{q}(a_2)\cdots\bar{q}(a_{n_q})$$

Collective indices: color, spinor, flavor and lattice site

As many quark interpolators as needed to represent a given system, e.g., 6 quarks for *NN(3S1)*.

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The wave-function must be totally anti-symmetric:

$$\frac{N!}{(N-n_q)!}$$

Removing permutations:

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More simplification is possible too:

$$\bar{\mathcal{N}}^h = \sum_{k=1}^{N_w} \tilde{w}_h^{(a_1,a_2\cdots a_{n_q}),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,\cdots,i_{n_q}} \bar{q}(a_{i_1})\bar{q}(a_{i_2})\cdots\bar{q}(a_{i_{n_q}})$$

New weight factors factoring in other constraints such as color singletness, parity, angular momentum, strangeness.

Easier to work with baryon blocks and tabulate the corresponding weights:

$$\bar{\mathcal{N}}^h = \sum_{k=1}^{M_w} \tilde{W}_h^{(b_1,b_2\cdots b_A),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,\cdots,i_A} \bar{B}(b_{i_1})\bar{B}(b_{i_2})\cdots\bar{B}(b_{i_A})$$

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Baryon interpolators

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Baryon interpolators

Example: A=2, *P*=+, *J*=0, *I*=1, *L*=0, *s*=0

$$\frac{1}{\sqrt{2}}(n_\uparrow n_\downarrow - n_\downarrow n_\uparrow) \qquad \frac{1}{2}(n_\uparrow p_\downarrow - n_\downarrow p_\uparrow + p_\uparrow n_\downarrow - p_\downarrow n_\uparrow) \qquad \frac{1}{\sqrt{2}}(p_\uparrow p_\downarrow - p_\downarrow p_\uparrow)$$

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Quark-level weight can then be obtained by equality:

$$\bar{B}(b) = \sum_{k=1}^{N_{B(b)}} \tilde{w}_b^{(a_1,a_2,a_3),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,i_3} \bar{q}(a_{i_1})\bar{q}(a_{i_2})\bar{q}(a_{i_3})$$

$$\begin{aligned}\mathcal{N}^h &= \sum_{k=1}^{M_w} \tilde{W}_h^{(b_1,b_2\cdots b_A),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,\cdots,i_A} \bar{B}(b_{i_1})\bar{B}(b_{i_2})\cdots\bar{B}(b_{i_A}) \\ &= \sum_{k=1}^{N_w} \tilde{w}_h^{(a_1,a_2\cdots a_{n_q}),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,\cdots,i_{n_q}} \bar{q}(a_{i_1})\bar{q}(a_{i_2})\cdots\bar{q}(a_{i_{n_q}})\end{aligned}$$

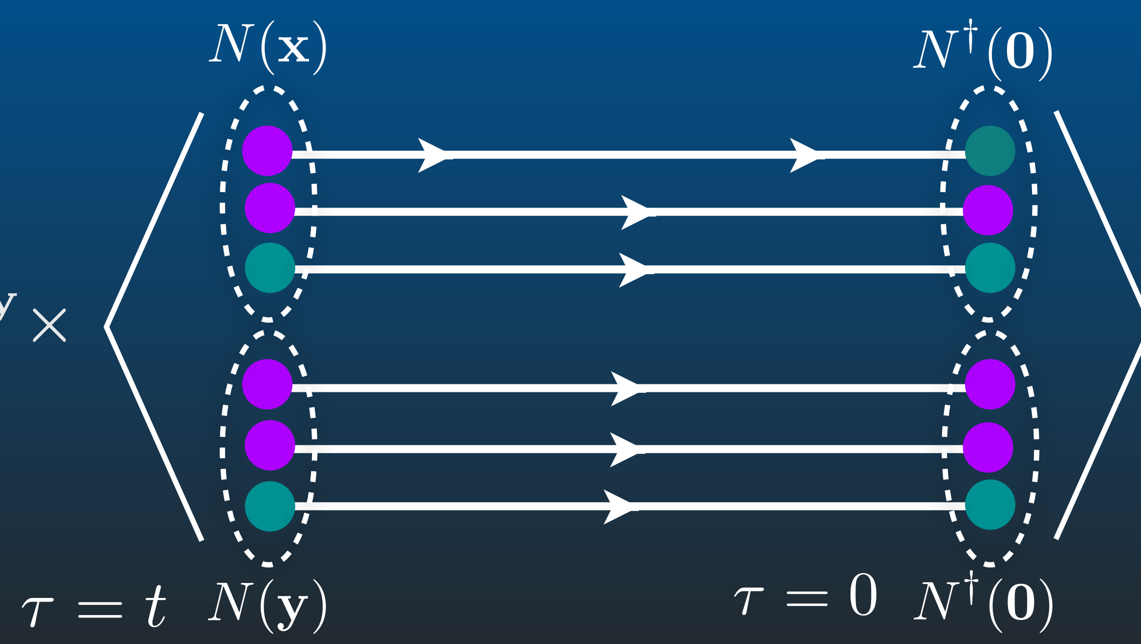
EXERCISE 1

Show that the number of terms in the simplest quark-level interpolating operator for the proton (constructed at a single point) is 9.

BONUS EXERCISE 1

Show that the number of terms in the simplest quark-level interpolating operator for the deuteron (constructed at a single point) is 21!

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



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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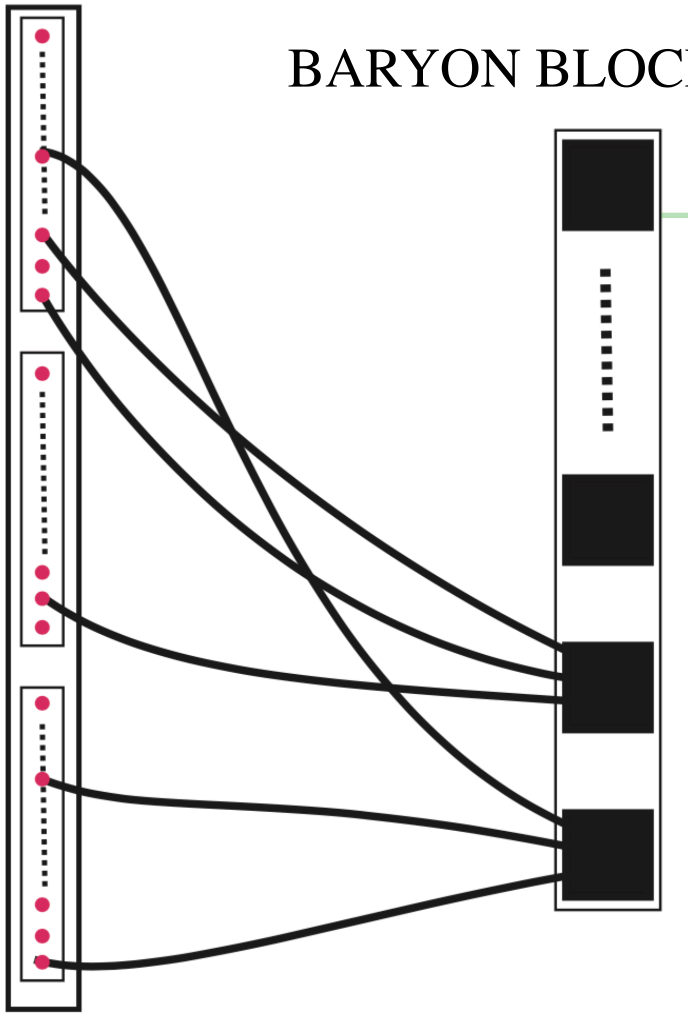
An example of a more efficient algorithm:



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

Can also start propagators at different locations.

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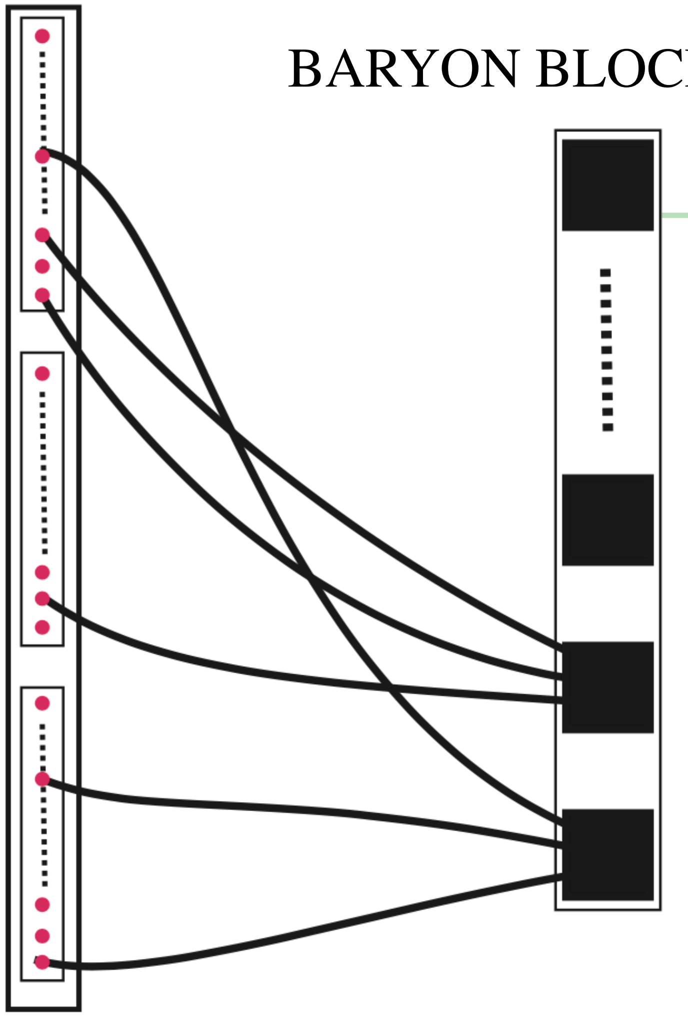


BARYON BLOCKS

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

Can also start propagators at different locations.

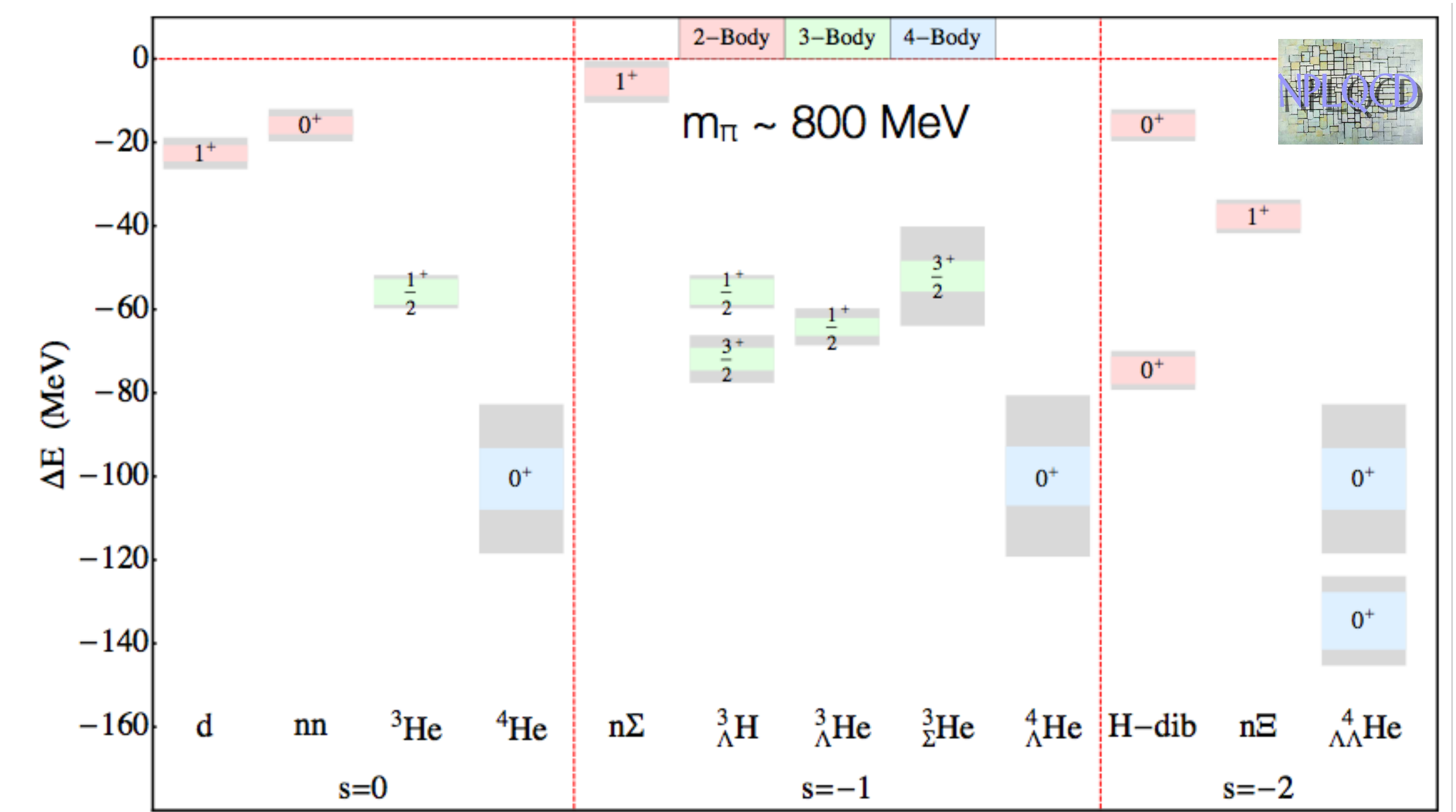
The new scaling is: $M_w \cdot N_w \cdot \dfrac{(3A)!}{(3!)^A}$

M_w: Number of terms in the sink

N_w: Number of terms in the source

NUCLEI OBTAINED FROM SUCH AN APPROACH (AT A HEAVIER QUARK MASSES)

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

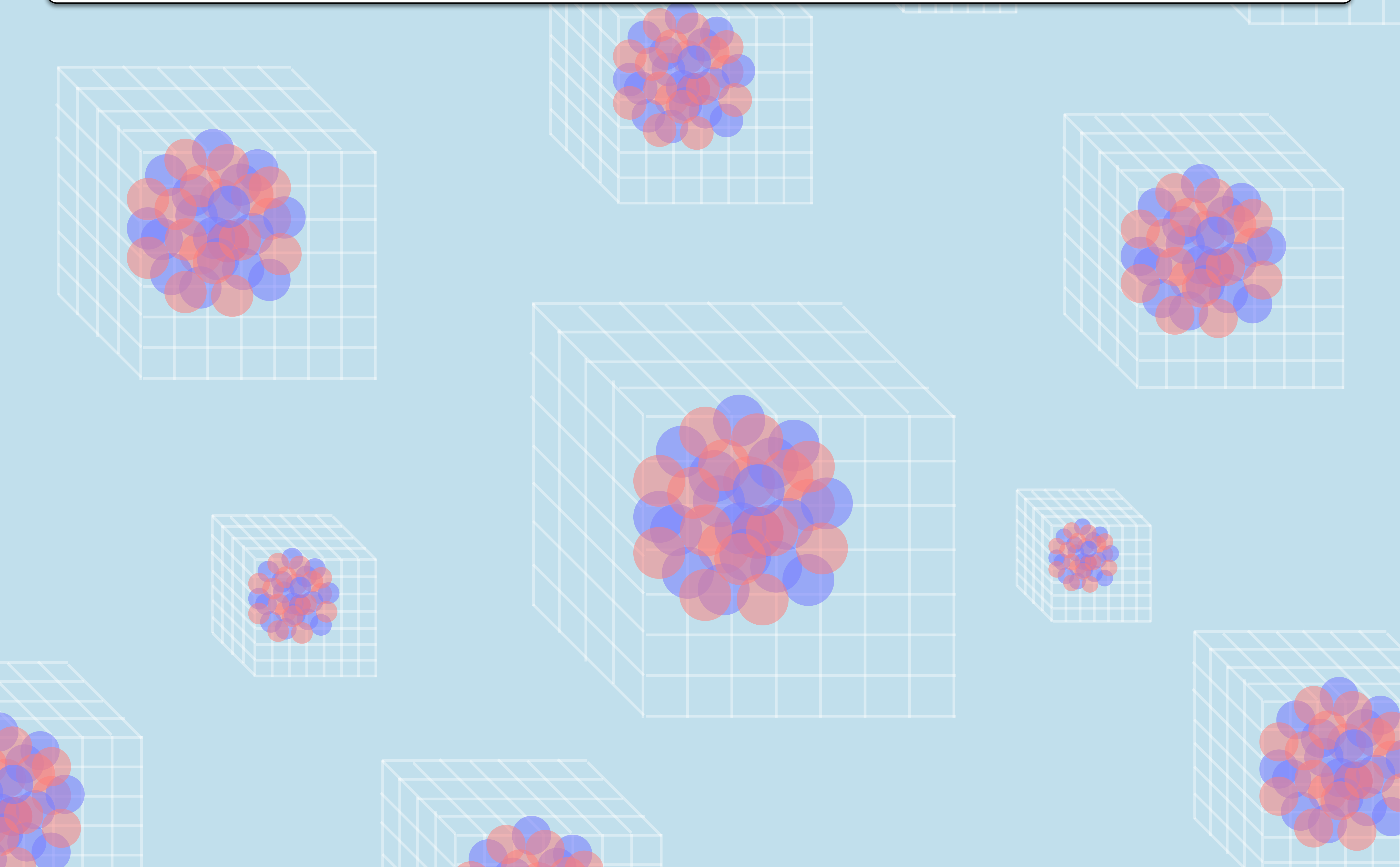


Beane, et al. (NPLQCD), Phys.Rev. D87 (2013) , Phys.Rev. C88 (2013)

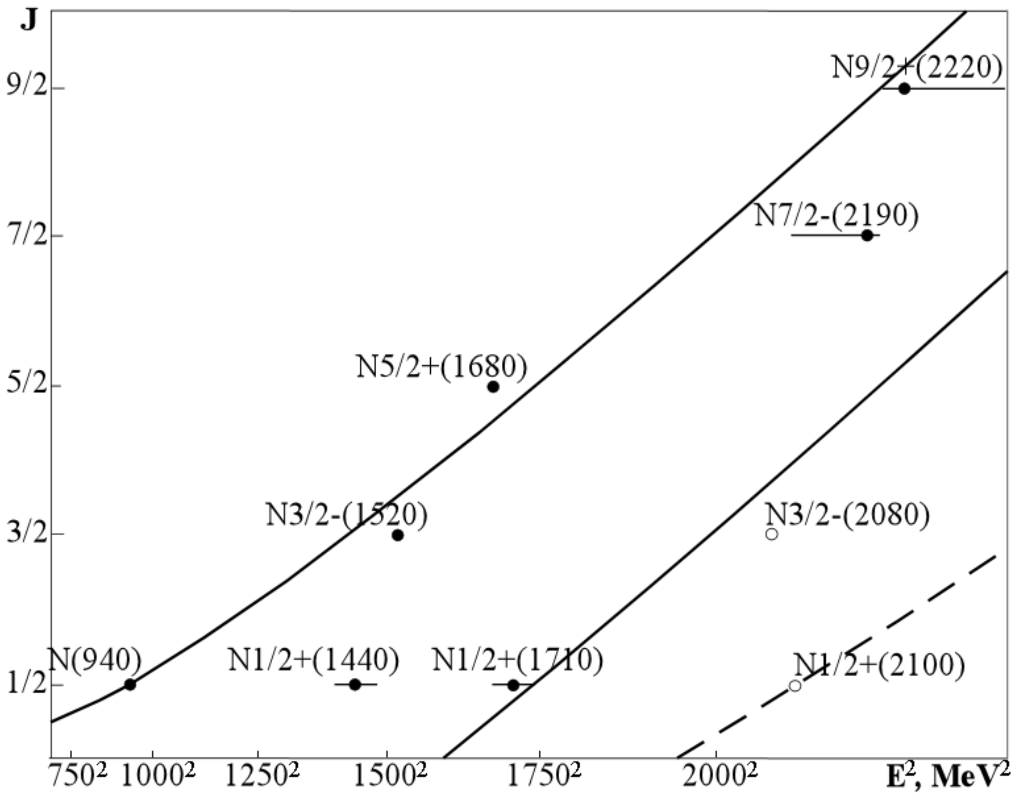
EXERCISE 2

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? There are even more optimal algorithms that lead to a polynomial scaling with the number of the quarks.

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) .

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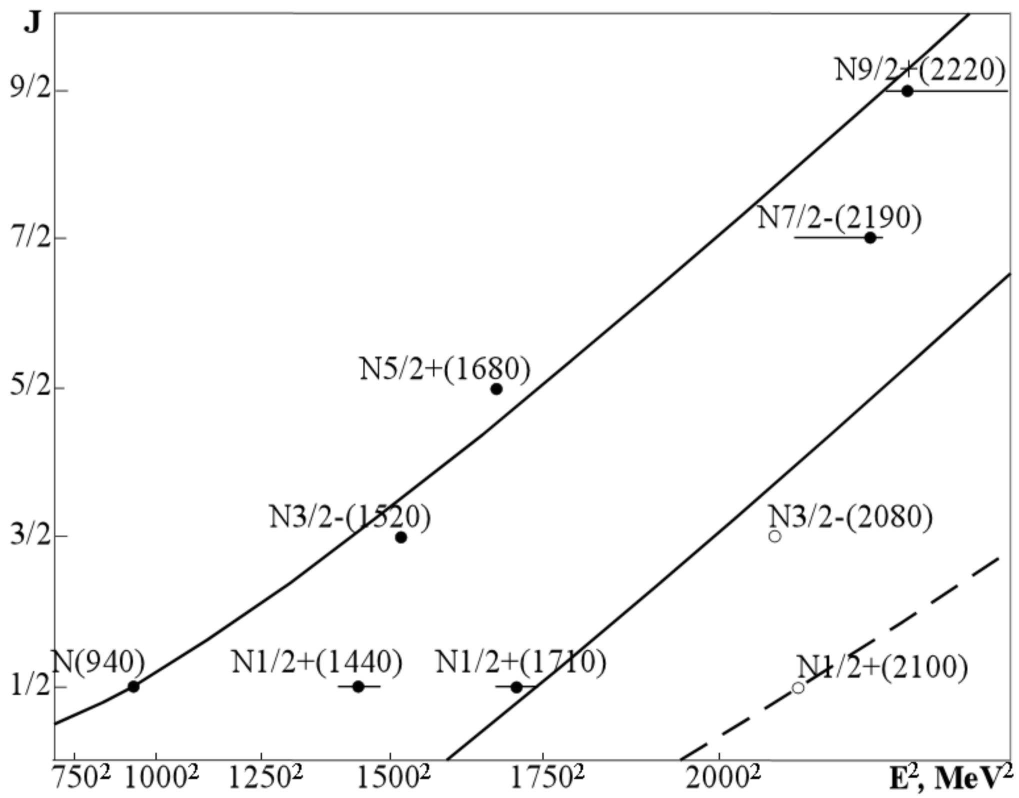

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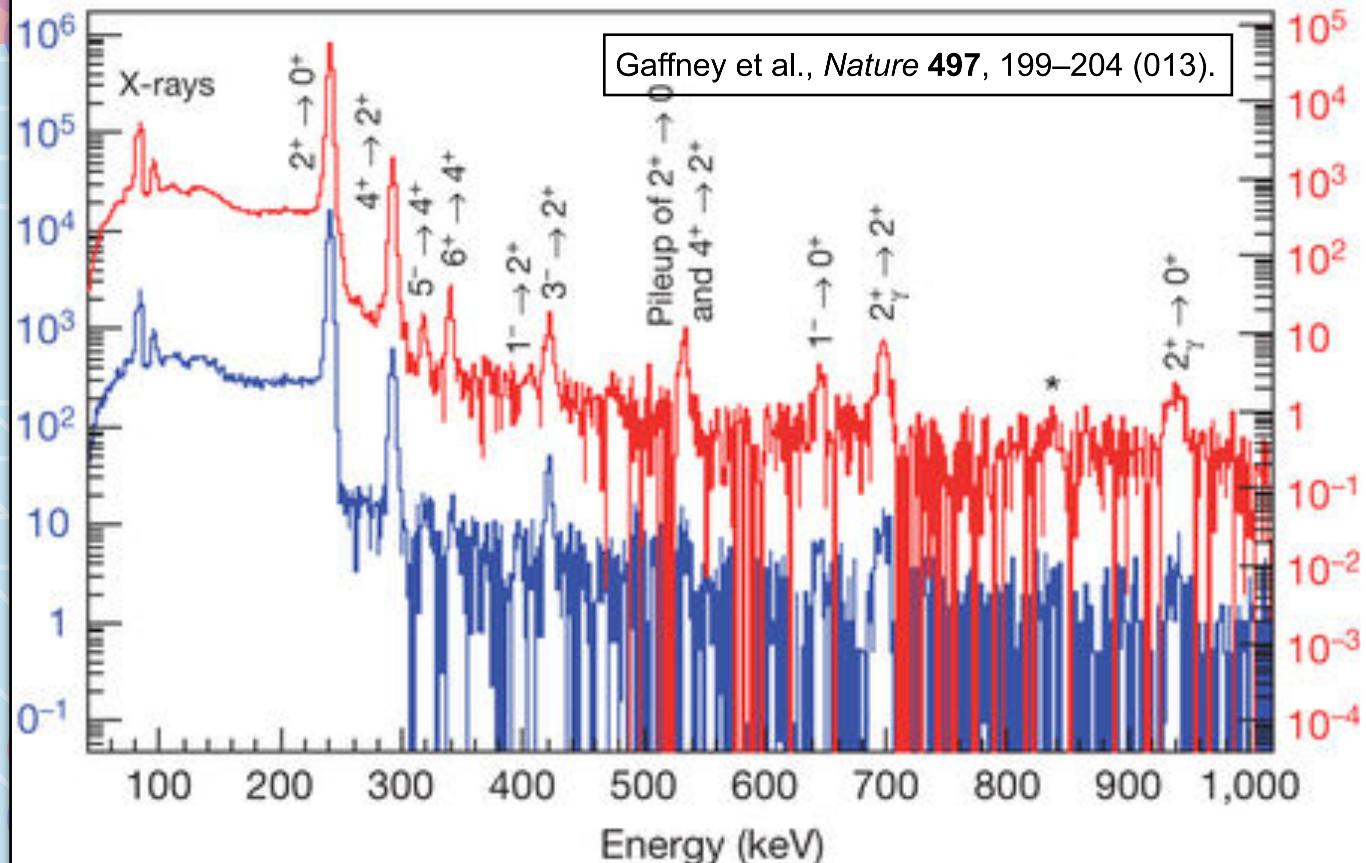
Nuclear excitations of two pear-shaped nuclei (radium and radon)



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

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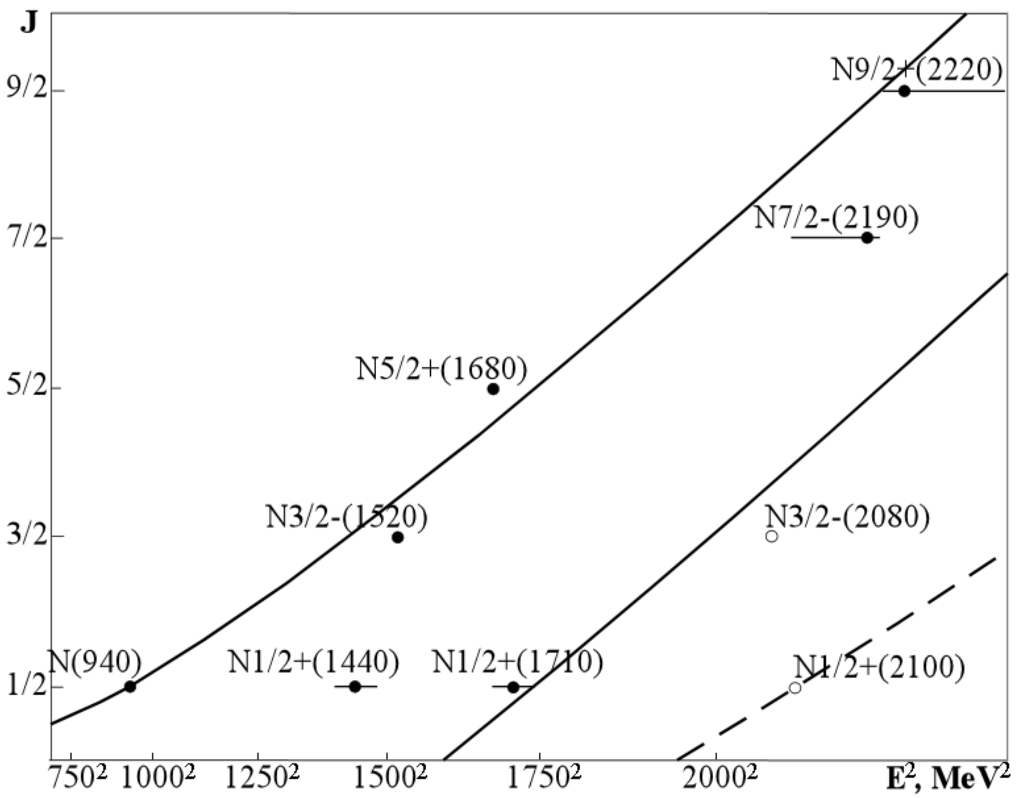

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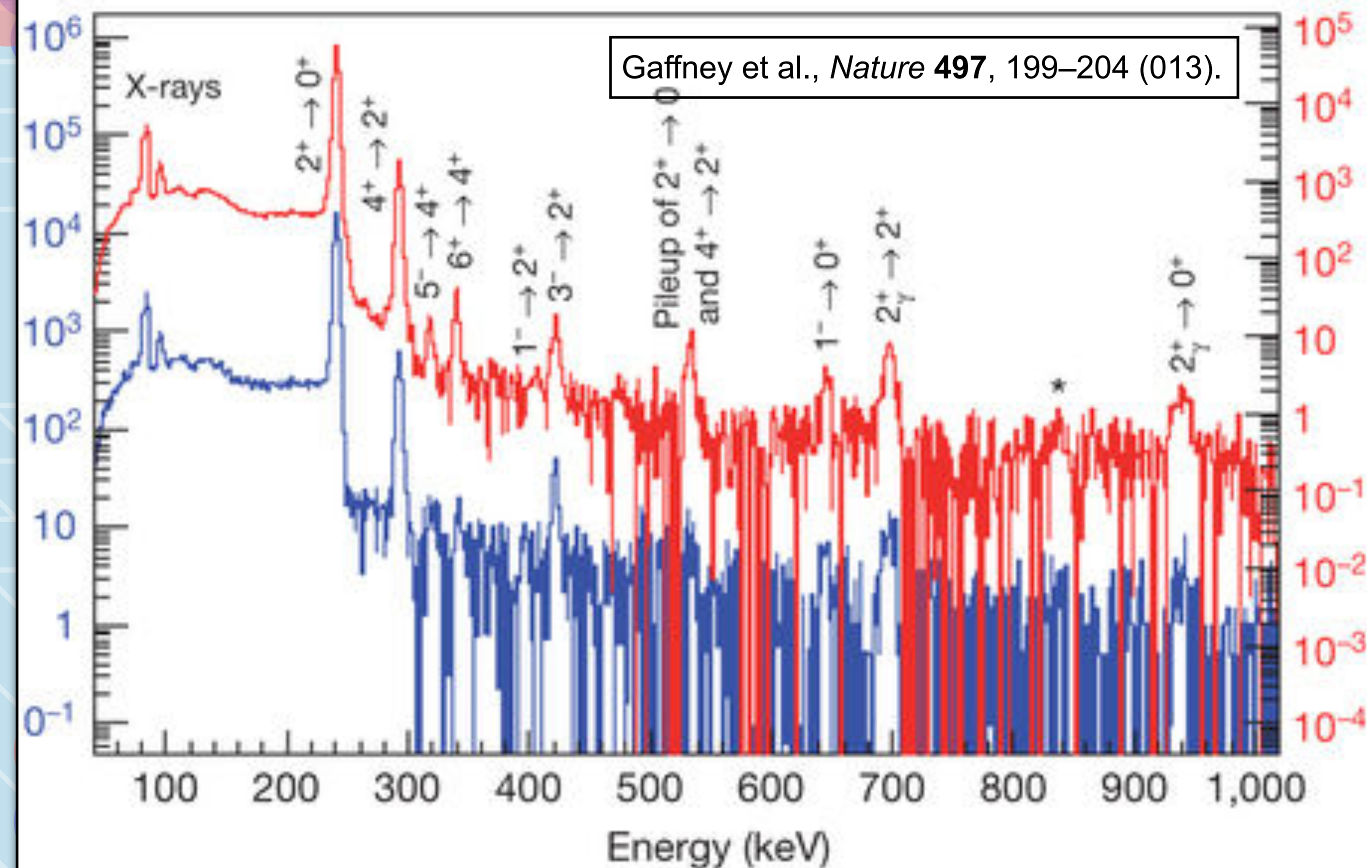

Getting radium directly from QCD will remain challenging for a long time! One should first compute A = 2, 3, 4 systems well. This is till not that easy: *B_d* = 2 MeV!

EXERCISE 3

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. `See exercise 4!`

- The key to success of this program is in the use of good interpolating operators for nuclei. Since nucleons retain their identity in nuclei, forming baryon blocks at the sink turns out to be very advantageous. `See the previous section.`

- Ideally need to use a large set of operators for a variational analysis, but this has remained too costly in nuclear calculations. `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 4

Consider a simple two-state model in the spectral decomposition of an 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.

VARIATIONAL METHOD

Form a matrix of correlation functions with a number of interpolators:

$$C_{i,j}(t) = \langle 0|\mathcal{O}_i(t)\mathcal{O}_j(0)|0\rangle$$

Michael (1985)
Luescher and Wolf (1990)

Solve the eigenvalue equation for a reasonably chosen initial time:

$$C(t)v_k = \lambda_k C(t_0)v_k \qquad \lim_{t-t_0\to\infty} \lambda_k = e^{-E_k t}$$

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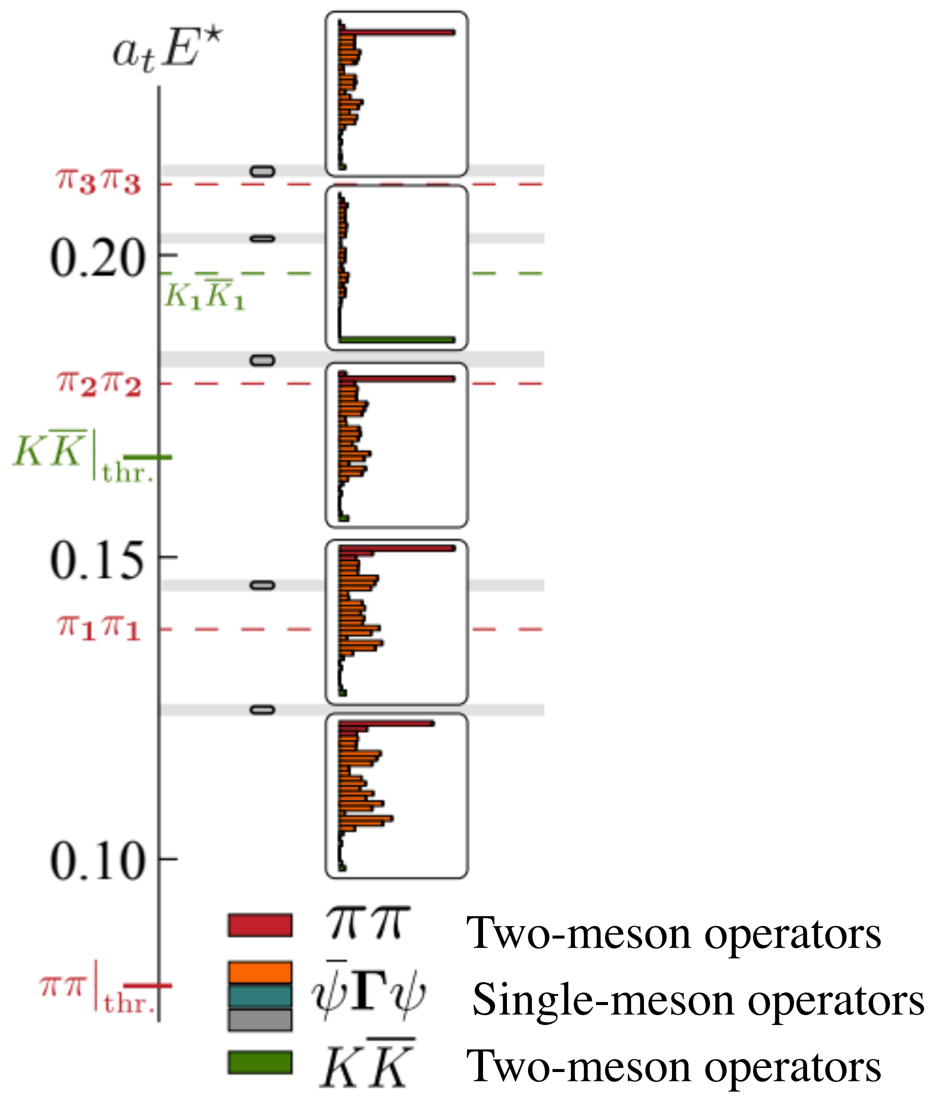
An example

Meson spectroscopy in the P-wave $\pi\pi - K\overline{K}$ channel:



Wilson et al (HadSpec), Phys. Rev. D 92, 094502 (2015). Briceno, Dudek and Young, Rev. Mod. Phys. 90 025001.

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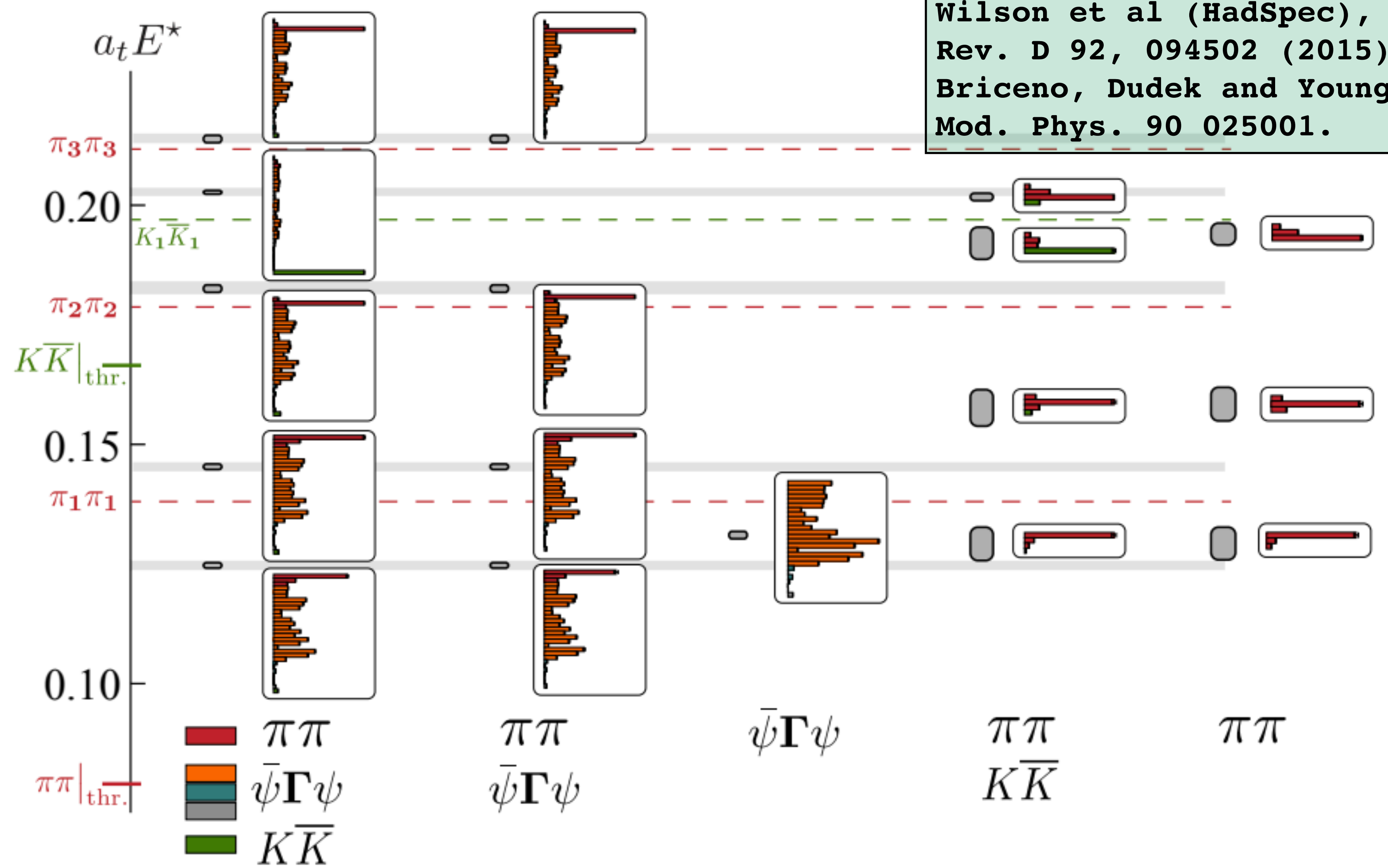

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MATRIX PRONY

de Prony (1795)

The method is useful when the correlation function matrix is not square or positive-definite matrix necessarily. It finds suitable linear combination of the correlates that are dominated by single exponentials.

Consider: $y(t) = \begin{pmatrix} C_{PS}(t) \\ C_{SS}(t) \end{pmatrix}$

With the ansatz: $y(t+\tau) = \hat{T}(\tau) y(t)$

A "transfer matrix" defined as: $\hat{T}(\tau) = M^{-1}(\tau) V$

This implies that: $M(\tau) y(t+\tau) y^T(t) = V y(t) y^T(t)$

Which can be satisfied by: $M(\tau) = \left(\sum_{t=t_0}^{t_0+\Delta t} y(t+\tau) y^T(t) \right)^{-1}, \quad V = \left(\sum_{t=t_0}^{t_0+\Delta t} y(t) y^T(t) \right)^{-1}$

Finally: $\hat{T}(\tau) q_n = (\lambda_n)^\tau q_n \,,$ with $\lambda_n = e^{-E_n}$

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Or: $$M(\tau) \sum_{t=t_0}^{t_0+\Delta t} y(t+\tau) y^T(t) = V \sum_{t=t_0}^{t_0+\Delta t} y(t) y^T(t)$$

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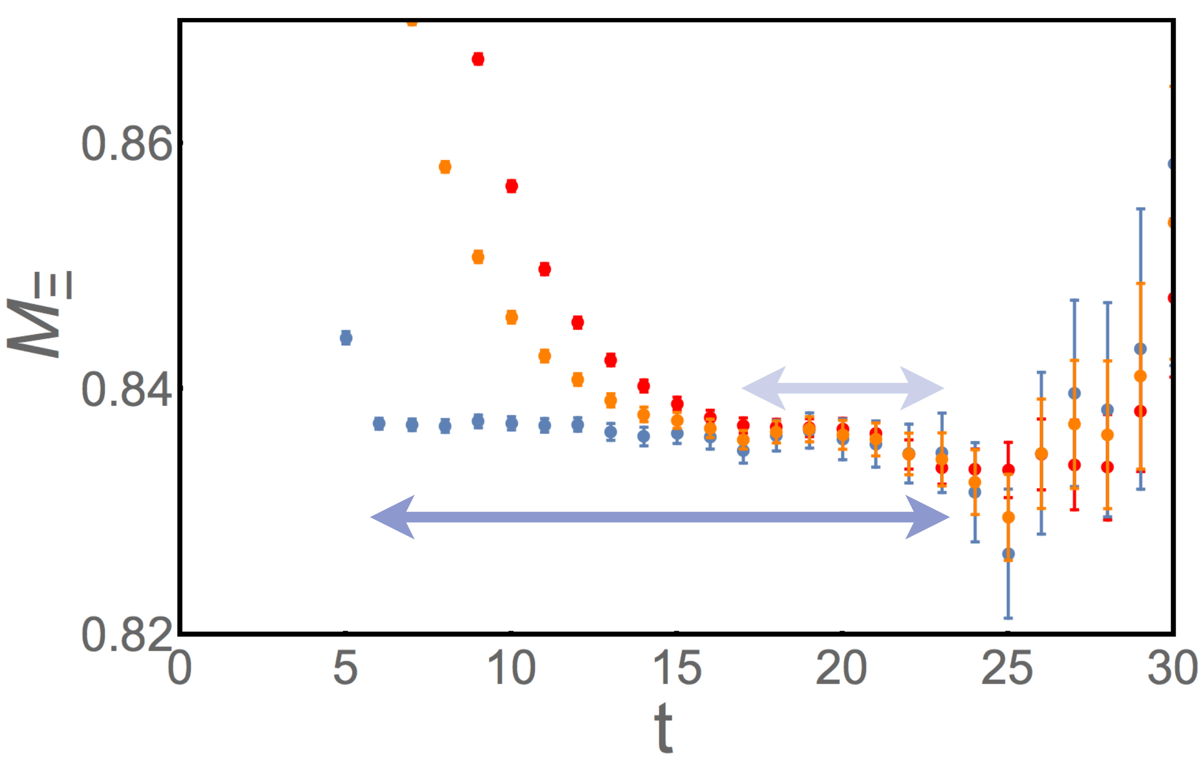
Finally: $$\hat{T}(\tau) q_n = (\lambda_n)^\tau q_n \,, \qquad \text{with } \lambda_n = e^{-E_n}$$

An example

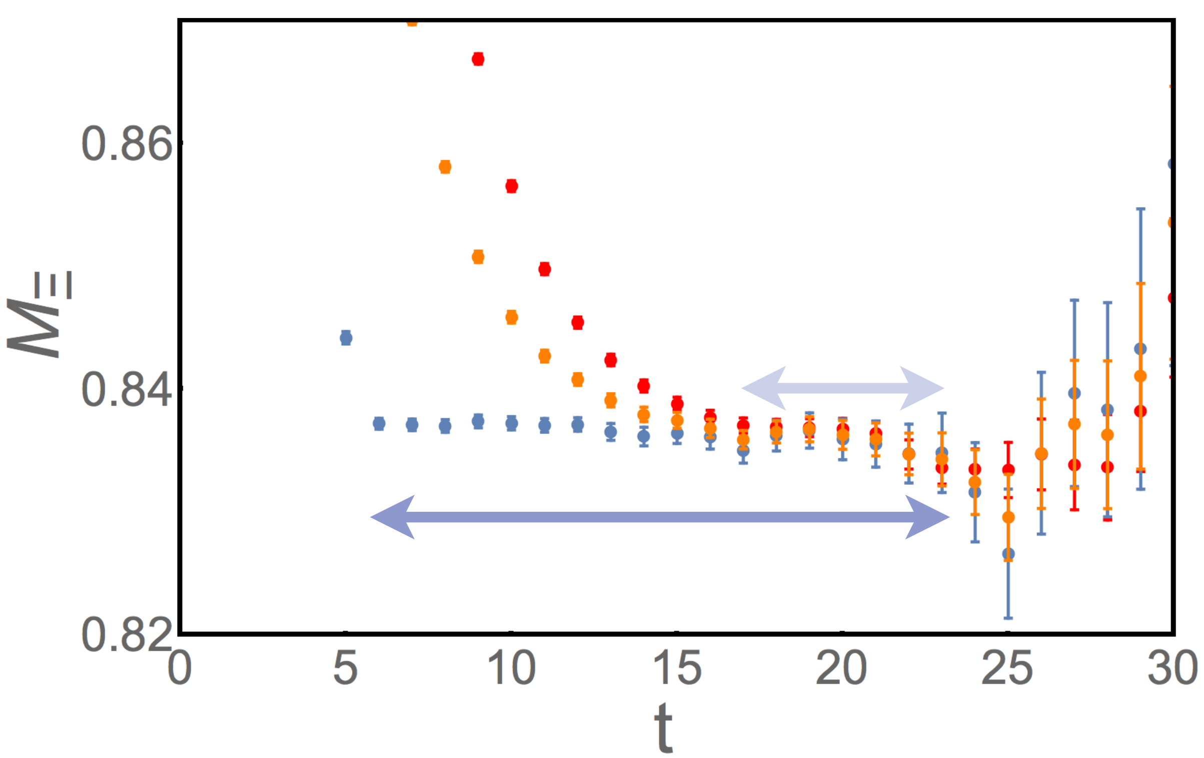
Linear combos. at the level of correlation functions



Beane et al (NPLQCD), Phys.Rev.D79:114502 (2009).

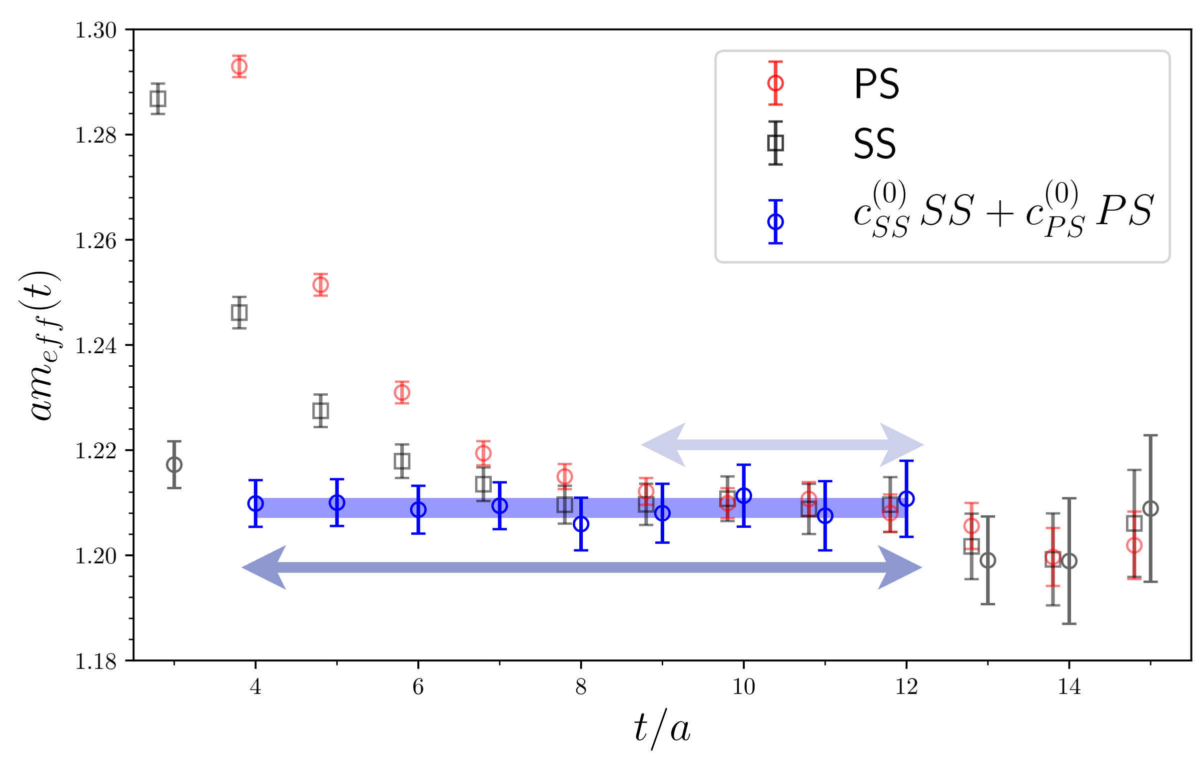
An example

Linear combos. at the level of correlation functions



Beane et al (NPLQCD), Phys.Rev.D79:114502 (2009).

Berkowitz et al (CalLatt), arXiv:1710.05642(2017).

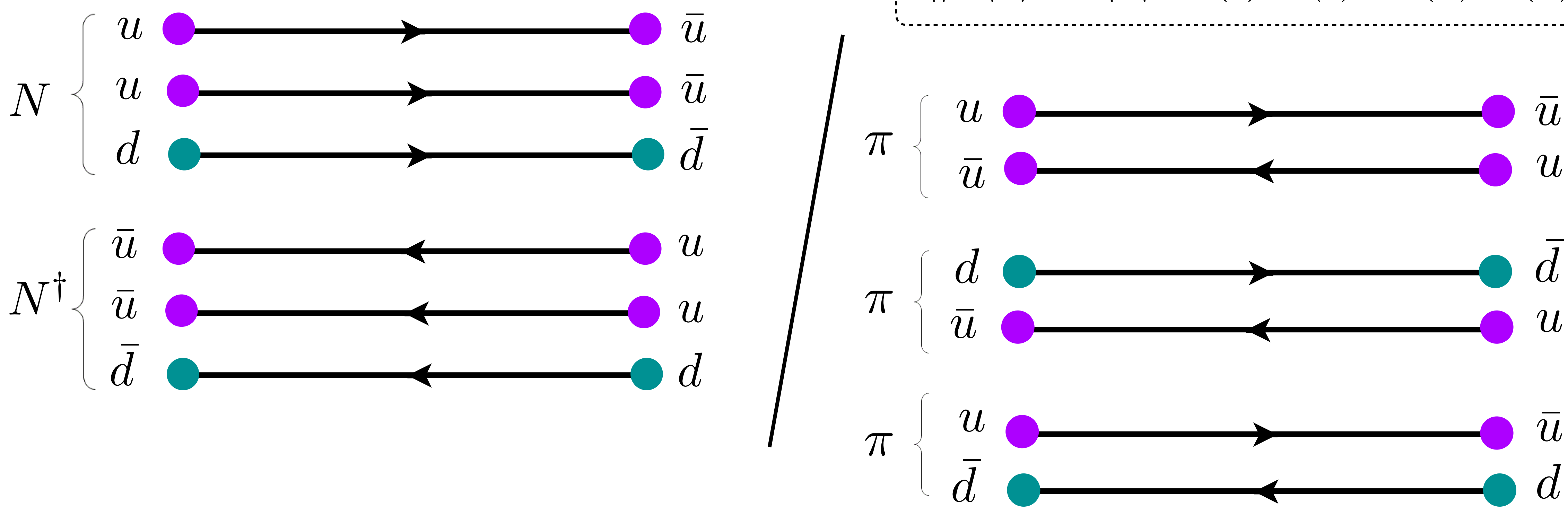


Linear combos. at the level of sink construction

iii) THERE IS A SEVERE SIGNAL-TO-NOISE DEGRADATION.

The origin of noise

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



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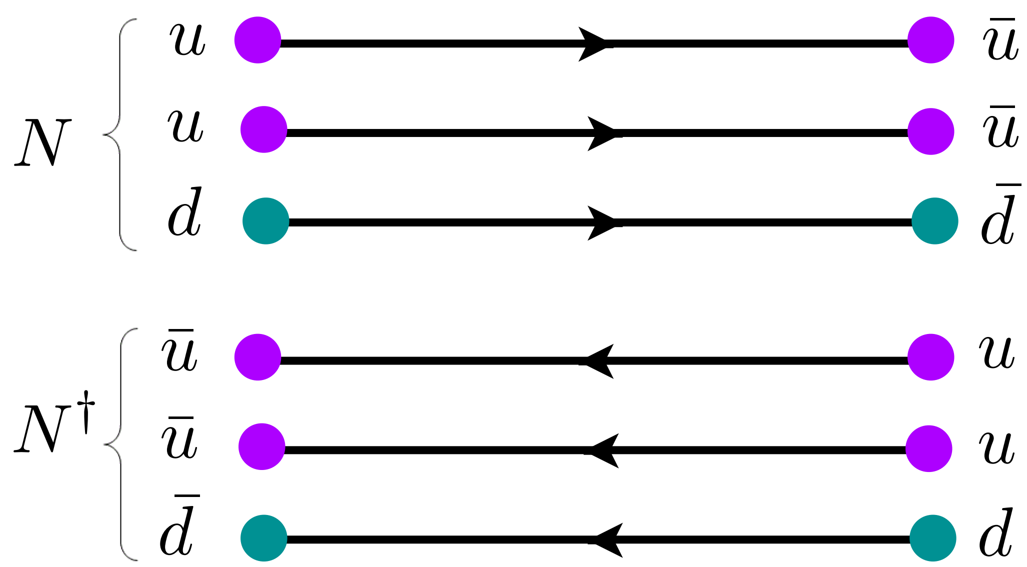
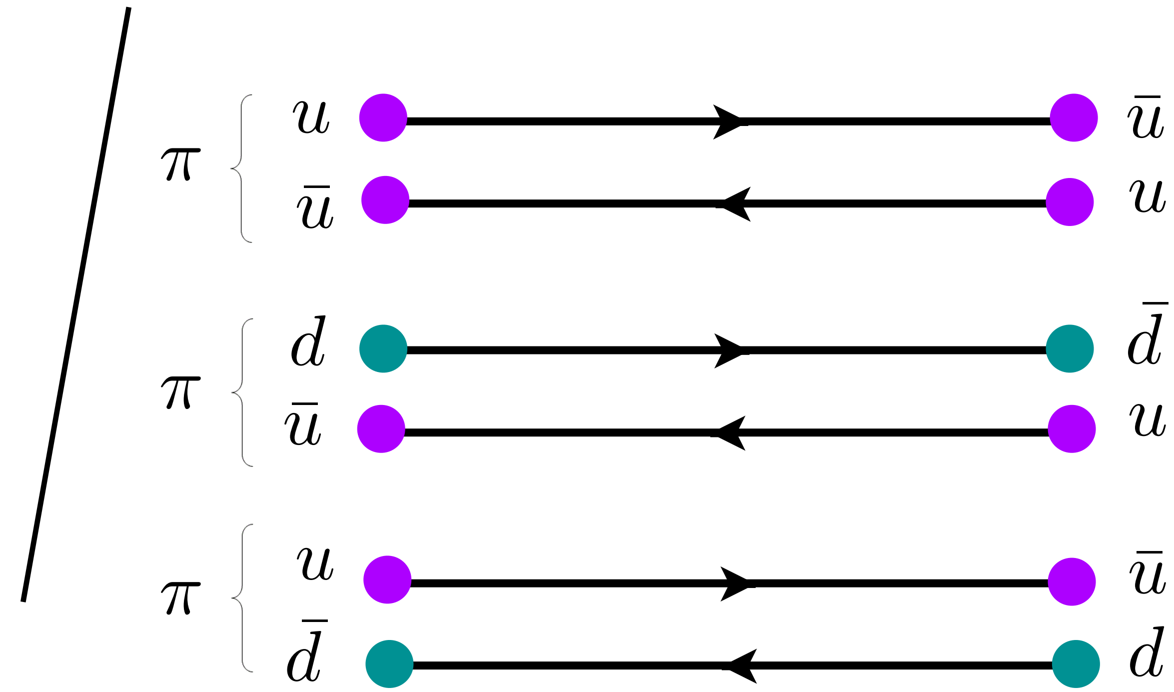
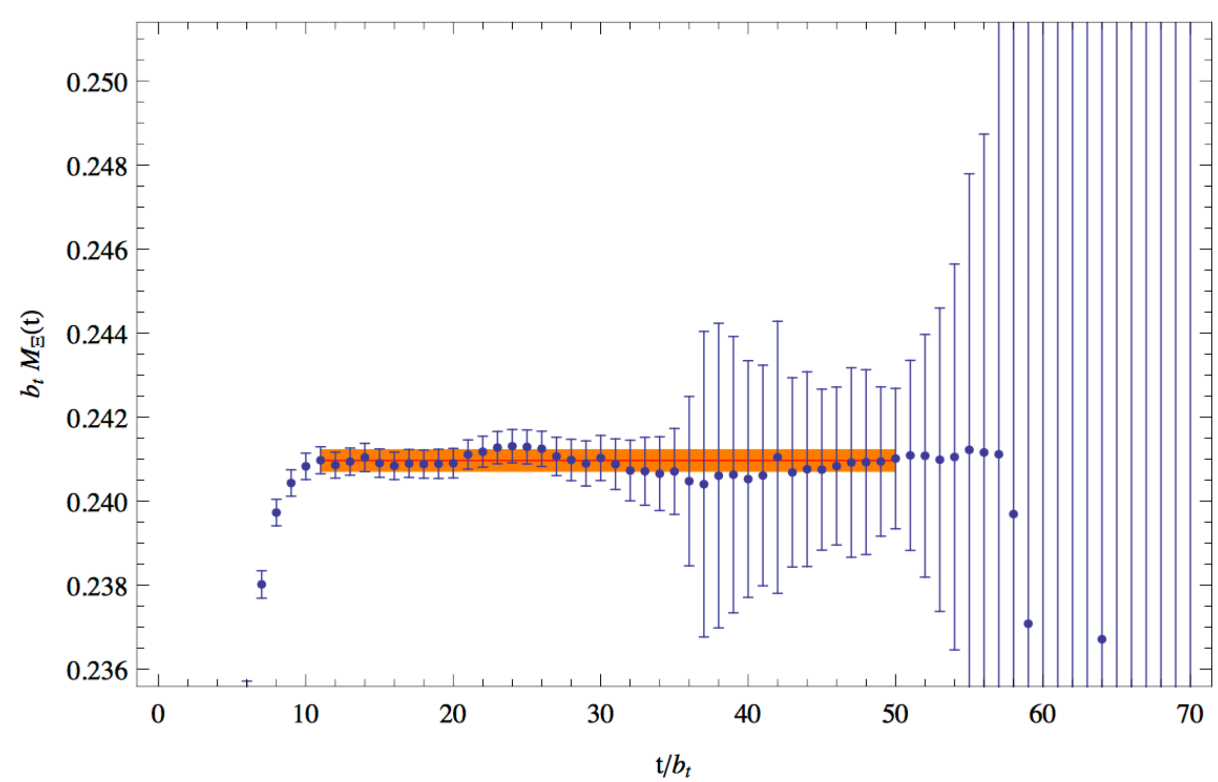




The ground-state of the variance correlator is three pions and not two nucleons:

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

`Parisi (1984) and Lepage (1989).`

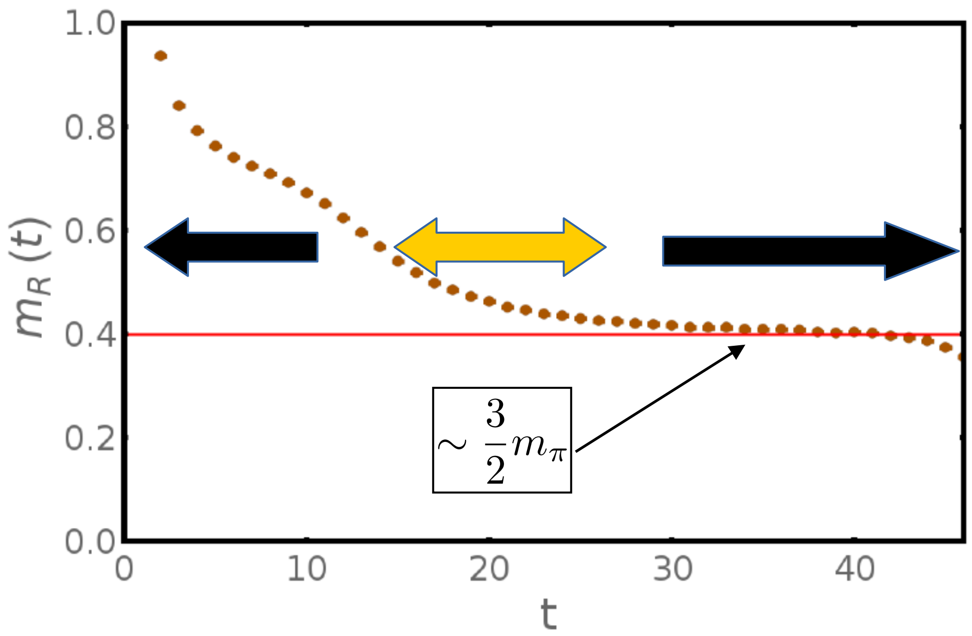


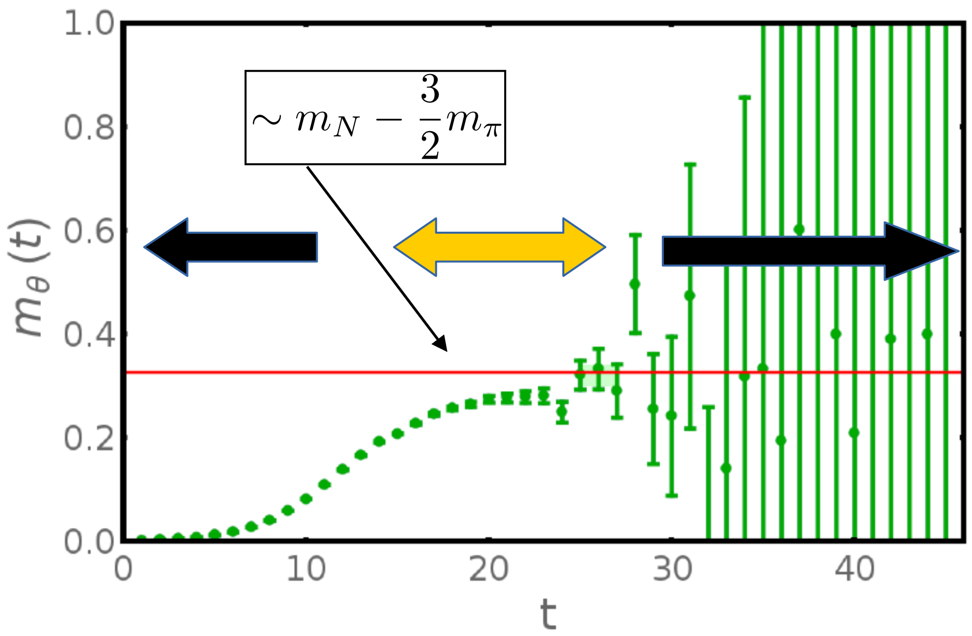
Can we understand better the noise in nuclear correlation function and control it?

$$\text{StN} \sim e^{-(m_N - \frac{3}{2}m_\pi)\Delta t}$$

Wagman and Savage (2016,2017).

Let's consider the magnitude and the phase of the correlation functions: $C_i(t) = e^{R_i(t)+i\theta_i(t)}$



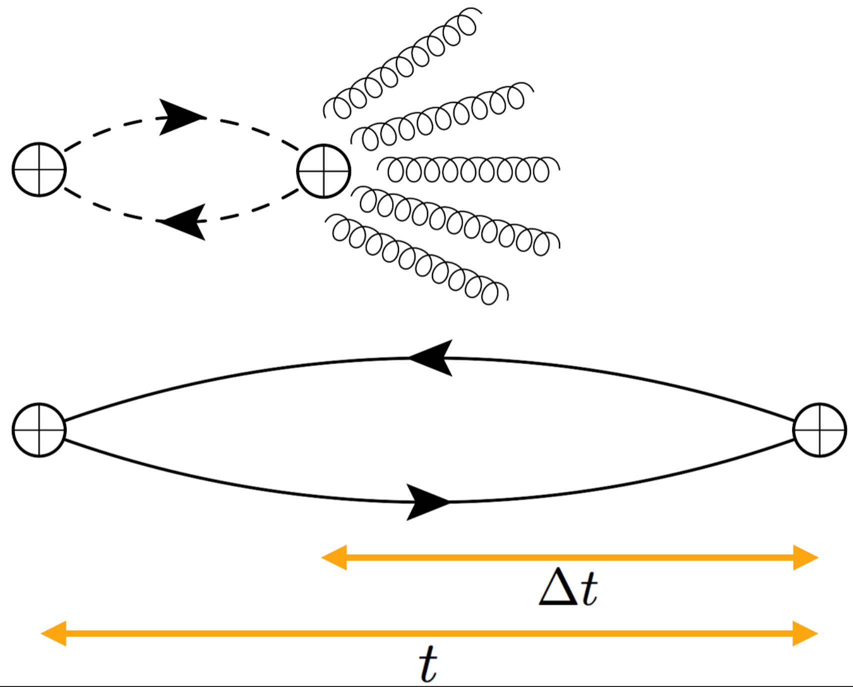


$$m_R(t) = \ln\left(\frac{\langle e^{R_i(t)}\rangle}{\langle e^{R_i(t+1)}\rangle}\right)$$

$$m_\theta(t) = \ln\left(\frac{\langle e^{i\theta_i(t)}\rangle}{\langle e^{i\theta_i(t+1)}\rangle}\right)$$

A phase reweighting method seems to work:

$$G^{\theta}(t, \Delta t) = \langle e^{-i\theta(t-\Delta t)} C(t) \rangle$$



$$M_{\rho}^{\theta}(t, \Delta t) \;=\; M_{\rho} \;+\; c\, \delta M_{\rho} e^{-\delta M_{\rho} \Delta t} \;+\; \ldots$$

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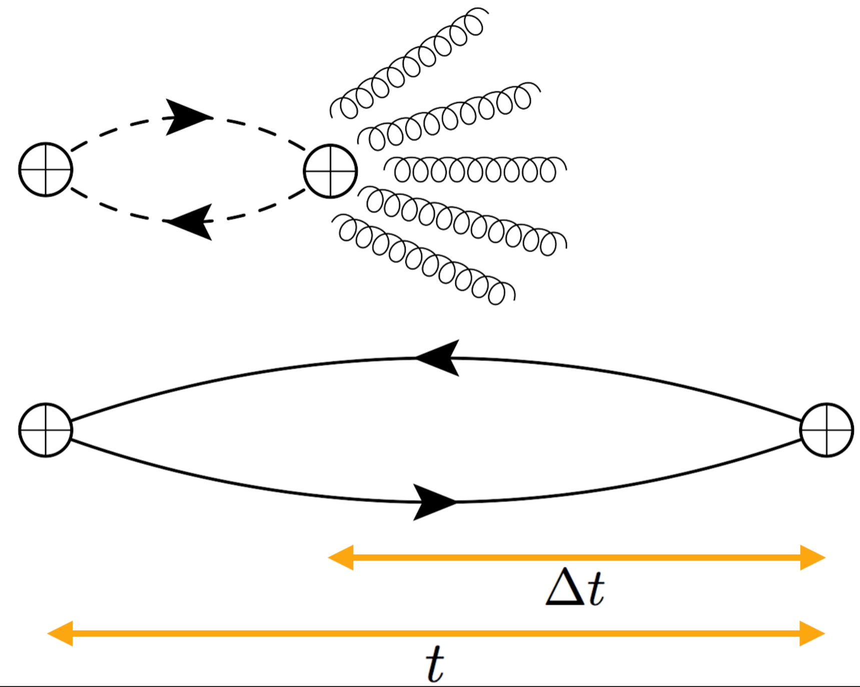
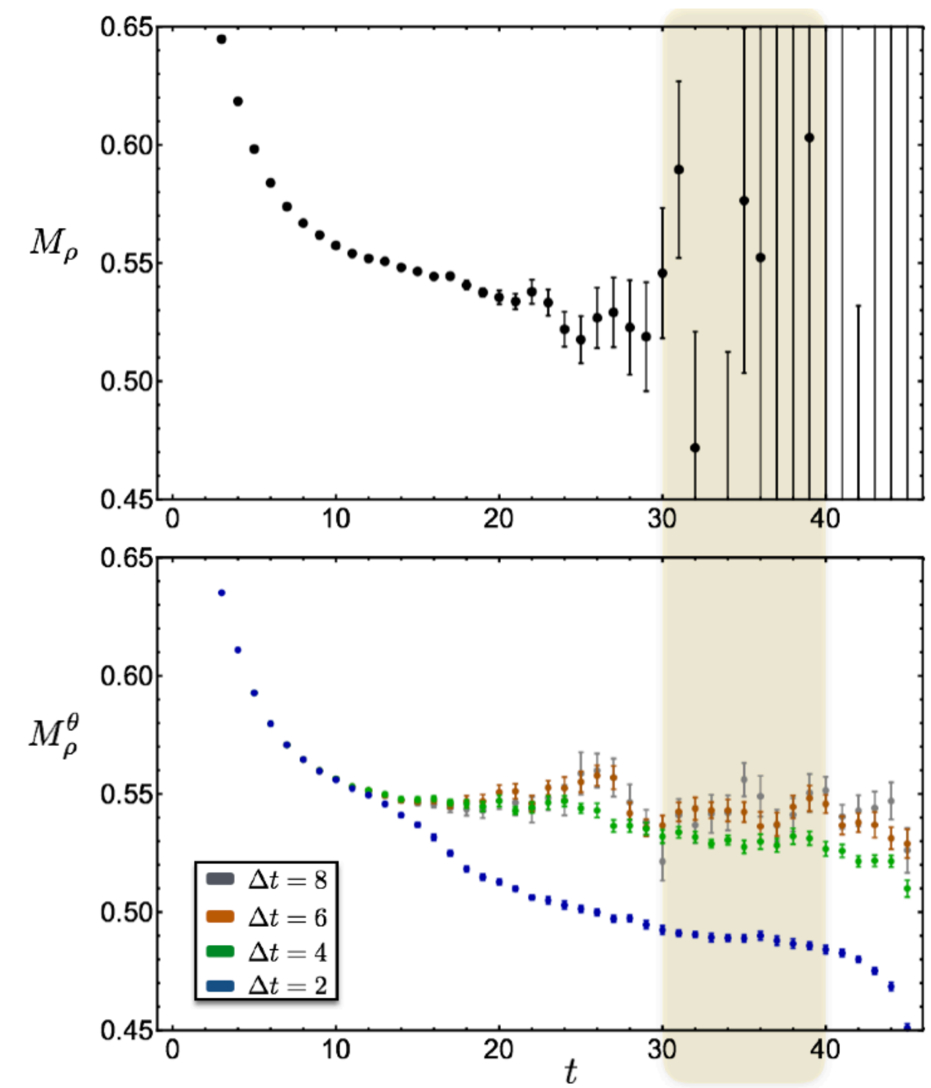
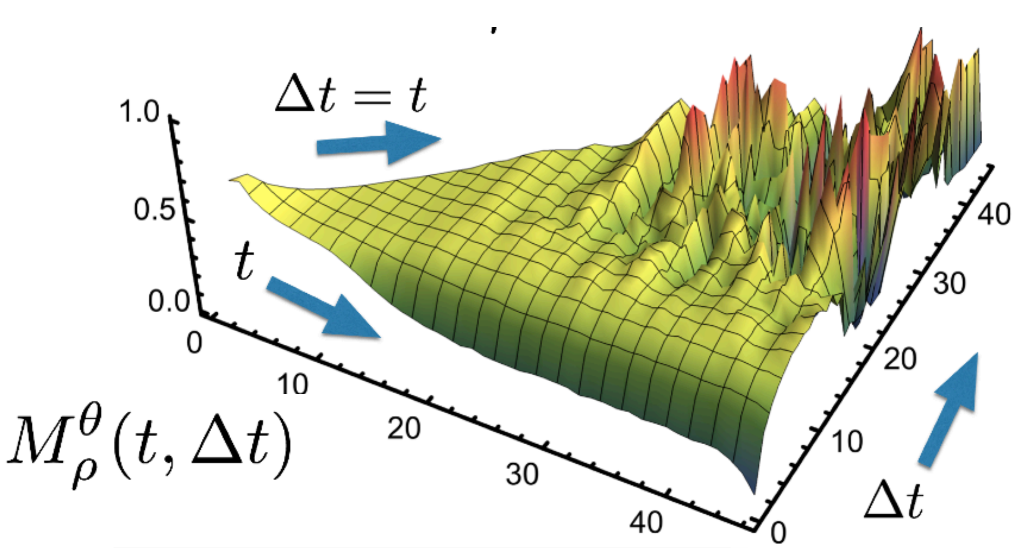
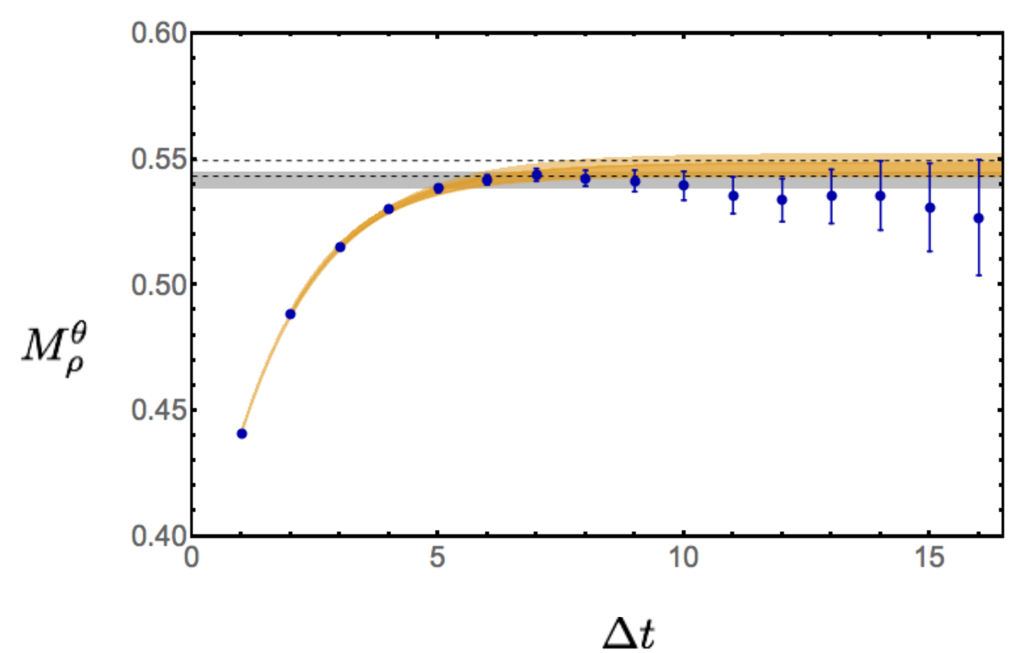


$$M_{\rho}^{\theta}(t, \Delta t) \;=\; M_{\rho} \;+\; c\,\delta M_{\rho} e^{-\delta M_{\rho} \Delta t} \;+\; \ldots$$







DESPITE CHALLENGES, PROGRESS HAS BEEN MADE. LQCD COMBINED WITH EFTS IS ON RIGHT TRACK TO DELIVER RESULTS ON IMPORTANT NUCLEAR PHYSICS QUANTITIES.

IN THE NEXT TWO LECTURES, WE WILL GO THROUGH A FEW EXAMPLES THAT DEMONSTRATE SUCH A PROGRESS.

QUESTIONS?