SORCERY

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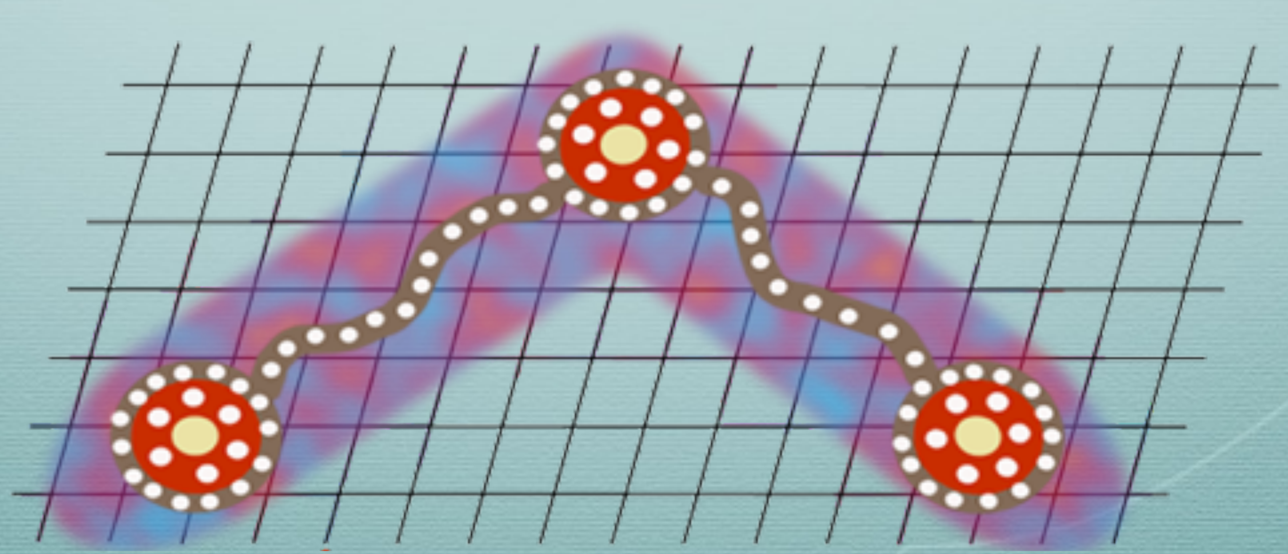


Hadron Interactions

Goals:

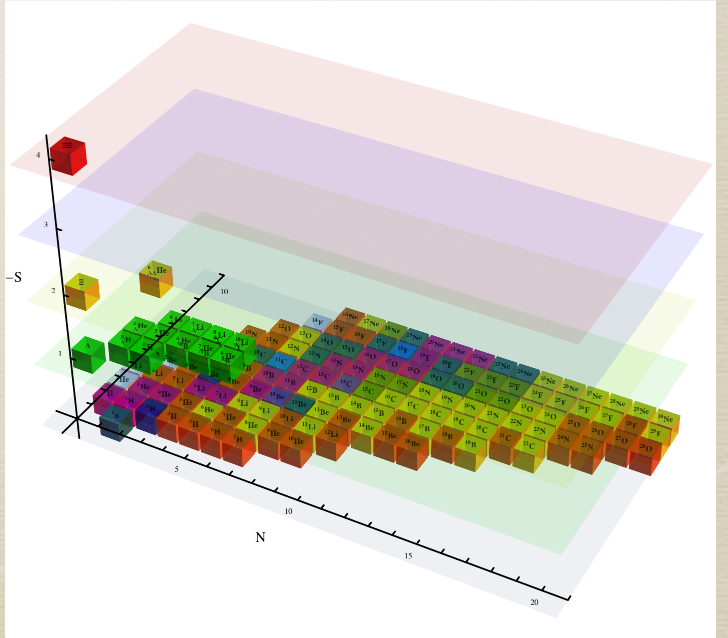
* Challenge: Compute properties of nuclei from QCD
    * Spectrum and structure
* Confirm well known experimental observations for two nucleon systems
* Explore the largely unknown territory of hyper-nuclear physics
* Provide input for the equation of state for nuclear matter in neutron stars
* Provide input for understanding the properties of multi-baryon systems

Jefferson Lab

FAIR

J-PARC

KEK
HIGH ENERGY ACCELERATOR RESEARCH ORGANIZATION



More than two body

* Construct interpolating fields
* Find efficient ways to perform the Wick contractions
* Address the signal to noise problem
* Extract the energy spectrum
* Interpret the energy spectrum

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Interpolating fields

Most general multi-baryon interpolating field

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

The indices a are composite including space, spin, color and flavor

- The goal is to calculate the tensors w
- The tensors w are completely antisymmetric
- Number of terms in the sum are $\dfrac{N!}{(N - n_q)!}$

Imposing the anti-symmetry:

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

Reduced weights

Totally anti-symmetric tensor

$$\epsilon^{1,2,3,4,\cdots,n_q} = 1$$

* Total number of reduced weights: $\dfrac{N!}{n_q!(N-n_q)!}$

Hadronic Interpolating field

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

hadronic reduced weights

baryon composite interpolating field

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

Basak et.al. PhysRevD.72.074501 (2005)

Calculation of weights

- Compute the hadronic weights
- Replace baryons by quark interpolating fields
- Perform Grassmann reductions
- Read off the reduced weights for the quark interpolating fields
- Computations done in: `algebra (C++)`

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

$$\downarrow$$

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

Interpolating fields

For a single point source

NPLQCD arXiv:1206.5219

Label	A	s	I	J^π	Local SU(3) irreps	int. field size
N	1	0	1/2	$1/2^+$	$\mathbf{8}$	9
Λ	1	-1	0	$1/2^+$	$\mathbf{8}$	12
Σ	1	-1	1	$1/2^+$	$\mathbf{8}$	9
Ξ	1	-2	1/2	$1/2^+$	$\mathbf{8}$	9
d	2	0	0	1^+	$\overline{\mathbf{10}}$	21
nn	2	0	1	0^+	$\mathbf{27}$	21
$n\Lambda$	2	-1	1/2	0^+	$\mathbf{27}$	96
$n\Lambda$	2	-1	1/2	1^+	$\mathbf{8}_A$, $\overline{\mathbf{10}}$	48, 75
$n\Sigma$	2	-1	3/2	0^+	$\mathbf{27}$	42
$n\Sigma$	2	-1	3/2	1^+	$\mathbf{10}$	27
$n\Xi$	2	-2	0	1^+	$\mathbf{8}_A$	96
$n\Xi$	2	-2	1	1^+	$\mathbf{8}_A$, $\mathbf{10}$, $\overline{\mathbf{10}}$	52,66,75
H	2	-2	0	0^+	$\mathbf{1}$, $\mathbf{27}$	90,132
^{3}H, ^{3}He	3	0	1/2	$1/2^+$	$\overline{\mathbf{35}}$	9
$^3_\Lambda$H$(1/2^+)$	3	-1	0	$1/2^+$	$\overline{\mathbf{35}}$	66
$^3_\Lambda$H$(3/2^+)$	3	-1	0	$3/2^+$	$\overline{\mathbf{10}}$	30
$^3_\Lambda$He, $^3_\Lambda\tilde{\mathrm{H}}$, $nn\Lambda$	3	-1	1	$1/2^+$	$\mathbf{27}$, $\overline{\mathbf{35}}$	30,45
$^3_\Sigma$He	3	-1	1	$3/2^+$	$\mathbf{27}$	21
^{4}He	4	0	0	0^+	$\overline{\mathbf{28}}$	1
$^4_\Lambda$He, $^4_\Lambda$H	4	-1	1/2	0^+	$\overline{\mathbf{28}}$	6
$^4_{\Lambda\Lambda}$He	4	-2	1	0^+	$\mathbf{27}$, $\overline{\mathbf{28}}$	15, 18
$\Lambda\Xi^0 pnn$	5	-3	0	$3/2^+$	$\overline{\mathbf{10}}$ + ...	1

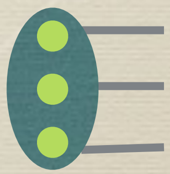
Hadronic interpolating field

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

Quark interpolating field

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

Baryon Block

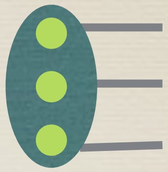


$$\mathcal{B}^{a_1,a_2,a_3}(b,\mathbf{p};x_0) = \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \sum_{k=1}^{N_{B(b)}} \tilde{w}_b^{(c_1,c_2,c_3),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,i_3} S(c_{i_1},\mathbf{x};a_1,x_0)S(c_{i_2},\mathbf{x};a_2,x_0)S(c_{i_3},\mathbf{x};a_3,x_0)$$

Quark propagator

Block construction

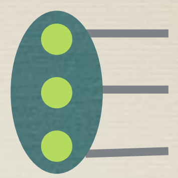
$$\mathcal{B}^{a_1,a_2,a_3}(b,\mathbf{p};x_0) = \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \sum_{k=1}^{N_{B(b)}} \tilde{w}_b^{(c_1,c_2,c_3),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,i_3} S(c_{i_1},\mathbf{x};a_1,x_0)S(c_{i_2},\mathbf{x};a_2,x_0)S(c_{i_3},\mathbf{x};a_3,x_0)$$



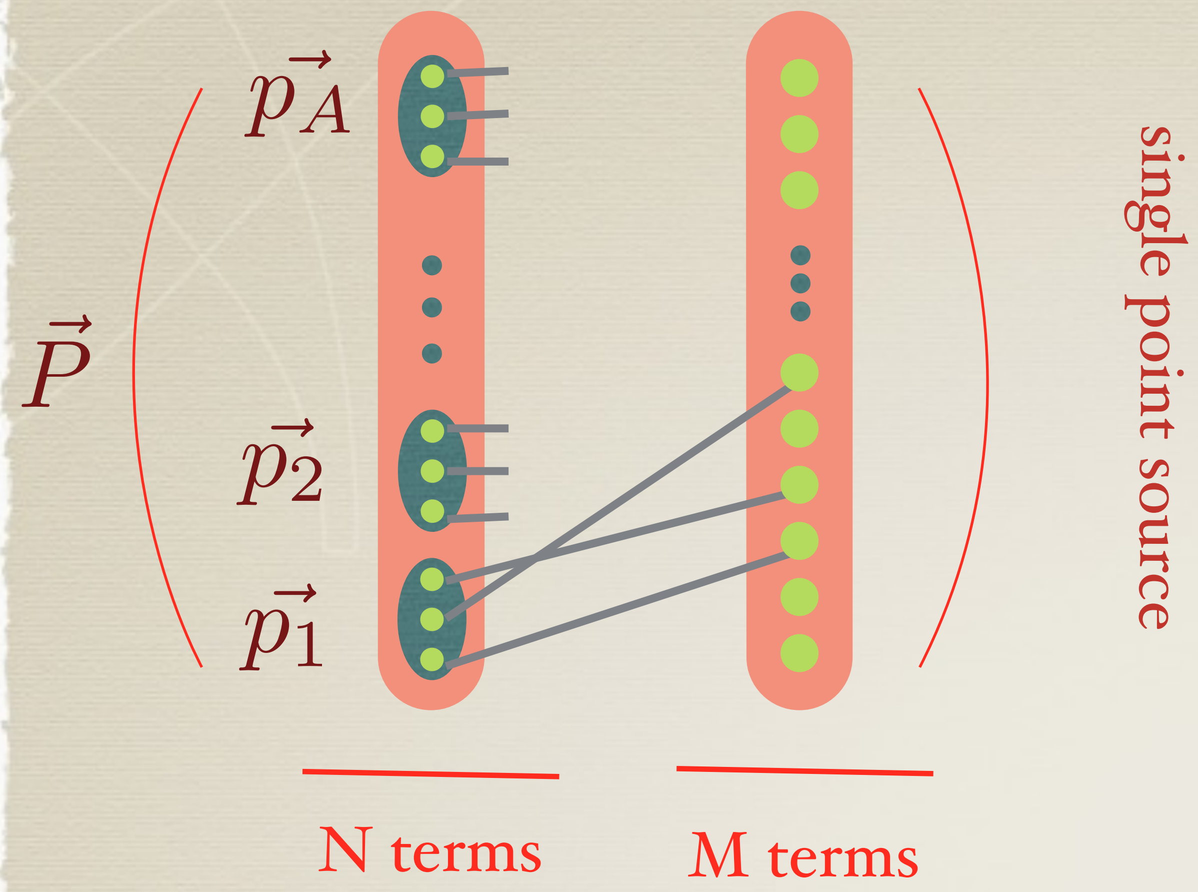
* This is parallel task
    * Requires global sums
    * Requires careful ordering of loops to minimize flops and memory access
    * Is vectorizable for both CPU and GPU
    * We break out of QDP++ for performance
    * QDP++ version exists

Block construction

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



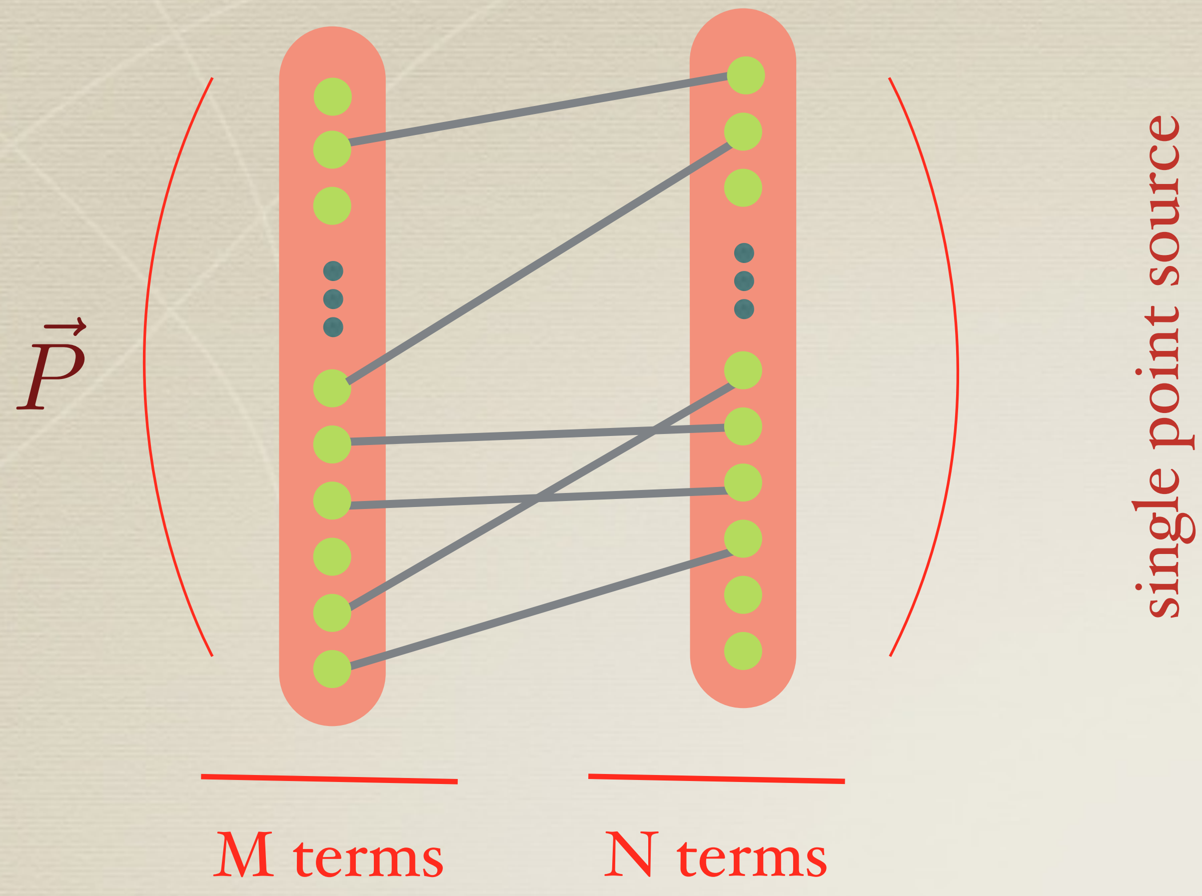
- Produces large data sets
  - Data need to be stored in disk
  - Data need to be accessed fast from disk or memory
  - Use the MapObject construct from QDP++
  - The code that uses these data is serial...



Quarks to Hadrons

Cost: $M \cdot N \frac{n_u! n_d! n_s!}{2^{(A - n_{\Sigma^0} - n_\Lambda)}}$

* Loop over all source and sink terms
* Connect each baryon in all possible ways to the source quarks (selecting the indices from the block)
* ^{4}He cost: 0.8 s per time slice on a single core of a Dual Core AMD Opteron 285 processor



Quarks to Quarks

Naive Cost: $n_u!n_d!n_s! \times NM$

Actual Cost: $n_u^3 n_d^3 n_s^3 \times MN$

- Loop over all source and sink terms
- Compute the determinant for each flavor
- Cost is polynomial in quark number

Quarks to Quarks

$$[\mathcal{N}_1^h(t)\bar{\mathcal{N}}_2^h(0)] = \int \mathcal{D}q\mathcal{D}\bar{q}\; e^{-\mathcal{S}_{QCD}} \sum_{k'=1}^{N'_w}\sum_{k=1}^{N_w} \tilde{w}_h'^{(a'_1,a'_2\cdots a'_{n_q}),k'}\;\; \tilde{w}_h^{(a_1,a_2\cdots a_{n_q}),k} \times$$

$$\times \sum_{\mathbf{j}}\sum_{\mathbf{i}} \epsilon^{j_1,j_2,\cdots,j_{n_q}}\epsilon^{i_1,i_2,\cdots,i_{n_q}} q(a'_{j_{n_q}})\cdots q(a'_{j_2})q(a'_{j_1}) \times \bar{q}(a_{i_1})\bar{q}(a_{i_2})\cdots\bar{q}(a_{i_{n_q}})$$

$$= \; e^{-\mathcal{S}_{eff}} \sum_{k'=1}^{N'_w}\sum_{k=1}^{N_w} \tilde{w}_h'^{(a'_1,a'_2\cdots a'_{n_q}),k'}\;\; \tilde{w}_h^{(a_1,a_2\cdots a_{n_q}),k} \times$$

$$\times \sum_{\mathbf{j}}\sum_{\mathbf{i}} \epsilon^{j_1,j_2,\cdots,j_{n_q}}\epsilon^{i_1,i_2,\cdots,i_{n_q}} S(a'_{j_1};a_{i_1})S(a'_{j_2};a_{i_2})\cdots S(a'_{j_{n_q}};a_{i_{n_q}})$$

Define the matrix:

$$G(j,i)^{(a'_1,a'_2\cdots a'_{n_q});(a_1,a_2\cdots a_{n_q})} = S(a'_j;a_i)$$

Quarks to Quarks

The matrix:

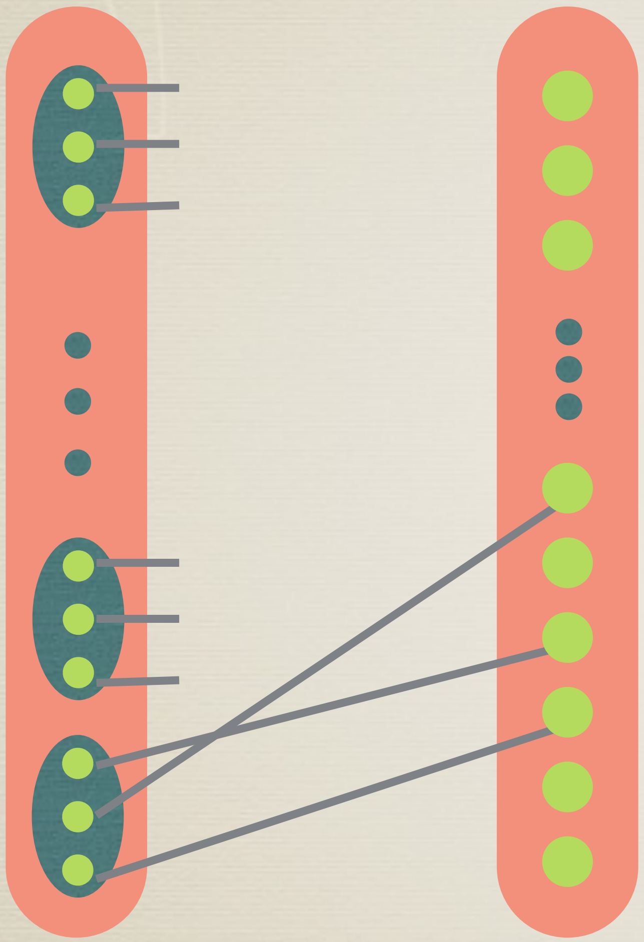
$$G(j,i)^{(a'_1,a'_2\cdots a'_{n_q});(a_1,a_2\cdots a_{n_q})} = S(a'_j;a_i)$$

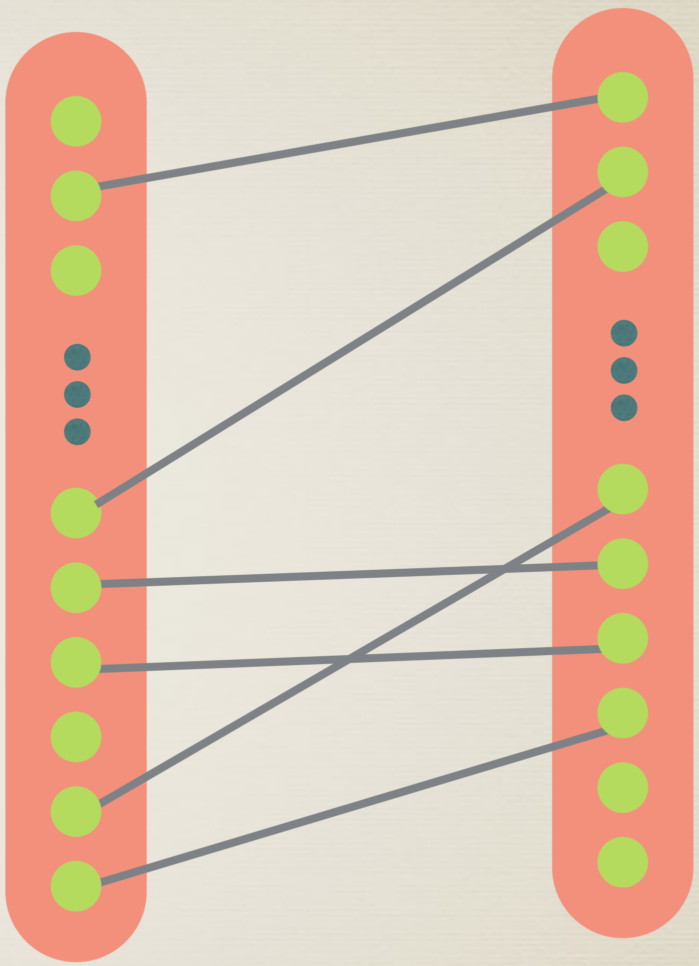
The Correlation function:

$$[\mathcal{N}_1^h(t)\bar{\mathcal{N}}_2^h(0)] = \sum_{k'=1}^{N'_w}\sum_{k=1}^{N_w} \tilde{w}_h^{\prime(a'_1,a'_2\cdots a'_{n_q}),k'} \; \tilde{w}_h^{(a_1,a_2\cdots a_{n_q}),k} \times \left| G^{(a'_1,a'_2\cdots a'_{n_q});(a_1,a_2\cdots a_{n_q})} \right|$$

Total momentum projection is implicit in the above

Contraction methods





- quark to hadronic interpolating fields
  - Better interpolating fields
  - Better correlation functions

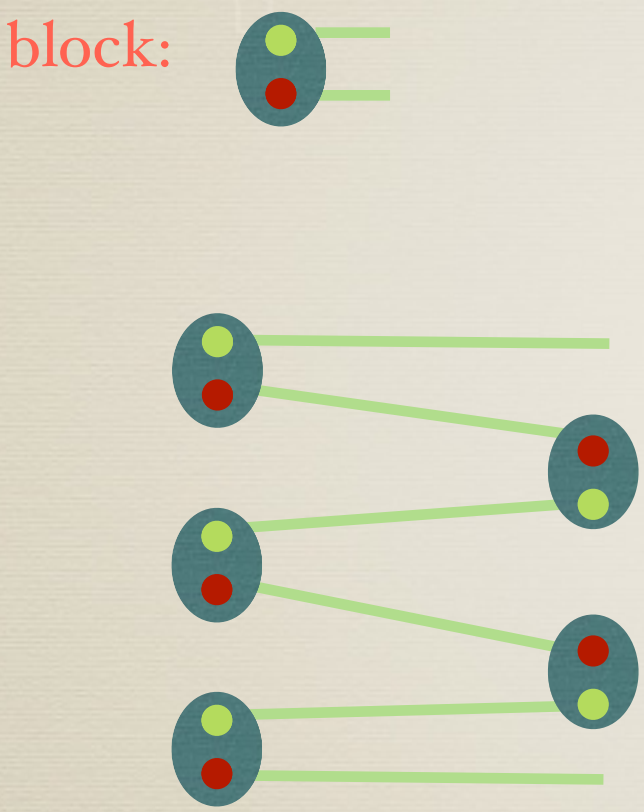
- quark to quark interpolating fields
  - Allow very large number of baryons
  - Correlators do not overlap with ground state well

Why are baryons hard

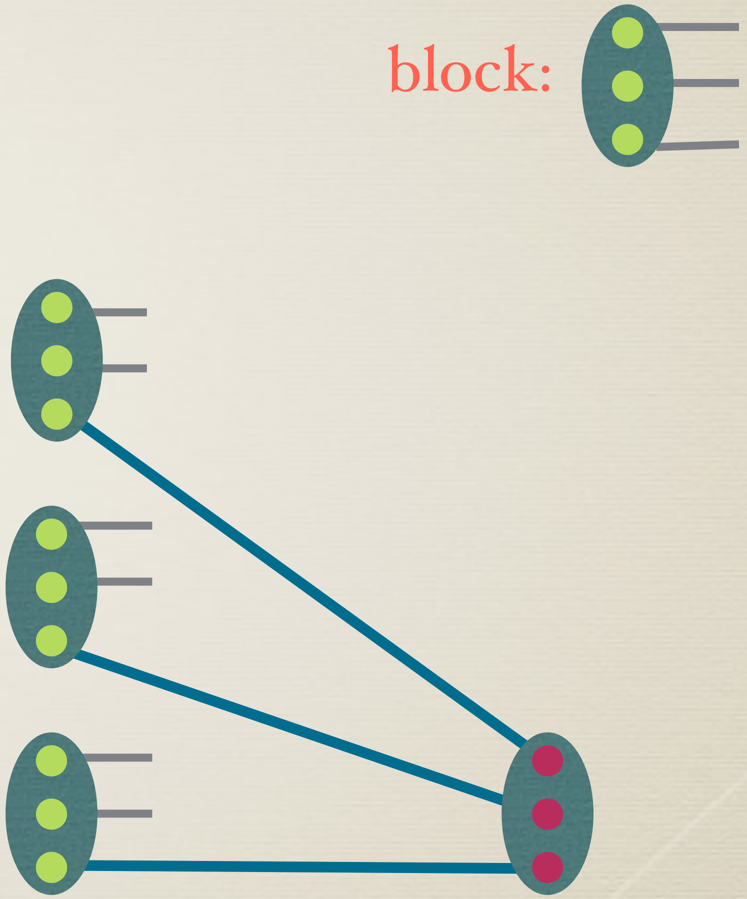
- We know that multi-meson contractions can be done fast:
  - Recursion relations for single point source [Detmold-Savage 2007]
  - Simpler and more efficient methods based on determinant evaluations exits [Shi,Detmold,KO 2012]
- Do recursion relations exist for baryons?
- Can we do as well as in the case of mesons?

Recursion relations

Mesons



Baryons



For baryons a proliferation of indices occur as baryons are added at the source

The tensor contraction engine

- Contractions no different than contactions of general tensors
    - For baryon we have 3-index tensors contracted (blocks) with the 3-index tensors (source interpolating fields)

The problem has been solved in a general way in chemistry

Lattice Setup

* Isotropic Clover Wilson with LW gauge action
  * Stout smeared (1-level)
  * Tadpole improved
* SU(3) symmetric point
  * Defined using m_π/m_Ω
* Lattice spacing 0.145fm
  * Set using Υ spectroscopy
* Large volumes
  * 24^3 x 48 32^3 x 48 48^3 x 64
  * 3.5fm 4.5fm 7.0fm

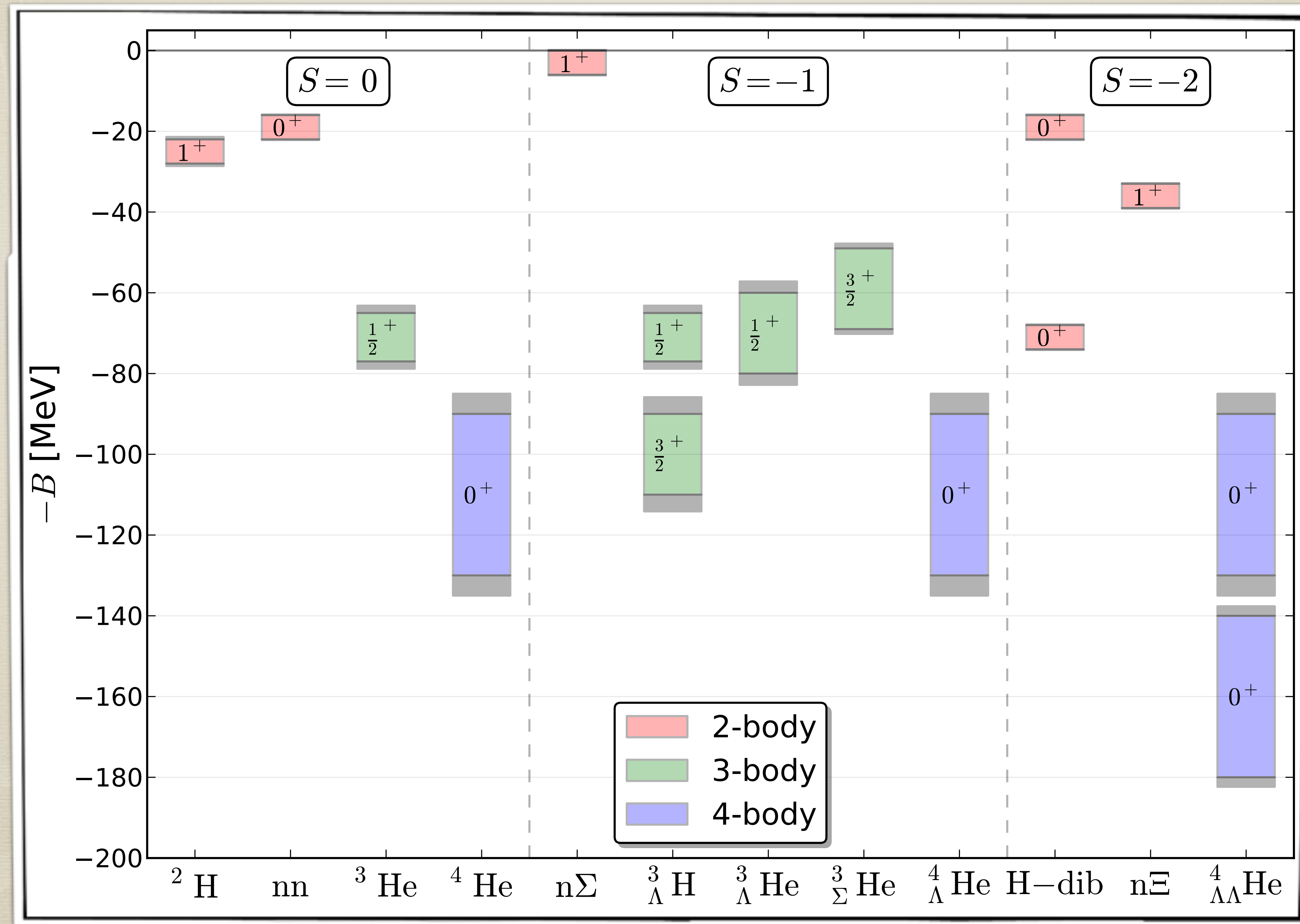
NPLQCD arXiv:1206.5219

Using Quark to Hadron contractions

* Calculate the spectrum of nuclei and hyper-hypernuclei
  * Work with A<6
* Use single point source for quark propagators
* In certain cases introduce nontrivial spatial wave function using a plane wave basis ($p^2<5$)
* Use boosted states interpolating fields to check for finite volume effects
* Hight statistics: 4K, 3K, 1.2K lattices with multiple correlators per lattice
* Cost of contractions negligible

Nuclear spectrum

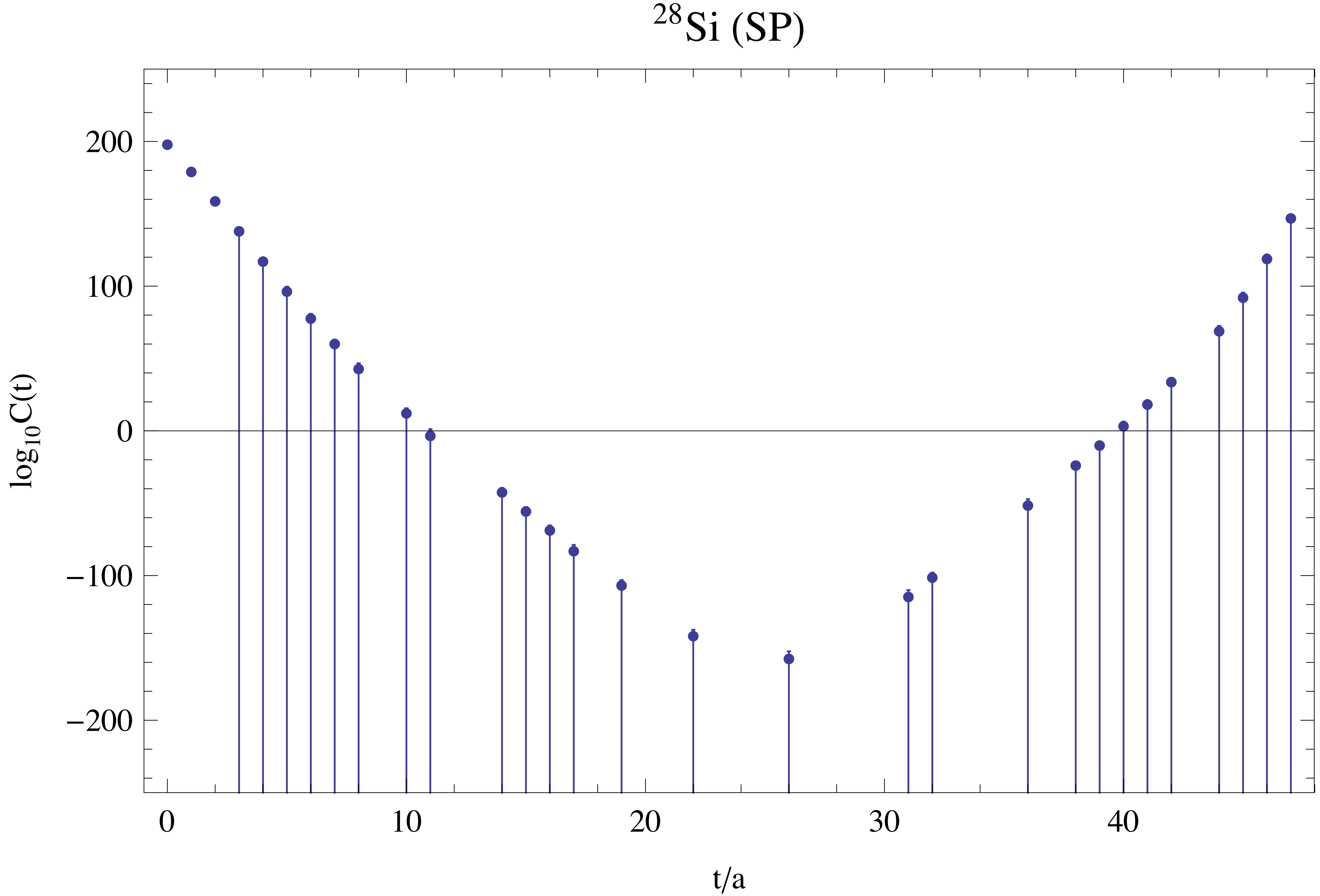
NPLQCD



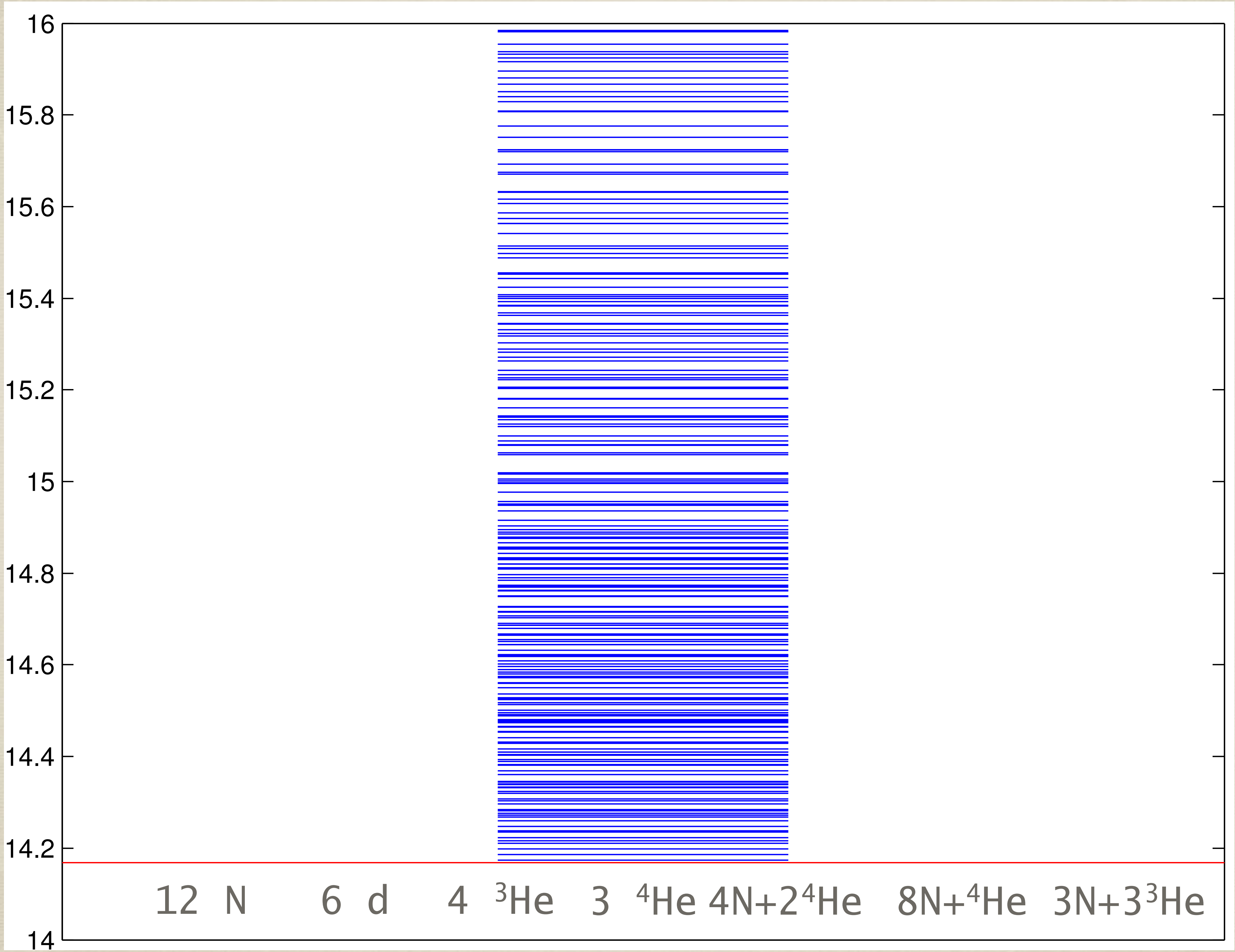
Using Quark to Quark contractions

* Push to large quark numbers
* Need to use more than one point for spacial wave function
  * Pauli exclusion principle ...
* Low statistics .... this was just a feasibility demonstration
* Only one volume: 32^3
* No attempt to extract physics

Correlators



Expected Carbon spectrum in the 32^3 box



Multi-meson contractions

Conclusions

* We have a systematic way of constructing all possible interpolating fields
* NPLQCD: Presented results for nuclei with A<5 and S>-3

  NPLQCD arXiv:1206.5219
* Special care needs to be given to the selection of interpolating fields
  * Minimize number of terms in the interpolating field and optimize the signal
* We have an algorithm for quark contractions in polynomial time