The Hyperspherical Harmonic basis for *ab-initio* nuclear theory

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Nuclear physics from first principles

Ab-initio approach

- How do we construct the Hamiltonian and the currents starting from first principles?

$$\hat{H}|\psi^N\rangle = E|\psi^N\rangle \qquad \hat{j}_\mu$$

- How do we compute the nuclear wave functions?

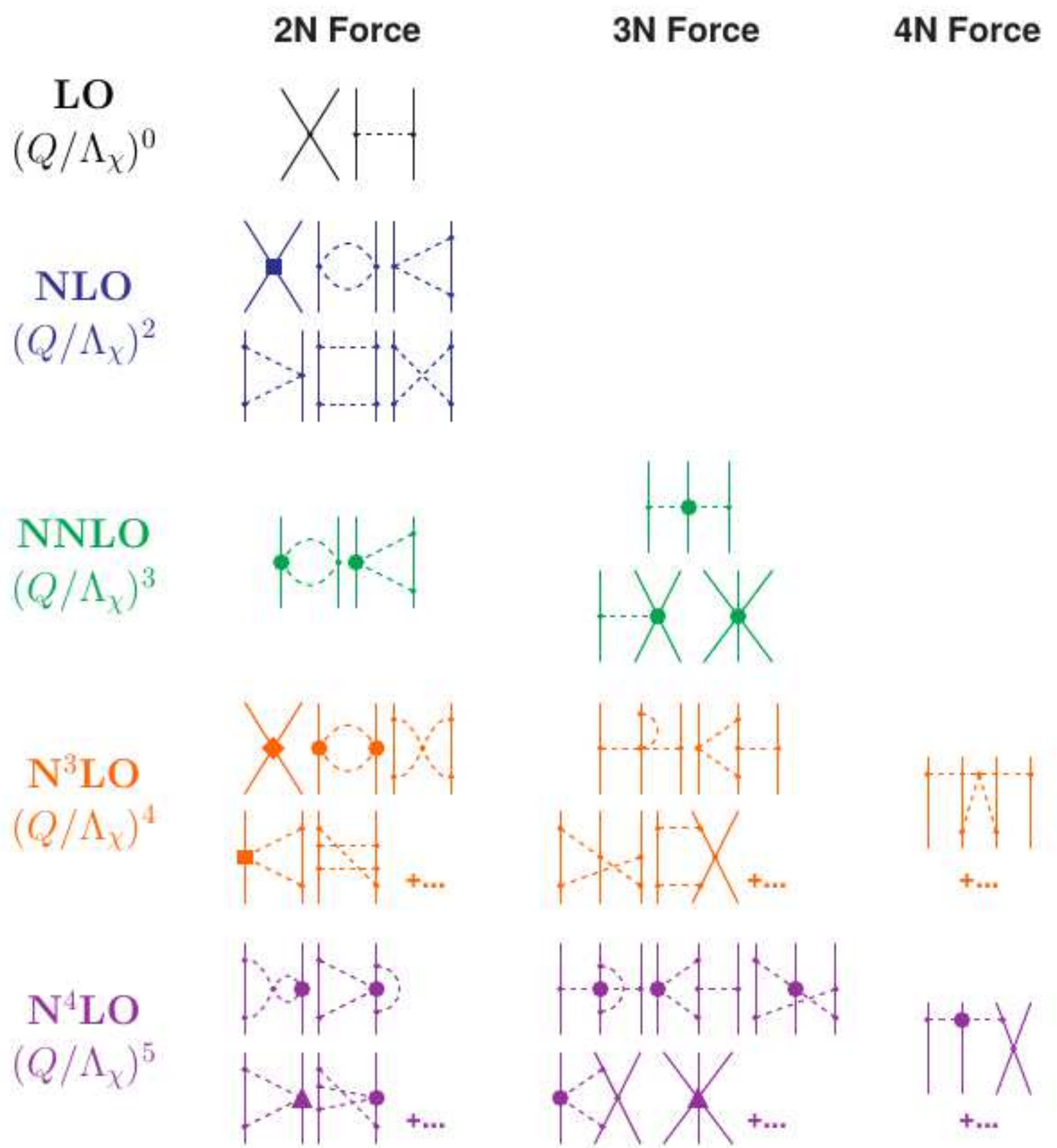
Overview

- **Chiral effective field theory**
- **The Hyperspherical Harmonics method**
- **Applications:**
    - The ^{6}Li wave function and the $\alpha + d$ clusterization
    - Magnetic form factors of light nuclei
- **Summary**

From QCD to nuclei

Chiral effective field theory (χEFT)

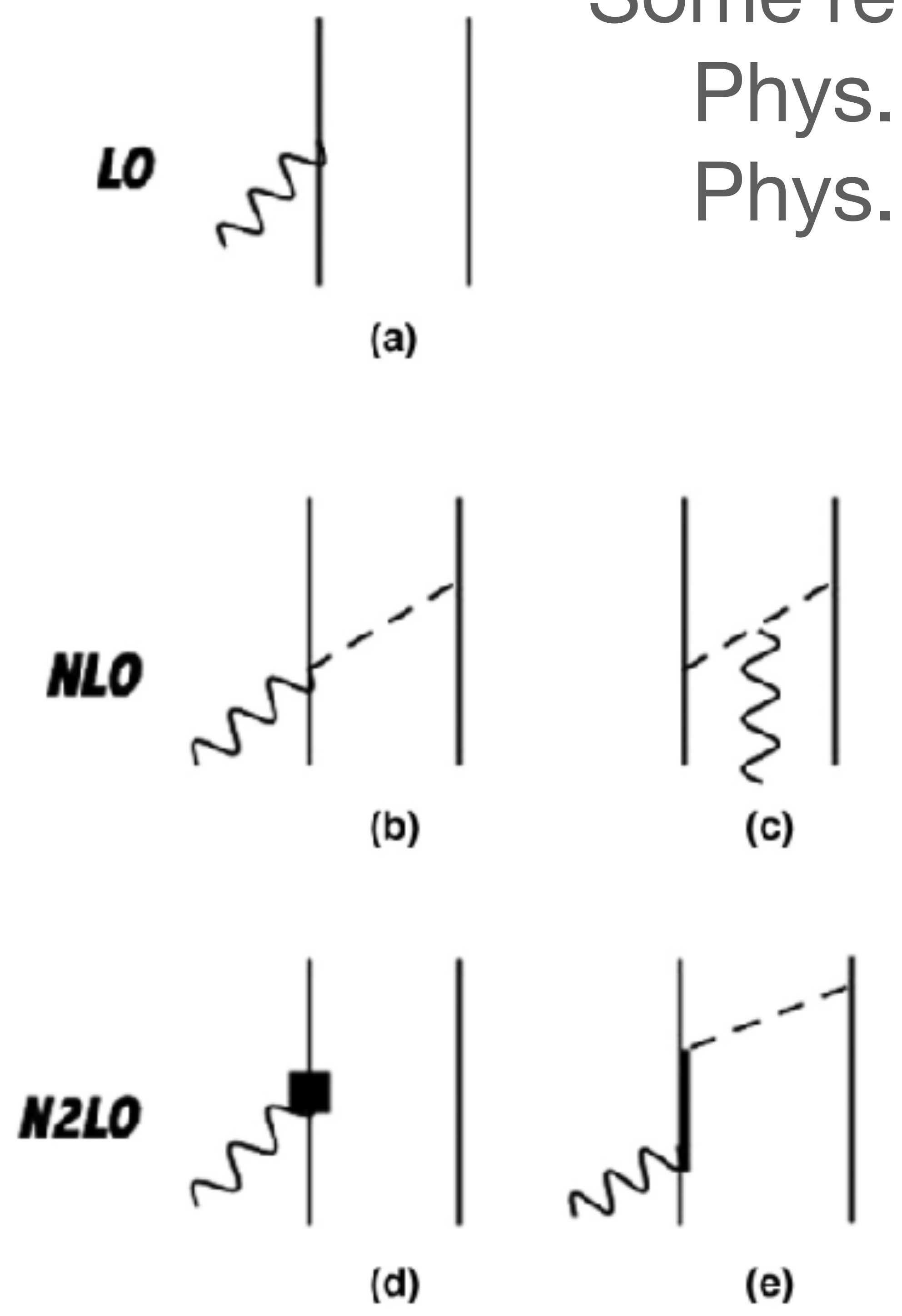
- Only Nucleons and Pions as degrees of freedom ($M_{QCD} \sim 1$ GeV)
- Direct connection with QCD: chiral symmetry (+ discrete symmetries + Lorentz invariance)
- Low Energy Constants (LECs): fitted on experimental data
- Organize the interaction as a power expansion Q/M_{QCD}



Phys. Rev. C **96**, 024004 (2017)
Phys. Rev. Lett. **115**, 122301 (2015)

Why chiral EFT?

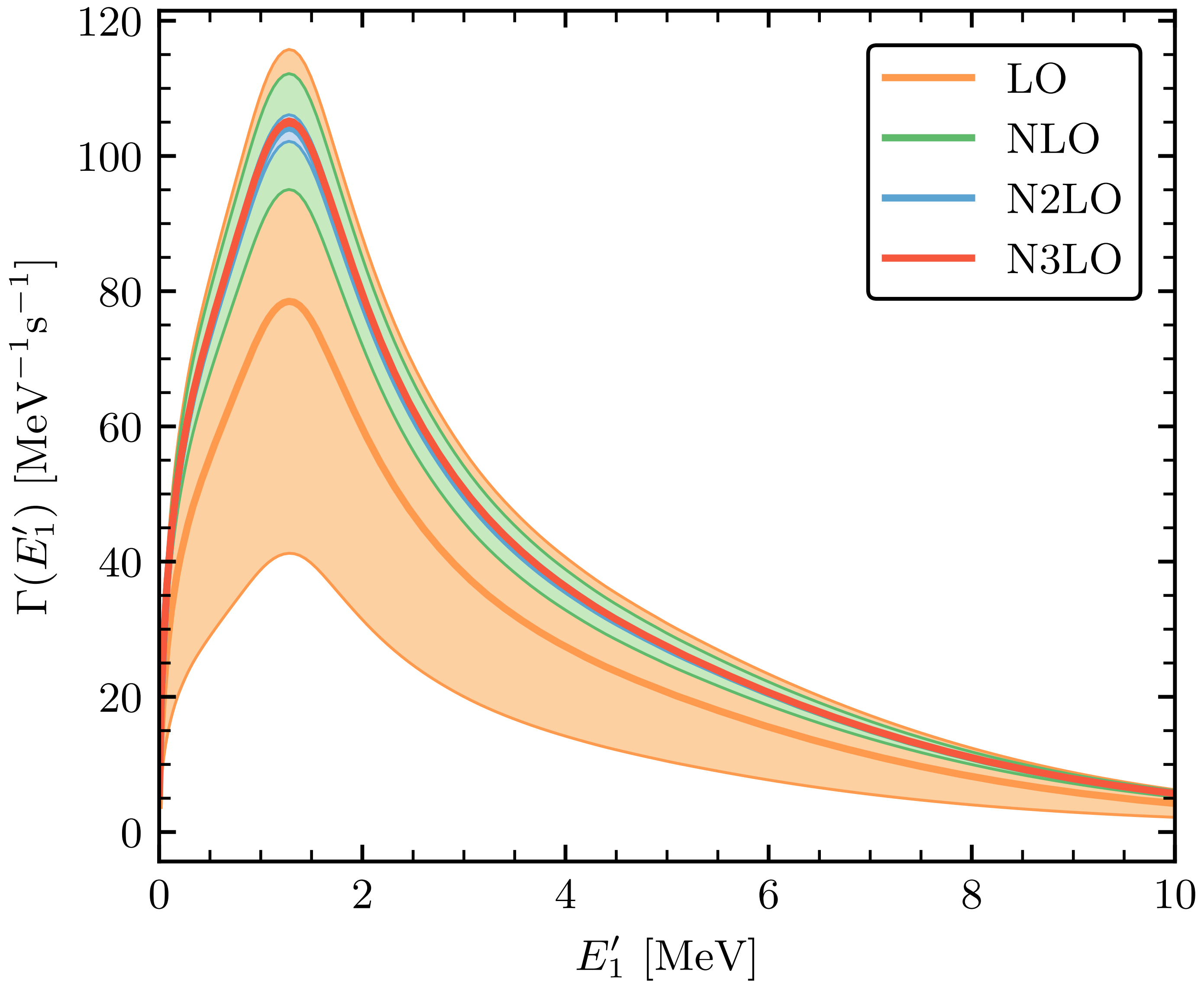
Some references for nuclear currents
Phys. Rev. C **80**, 034004 (2009)
Phys. Rev. C **99**, 034005 (2019)



- Consistent treatment of interactions with external probes

- You can add even BSM particles (i.e. dark matter, axions,…)

- Reliable estimate of the uncertainties generated by the theory



Spectra of muon capture

$$\mu^- + d \to n + n + \nu_\mu$$

Order-by-order expansion: control of the truncation errors

AG et al., arXiv:2305.07568

Computing the nuclear wave function

$$H = \sum_i \frac{p_i^2}{2M} + \sum_{i<j} V_{ij} + \sum_{i,j,k} V_{ijk} + \cdots$$

Solving the many-body problems for bound states

- A couple of examples
  - Hyperspherical Harmonic method

A. Kievsky, *et al.*, J. Phys. G, **35**, 063101 (2008)
L.E. Marcucci, *et al.*, Front. Phys. **8**, 69 (2020)

  - Neural Network quantum states

A. Lovato et al., Phys. Rev. Res. **4**, 041378 (2022)
AG et al., arXiv:2308.16266 (2023)

Eigenvalue problem for bound state

- **Rayleigh-Ritz variational principle**

$$E = \min_{c} \frac{\langle \Psi(c) | \hat{H} | \Psi(c) \rangle}{\langle \Psi(c) | \Psi(c) \rangle}$$

- A possible choice for the variational wave function is

$$|\psi(c)\rangle = \sum_i c_i \boxed{|f_i\rangle}$$

Complete orthonormal basis → **Hyperspherical Harmonics**

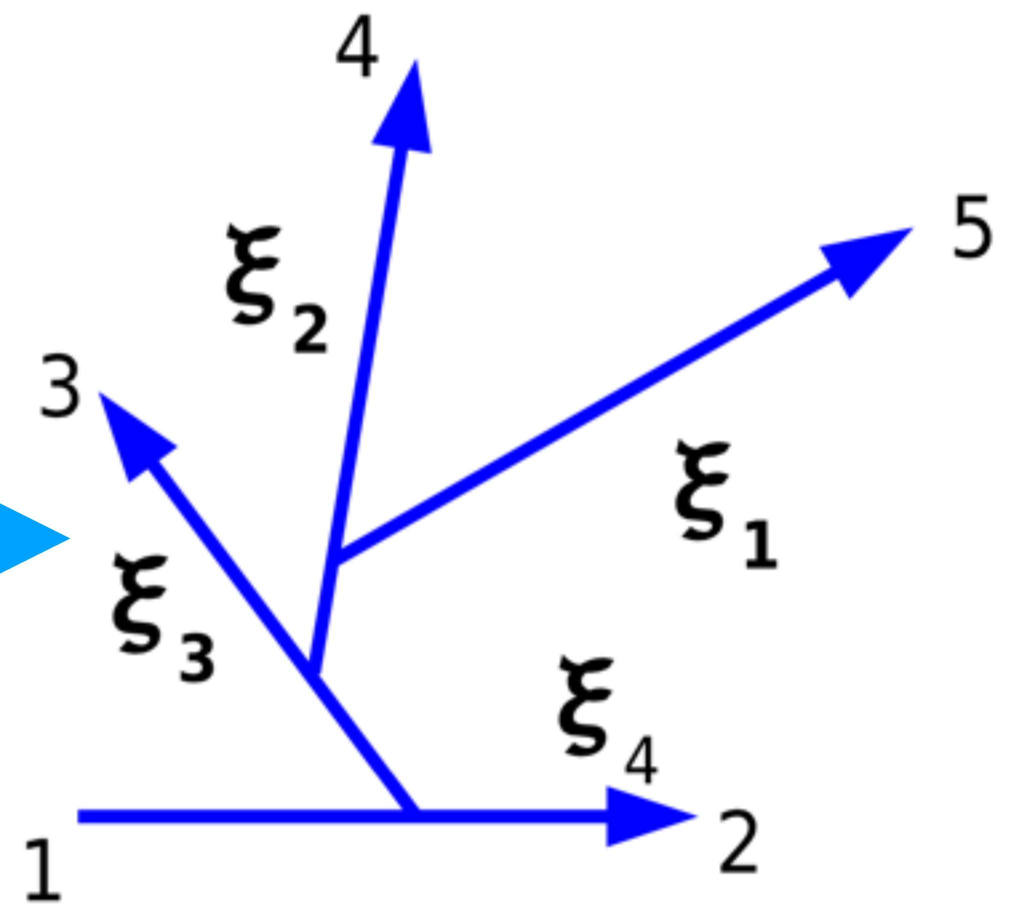
- **(Generalized) Eigenvalue problem**

$$\sum_j c_j \langle f_i | \hat{H} | f_j \rangle = E c_i$$

Hypersperical coordinates

- **Kinetic energy in Jacobi vectors**

$$T = -\frac{\hbar^2}{2m}\sum_{i=1}^{A}\nabla^2_{\vec{r}_i} = T_{CM} - \frac{\hbar^2}{m}\sum_{i=1}^{A-1}\nabla^2_{\vec{\xi}_i}$$



- **Kinetic energy in hyperspherical coordinates**

$\vec{\xi}_i$ →
- Angular part of the Jacobi vec. $\hat{\xi}_i$
- Angles between Jacobi vec. ϕ_i
- Hyperradius $\rho^2 = \sum_i \xi_i^2$

$$T_0 = -\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{3A-4}{\rho}\frac{\partial}{\partial\rho} - \frac{L^2(\Omega)}{\rho^2}\right)$$

The Hyperspherical Harmonic basis

- Eigenstates of the $L^2(\Omega)$ operator

$$L^2(\Omega)\mathscr{Y}_{[K]}(\Omega) = K(K + 3A - 5)\mathscr{Y}_{[K]}(\Omega)$$

Eigenvalue

The parameter we use to control our expansion

- The trivial case (A=2)

$$\hat{L}^2(\theta, \phi)\mathscr{Y}_{[K]}(\Omega) = K(K+1)\mathscr{Y}_{[K]}(\Omega)$$

$$\hat{L}^2 Y_{L,M}(\theta, \phi) = L(L+1)Y_{L,M}(\theta, \phi)$$

The HH wave function

Expansion on ρ
Laguerre polynomials

Spin and Isospin states

HH states

$$\psi_A^{J,J_z} = \sum_p \sum_{l,[KST]} c_{l,[KST]} f_l(\rho) \underbrace{\left[\mathcal{Y}_{[K]}(\Omega^p_{A-1}) \left[\chi^p_{[S]} \otimes \chi^p_{[T]}\right]\right]_{JJ_z}}_{\Phi^p_{[\alpha]}}$$

Unknown variational coefficients

Sum over the even permutations

This permits to antisymmetrize the wave function selecting specific quantum numbers

Construction of the basis I

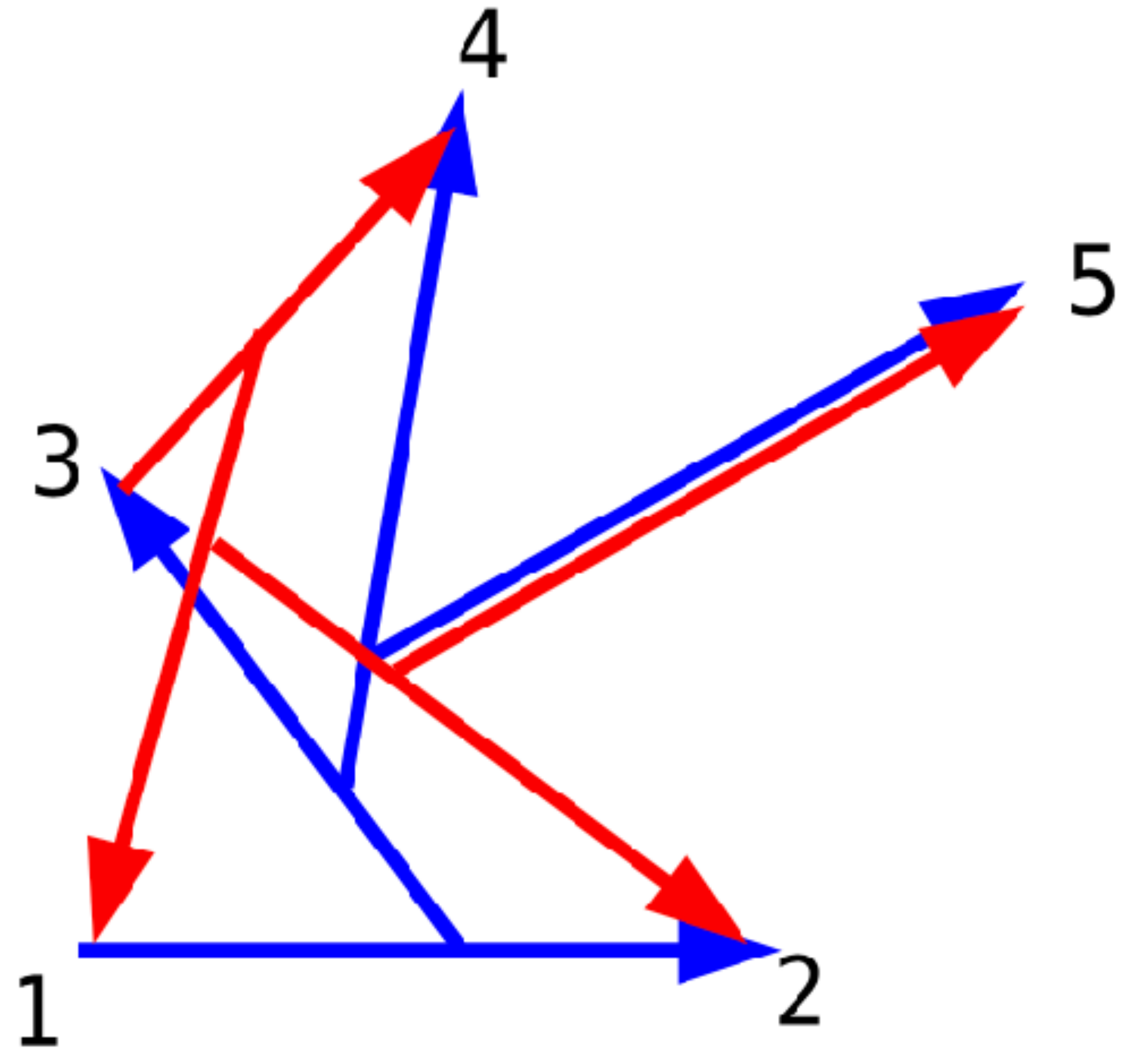
- Geometric property of the HH

$$\mathcal{Y}_{[K]}(\Omega^p) = \sum_{[K'](K=K')} a^{p\to 1}_{[K],[K']} \mathcal{Y}_{[K']}(\Omega^1)$$

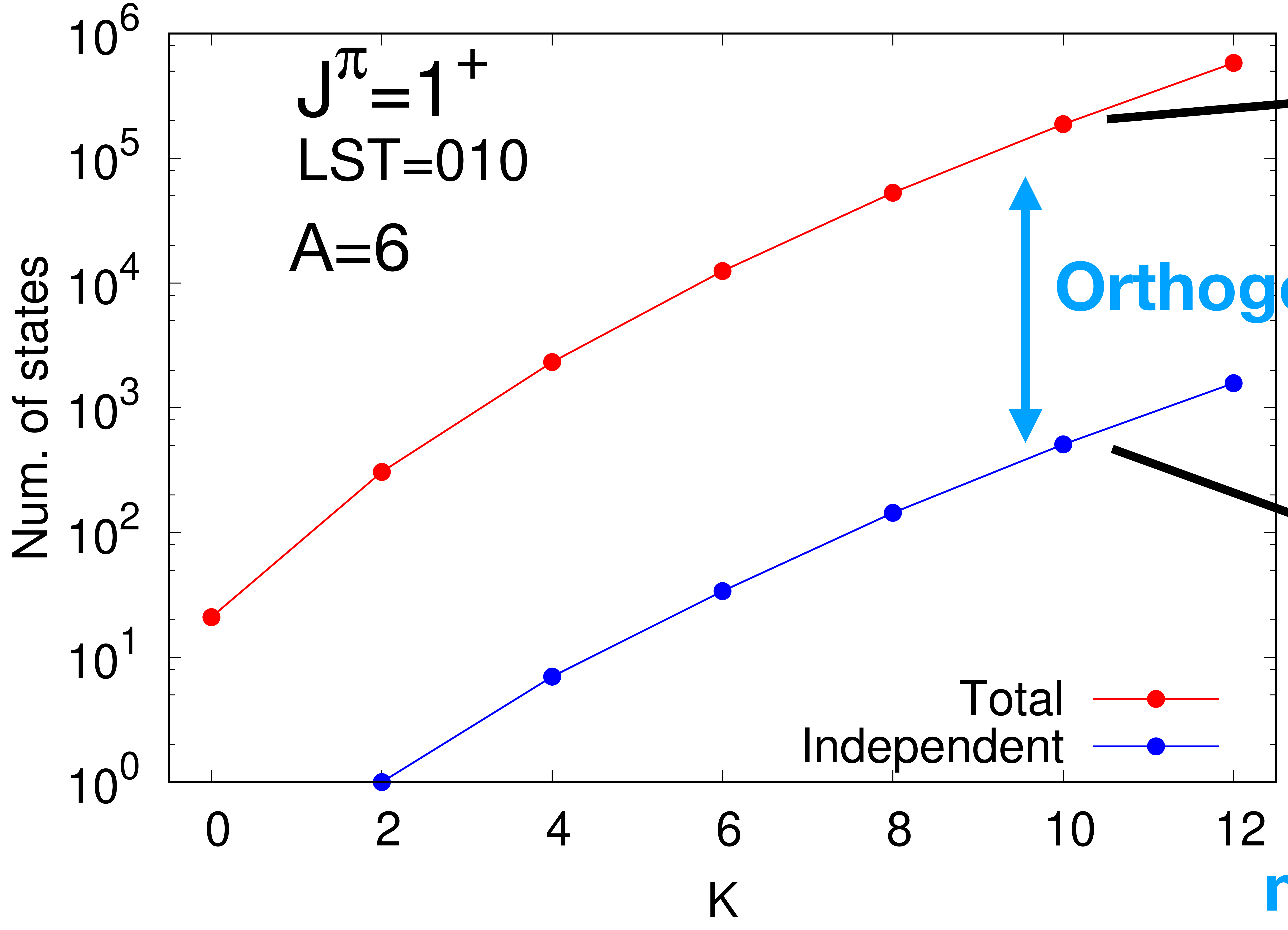
- Transform the sum over the permutations on sum of geometric coefficients

$$\sum_{\text{even}\, p} \Phi^p_{[\alpha]} = \sum_{\text{even}\, p} \sum_{[\alpha']} a^{p\to 1}_{[\alpha],[\alpha']} \Phi^1_{[\alpha']} = \sum_{[\alpha']} \boxed{A_{[\alpha],[\alpha']}} \Phi^1_{[\alpha']}$$

Knowing the coefficients is knowing the entire basis

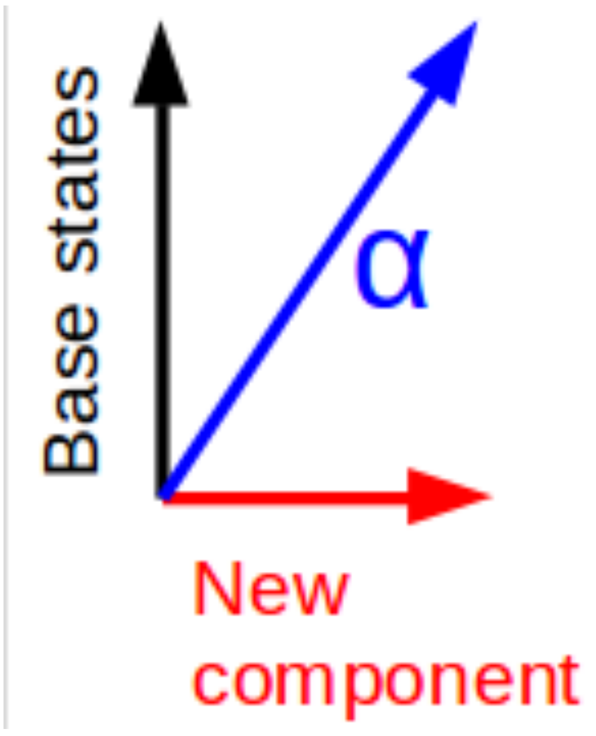


Construction of the basis II



Orthogonalization

Total number of non orthogonal states



Total number of orthogonal states

The dimension of the final matrix to diagonalize is small

Matrix elements

- For any operator is possible to write it in the following way

$$\langle HH_{[\alpha]} | \sum_{i<j} \hat{O}_{ij} | HH_{\beta} \rangle = \frac{A(A-1)}{2} \langle HH_{[\alpha]} | \hat{O}_{12} | HH_{\beta} \rangle =$$

$$= \frac{A(A-1)}{2} \sum_{[\alpha'],[\beta']} \boxed{A_{[\alpha],[\alpha']} A_{[\beta],[\beta']}} \boxed{\langle \Phi^1_{[\alpha']} | \hat{O}_{12} | \phi^1_{[\beta']} \rangle}$$

Only geometric (operator independent)
Computationally expensive

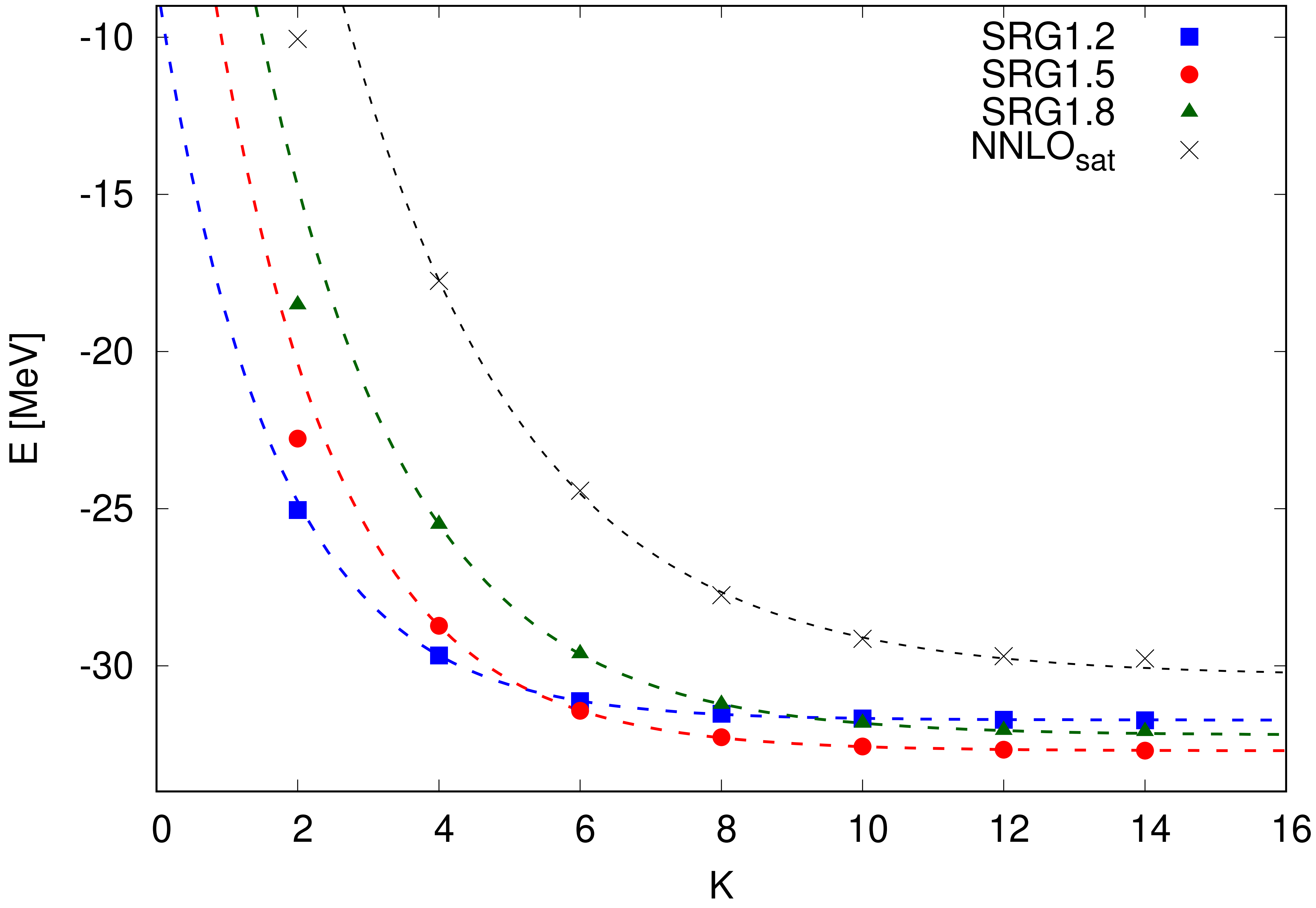
Depends on the operator
Implies few numerical integrations

The ^{6}Li wave function in the HH basis

A. G., M. Viviani and L.E. Marcucci, Phys. Rev. C **102**, 014001 (2020)

Convergence of the HH basis

^{6}Li ground state



- Interaction N3LO500 [1] SRG evolved [2]
- No 3-body forces are considered
- Extrapolation is needed

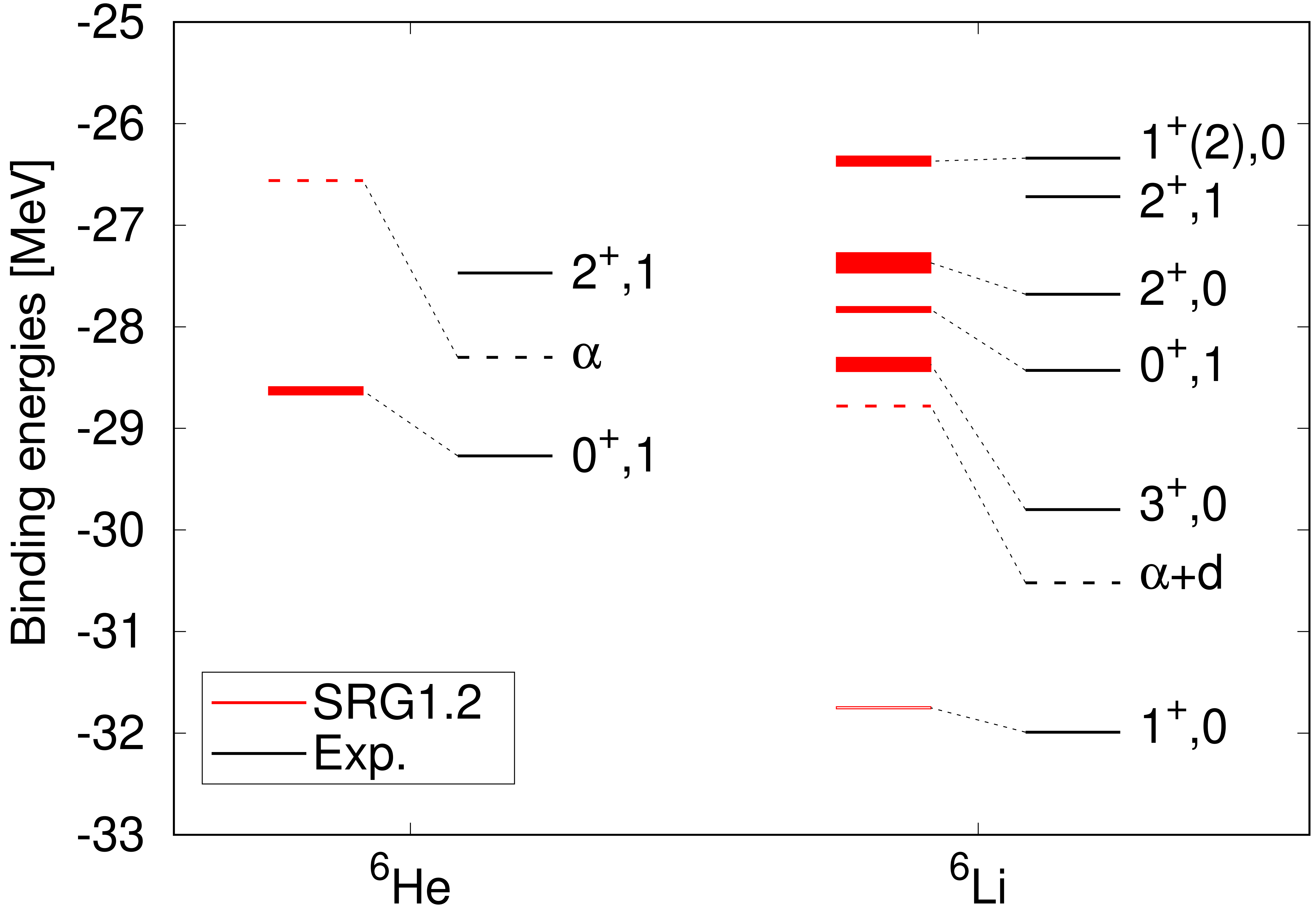
$$E(K) = E(\infty) + e^{-bK}$$

SRG 1.2	SRG 1.5	SRG 1.8	NNLO_sat	Exp.
-31.81(1)	-32.91(2)	-32.68(9)	-30.71(15)	-31.99

[1] D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001(R) (2003)
[2] S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. C **75**, 061001(R) (2007)

The A=6 spectra

By fixing J it is possible to obtain also the excited states



^{6}Li

J^π, T	Exp.	SRG1.2
$1^+, 0$	-31.99	-31.78(1)
$\alpha + d$	-30.52	-28.78
$3^+, 0$	-29.80	-28.37(7)
$0^+, 1$	-28.43	-26.37(5)
$2^+, 0$	-27.86	-27.4(1)
$2^+, 1$	-26.72	–
$1^+_2, 0$	-26.34	-27.83(3)

^{6}He

J^π, T	Exp.	SRG1.2
$0^+, 1$	-29.27	-28.63(4)
α	-28.30	-26.56
$2^+, 1$	-27.47	–

K=12

K=8

The $\alpha + d$ clusterization

- The simplest approach is to consider the ^{6}Li as an α and a deuteron

$$\psi_{^6Li} \simeq \sum_{L,S} \frac{\mathscr{A}}{\sqrt{15}} \left[\left(\Psi_\alpha \otimes \Psi_d \right)_S Y_L(\hat{r}) \right]_{J=1} \frac{f_L(r)}{r}$$

Antisymmetry operator

S=1

L=0,2
(positive parity)

Cluster form factor

$$\frac{f_L(r)}{r} = \langle \frac{\mathscr{A}}{\sqrt{15}} \left[\left(\Psi_\alpha \otimes \Psi_d \right)_S Y_L(\hat{r}) \right]_J | \Psi_{^6Li} \rangle$$

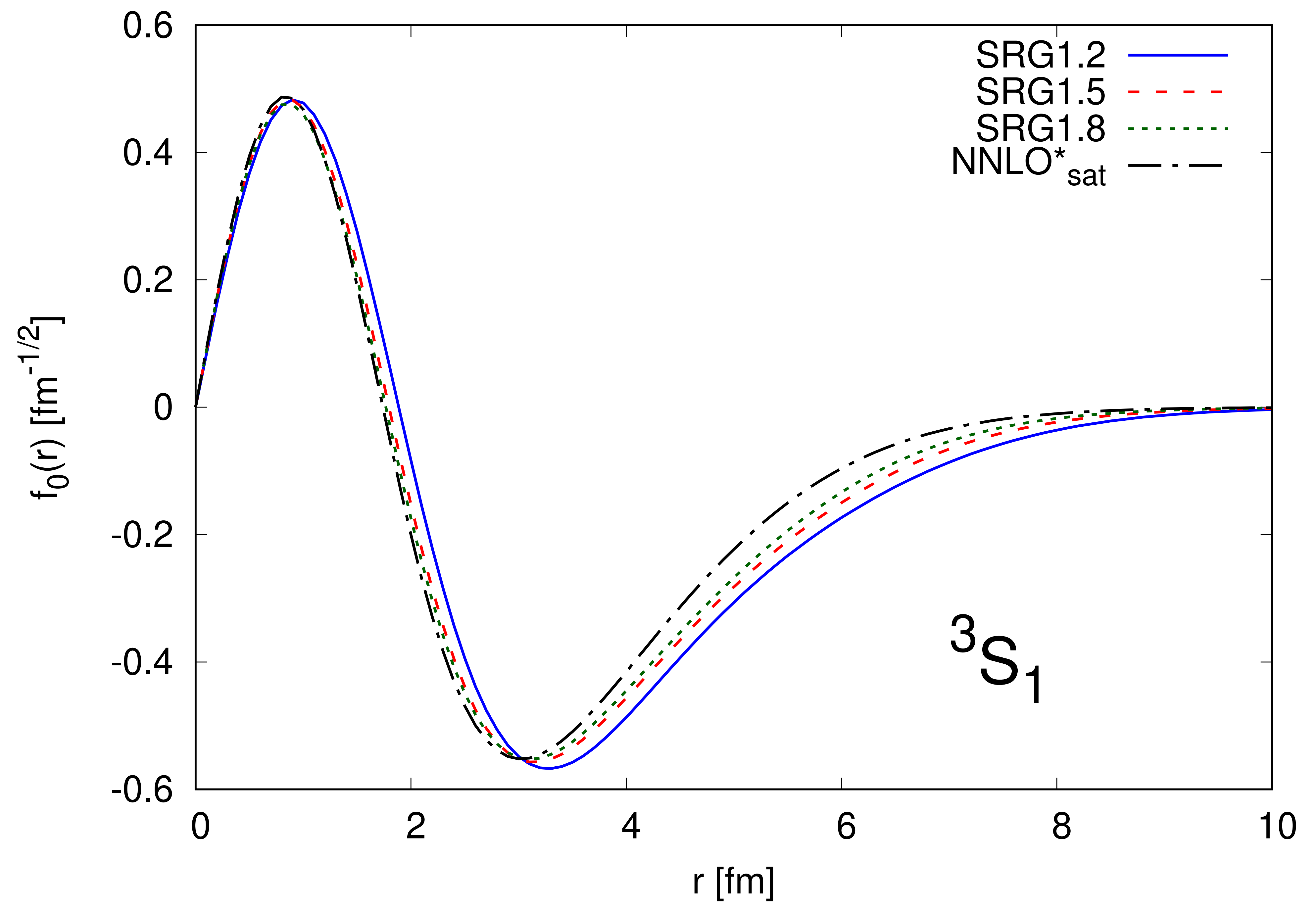
Cluster form factor

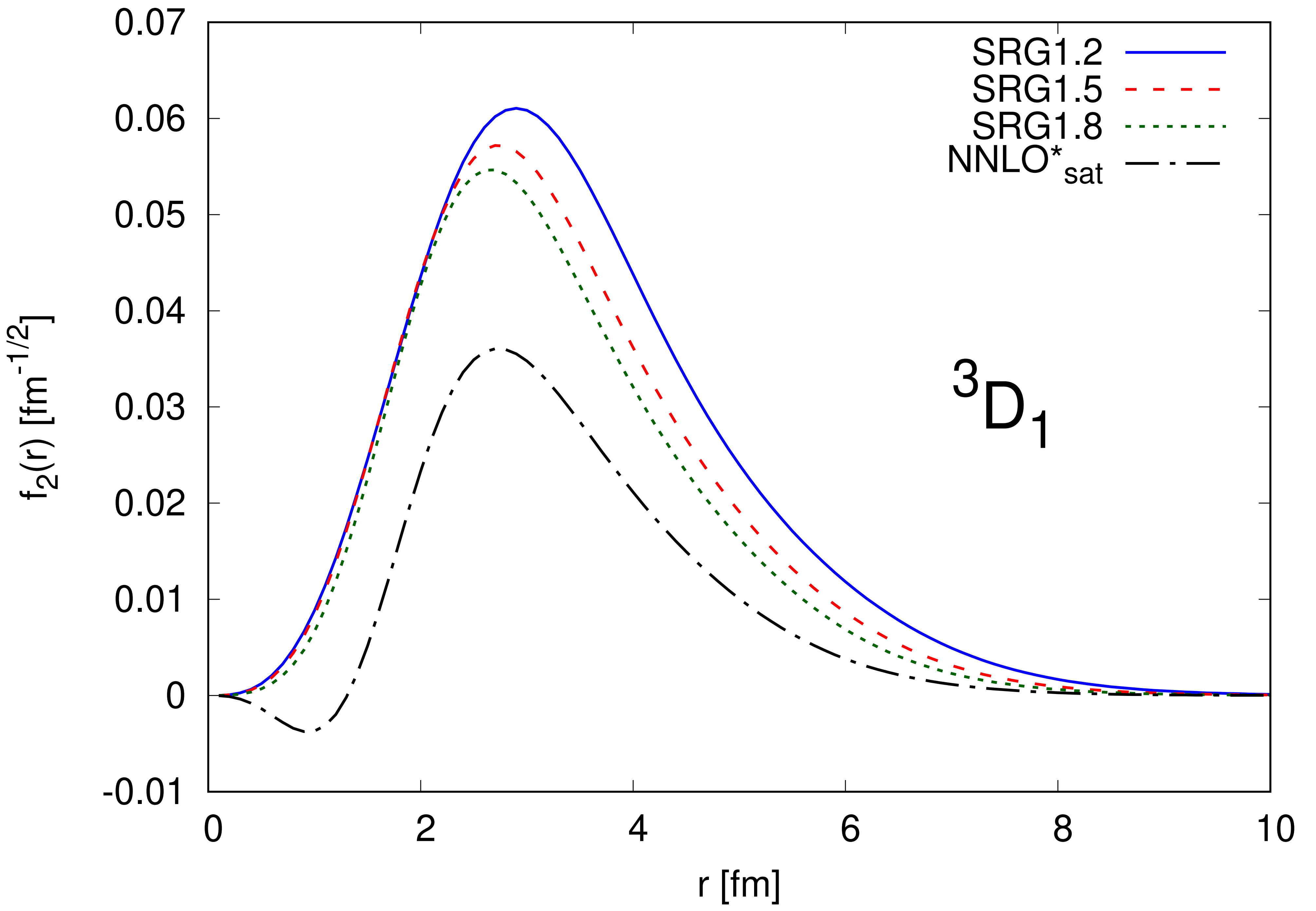
Which kind of information can we extract?

Spectroscopic factor

$$\mathcal{S}_L = \int_0^\infty dr\,|f_L(r)|^2$$

	$\mathcal{S}_0$	$\mathcal{S}_2$	$\mathcal{S}_0 + \mathcal{S}_2$
SRG 1.2	0.909	0.008	0.917
SRG 1.5	0.868	0.007	0.875
SRG 1.8	0.840	0.006	0.846
NNLO(sat)	0.805	0.002	0.807
Exp.	—	—	0.85(4)



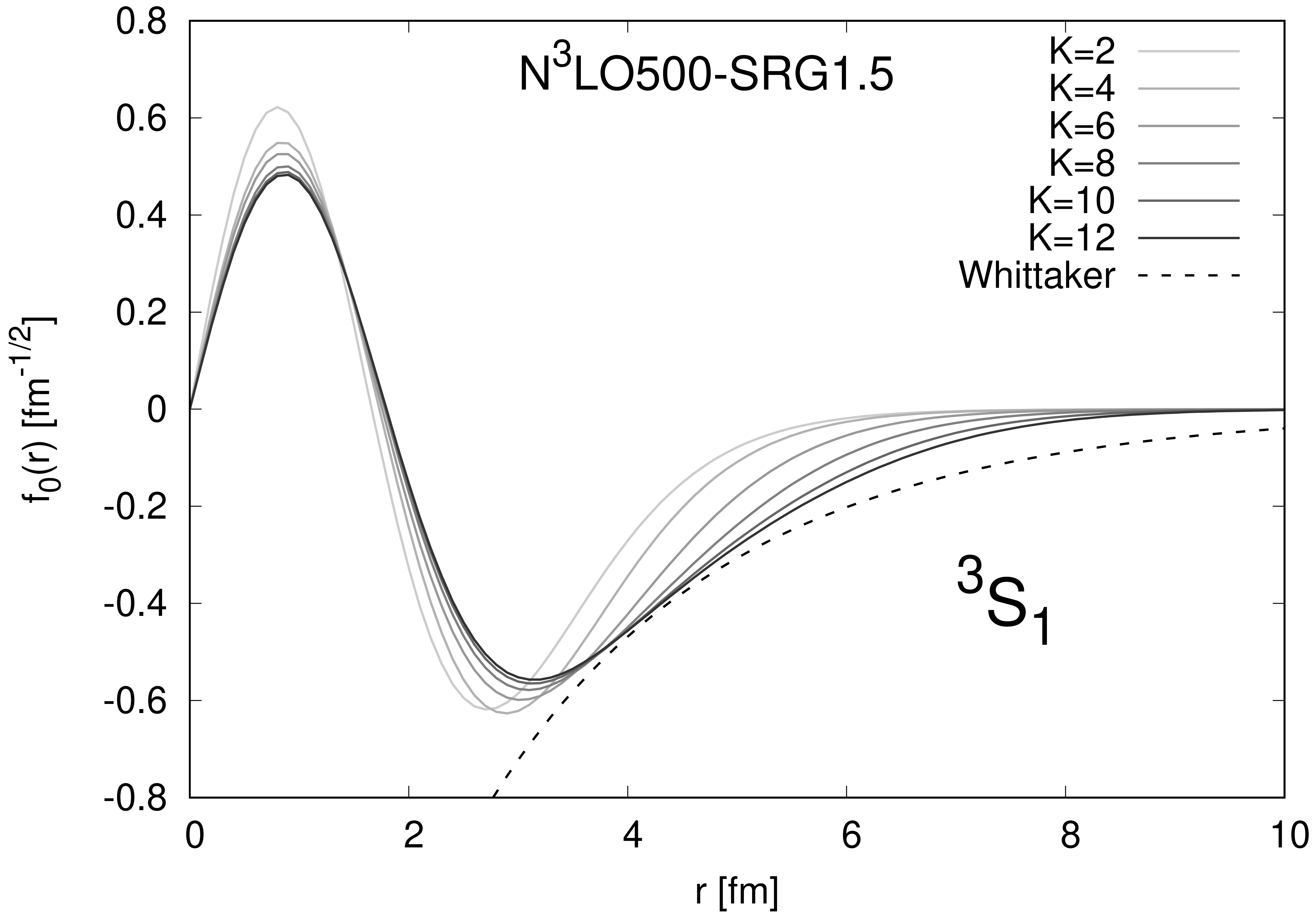


Cluster form factor

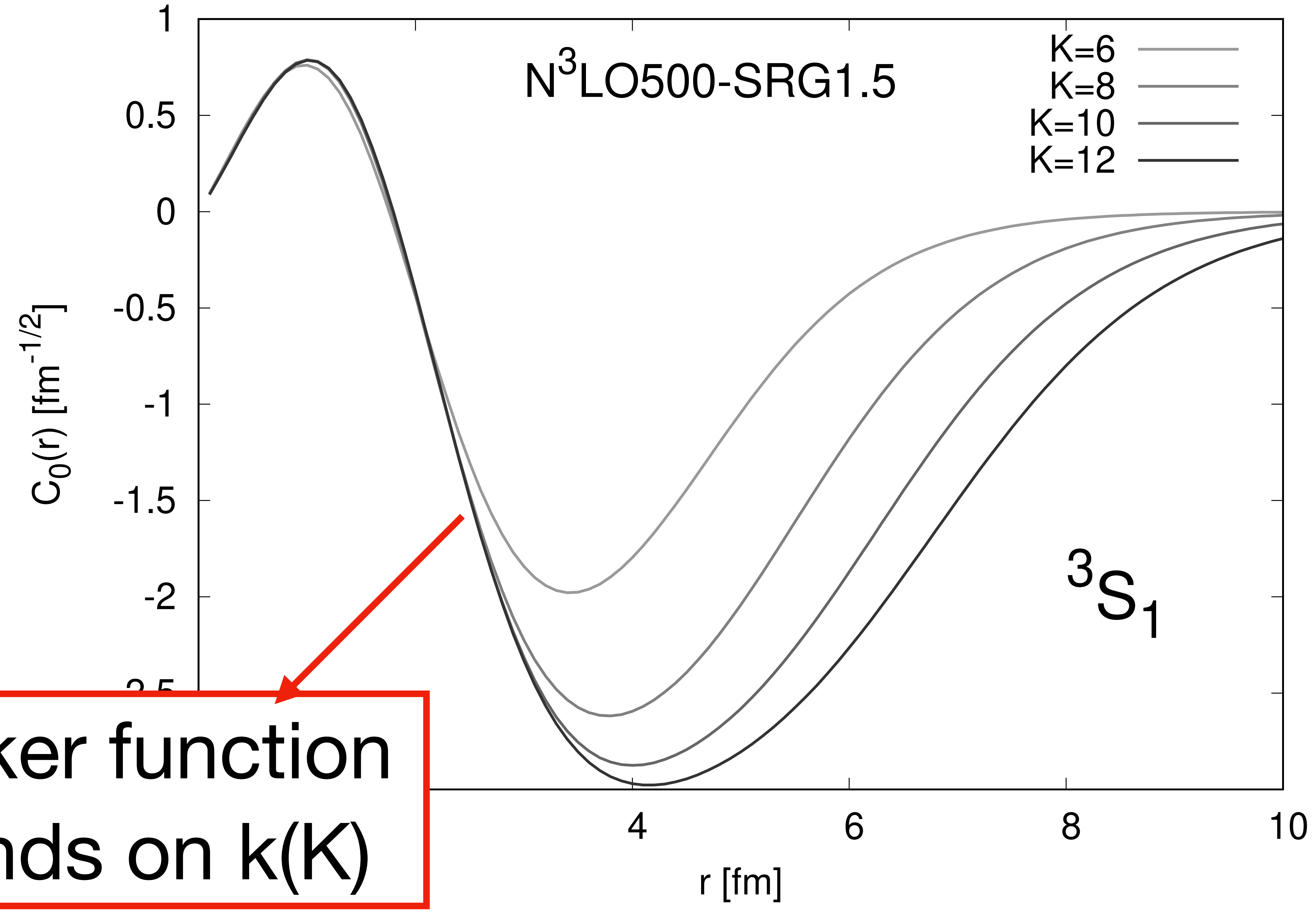
Which kind of information can we extract?

Asymptotic Normalization Coefficient

$$C_L(r) = \frac{f_L(r)}{W_{-\eta,L+1/2}(2kr)} \xrightarrow{r\to\infty} C_L$$



Doing the ratio



Whittaker function depends on k(K)

An equation for the cluster form factor

- It is possible to derive an equation for the cluster form factor by sandwiching $\langle \psi_{\alpha+d} | \hat{H} - E_{^6Li} | \psi_{^6Li} \rangle = 0$ [1,2]

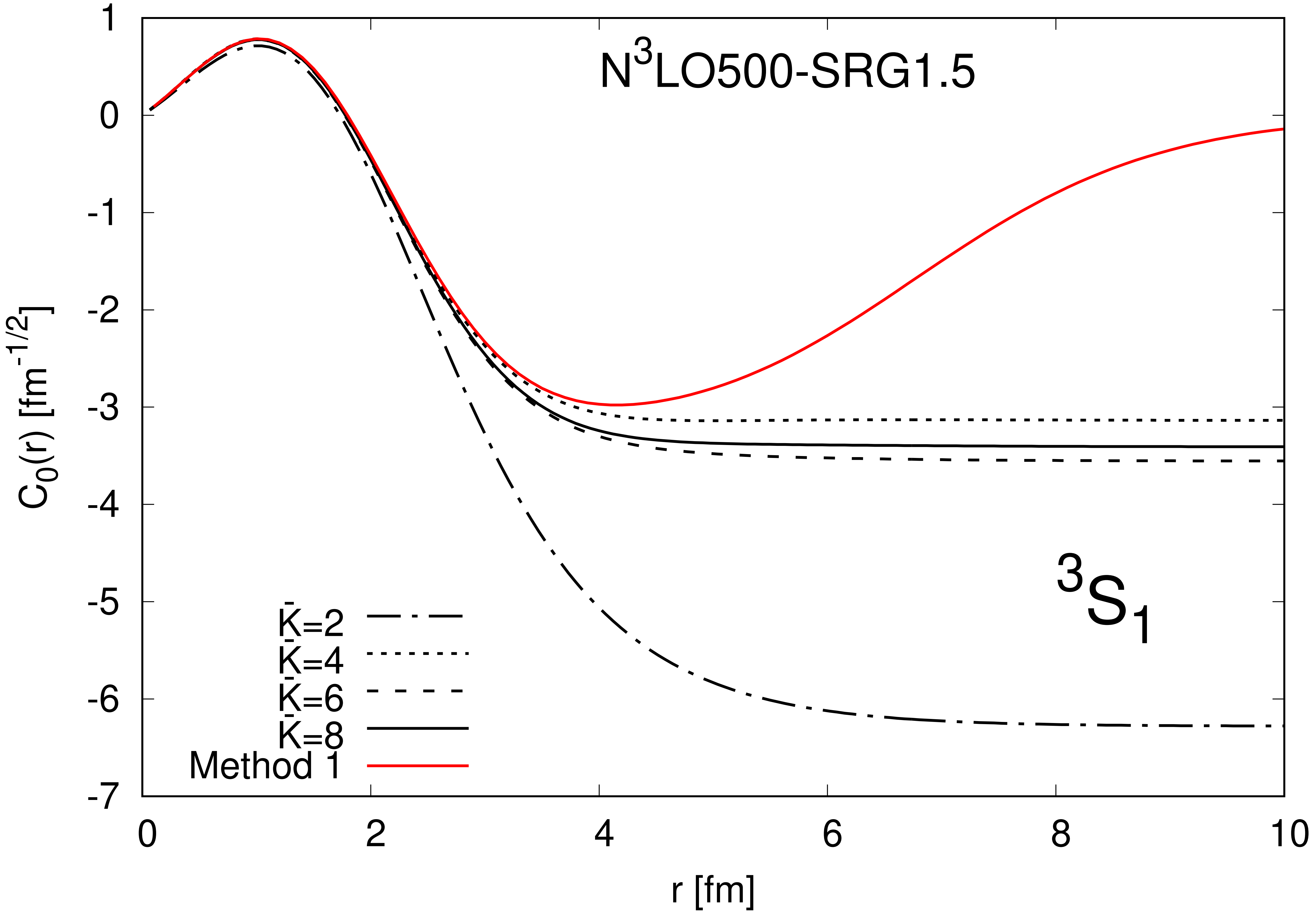
$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} \right) + \frac{2e^2}{r} + B_c \right] f_L(r) + g_L(r) = 0$$

Source term → $$g_L(r) = \langle \left(\psi_\alpha \times \psi_d \right)_S Y_L(\hat{r}) | \left(\sum_{i \in \alpha} \sum_{j \in d} V_{ij} - \frac{2e^2}{r} \right) | \Psi_{^6Li} \rangle$$

Insert a complete basis set $\sum_{[K]} | HH_{[K]} \rangle \langle HH_{[K]} |$ up to $\overline{K}$

[1] N. Timofeyuk, Nucl. Phys. A **632**, 19 (1998)
[2] M. Viviani et al., Phys. Rev. C **71**, 024006 (2005)

Extraction of the ANC



$$C_L(r) = \frac{f_L(r)}{W_{-\eta,L+1/2}(2kr)} \xrightarrow{r\to\infty} C_L$$

- Correct extrapolation of the ANCs
- Same short range behavior as before

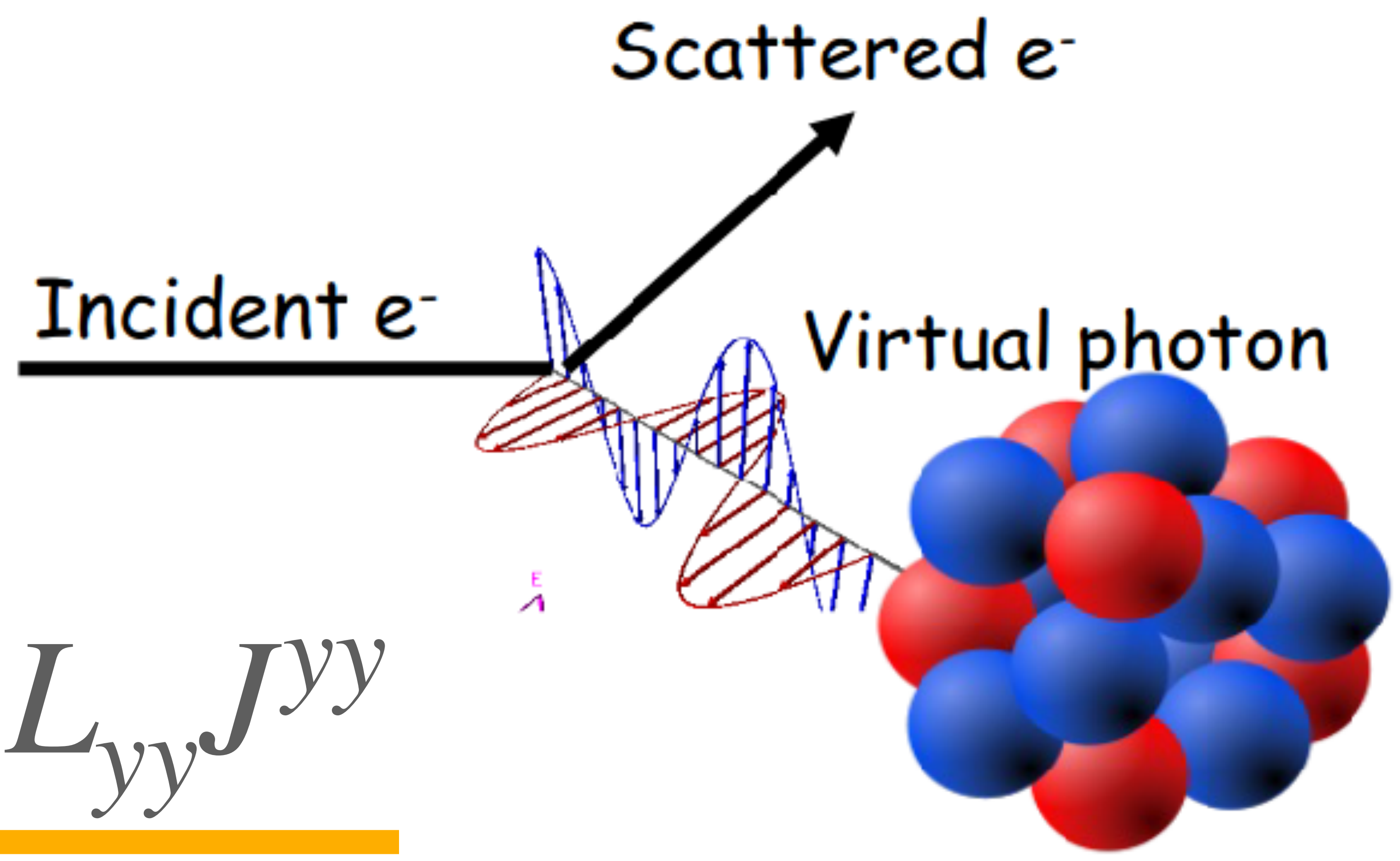
	B_c	C_0	C_2
SRG 1.2	-3.00(1)	-4.2(1)	0.12(2)
SRG 1.5	-2.46(2)	-3.44(7)	0.07(2)
SRG 1.8	-2.02(9)	-3.01(7)	0.05(1)
NNLO(sat)	-1.15	-2.8(2)	0.03(1)
Exp.	-1.4743	-2.91(9)	0.077(18)

Magnetic form factors of light nuclei

A. G., and R. Schiavilla, Phys. Rev. C **106**, 044001 (2022)

Elastic scattering of electrons on nuclei

$$\langle f | \hat{O} | i \rangle = \langle \psi_f^L | l_\mu | \psi_i^L \rangle \langle \psi_f^N | j^\mu | \psi_i^N \rangle$$



$$| \langle f | \hat{O} | i \rangle |^2 = L_{\mu\nu} J^{\mu\nu} = L_{00} J^{00} + L_{xx} J^{xx} + L_{yy} J^{yy}$$

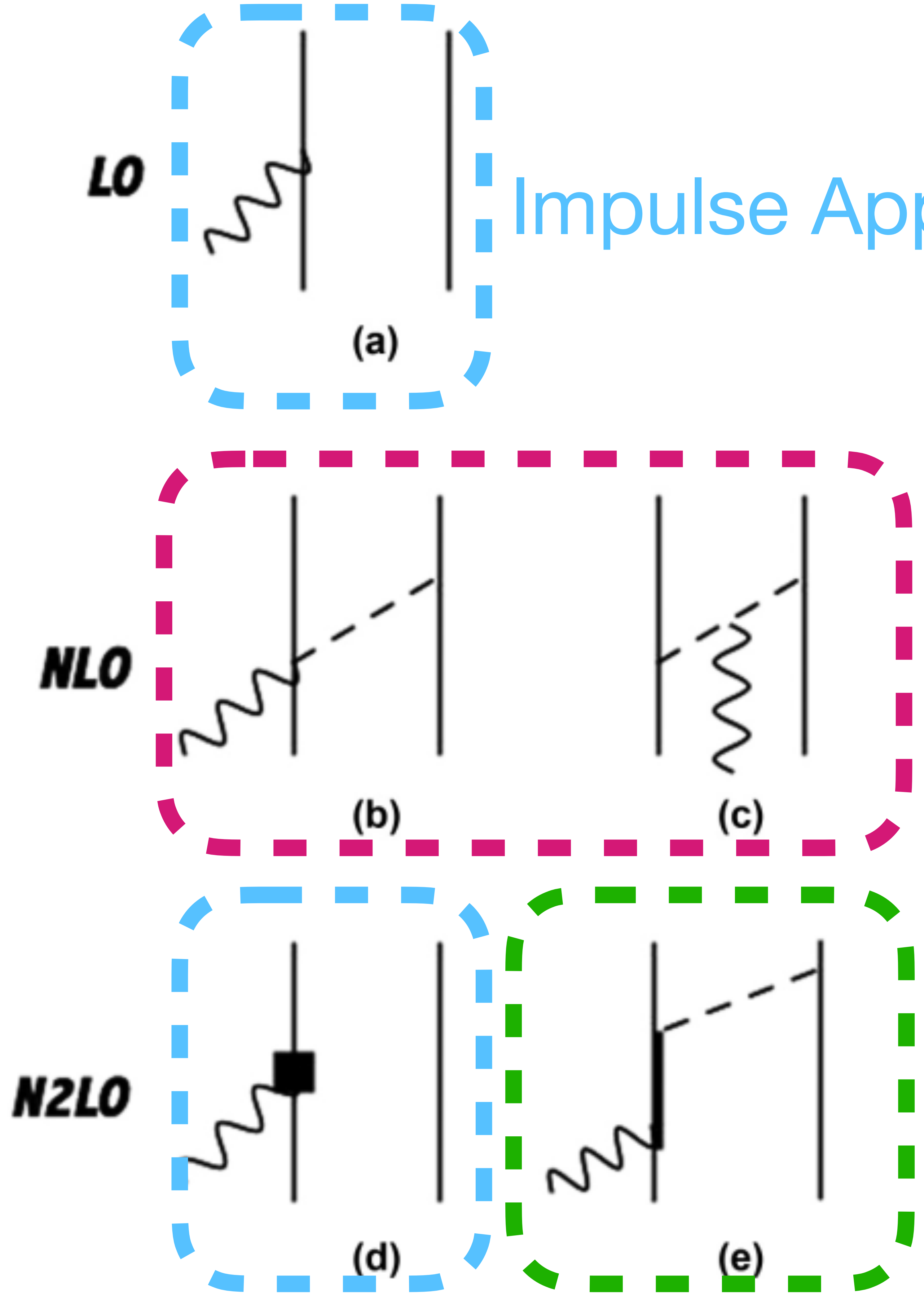
$$\frac{d\sigma}{d\Omega} = 4\pi\sigma_M f_{\text{rec}}^{-1} \left[\frac{Q^4}{q^4} F_L^2(q) + \left(\frac{Q^2}{2q^2} + \tan^2 \theta_e/2 \right) F_T^2(q) \right]$$

F_L longitudinal form factor

F_T transverse form factor

Mott's cross section (scattering of electrons from a point-like charge)

The electromagnetic currents

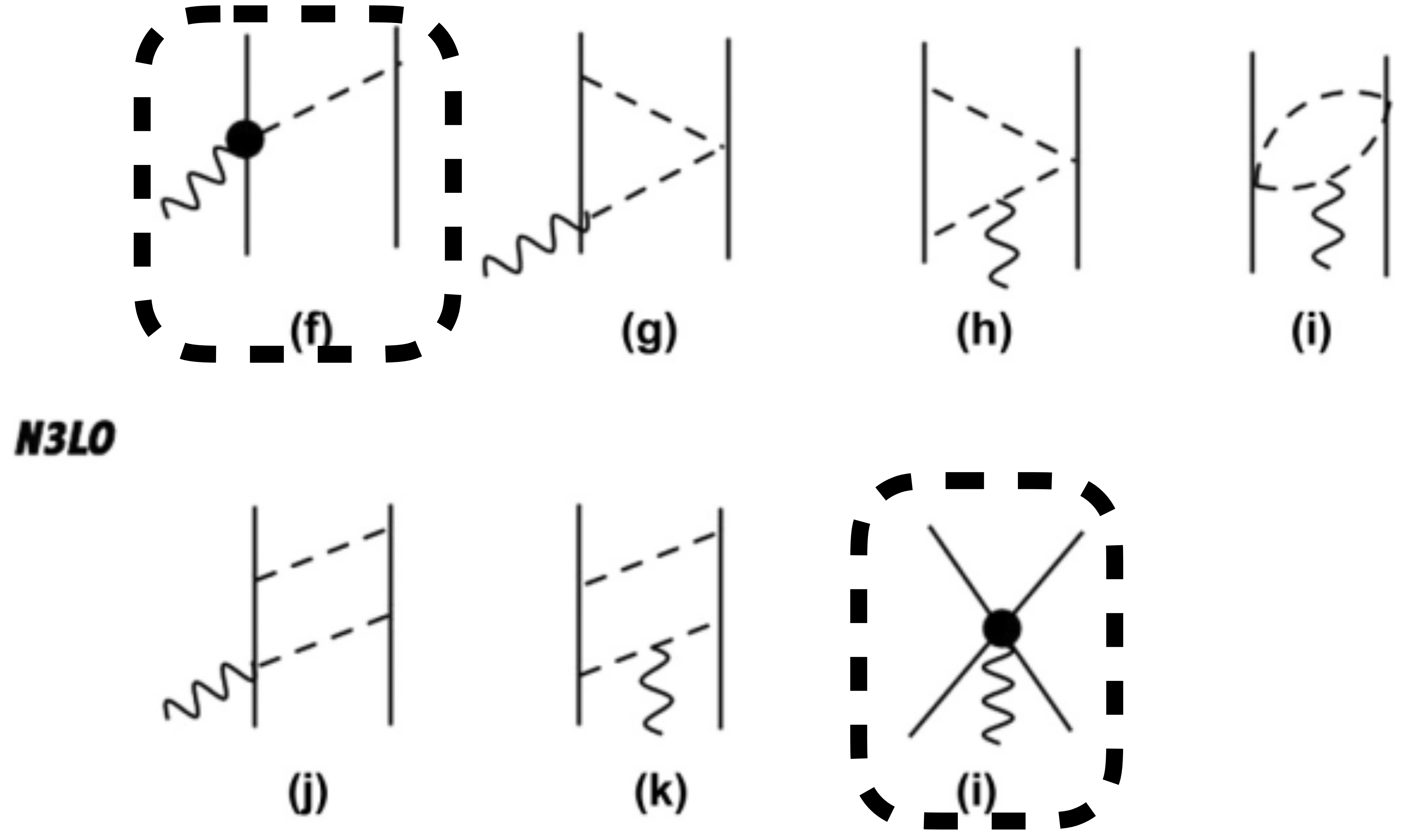


Impulse Approximation

OPE

Δ-N2LO

d_2^V d_3^V d_2^S N3LO-OPE

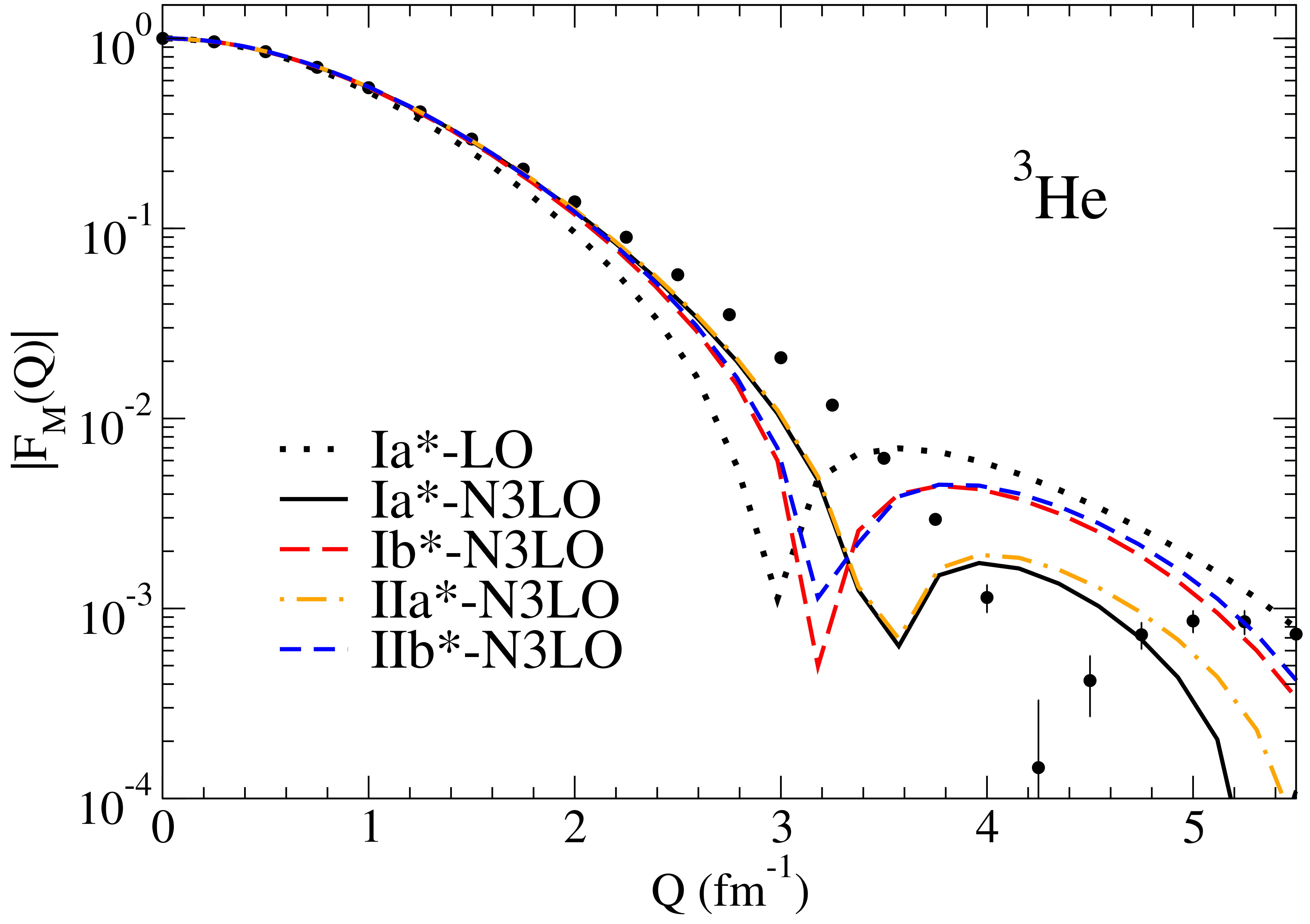


d_1^V d_1^S contact terms

How to fix the LECs I

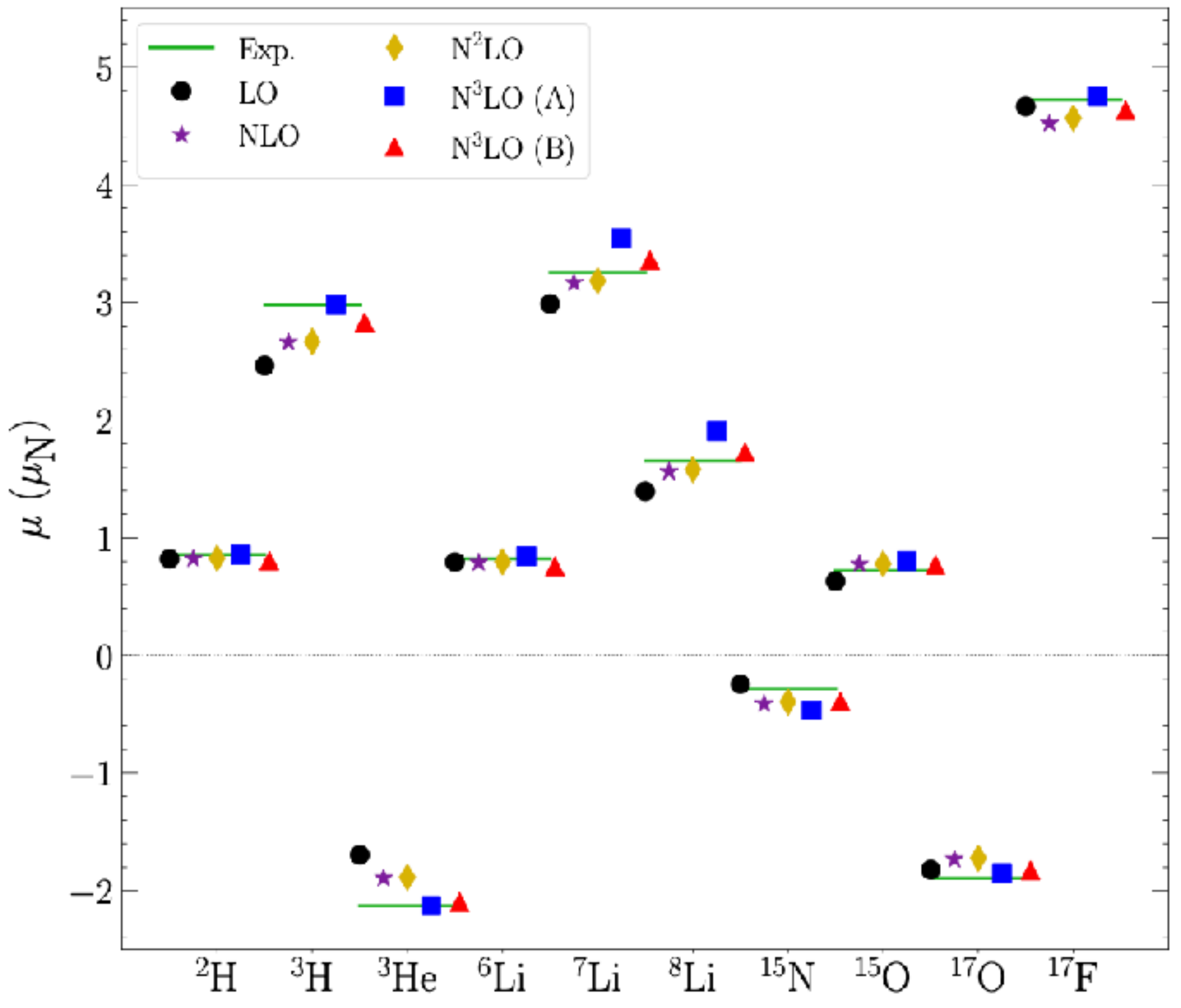
Using the magnetic moments

Δ saturation (fix d_2^V d_3^V)



[R. Schiavilla et al., PRC 99, 034005 (2019)]

Not including (d_1^V d_2^V d_3^V d_1^S d_2^S)



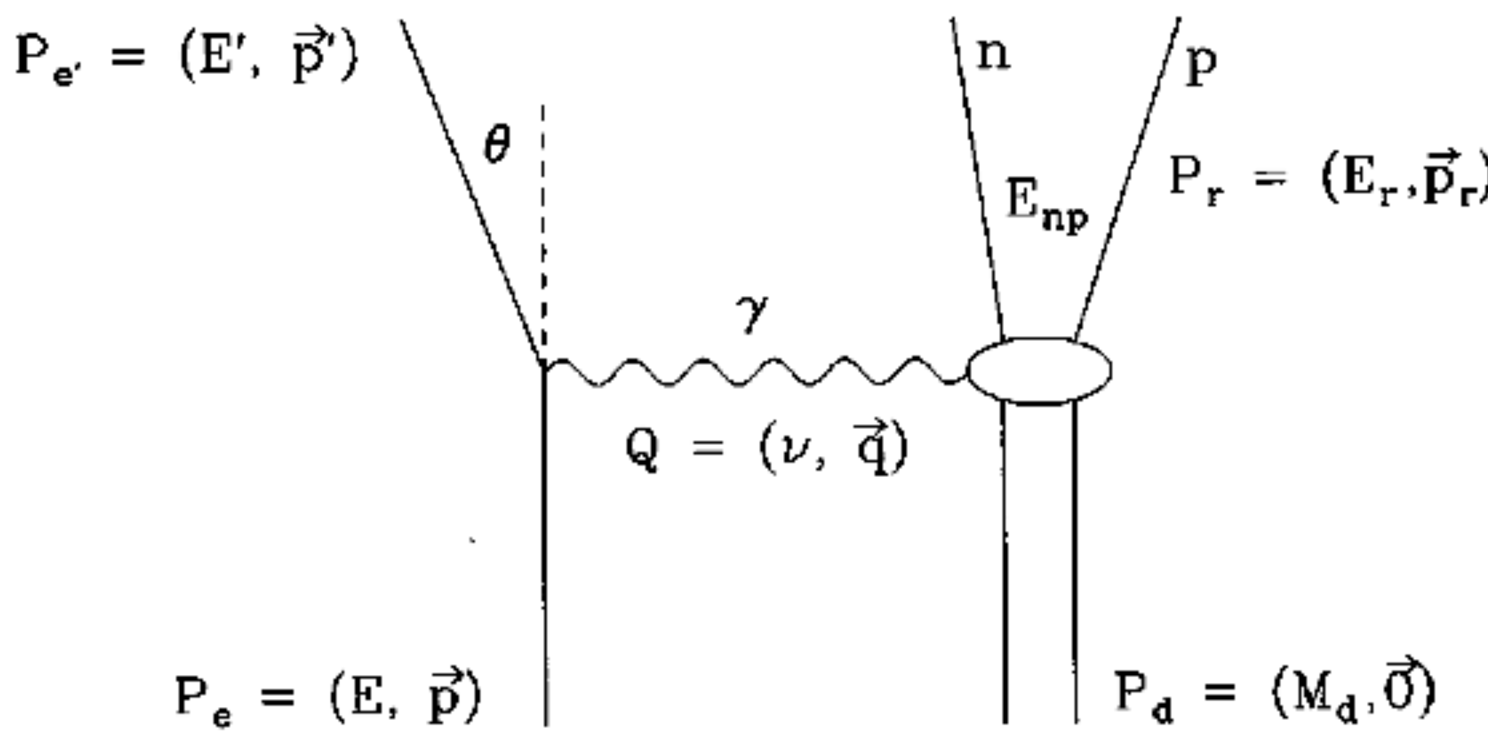
[J.D. Martin *et al.*, PRC 108, L031304 (2023)]

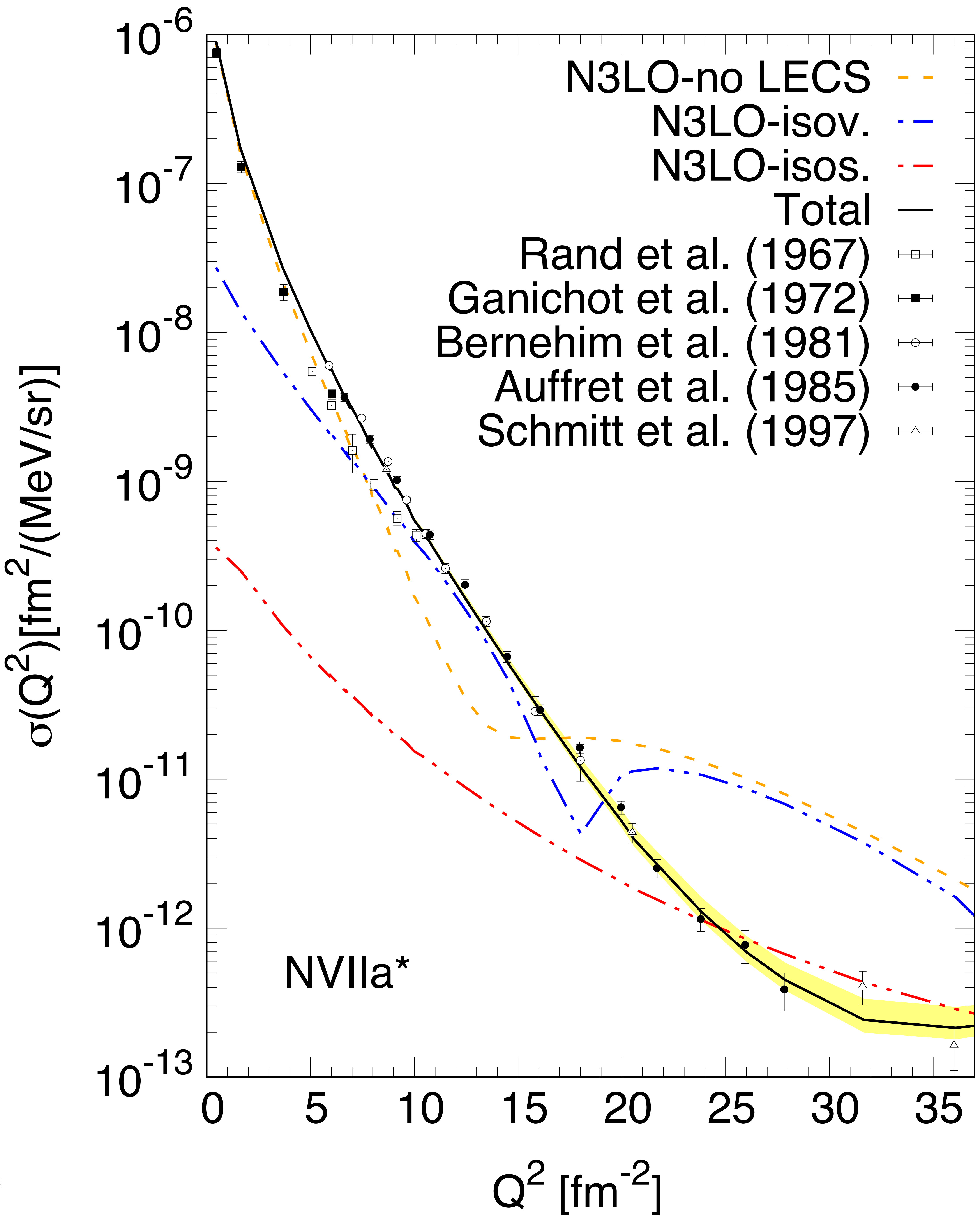
Diffraction generated by tensor forces

How to fix the LECs II

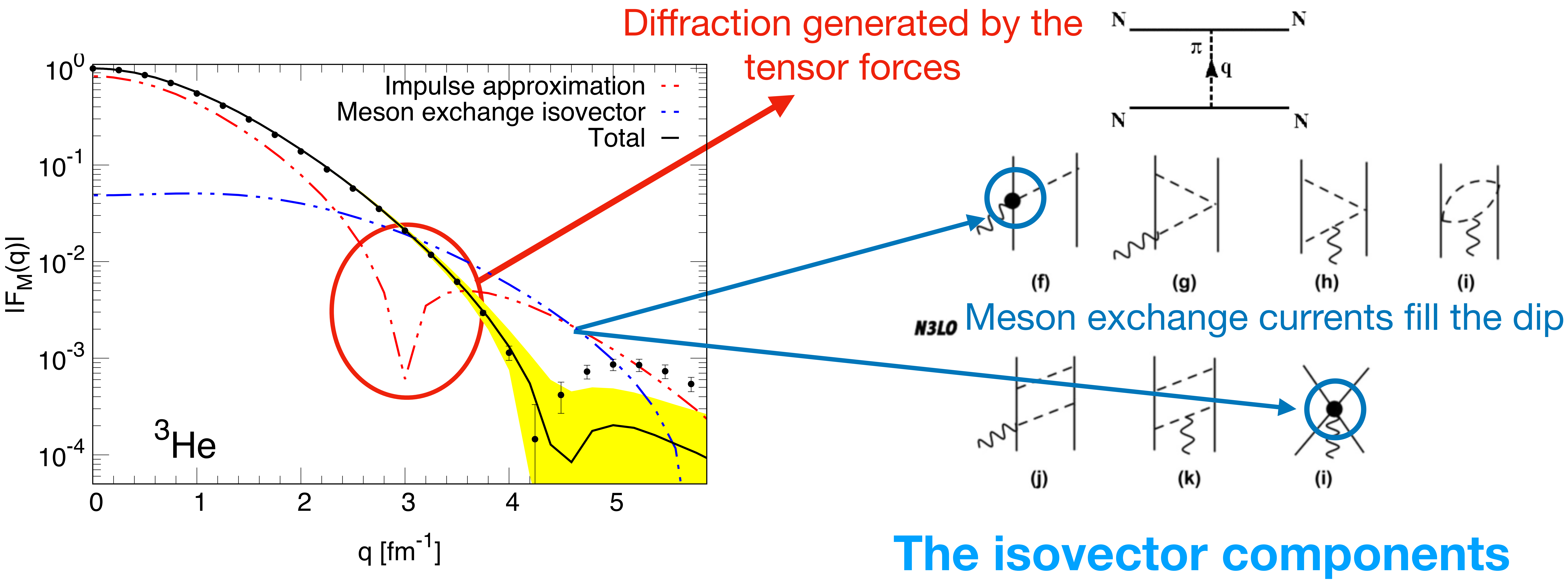
This work

- Magnetic moments of d, ^{3}He, ^{3}H (fix normalization)
- deuteron-threshold electrodisintegration at backward angles (fix dynamics)





Prediction of A=3 Magnetic Form Factor



The isovector components fill/generates the diffraction

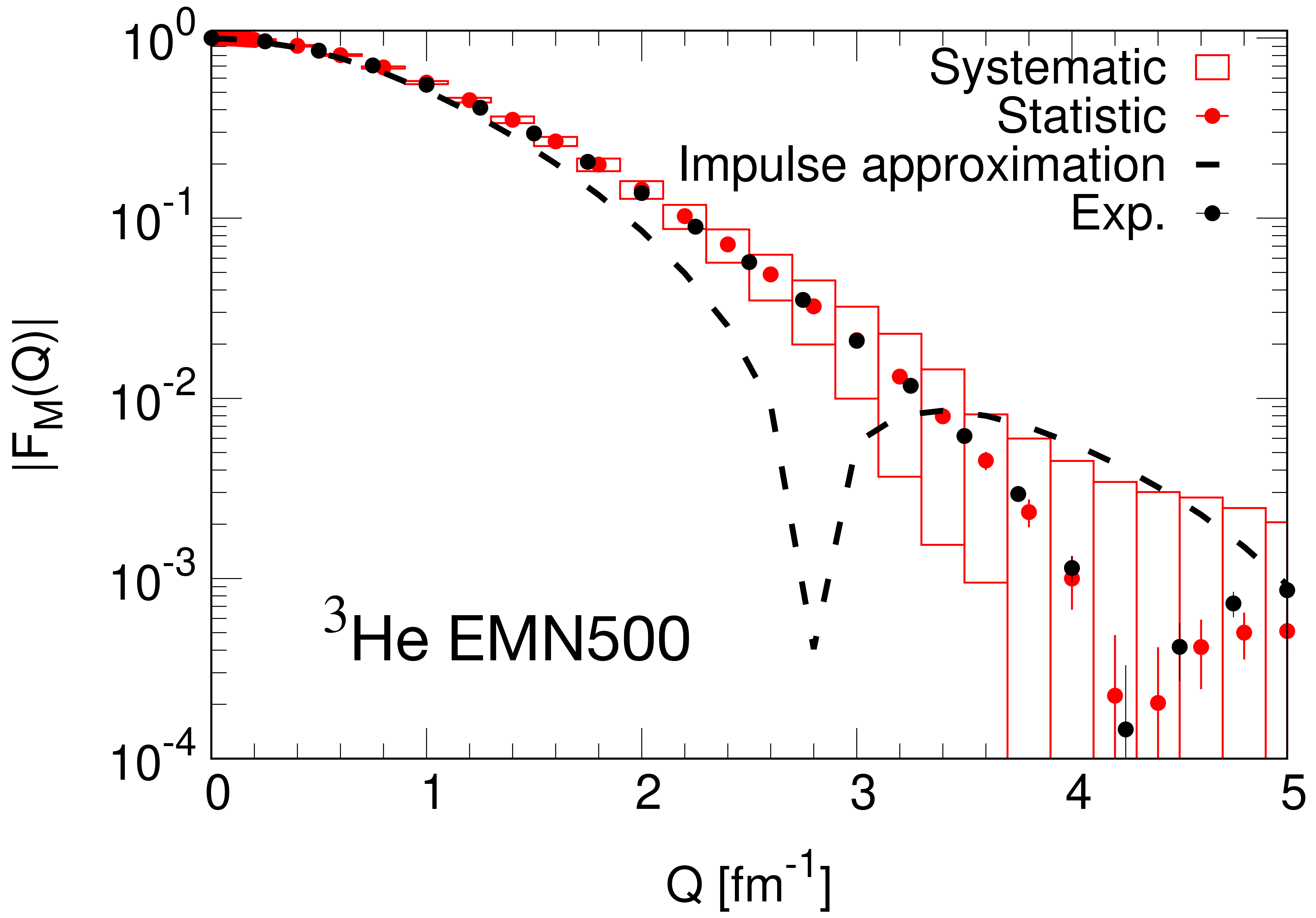
Naive truncation error estimate

Is χEFT able to describe large Q?

- Truncation errors (as [EPJA 51, 53 (2015)])

$$\alpha = \max\left\{\frac{Q}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right\} \quad \Lambda_b = 1 \text{ GeV}$$

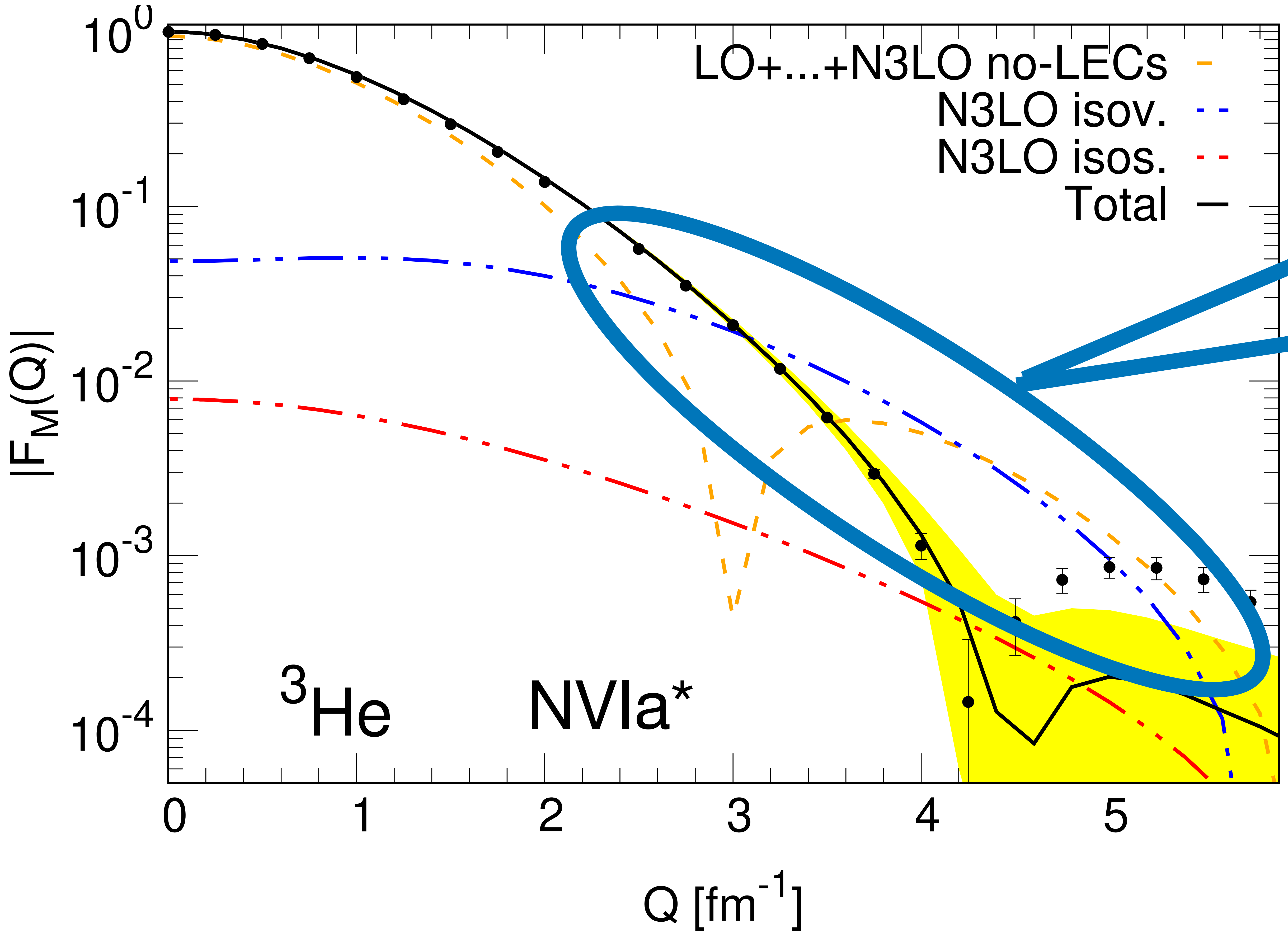
- Nuclear interaction + currents
- Bayesian analysis (slowly) in progress



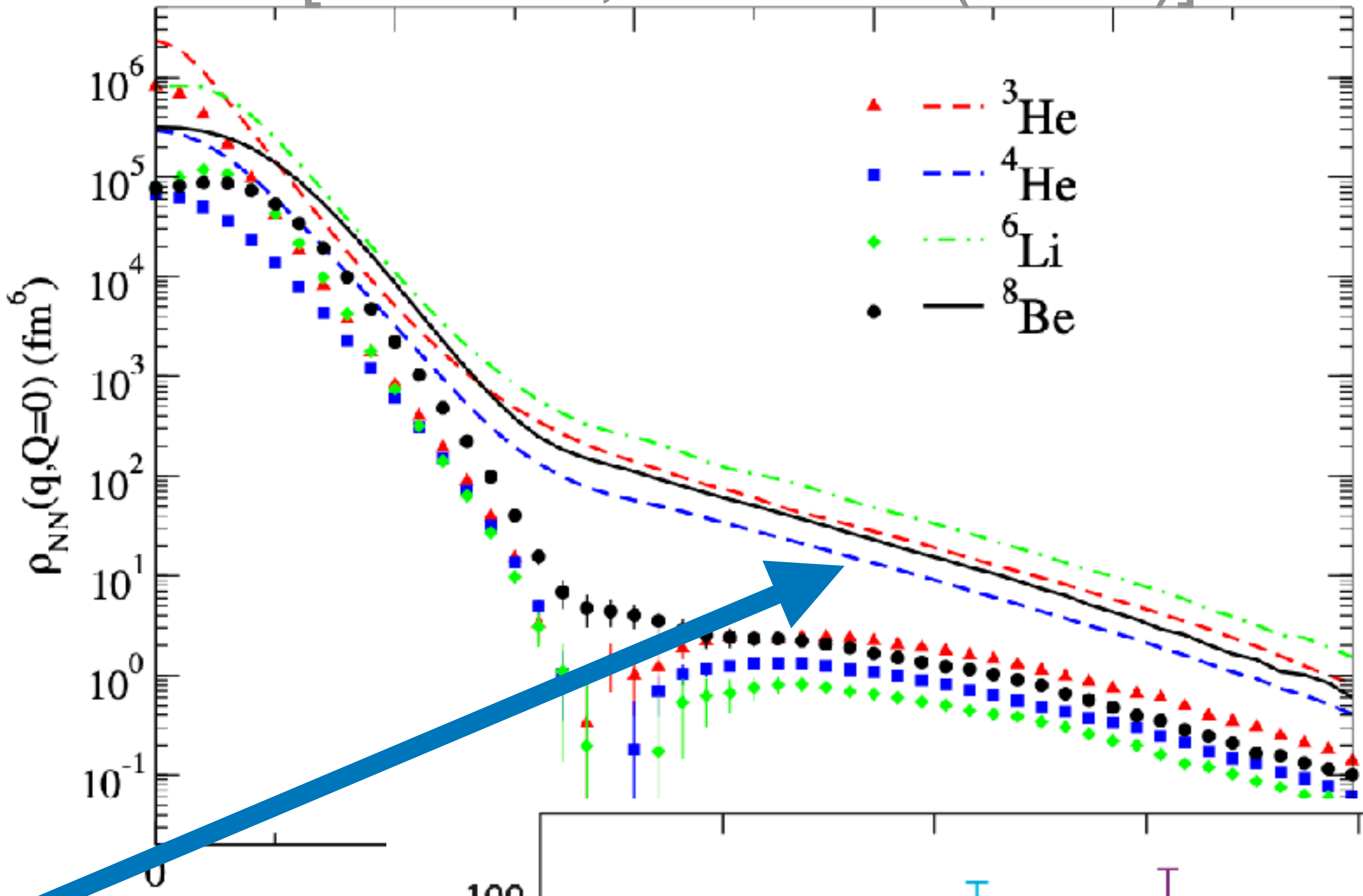
Why does it work?

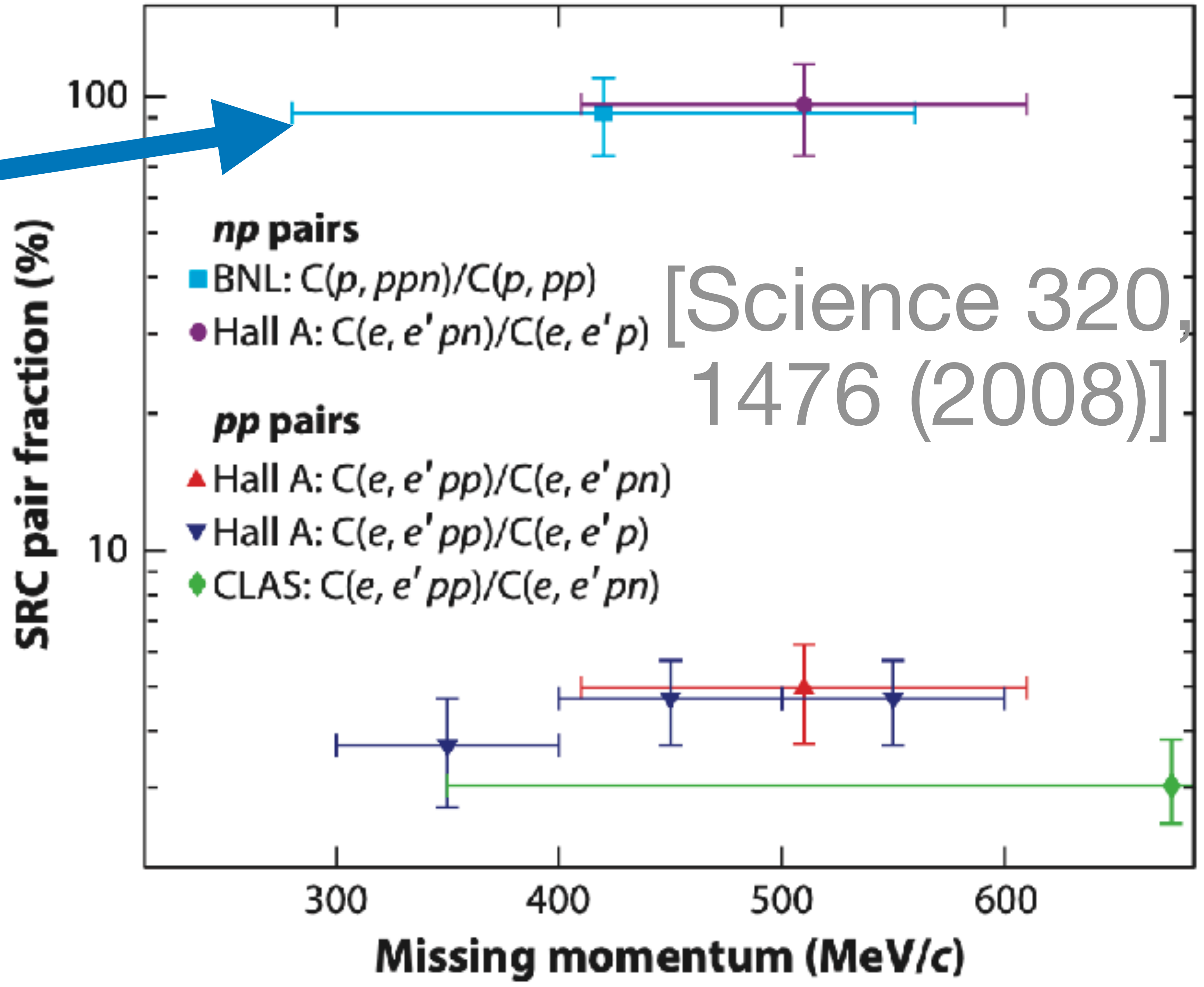
Isovector currents transform S/T=0/1 in S/T=1/0 pairs

np dominance



[PRL 98, 132501 (2007)]



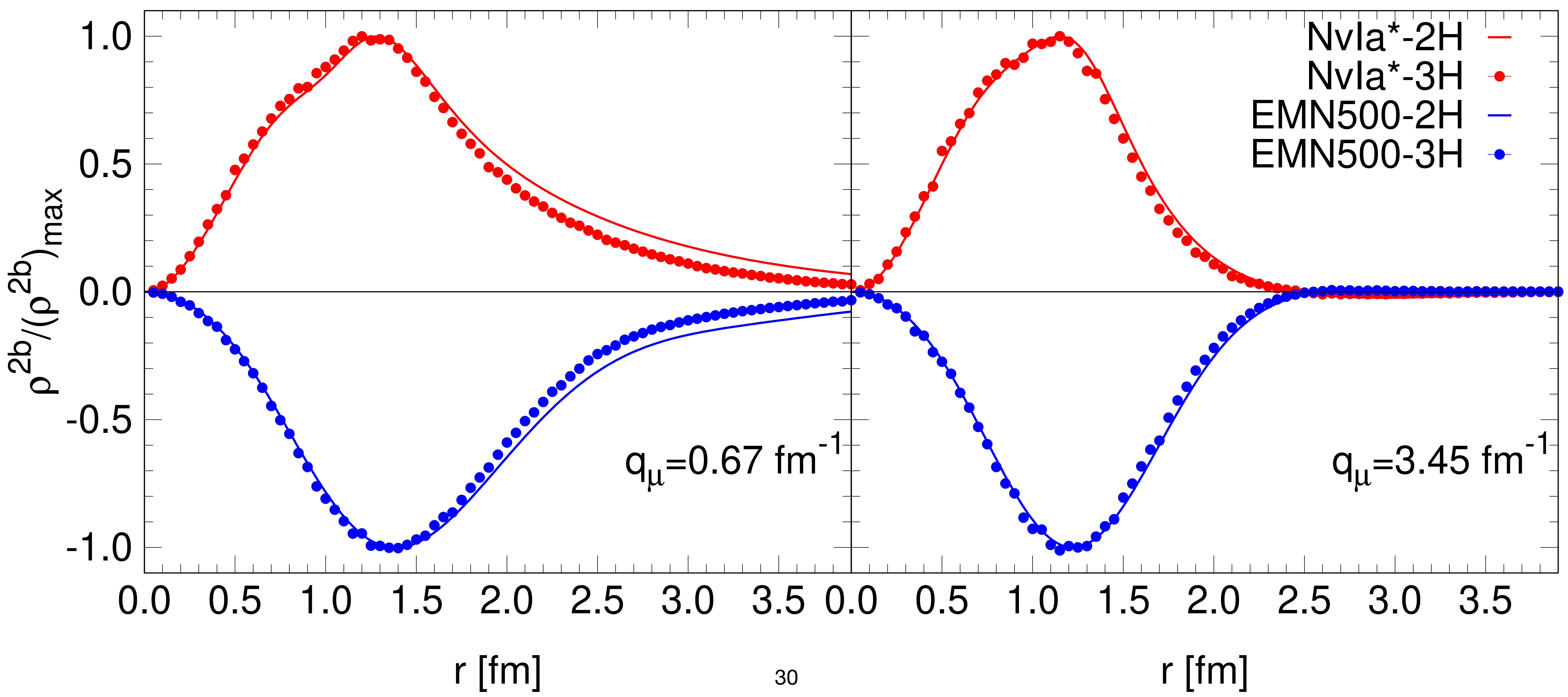


[Science 320, 1476 (2008)]

Why does it work?

Universal behavior of isovector transitions

Correlated np pairs ⟷ **Universal 2-body wave functions** ⟷ **Universal 2-body transition densities**



Summary

- **The HH method is a powerful few-body approach for studying light nuclei and their interactions with external probes.**
  - Calculation of ^{6}Li properties relevant for reactions (Spectroscopic factor and ANCs)
  - Study of electromagnetic currents in chiral EFT
- The HH method has been used in combination of the Kohn variational principle for studying three and four-body scattering states
- And many more…

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