Breaking symmetries into Self-Consistent Green's functions theory

CEA ESNT Workshop - Nuclear *ab initio* spectroscopy

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NUMERICS

International PhD Program in Numerical Simulation at CEA

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Papers to be published presented in this talk

1. Impact of correlations on nuclear binding energies [Scalesi, Duguet, Demol, Frosini, Somà, Tichai]

2. Deformed Self-Consistent Green's functions at second order [Scalesi, Duguet, Frosini, Somà]

3. Deformed natural orbitals for *ab initio* calculations [Scalesi, Duguet, Frosini, Somà]

Outline

- Basic ingredients of Self-Consistent Green's function theory
- Symmetry-breaking Green's functions - 1. Particle number
- Role of Many-Body correlations
- Symmetry-breaking Green's functions - 2. Rotational symmetry
- dDSCGF(2) results
- Deformed Natural Orbitals
- Conclusions and future perspectives

Many-body Green's functions

A-body wave function

$$|\Psi_k^A\rangle$$

Green's functions

$$\mathrm{i}\, g_{\alpha\beta}(t_\alpha, t_\beta) \equiv \langle \Psi_0^A | \mathcal{T}[a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta)] | \Psi_0^A \rangle$$

$$\mathrm{i}\, g^{4-\mathrm{pt}}_{\alpha\gamma\beta\delta}(t_\alpha, t_\gamma, t_\beta, t_\delta) \equiv \langle \Psi_0^A | \mathcal{T}[a_\gamma(t_\gamma) a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta) a_\delta^\dagger(t_\delta)] | \Psi_0^A \rangle$$

$$\ldots$$

A-body Schrödinger equation

$$H|\Psi_k^A\rangle = E_k^A |\Psi_k^A\rangle$$

Martin-Schwinger equations

$$g_{\alpha\beta}(\omega) = g_{0\,\alpha\beta}(\omega) - \sum_{\gamma\delta} g_{0\,\alpha\gamma}(\omega)\, u_{\gamma\delta}\, g_{\delta\beta}(\omega) - \frac{1}{2} \sum_{\substack{\gamma\epsilon \\ \delta\mu}} g_{0\,\alpha\gamma}(\omega)\, v_{\gamma\epsilon,\delta\mu} \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} g^{4-\mathrm{pt}}_{\delta\mu,\beta\epsilon}(\omega_1, \omega_2; \omega, \omega_1 + \omega_2 - \omega)$$

$$\ldots$$

Decouple via Σ

Observables: exp. values

$$\mathrm{O} = \langle \Psi_0^A | O | \Psi_0^A \rangle$$

Many-body Green's functions

A-body wave function → **Green's functions**

$$|\Psi_k^A\rangle$$

$$\mathrm{i}\, g_{\alpha\beta}(t_\alpha, t_\beta) \equiv \langle \Psi_0^A | \mathcal{T}[a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta)] | \Psi_0^A \rangle$$

$$\mathrm{i}\, g^{4-\mathrm{pt}}_{\alpha\gamma\beta\delta}(t_\alpha, t_\gamma, t_\beta, t_\delta) \equiv \langle \Psi_0^A | \mathcal{T}[a_\gamma(t_\gamma) a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta) a_\delta^\dagger(t_\delta)] | \Psi_0^A \rangle$$

$$\dots$$

A-body Schrödinger equation → **Dyson equation**

$$H|\Psi_k^A\rangle = E_k^A |\Psi_k^A\rangle$$

$$g_{\alpha\beta}(\omega) = g_{0\,\alpha\beta}(\omega) + \sum_{\gamma\delta} g_{0\,\alpha\gamma}(\omega)\, \Sigma^\star_{\gamma\delta}(\omega)\, g_{\delta\beta}(\omega)$$

Self-energy expansion → Many-body approximations

Observables: exp. values → **Observables: convolutions with GFs**

$$\mathrm{O} = \langle \Psi_0^A | O | \Psi_0^A \rangle$$

$$\langle \Psi_0^A \,|\, O^{1\mathrm{B}} \,|\, \Psi_0^A \rangle = \sum_{\alpha\beta} \int \frac{d\omega}{2\pi i}\, g_{\beta\alpha}(\omega)\, o_{\alpha\beta}$$

+ Koltun sum rule

$$E_0 = \langle \Psi_0^A \,|\, H \,|\, \Psi_0^A \rangle = \frac{1}{2} \sum_{\alpha\beta} \int \frac{d\omega}{2\pi i}\, g_{\beta\alpha}(\omega)\, [t_{\alpha\beta} + \omega\, \delta_{\alpha\beta}]$$

Källén-Lehmann representation

One-body propagator displays **spectral representation (Källén-Lehmann)**

$$g_{\alpha\beta}(\omega) = \sum_n \frac{(\mathcal{X}_\alpha^n)^* \mathcal{X}_\beta^n}{\omega - \varepsilon_n^+ + i\eta} + \sum_k \frac{\mathcal{Y}_\alpha^k (\mathcal{Y}_\beta^k)^*}{\omega - \varepsilon_k^- - i\eta}$$

Separation energies

$$\varepsilon_n^+ = E_n^{A+1} - E_0^A$$
$$\varepsilon_k^- = E_0^A - E_k^{A-1}$$

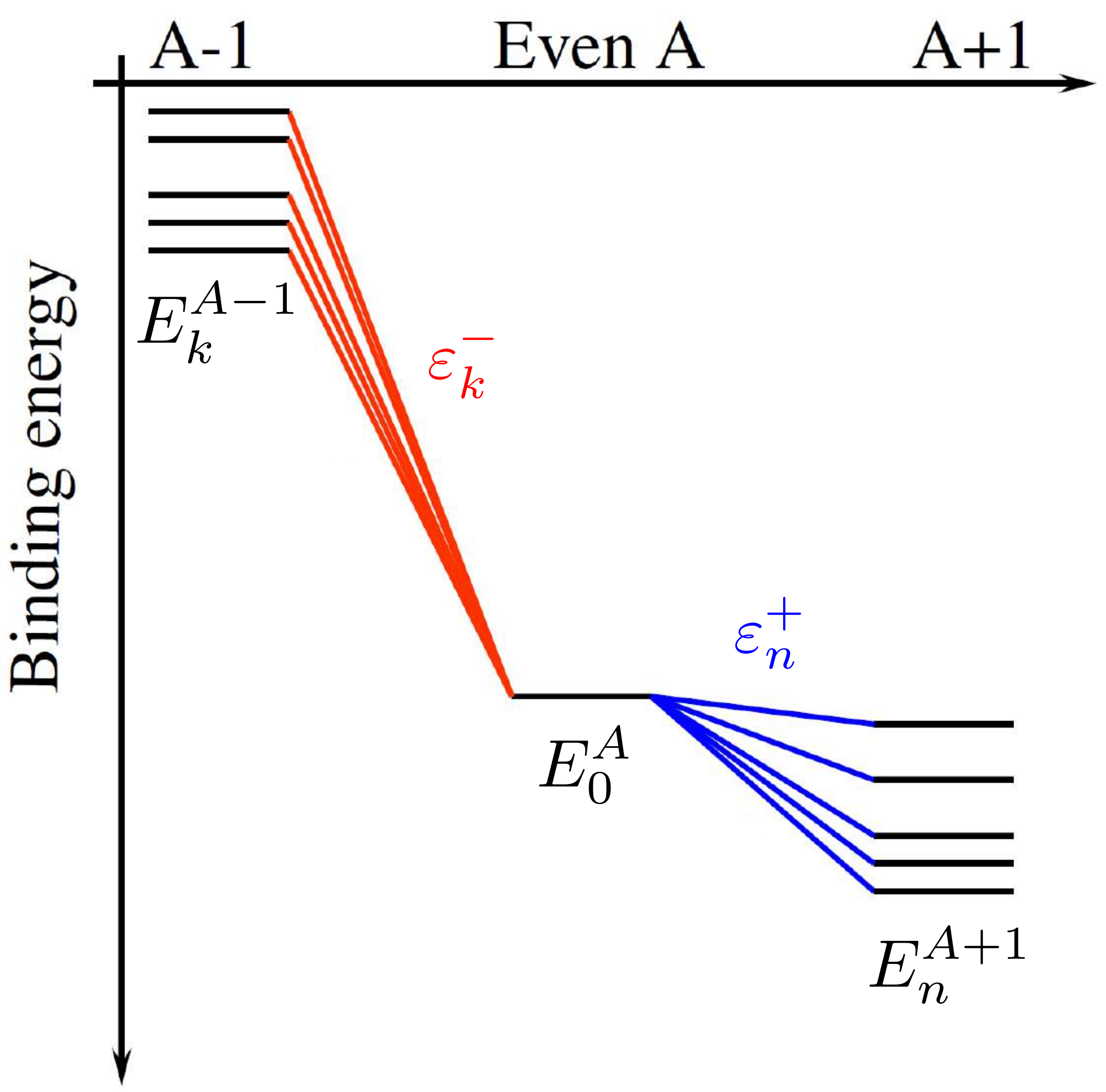
Transition amplitudes

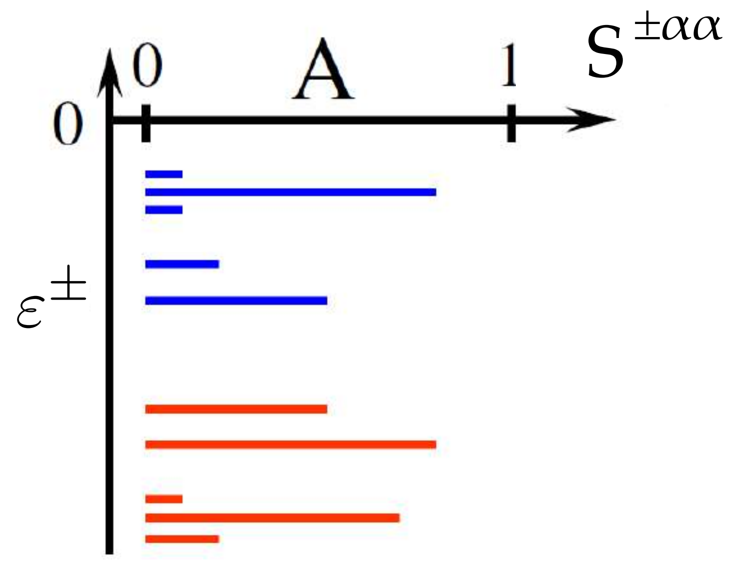
$$\mathcal{X}_\alpha^n = \langle \Psi_n^{\text{A+1}} | a_\alpha^\dagger | \Psi_0^{\text{A}} \rangle$$
$$\mathcal{Y}_\alpha^k = \langle \Psi_k^{\text{A-1}} | a_\alpha | \Psi_0^{\text{A}} \rangle$$

Spectroscopic factors

$$SF_n^+ = \sum_{\alpha \in \mathcal{H}_1} |\mathcal{X}_\alpha^n|^2$$
$$SF_k^- = \sum_{\alpha \in \mathcal{H}_1} |\mathcal{Y}_\alpha^k|^2$$

Numerator + denominator





Spectral strength distribution

$$\mathcal{S}(\omega) = \sum_{n \in \mathcal{H}_{A+1}} SF_n^+ \, \delta(\omega - \varepsilon_n^+) + \sum_{k \in \mathcal{H}_{A-1}} SF_k^- \, \delta(\omega - \varepsilon_k^-)$$

Algebraic Diagrammatic Construction

Exact self-energy can be decomposed as $\Sigma^{*}_{\alpha\beta}(\omega) = \Sigma^{(n=1)}_{\alpha\beta}(\omega) + \Sigma^{(n>1)}_{\alpha\beta}(\omega) \equiv \Sigma^{(\infty)}_{\alpha\beta} + \tilde{\Sigma}_{\alpha\beta}(\omega)$

Static self-energy

Dynamic self-energy

Dynamic (energy-dependent) self-energy displays a spectral representation

$$\widetilde{\Sigma}_{\alpha\beta}(\omega) = \sum_{j} \frac{\mathcal{M}^{\dagger}_{\alpha j}\,\mathcal{M}_{j\beta}}{\omega - \mathcal{E}^{+}_{j} + \mathrm{i}\eta} + \sum_{k} \frac{\mathcal{N}_{\alpha k}\,\mathcal{N}^{\dagger}_{k\beta}}{\omega - \mathcal{E}^{-}_{k} - \mathrm{i}\eta}$$

A+1 configurations

A-1 configurations

Dyson eq. in matrix form

$$\varepsilon_i \begin{pmatrix} \mathcal{Z}^i_\alpha \\ \mathcal{W}^i_j \\ \mathcal{W}^i_k \end{pmatrix} = \begin{pmatrix} h^{(0)}_{\alpha\delta} + \Sigma^{(\infty)}_{\alpha\delta} & \mathcal{M}^{\dagger}_{\alpha j} & \mathcal{N}_{\alpha k} \\ \mathcal{M}_{j\delta} & \mathcal{E}^{+}_{j} & 0 \\ \mathcal{N}^{\dagger}_{k\delta} & 0 & \mathcal{E}^{-}_{k} \end{pmatrix} \begin{pmatrix} \mathcal{Z}^i_\delta \\ \mathcal{W}^i_j \\ \mathcal{W}^i_k \end{pmatrix}$$

Algebraic Diagrammatic Construction (ADC)

1. Rewrite exact self-energy as $\widetilde{\Sigma}^{(\mathrm{ADC})}_{\alpha\beta}(\omega) = \sum_{jj'} M^{\dagger}_{\alpha j} \left[\frac{1}{\omega\mathbb{1} - (E^{>} + C) + \mathrm{i}\eta\mathbb{1}} \right]_{jj'} M_{j'\beta} + \sum_{kk'} N_{\alpha k} \left[\frac{1}{\omega\mathbb{1} - (E^{<} + D) - \mathrm{i}\eta\mathbb{1}} \right]_{kk'} N^{\dagger}_{k'\beta}$

Non-diagonal energy matrices

2. Expand *M*, *N*, *C* & *D* in perturbation → Combine them to construct ADC at order *n*, i.e. **ADC(*n*)**

3. Determine *M*, *N*, *C* & *D* by matching ADC(*n*) to the **perturbative expansion at order *n***

[Schirmer 1982]

Algebraic Diagrammatic Construction

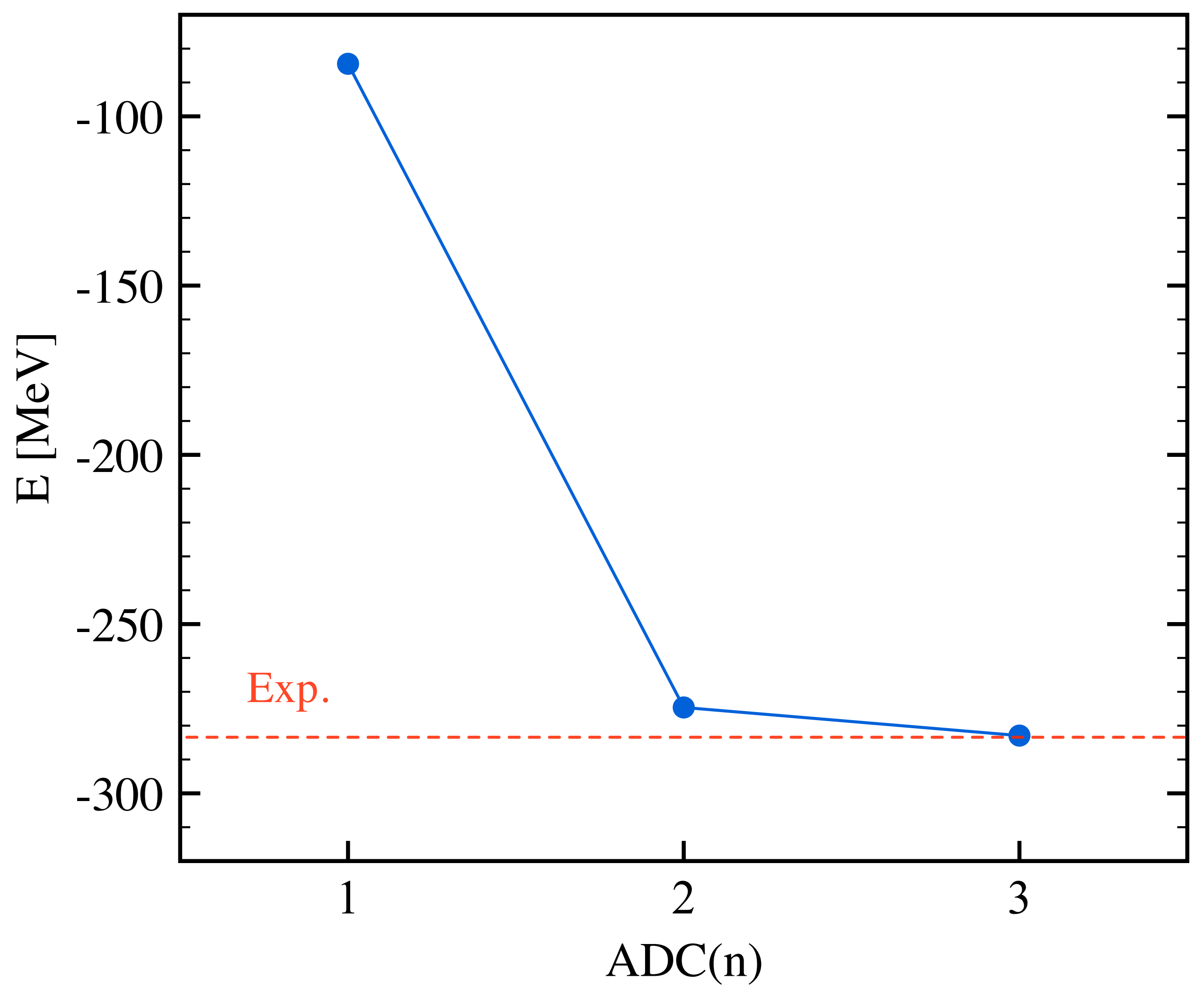
Convergence of ADC expansion

^{34}**Si**, NNLO$_{sat}$, e$_{max}$=13

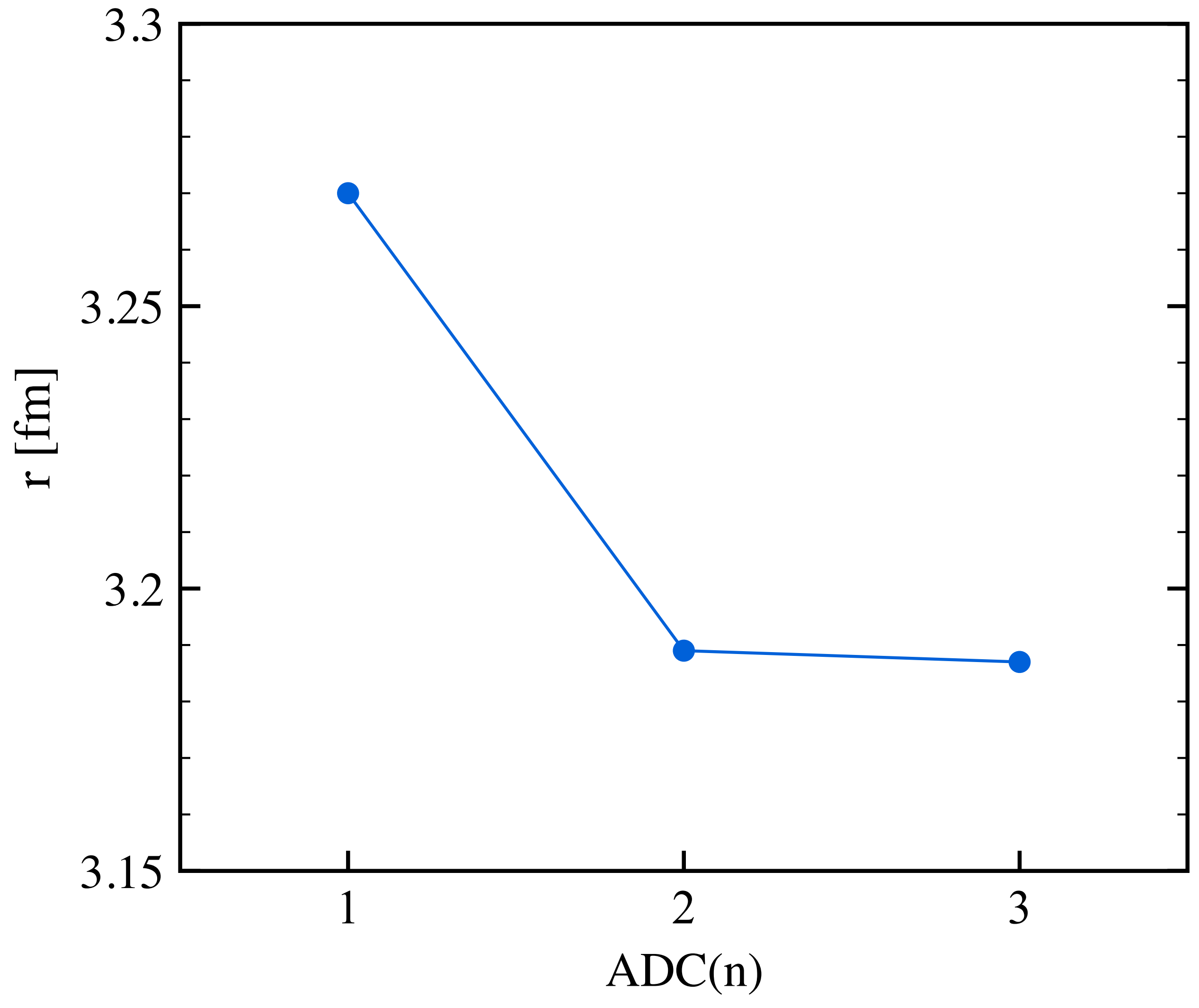
ADC(3)

[Duguet *et al.* 2017]

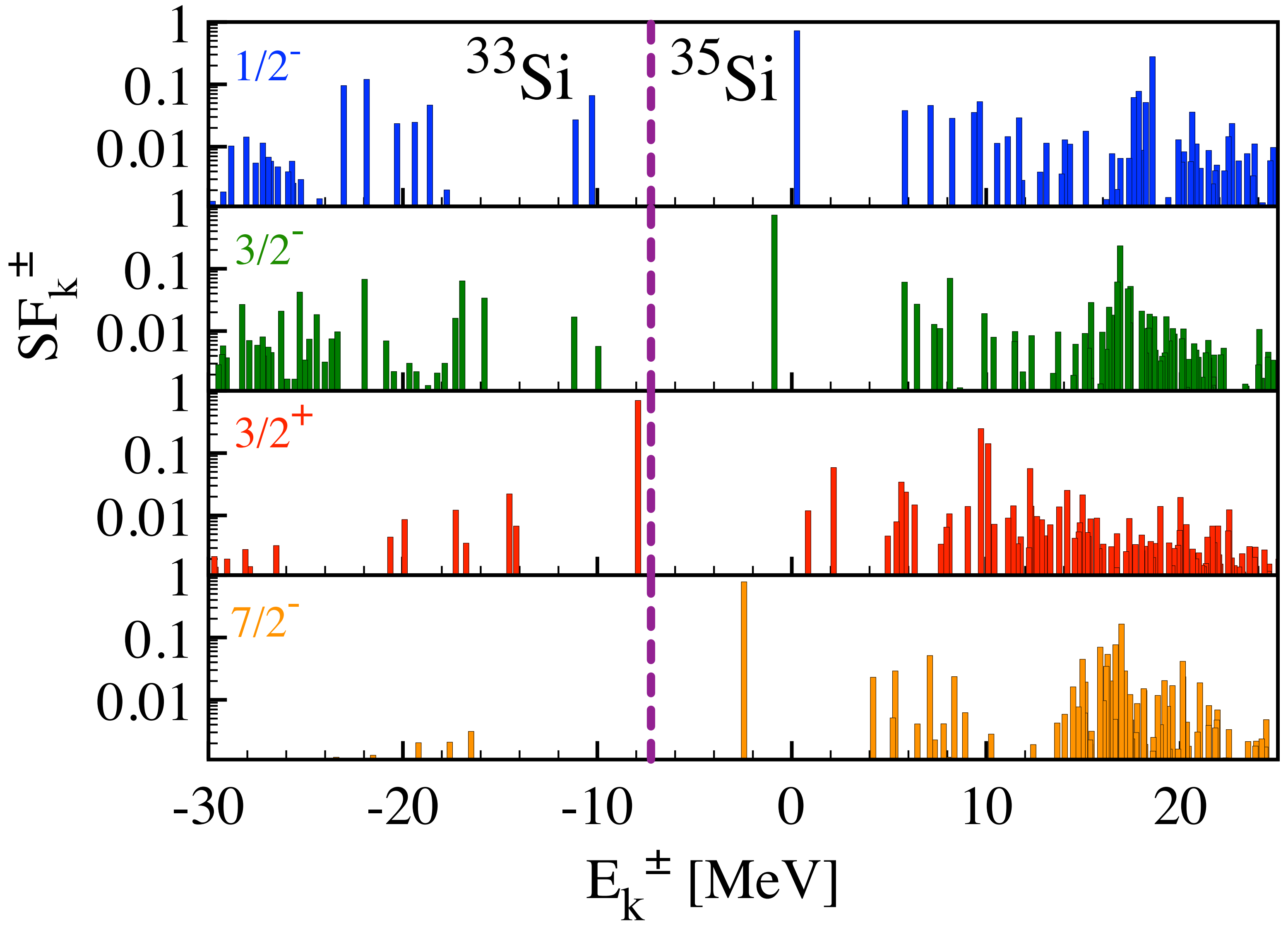
Binding energy



Charge radius



Spectral strength distribution

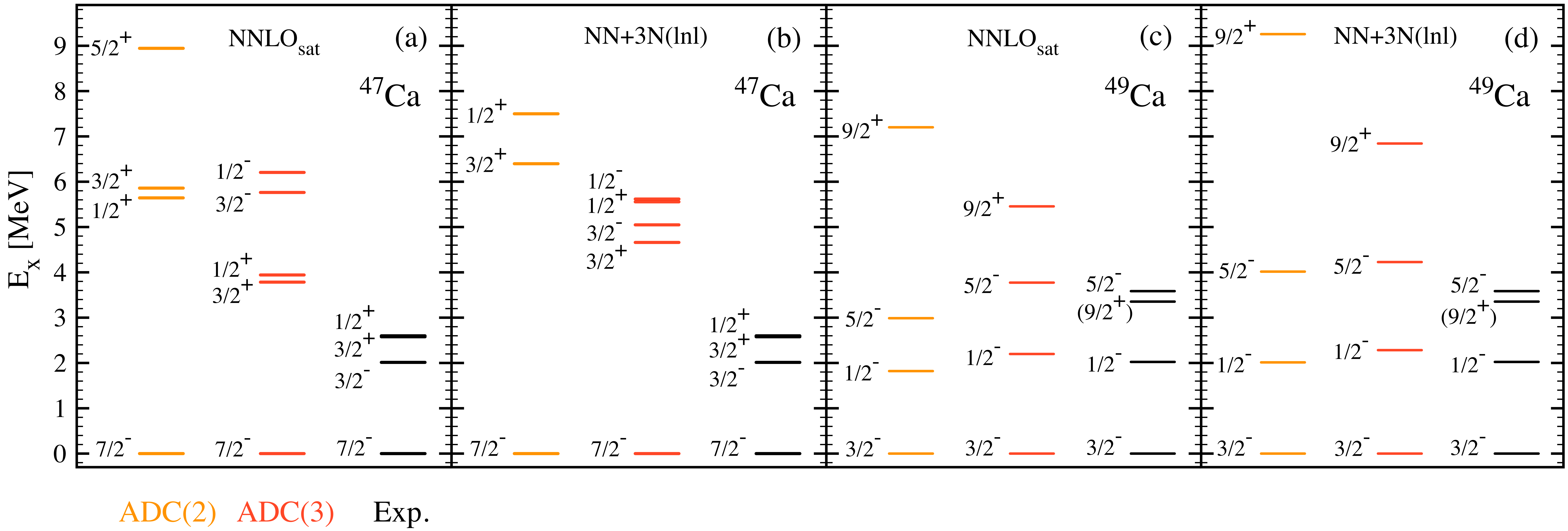


Energies → ADC(3) brings additional 5-10% correlation energy

Radii → Nearly converged already at ADC(2) level

Spectral distribution → ADC(3): more fragmentation, position of main peaks stabilised, smaller peaks qualitatively correct

Application: spectroscopy of Ca & neighbours



^{47}Ca

Footprint of too large N=20 gap

ADC(3) helps but not there yet

^{49}Ca

Good reproduction at ADC(2,3)

ADC(3) brings down higher-lying states

[Somà *et al.* 2020]

Symmetry-breaking Green's functions - 1. Particle number

Open-shell nuclei degenerate w.r.t. particle-hole excitations → Reopen gap via **symmetry breaking**

(BMBPT) [Tichai et al. 2018]
(BCC) [Signoracci et al. 2014]

Pairing correlations ➪
$$E_0^{A\pm 2n}(Z\pm 2n, N) - E_0^A(Z,N) \approx \ \pm\ 2n\mu_Z$$
$$E_0^{A\pm 2n}(Z, N\pm 2n) - E_0^A(Z,N) \approx \ \pm\ 2n\mu_N$$

Degeneracy associated to creating/annihilating pairs

Hamiltonian → Grand-canonical potential

$$\Omega \equiv H - \mu_Z Z - \mu_N N$$

G.s. wave function in equilibrium with a reservoir of Cooper pairs

Symmetry-breaking wave function

$$|\Psi_0\rangle = \sum_A^{\text{even}} |\Psi_0^A\rangle$$

Generalised one-body GFs

$$\mathrm{i}\, g^{11}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\ T[a_\alpha(t) a^\dagger_\beta(t')]\ |\Psi_0\rangle$$
$$\mathrm{i}\, g^{12}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\ T[a_\alpha(t) \bar{a}_\beta(t')]\ |\Psi_0\rangle$$
$$\mathrm{i}\, g^{21}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\ T[\bar{a}^\dagger_\alpha(t) a^\dagger_\beta(t')]\ |\Psi_0\rangle$$
$$\mathrm{i}\, g^{22}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\ T[\bar{a}^\dagger_\alpha(t) \bar{a}_\beta(t')]\ |\Psi_0\rangle$$

Nambu notation

$$\mathrm{i}\,\mathbf{g}_{\alpha\beta}(t-t') \equiv \langle\Psi_0| T\left\{\mathbf{A}_\alpha(t)\mathbf{A}^\dagger_\beta(t')\right\}|\Psi_0\rangle = \mathrm{i}\begin{pmatrix} g^{11}_{\alpha\beta}(t-t') & g^{12}_{\alpha\beta}(t-t') \\ g^{21}_{\alpha\beta}(t-t') & g^{22}_{\alpha\beta}(t-t') \end{pmatrix}$$

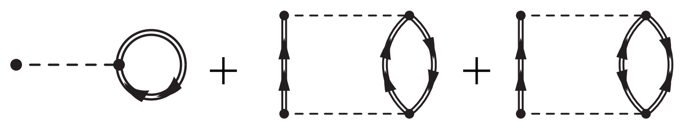
Gorkov equation

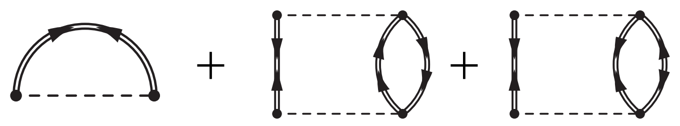
$$\mathbf{g}_{\alpha\beta}(\omega) = \mathbf{g}_{0\,\alpha\beta}(\omega) + \sum_{\gamma\delta} \mathbf{g}_{0\,\alpha\gamma}(\omega)\,\mathbf{\Sigma}^\star_{\gamma\delta}(\omega)\,\mathbf{g}_{\gamma\beta}(\omega)$$

Self-energy matrix

$$\mathbf{\Sigma}^\star_{\alpha\beta}(\omega) \equiv \begin{pmatrix} \Sigma^{\star\,11}_{\alpha\beta}(\omega) & \Sigma^{\star\,12}_{\alpha\beta}(\omega) \\ \Sigma^{\star\,21}_{\alpha\beta}(\omega) & \Sigma^{\star\,22}_{\alpha\beta}(\omega) \end{pmatrix}$$

Perturbative expansion

$\Sigma^{\star\,11}_{\alpha\beta}(\omega) =$ 

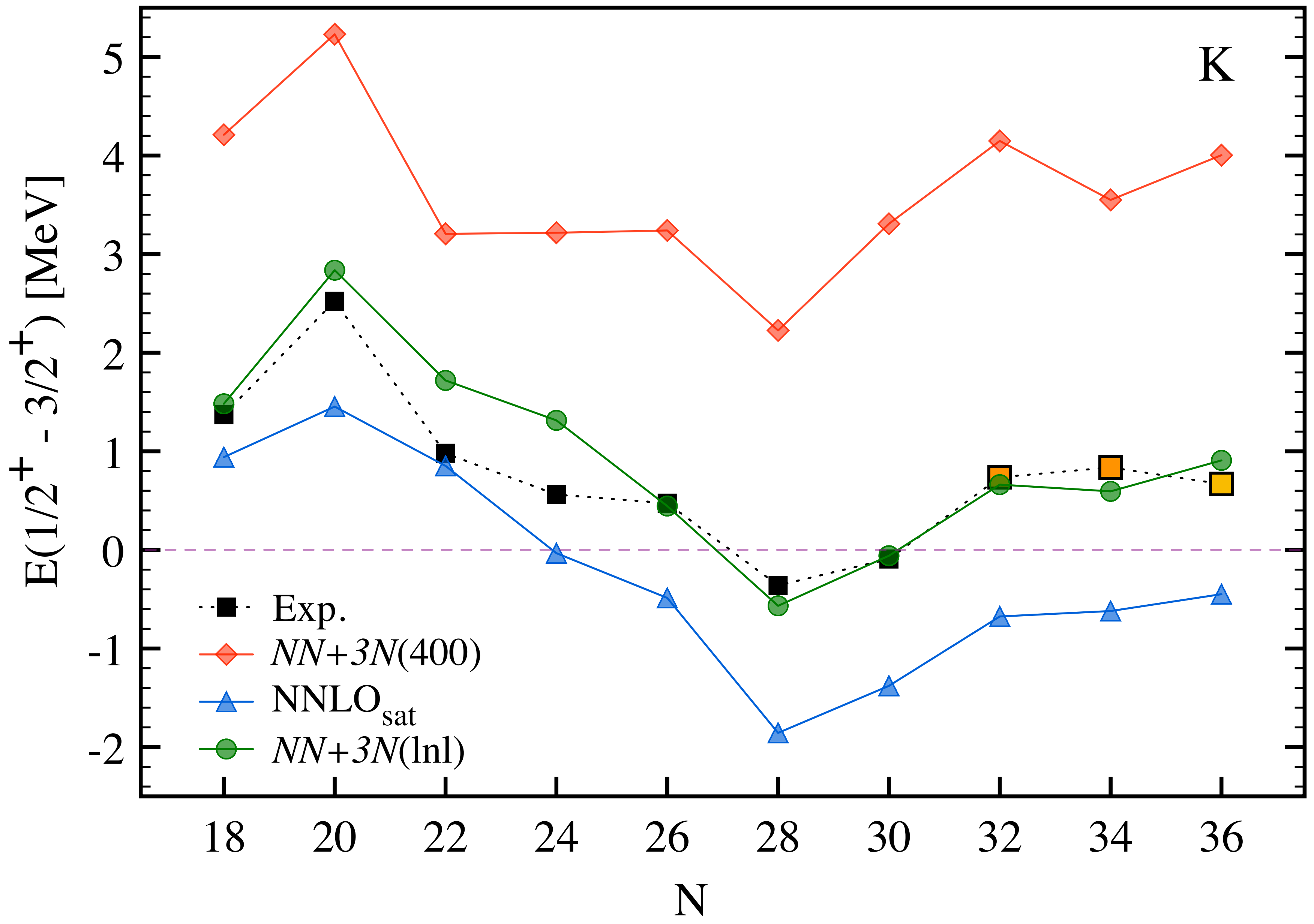
$\Sigma^{\star\,21}_{\alpha\beta}(\omega) =$ 

[Somà, Duguet, Barbieri 2011]

Application: spectroscopy of K and Cl chains

Spectroscopy through full isotopic chains becomes in reach

→ Case of **inversion & re-inversion of g.s. spin in K isotopes**

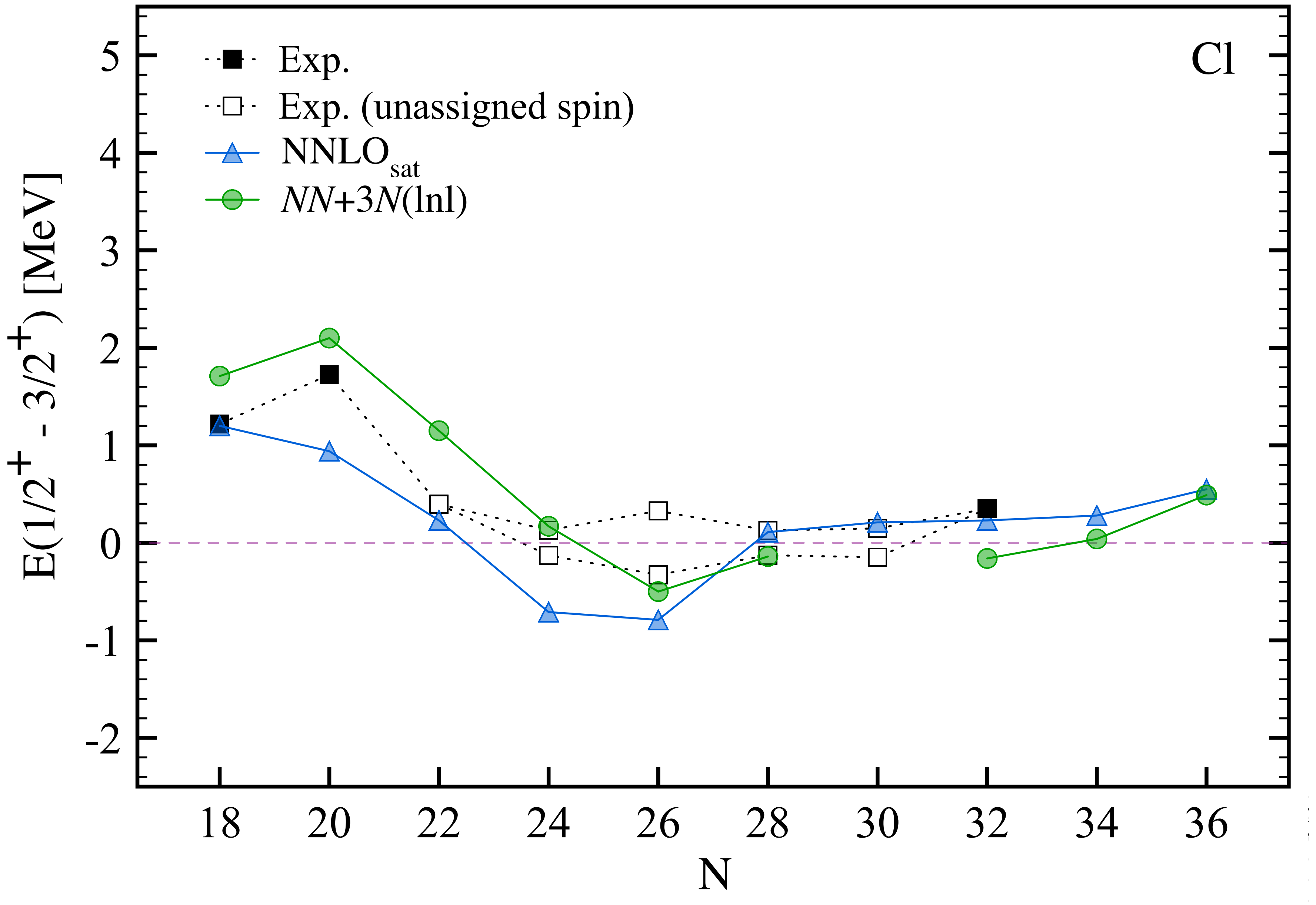


[Somà *et al.* 2020]

[Sun *et al.* 2020]

[Koiwai *et al.* 2022]

Extension to **Cl** chain



[Linh *et al.* 2021]

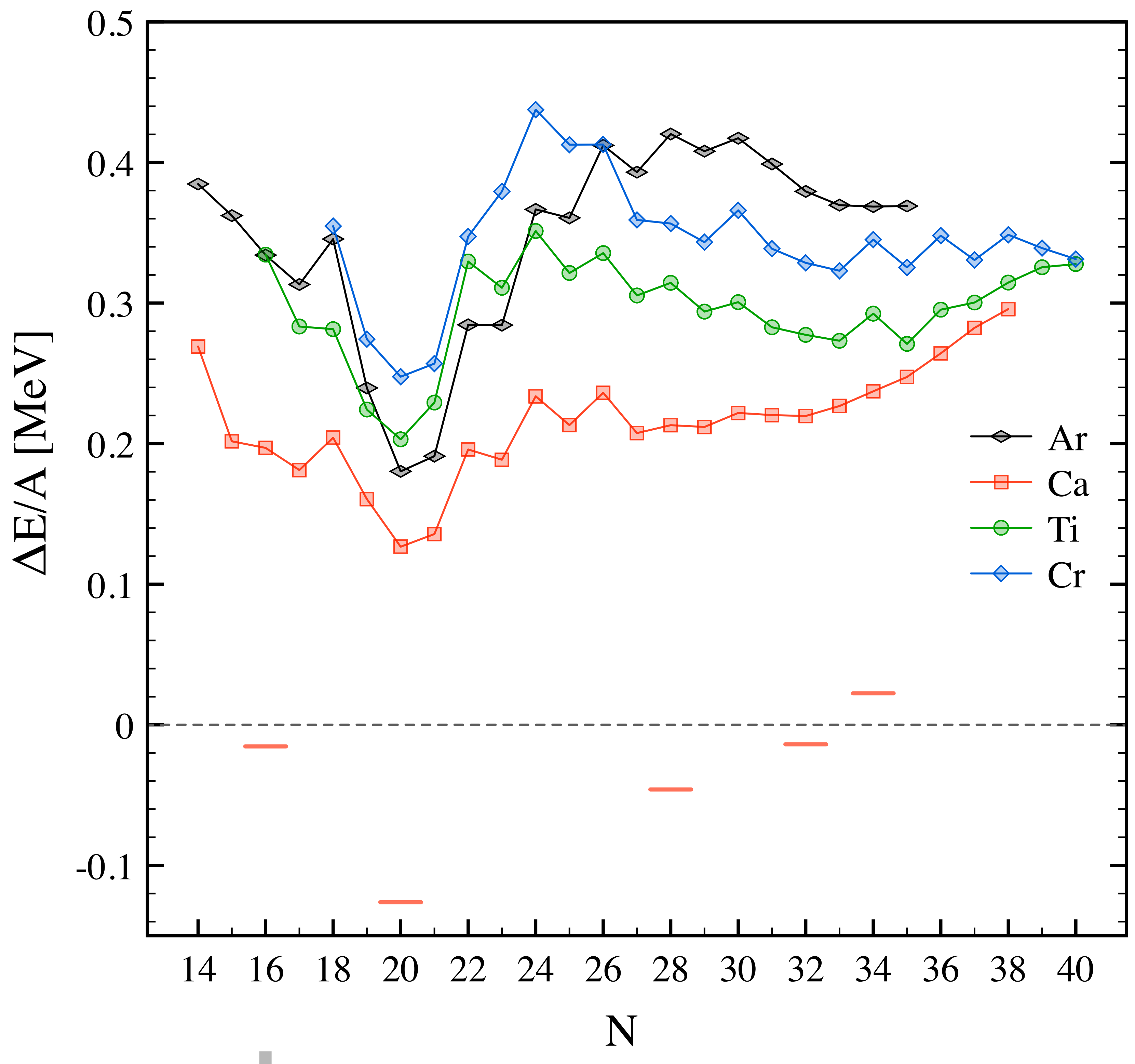
→ Gorkov ADC(2) calculations capable of grasping main evolution in K

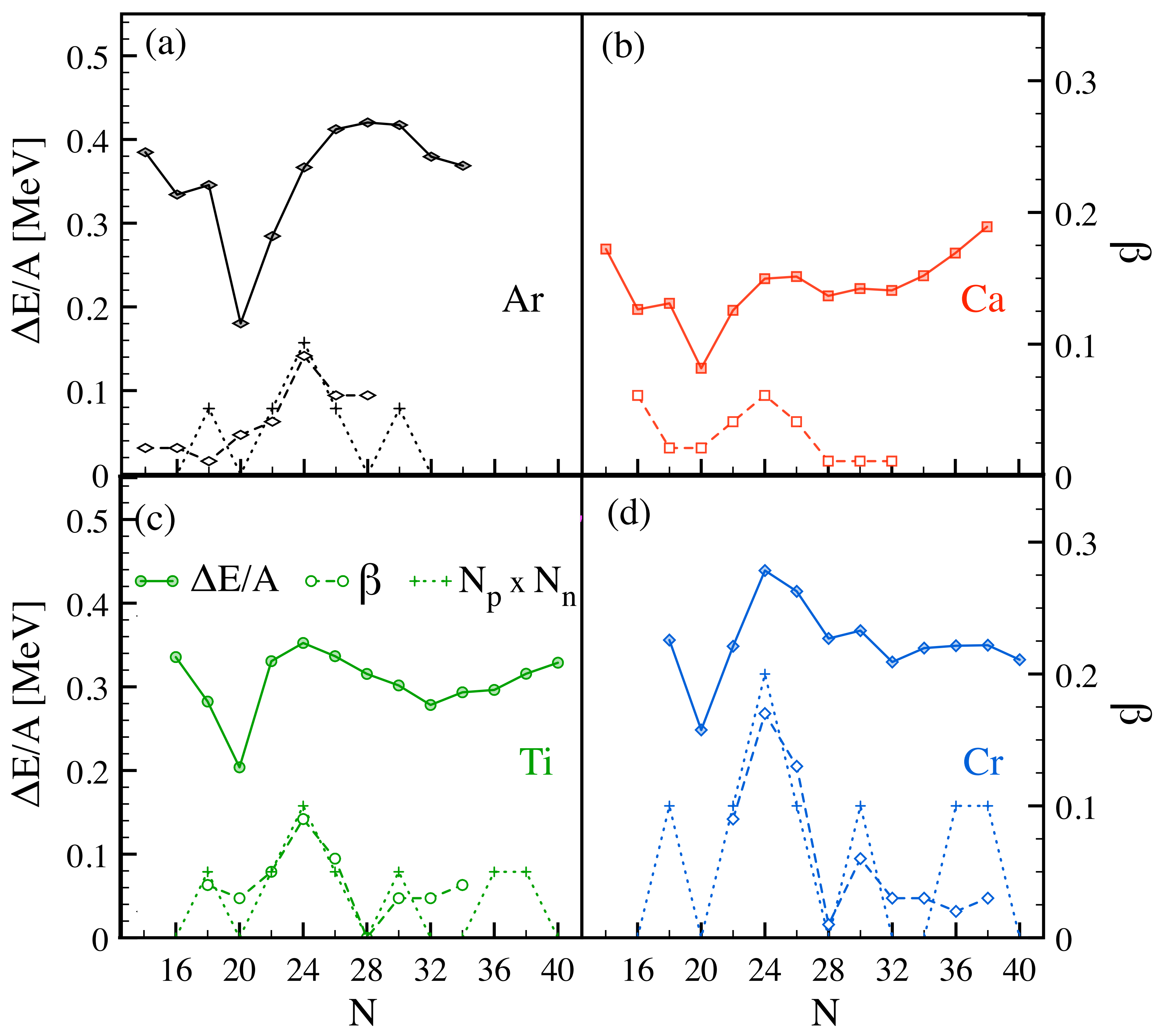
→ **Cl** case more complicated because of increased collectivity

Footprint of deformation

Impact of missing correlations visible **moving away from semi-magic** calcium chain

[Somà *et al.* 2021]





Behaviour consistent throughout isotopic chains

Correlation with measures of **deformation**

→ Calls for **extension to SU(2)-breaking scheme** when addressing doubly open-shell nuclei

Role of many-body correlations

How **SU(2)-breaking schemes** help in the description of open-shell nuclei?

- **Pedagogical analysis** of how MB correlations work out in *ab initio*
- Step-by-step study of the contribution of MB correlations to the total energy
- Understand the **best strategy to capture correlations** with different methods:

Symmetry Conserving vs **Symmetry Breaking**

Systems under study:

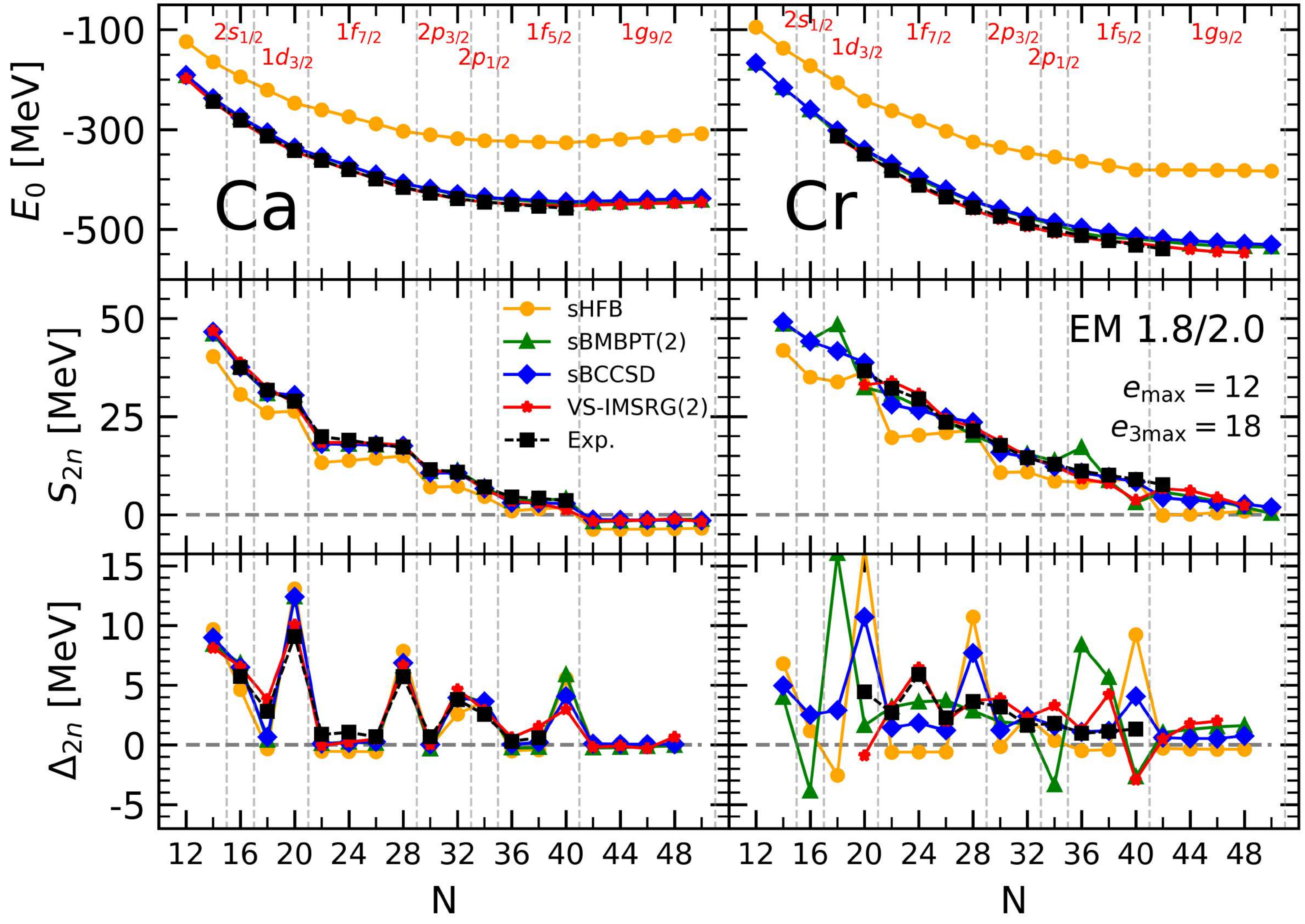
Medium-mass singly-closed shell → **Ca**

Medium-mass doubly-closed shell → **Cr**

Methods:

sHFB	dHFB
sBMBPT(2)	dBMBPT(2)
sBCCSD	
sVS-IMSRG(2)	

Role of many-body correlations



Ca $\longrightarrow$ wrong curvature with sHFB

- **low effective mass**
- **attractive valence-space MEs**

MB correlations corrections:

- increase of effective mass
- make valence-space MEs **repulsive**

Cr $\longrightarrow$ wrong curvature with sHFB

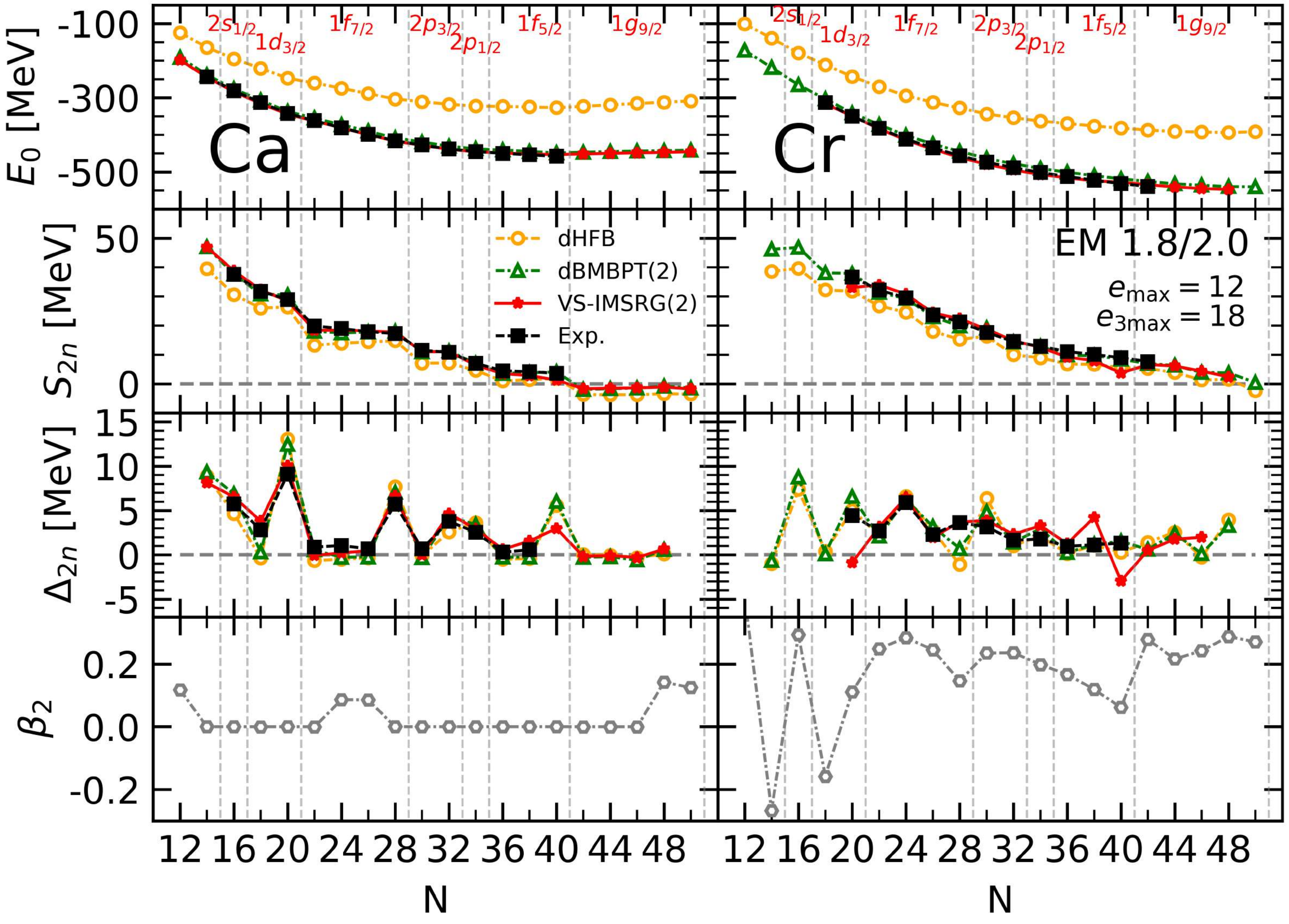
For symm. conserving methods

$\Big\downarrow$

higher MB orders needed

[Scalesi *et al.* n°1]

Role of many-body correlations



- deformation doesn't change res. in **Ca**
- dHFB **corrects curvature** in **Cr**

↓

Activation of **quadrupole MEs**

[Scalesi *et al.* n°1]

Role of many-body correlations

- **Deformation is necessary** to correctly describe doubly-open shell nuclei at polynomial cost

- It is **sufficient** since most of nuclei when deformed have no pairing with current χEFT interactions

  w.r.t. $U(1)$ sym. break.

$$\downarrow$$

- It is a good strategy to set up methods breaking $SU(2)$ and not $U(1)$

- Necessity of a **non-perturbative deformed theory** to go beyond perturbation theory

$\longrightarrow$ calls for **Dyson formalism** in **deformed SCGF** calculations!

[Hagen *et al.* 2014]

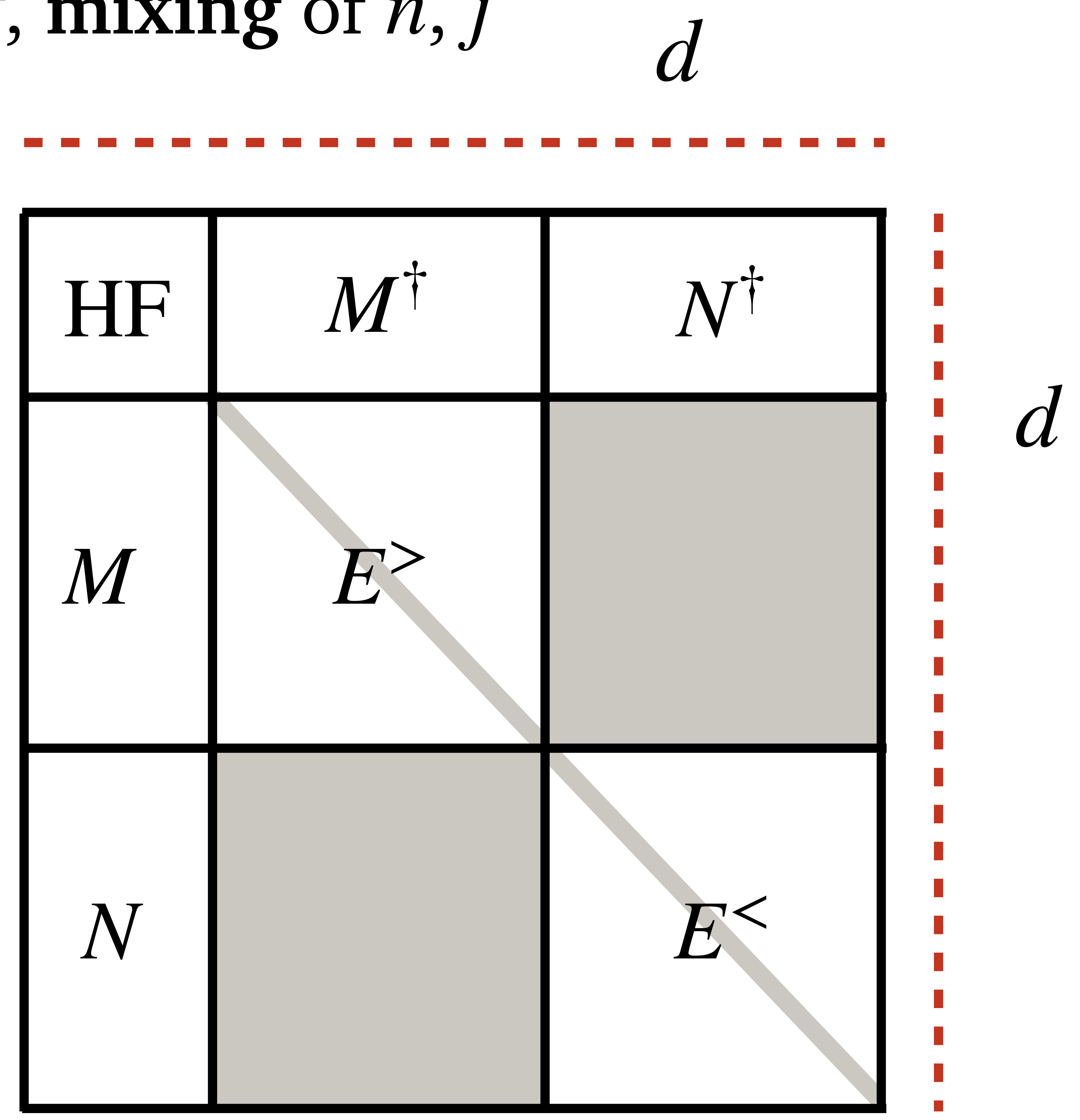
[Frosini *et al.* 2021]

See also T Papenbrock and J. M. Yao talks!

Symmetry-breaking Green's functions - 2. Rotational symmetry

- **Dyson** formalism
- **m-scheme** based
- **Symmetry blocks** of m, π, t, **mixing** of n, j

For every (m, π, t)



e_{max}	biggest d (^{16}O)
2	629
4	6480
6	35001
8	112016
10	285429
12	617580

- Dyson matrix decomposed in bigger blocks than spherical case

[Scalesi *et al.* n°2]

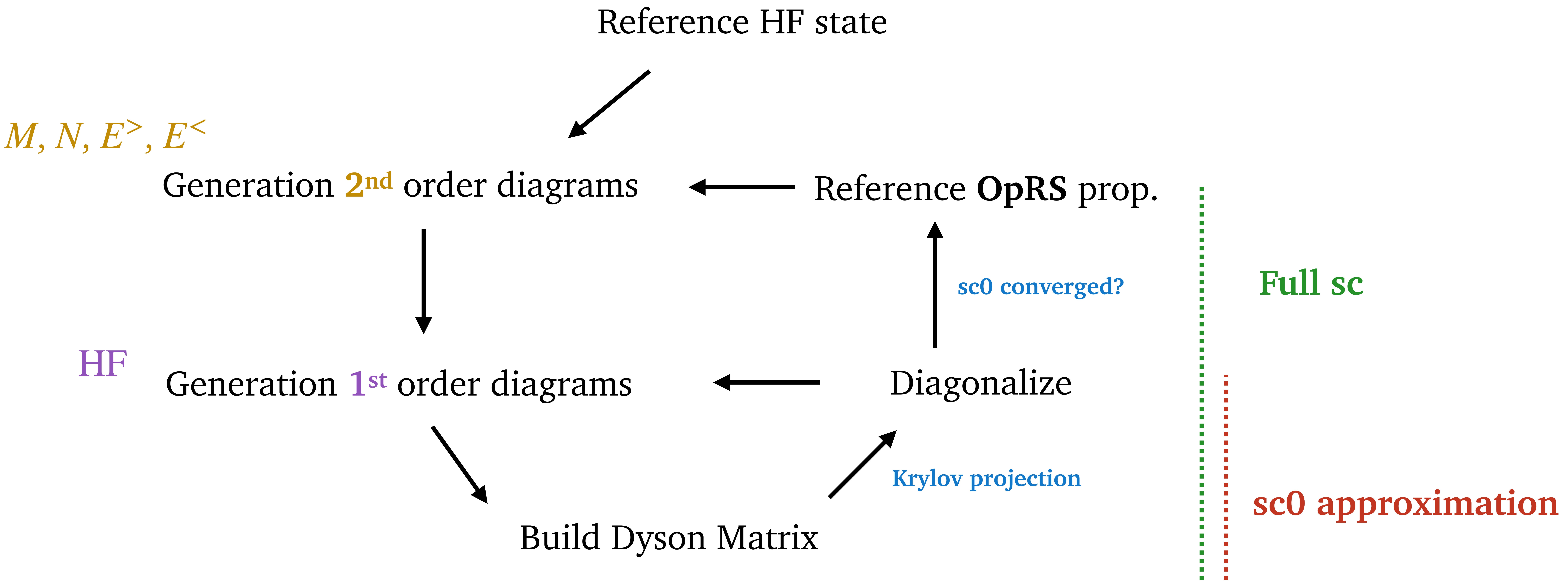
New Numerical Code for *ab initio* deformed calculations

- Axially **deformed HF reference state**
- **Eigen C++** library to handle 1- and 2-body tensors 
- **OpenMP** parallelization (multi-node MPI will be needed for future developments)
- Three-body forces included through rank reduction of operators
- Works with any generic spherical basis read from file
- Implements multi-pivot **Lanczos** algorithm for Krylov projection, **OpRS** for full SC calculations

[Frosini *et al.* 2021]

[Scalesi *et al.* 2024] [Scalesi *et al.* n°2]

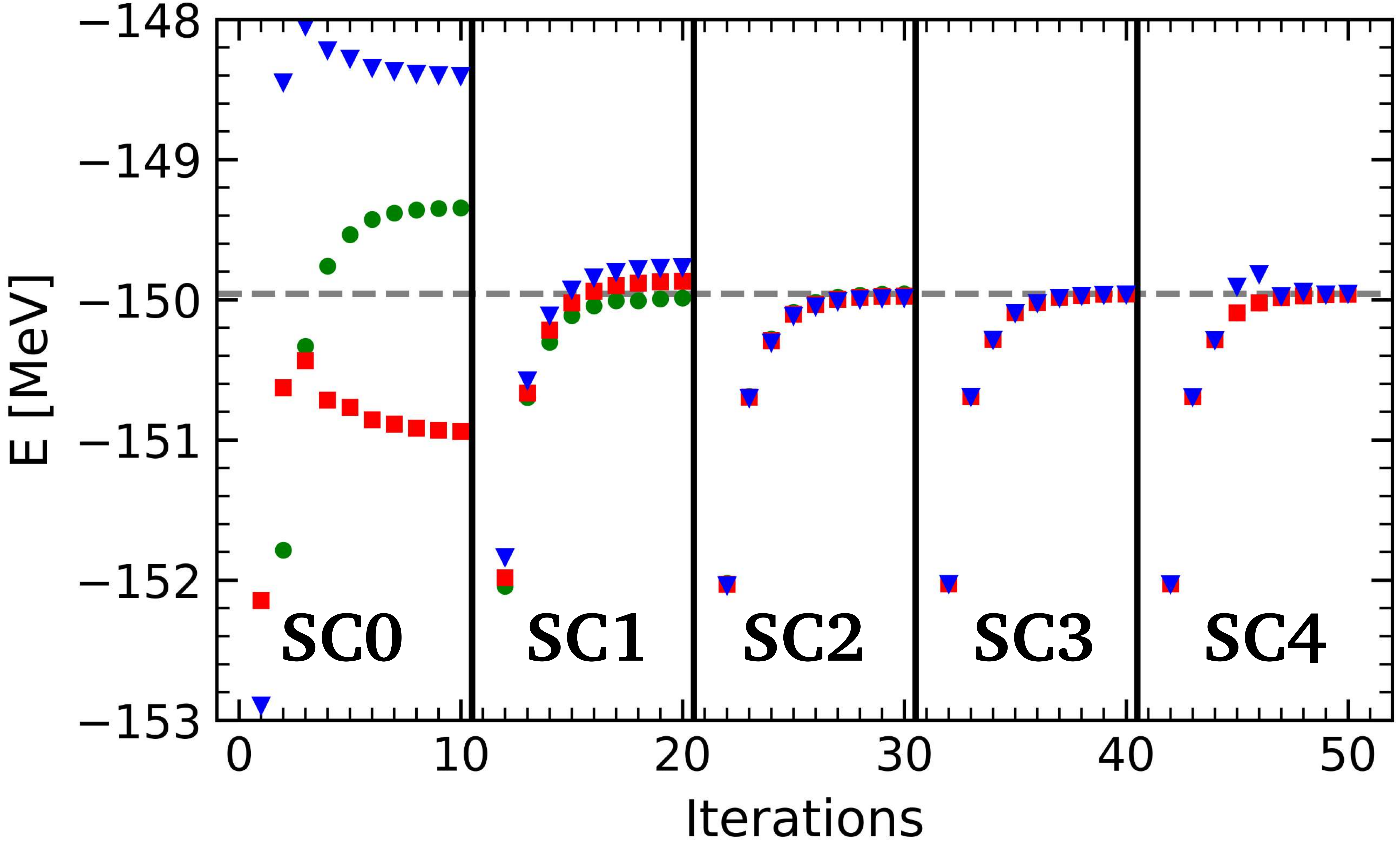
The Self-Consistent loop



[Scalesi *et al.* n°2]

dDSCGF(2) results - A numerical proof of Self-Consistency

Calculation: ADC(2), ^{20}Ne, ΔNNLO$_{go}$(394)

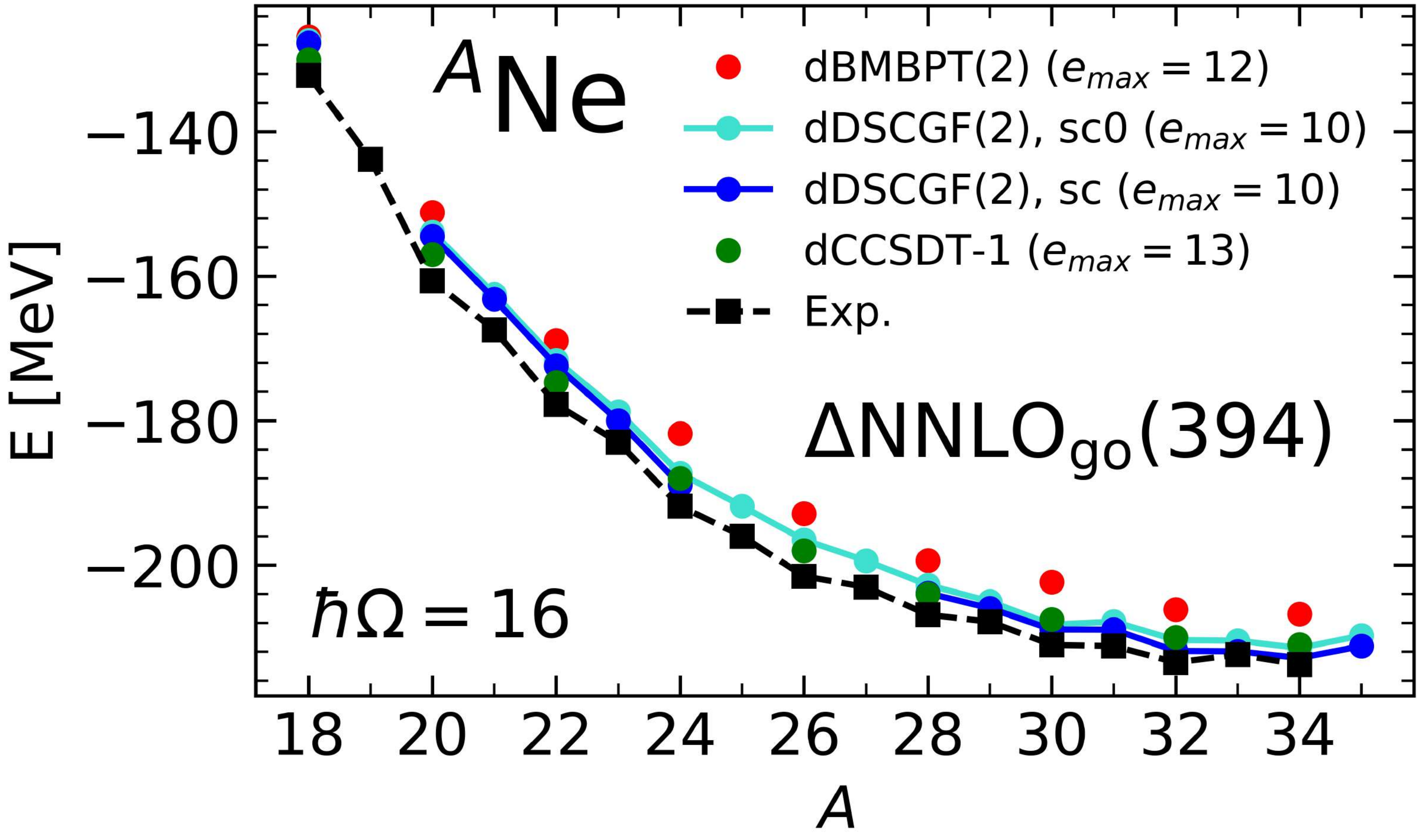


Reference HF state:

- ^{20}Ne, ΔNNLO$_{go}$(394)
- ^{20}Ne, NNLO$_{sat}$(bare)
- ^{24}Mg, NNLO$_{sat}$(bare)

[Scalesi *et al.* n°2]

dDSCGF(2) results - Total Energy



GMK sum rule

$$E_0^A = \frac{1}{2\pi}\int_{-\infty}^{\epsilon_F^-} d\omega \sum_{\alpha\beta} (t_{\alpha\beta} + \omega\, t_{\alpha\beta})\ \mathrm{Im}\, g_{\beta\alpha}$$

2-Body

$$- \frac{1}{2} \sum_{\alpha\gamma\epsilon\beta\delta\eta} w_{\alpha\gamma\epsilon\beta\delta\eta}\ \rho_{\beta\delta\eta\alpha\gamma\epsilon}$$

3-Body

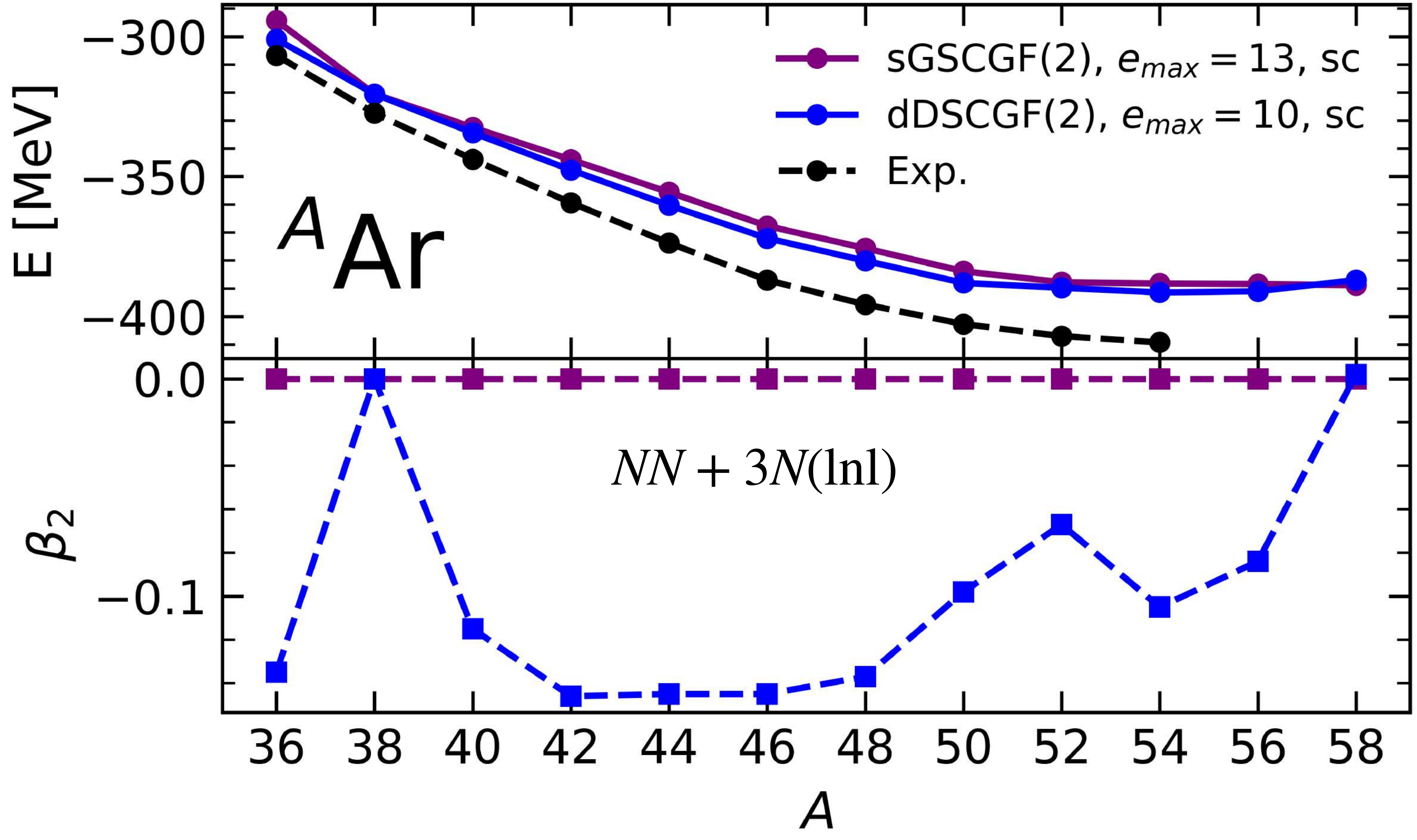
$$\sim \rho_{\beta_\alpha}\rho_{\delta\gamma}\rho_{\eta\epsilon}$$

- $\approx$ 4 MeV overall **gain from dBMBPT(2)**
- $\approx$ 1.5 MeV difference w.r.t. dCCSDT-1
- **sc** gain w.r.t. **sc0** increases with mass
- access to **odd-even isotopes**

Particle **addition/removal** GF formalism

[Novario *et al.* 2020]
[Scalesi *et al.* n°2]

dDSCGF(2) results - Comparison with spherical results



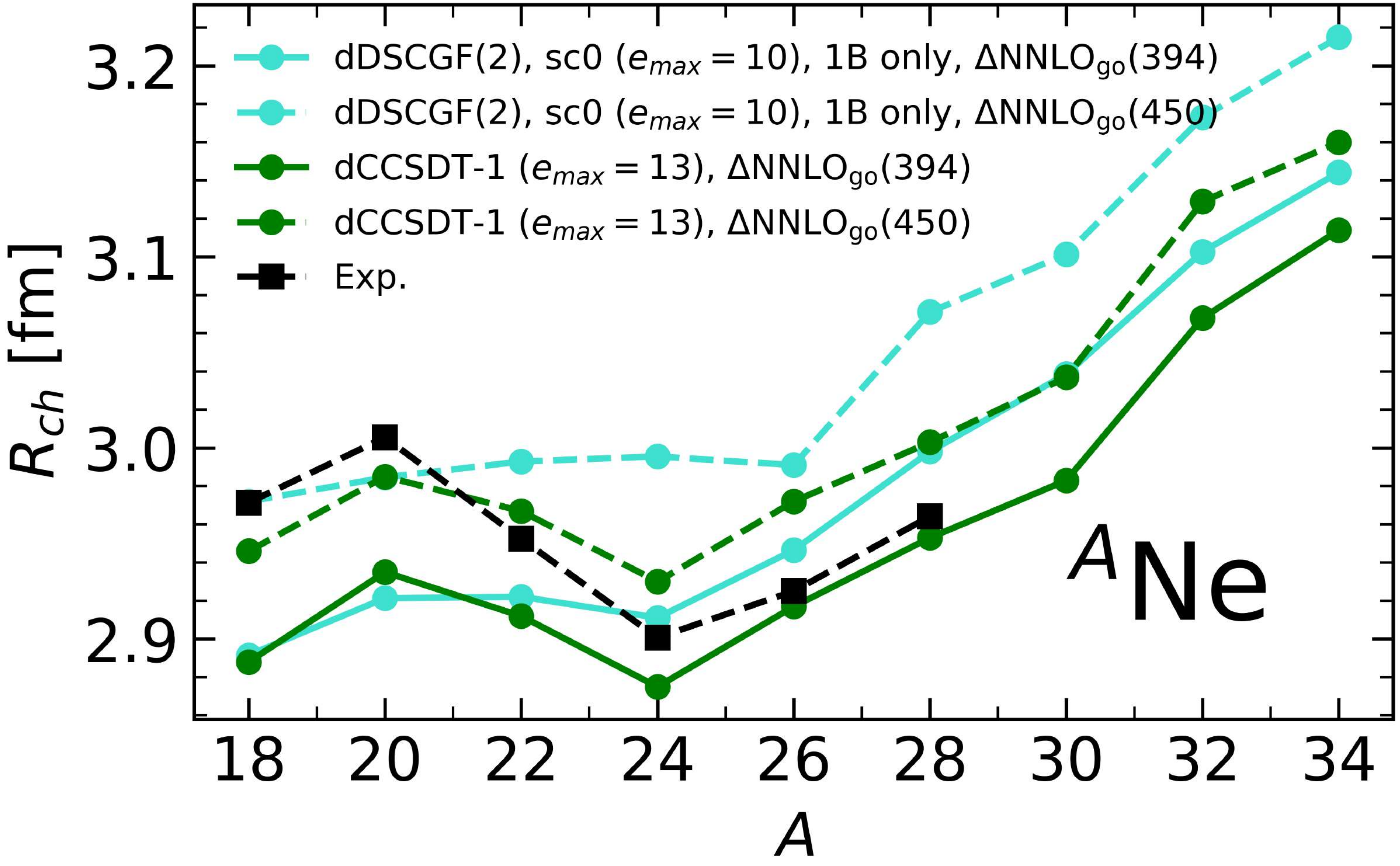
- **oblate** isotopic chain
- sphericity recovered at shell closures
- **correlation** of difference **w.r.t. def.**
- $\approx$ 3.5 MeV overall gain
- Further MeV to be gained for dDSCGF

→ **Improved description** of collectivity

[Somà *et al.*, *in preparation*]

[Scalesi *et al.* n°2]

dDSCGF(2) results - Charge Radii



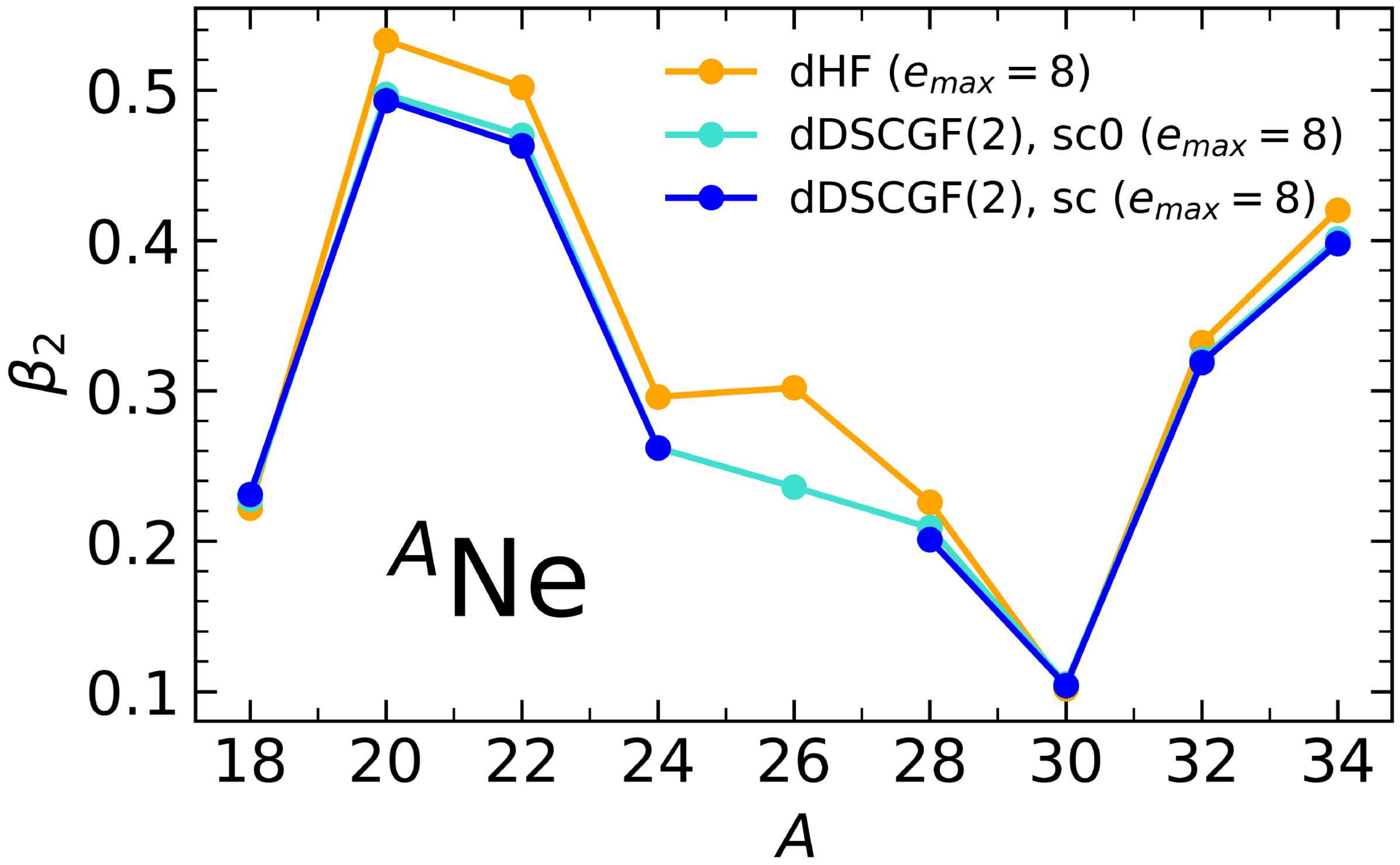
1B + 2B CoM corrections

$$R_{ch}^2 = R_p^2 + \langle r_p^2 \rangle + \frac{N}{Z}\langle r_n^2 \rangle + \langle r_{\mathrm{DF}}^2 \rangle + \langle r_{\mathrm{SO}}^2 \rangle$$

- Overall trend follows dCCSDT-1
- 2B CoM corrections missing in dDSCGF

[Novario *et al.* 2020]
[Scalesi *et al.* n°2]

dDSCGF(2) results - β_2 deformation



$$\langle \alpha | Q_{20} | \beta \rangle = \langle \alpha | r^2 \, Y_{20} | \beta \rangle$$

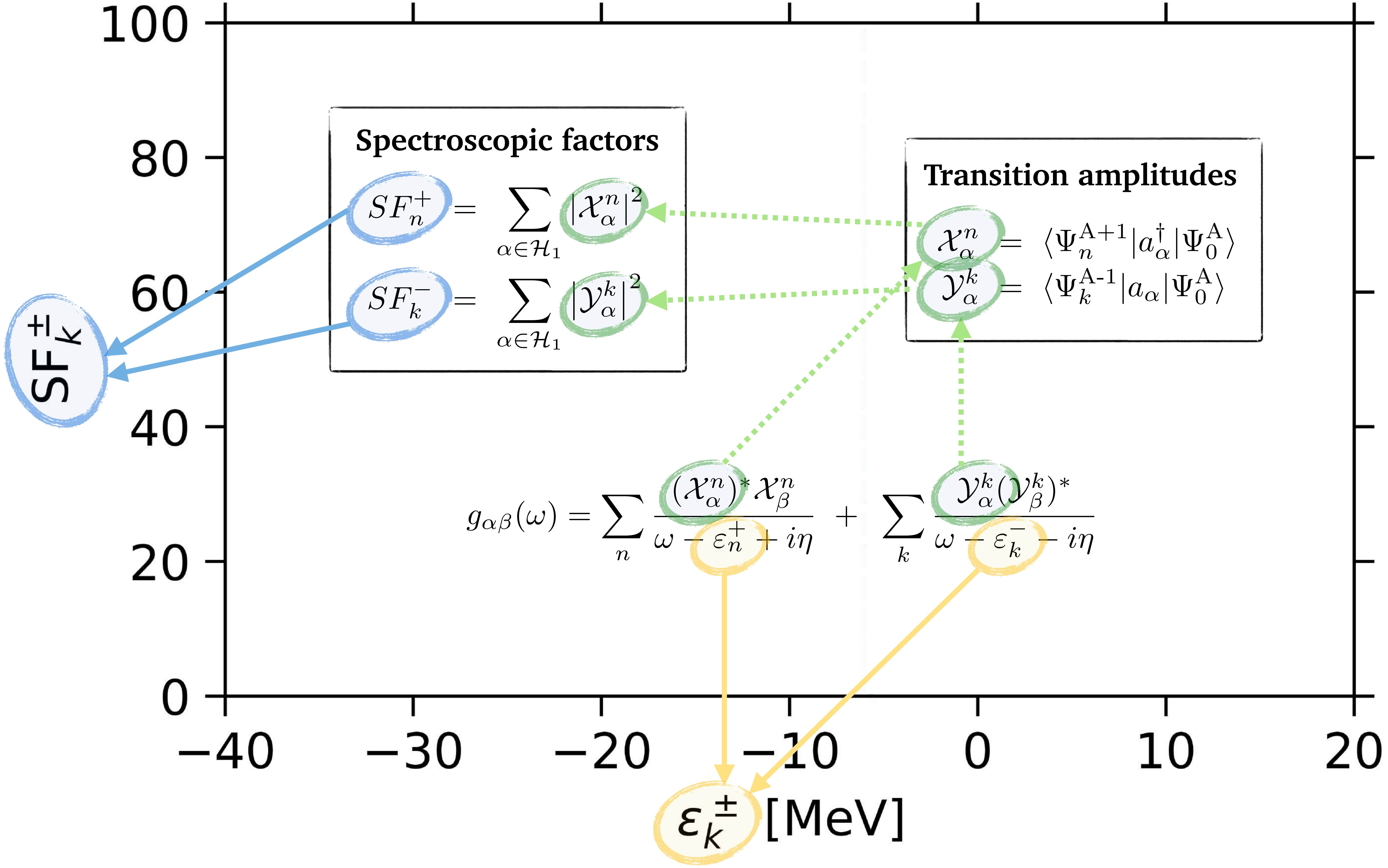
$$q_{20} = \sum_{\alpha\beta} \langle \alpha | Q_{20} | \beta \rangle \rho_{\beta\alpha}$$

$$\beta_2 = \frac{4}{3} \pi \, q_{20} \, \frac{1}{A \, R_0^2}$$

$\longrightarrow$ **Deformation decreases** with MB correlations

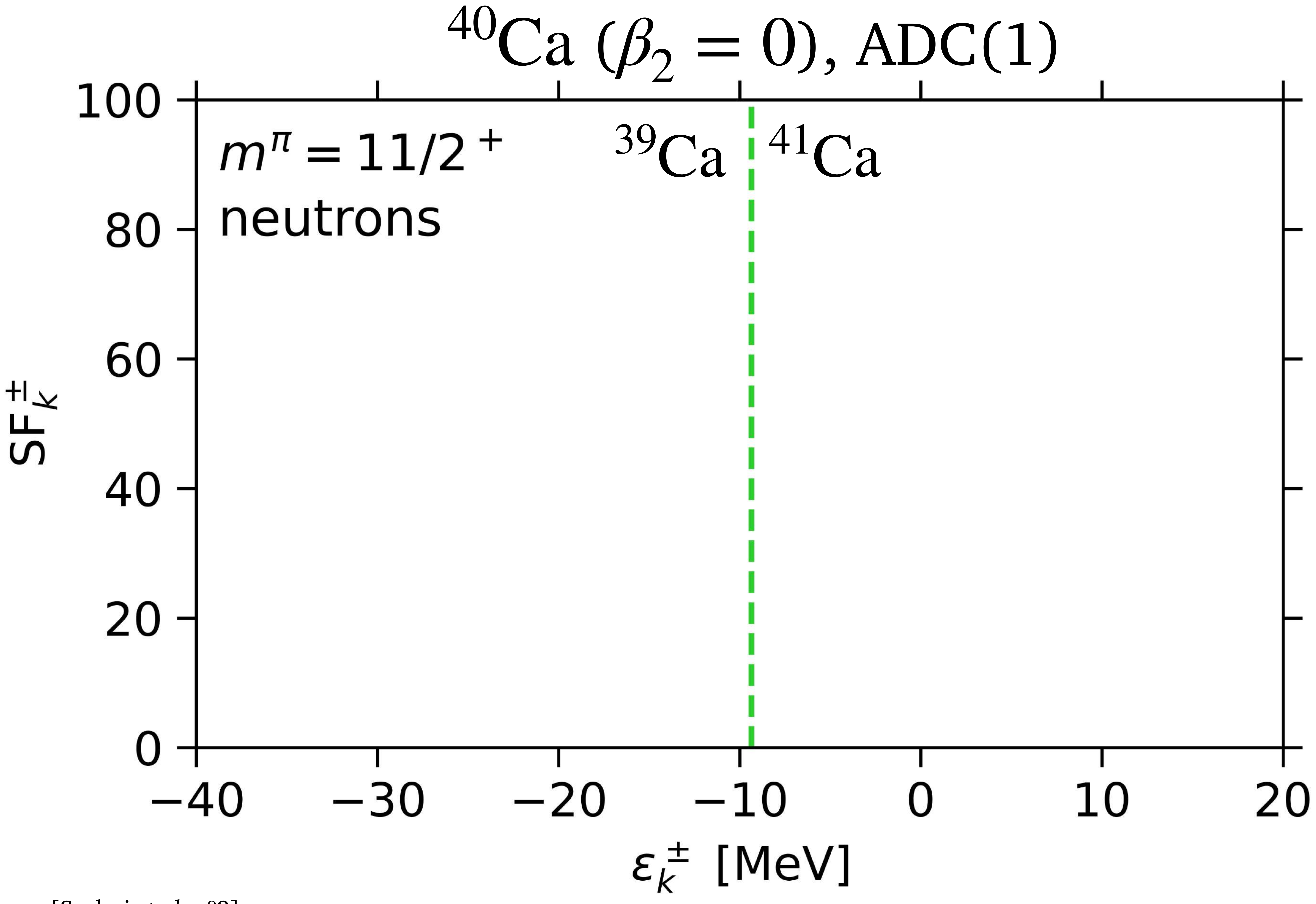
[Scalesi *et al.* n°2]

dDSCGF(2) results - Spectroscopic Amplitudes



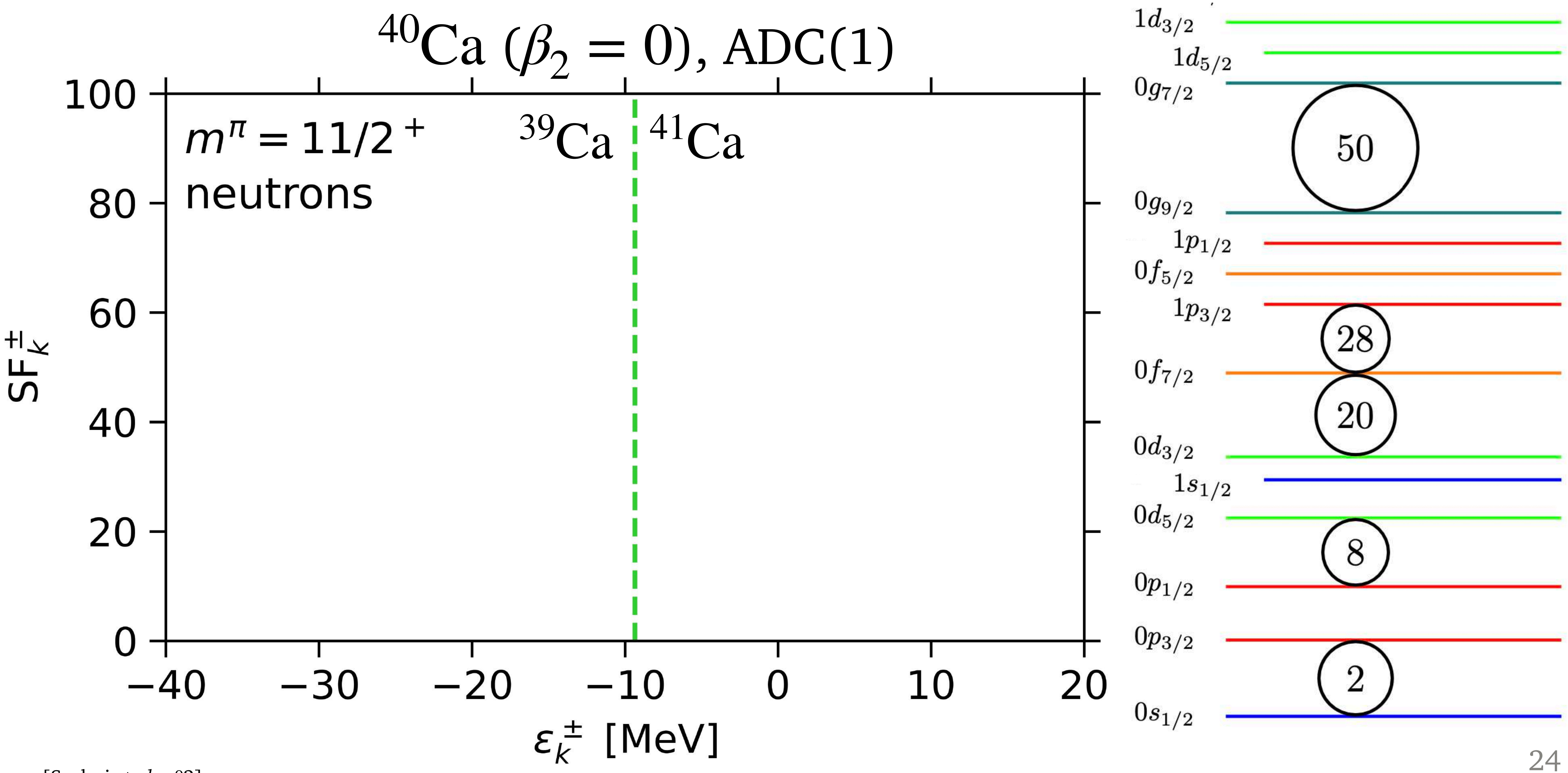
Reminder

dDSCGF(2) results - Spectroscopic Amplitudes



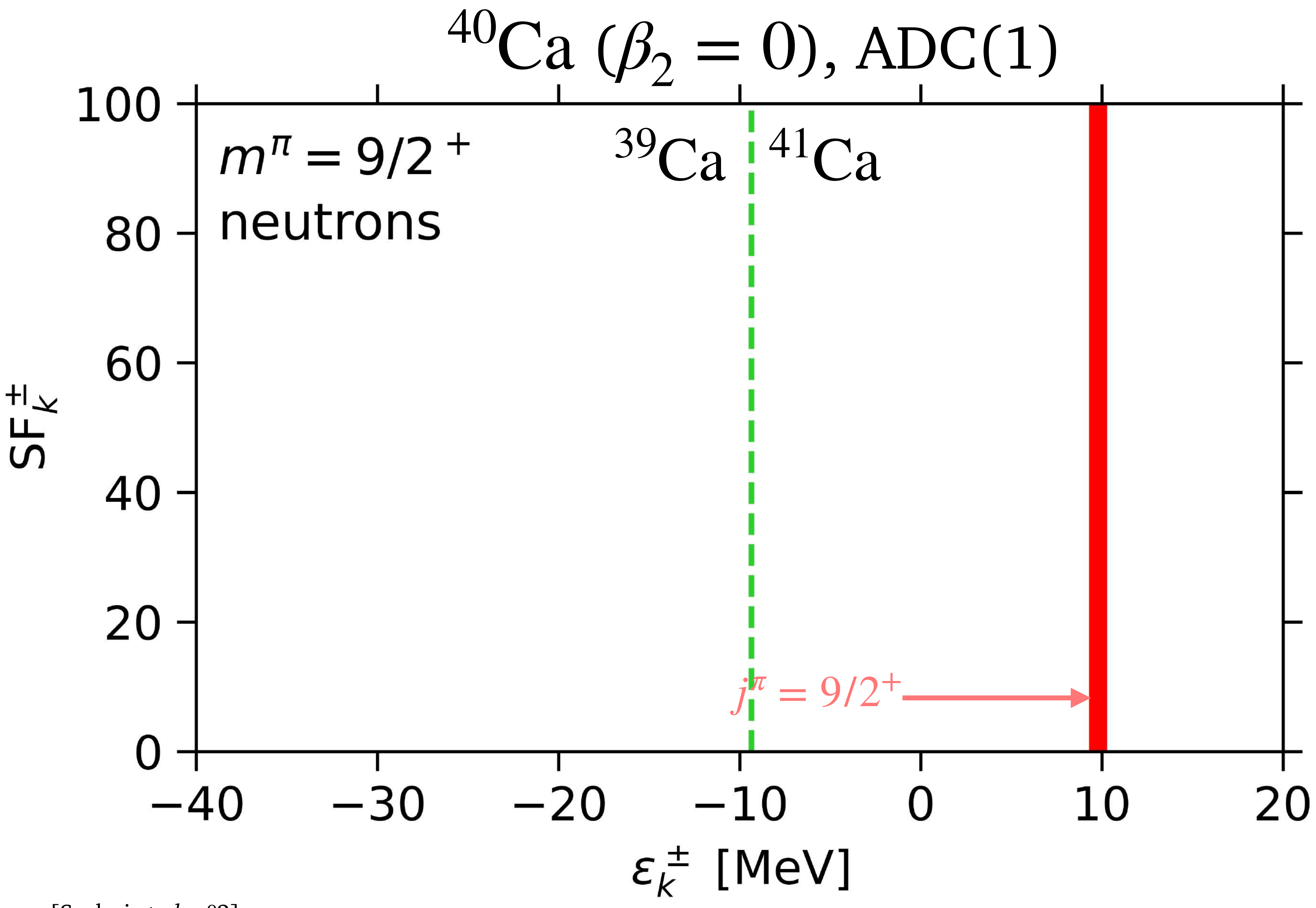
[Scalesi *et al.* n°2]

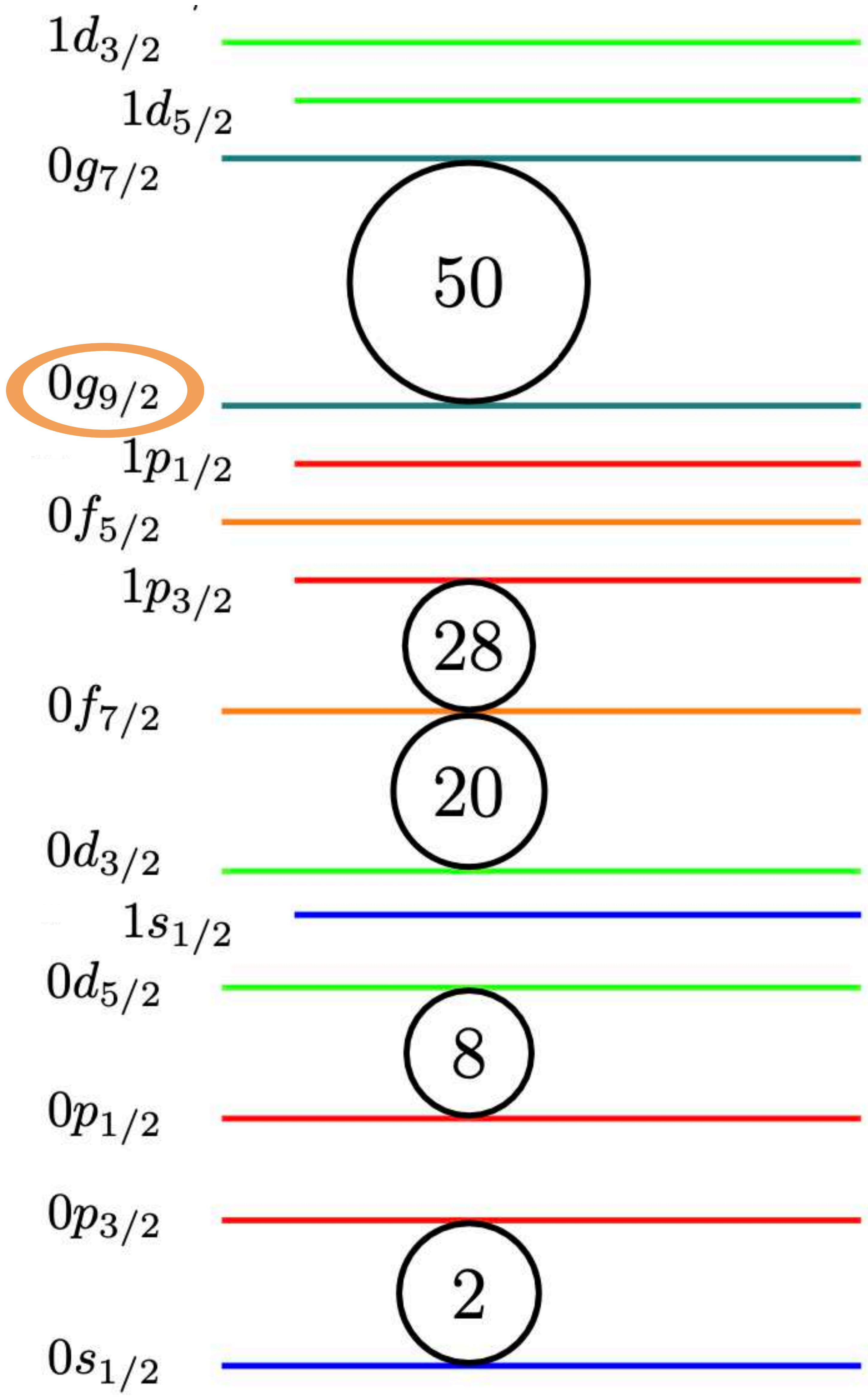
dDSCGF(2) results - Spectroscopic Amplitudes



[Scalesi *et al.* n°2]

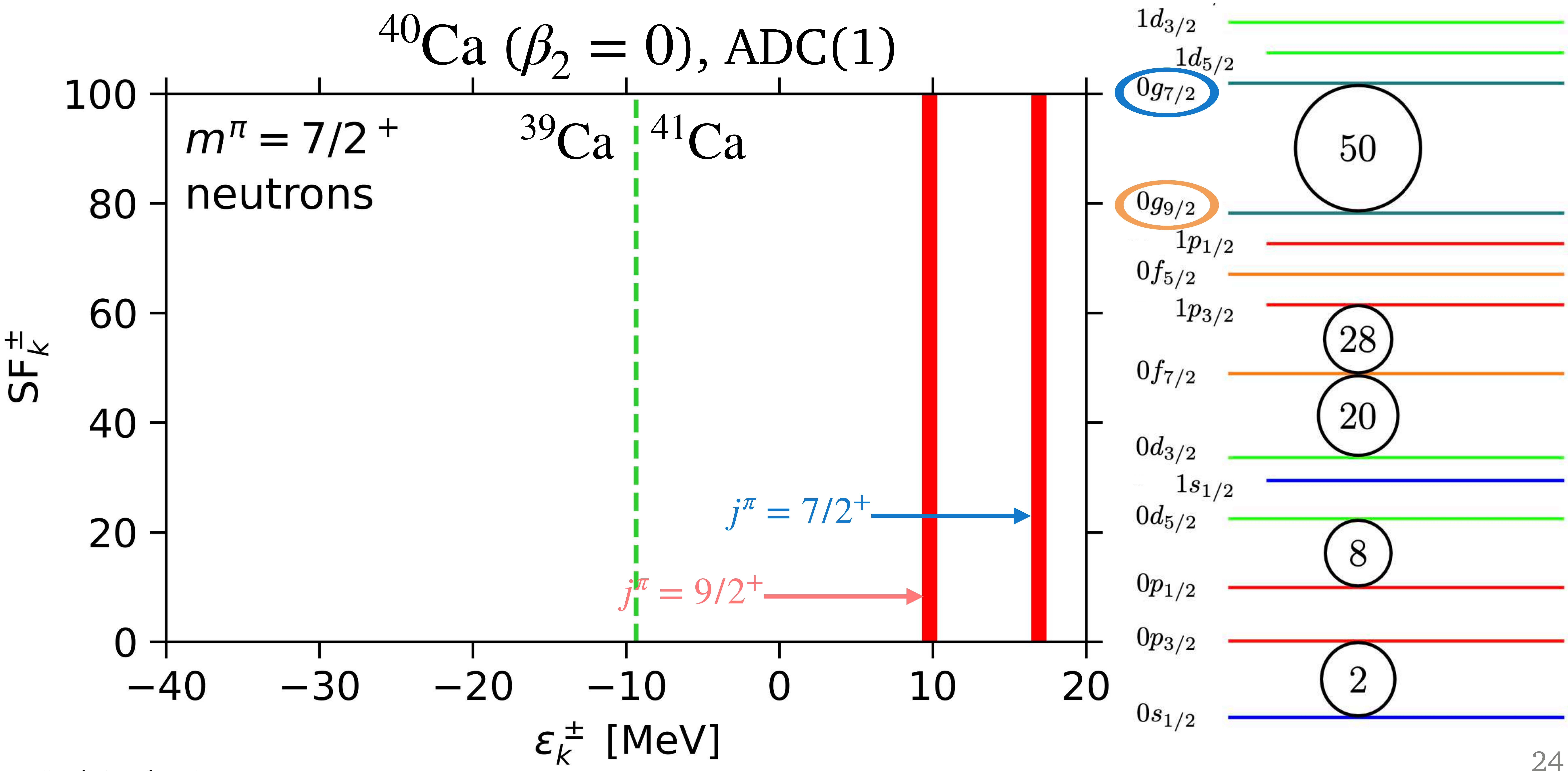
dDSCGF(2) results - Spectroscopic Amplitudes





[Scalesi *et al.* n°2]

dDSCGF(2) results - Spectroscopic Amplitudes



[Scalesi *et al.* n°2]

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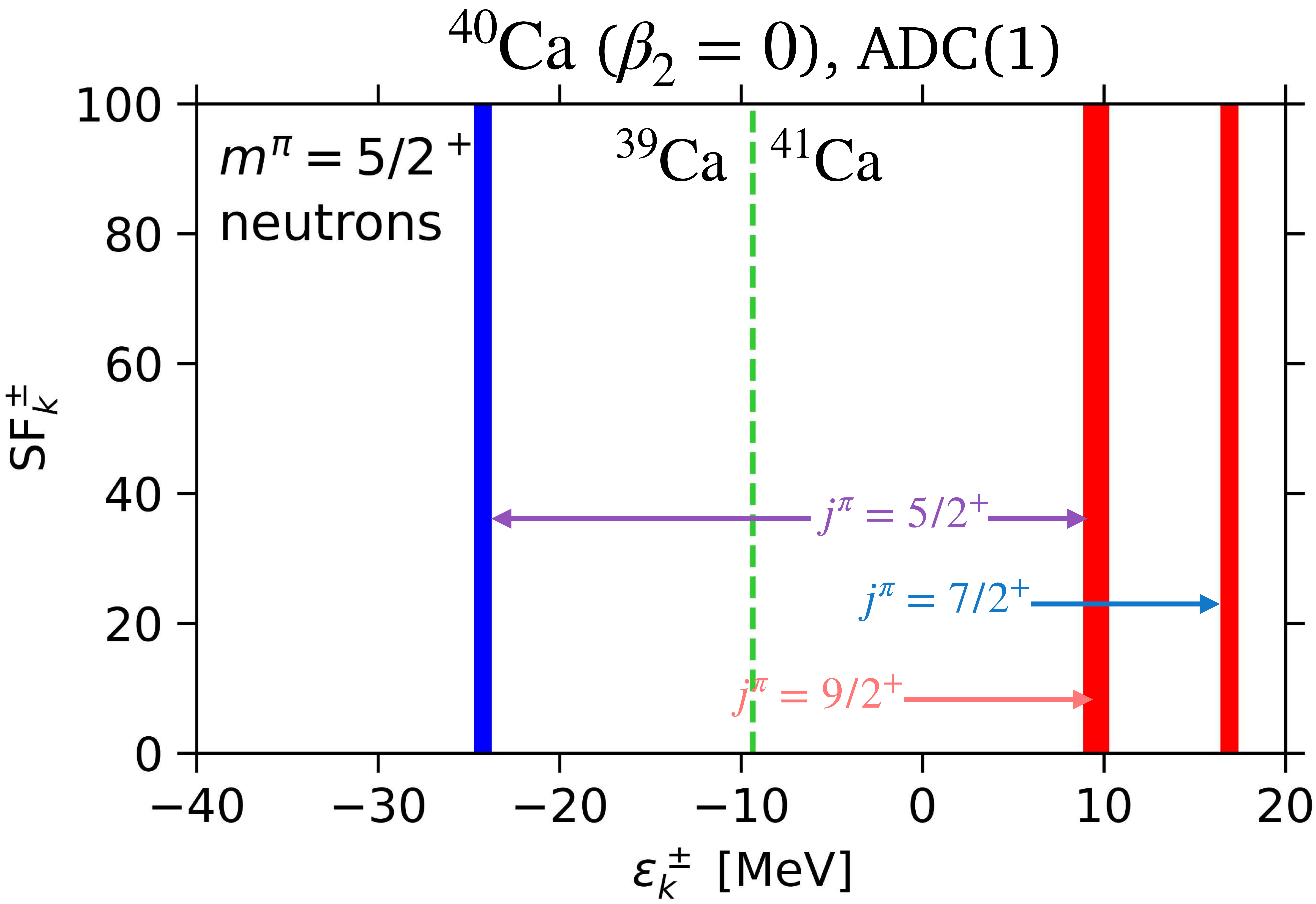

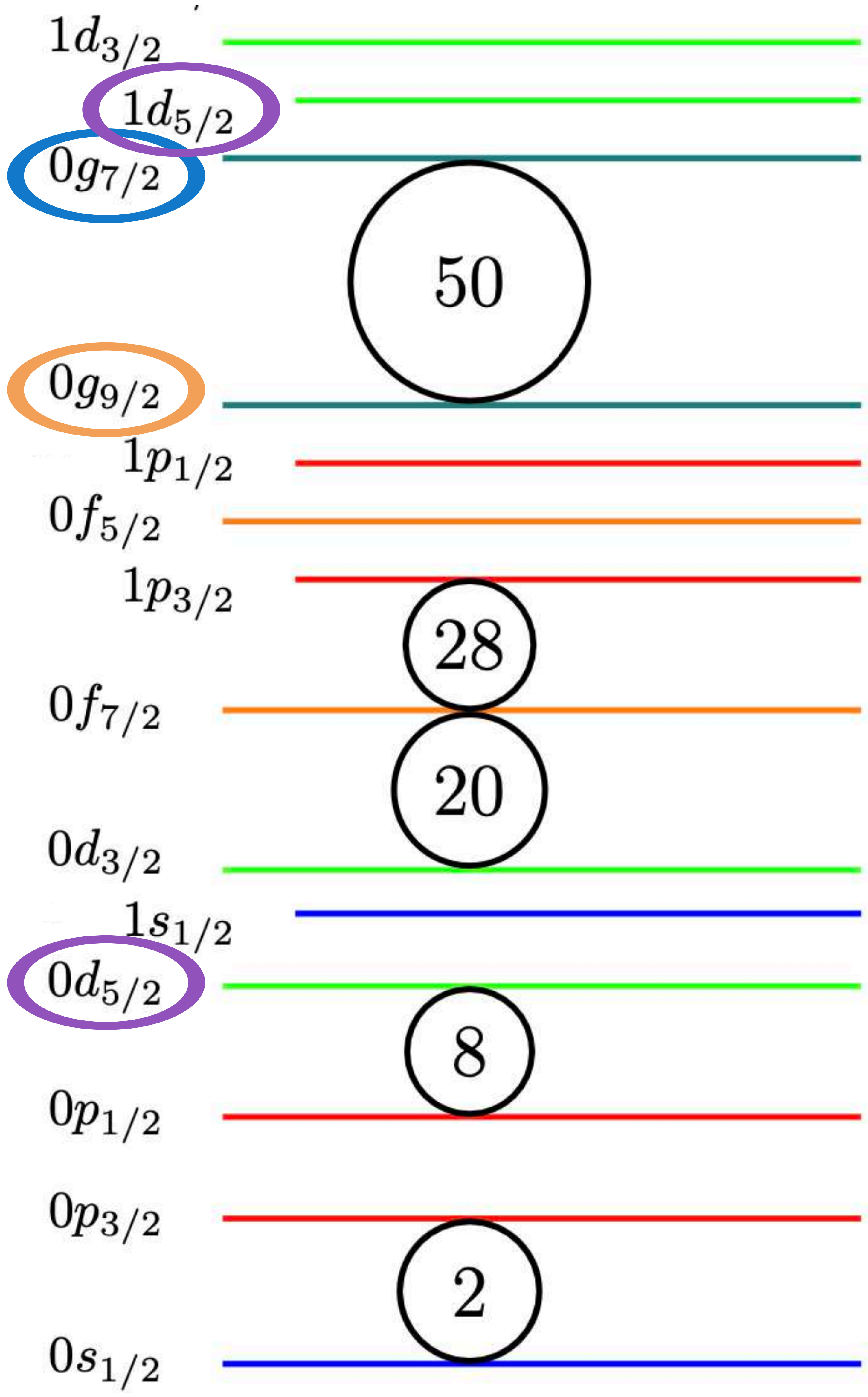

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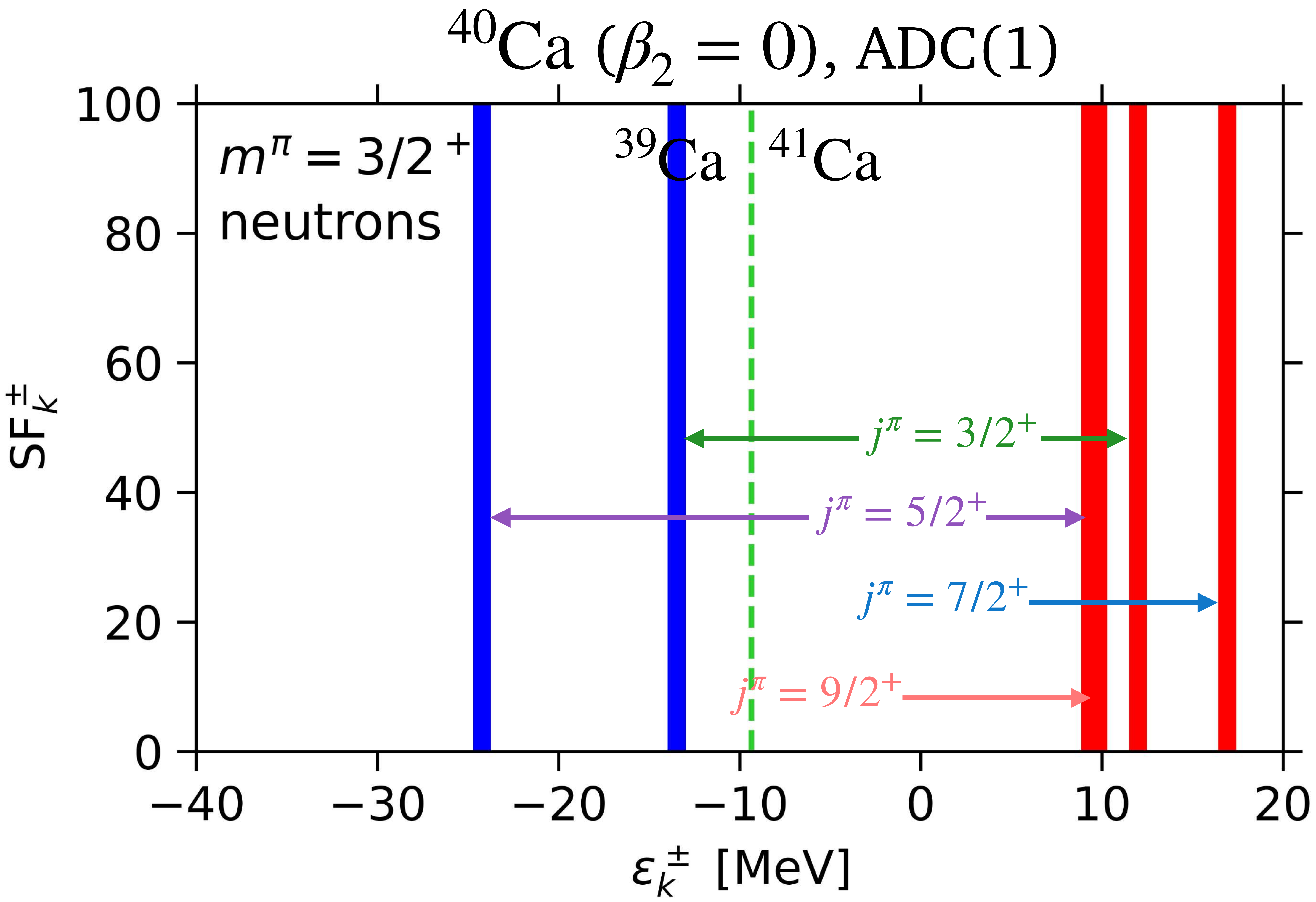

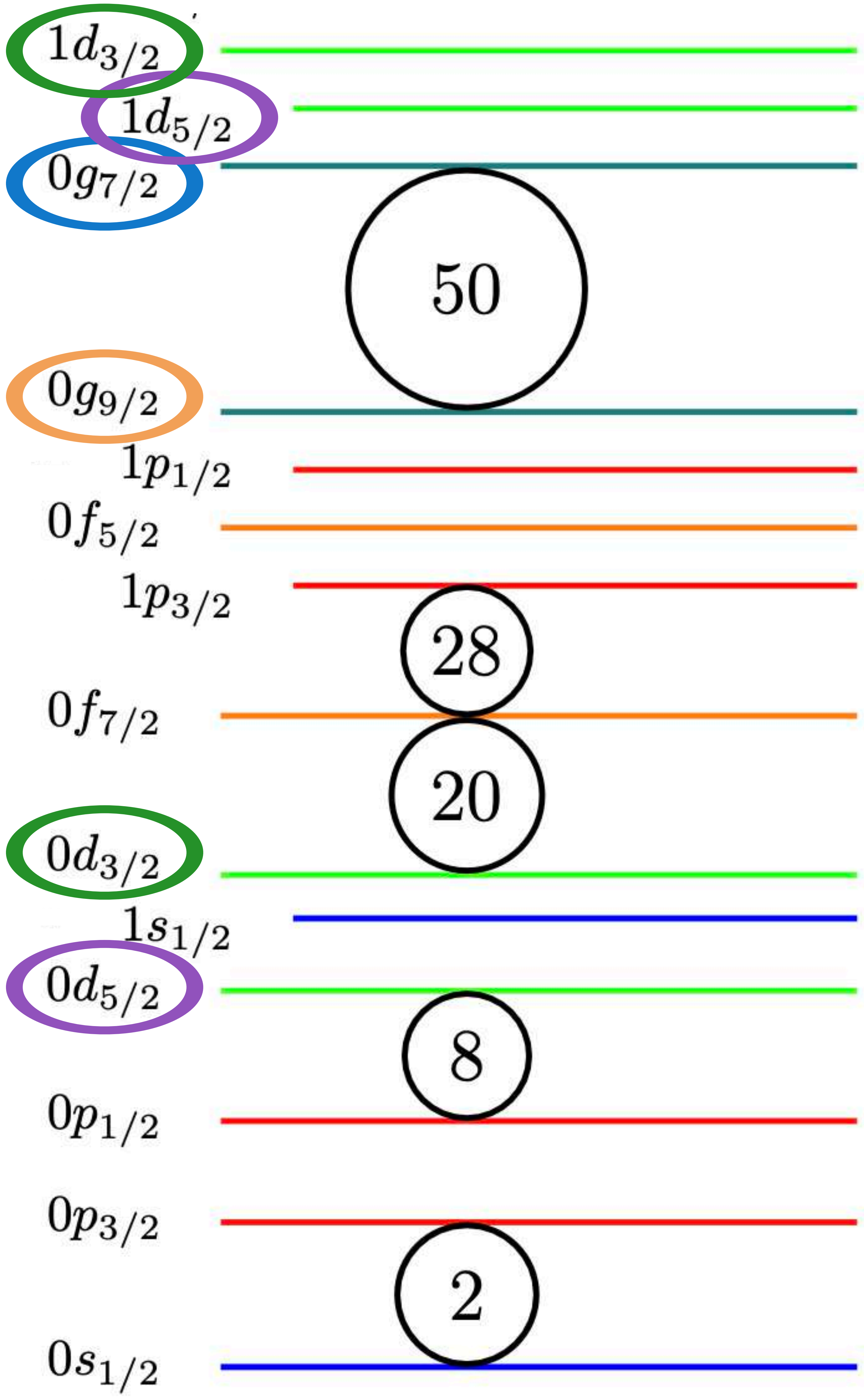

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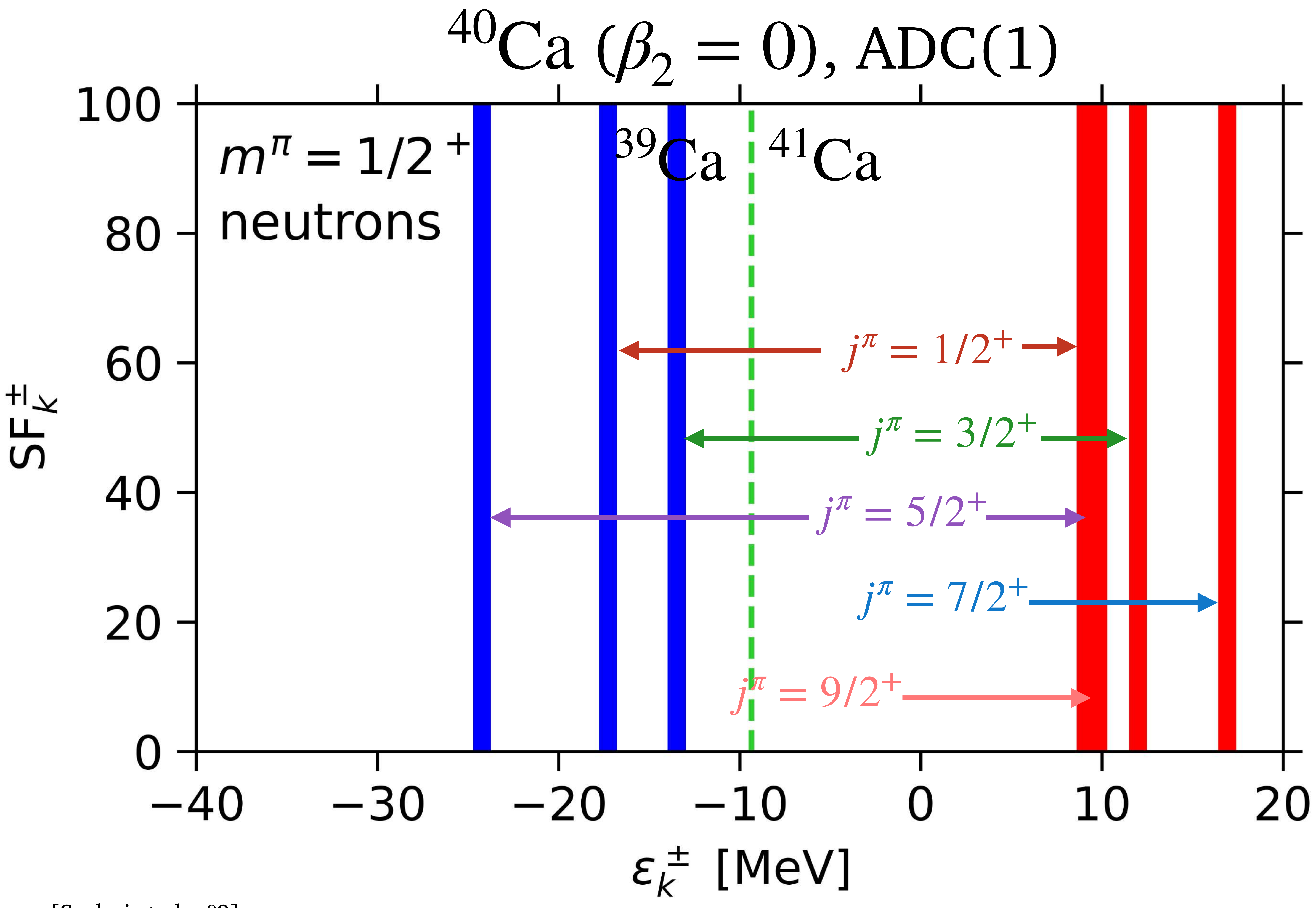
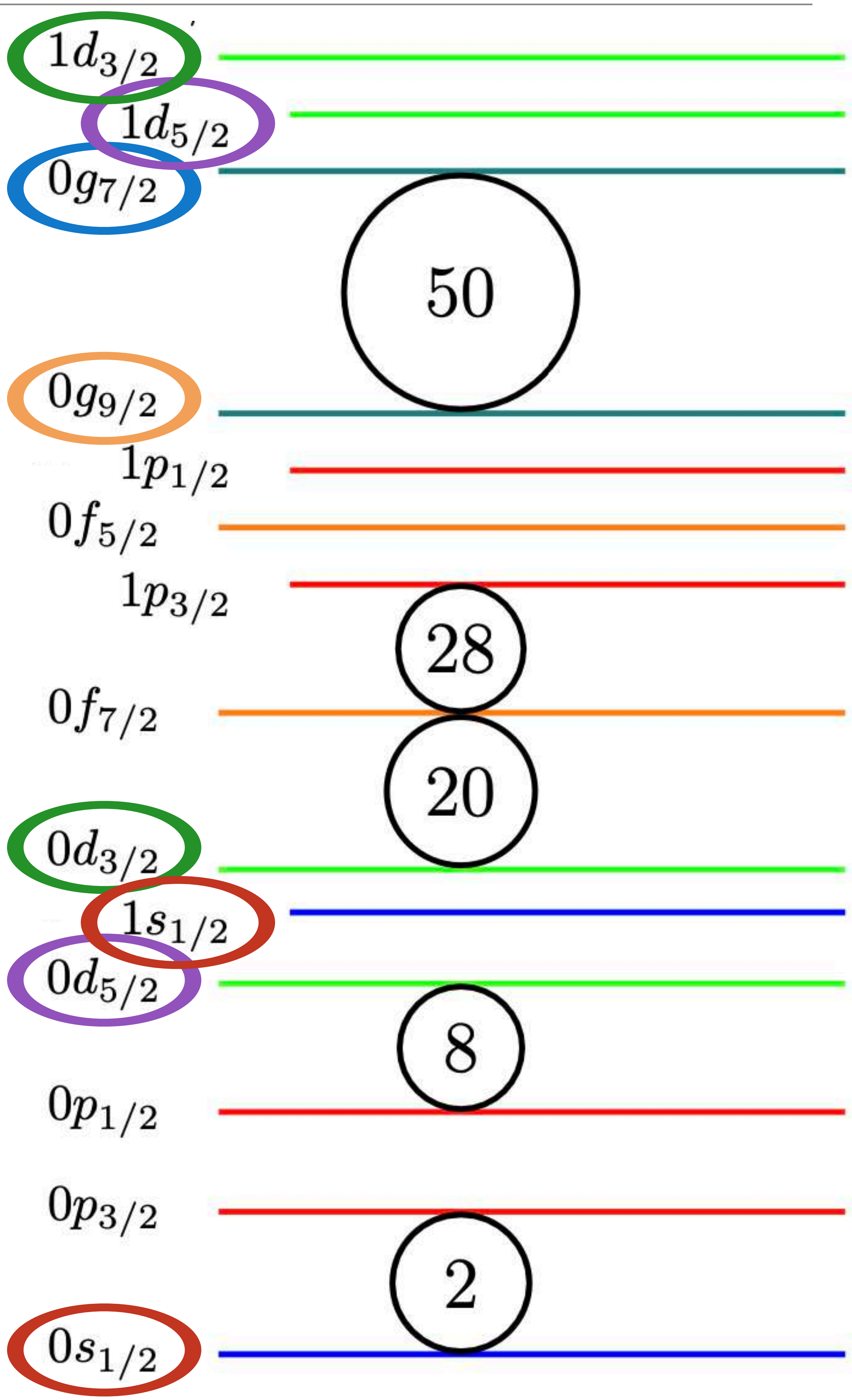
dDSCGF(2) results - Spectroscopic Amplitudes

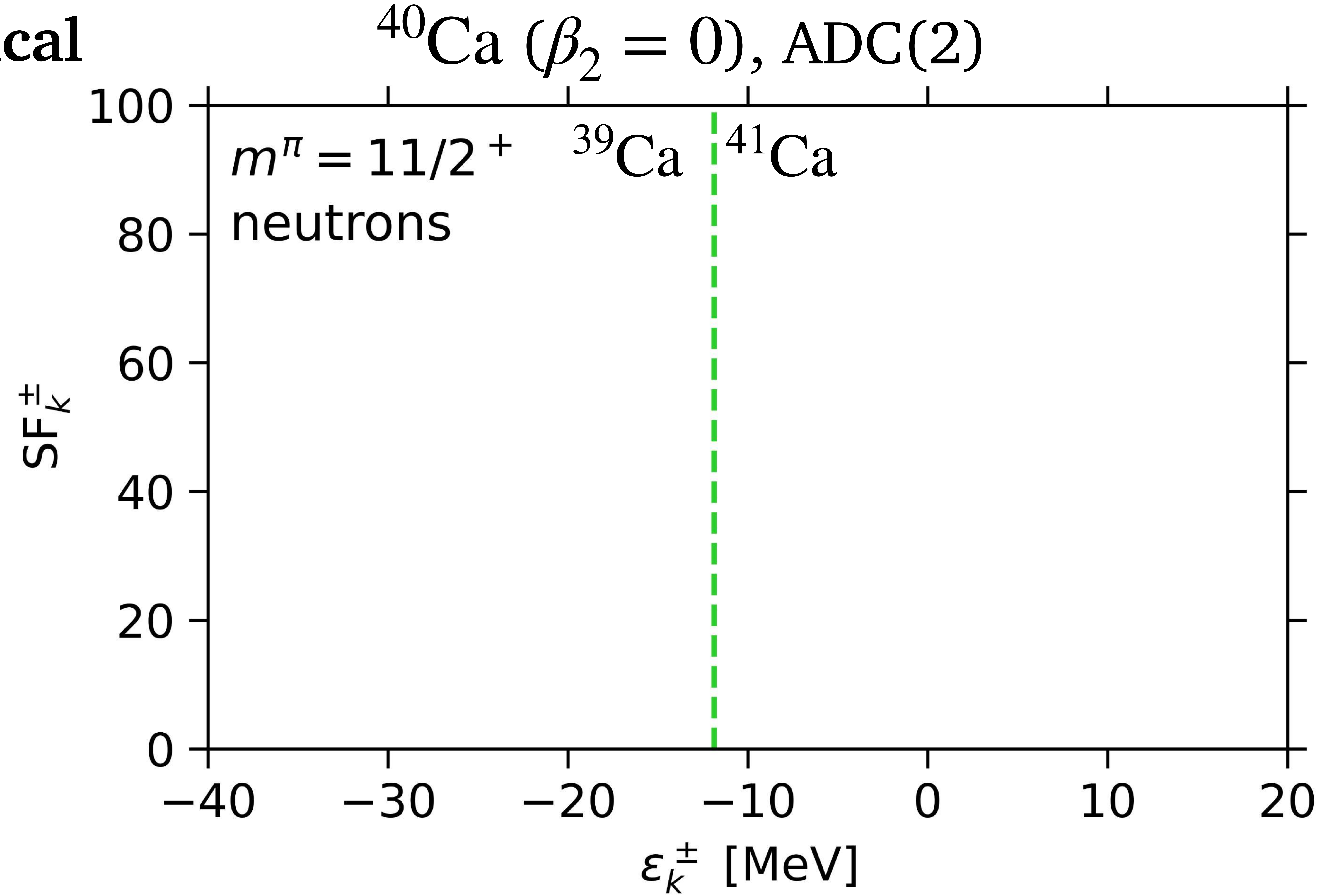




[Scalesi *et al.* n°2]

dDSCGF(2) results - Spectroscopic Amplitudes

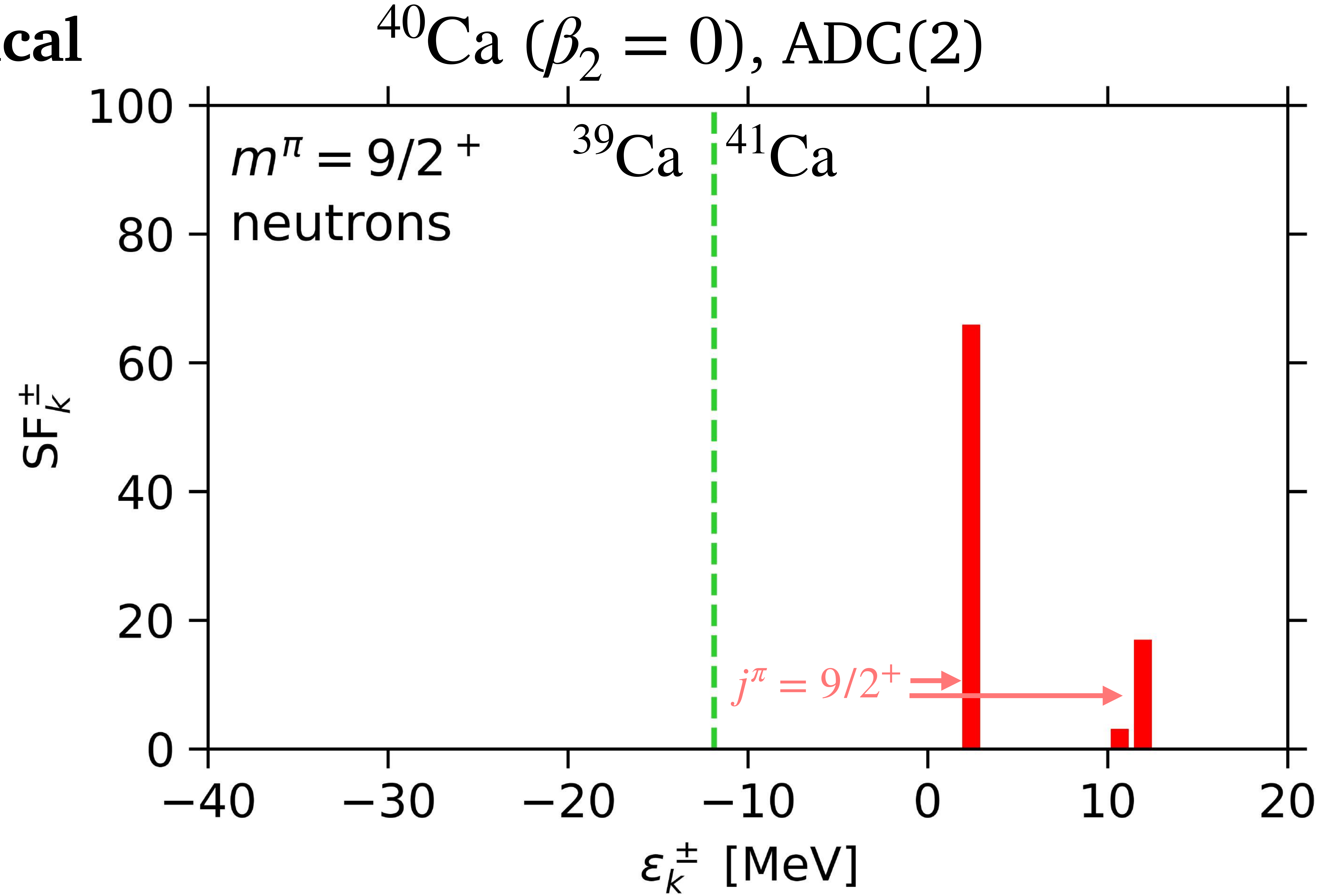
spherical



[Scalesi *et al.* n°2]

dDSCGF(2) results - Spectroscopic Amplitudes

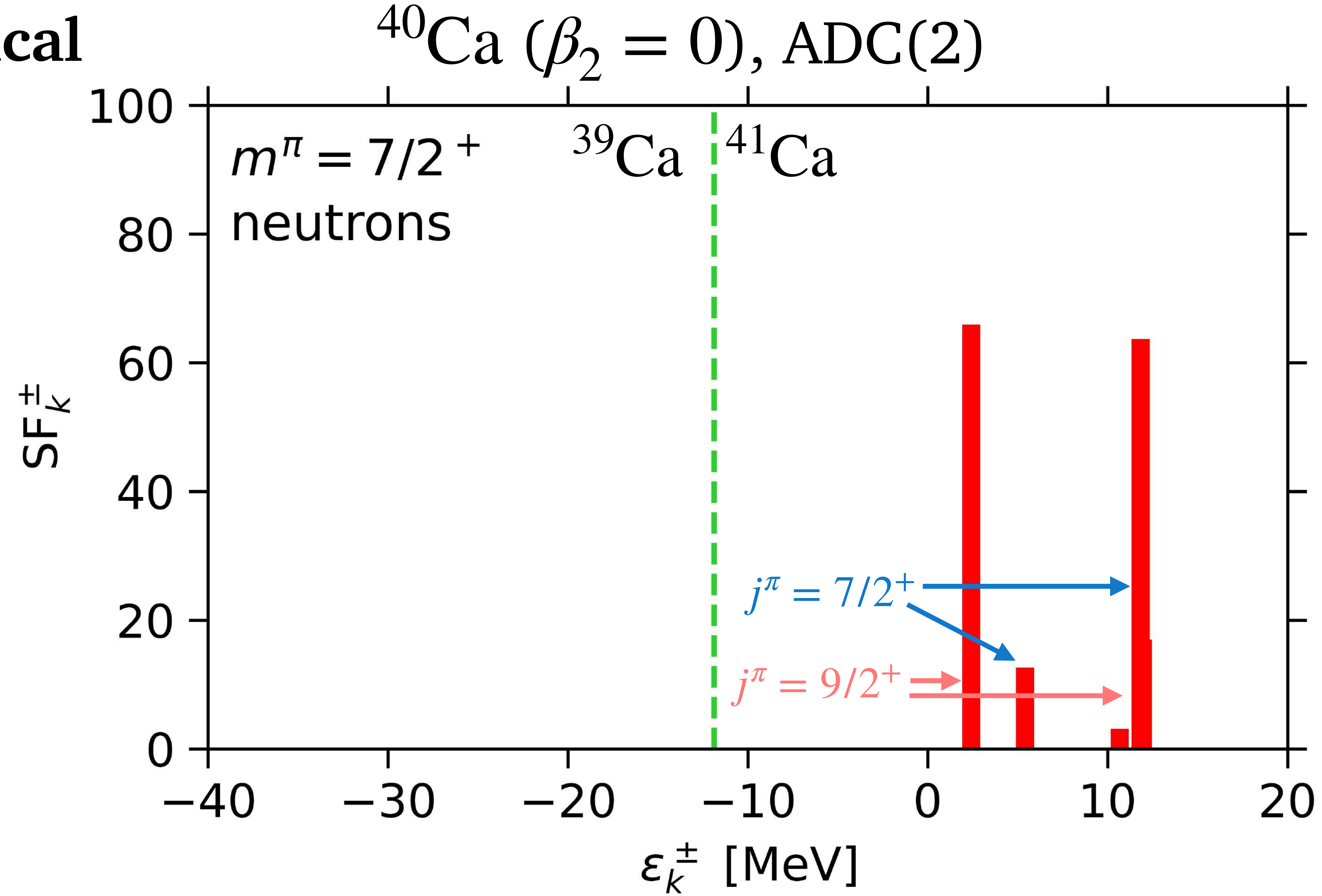
spherical



[Scalesi *et al.* n°2]

dDSCGF(2) results - Spectroscopic Amplitudes

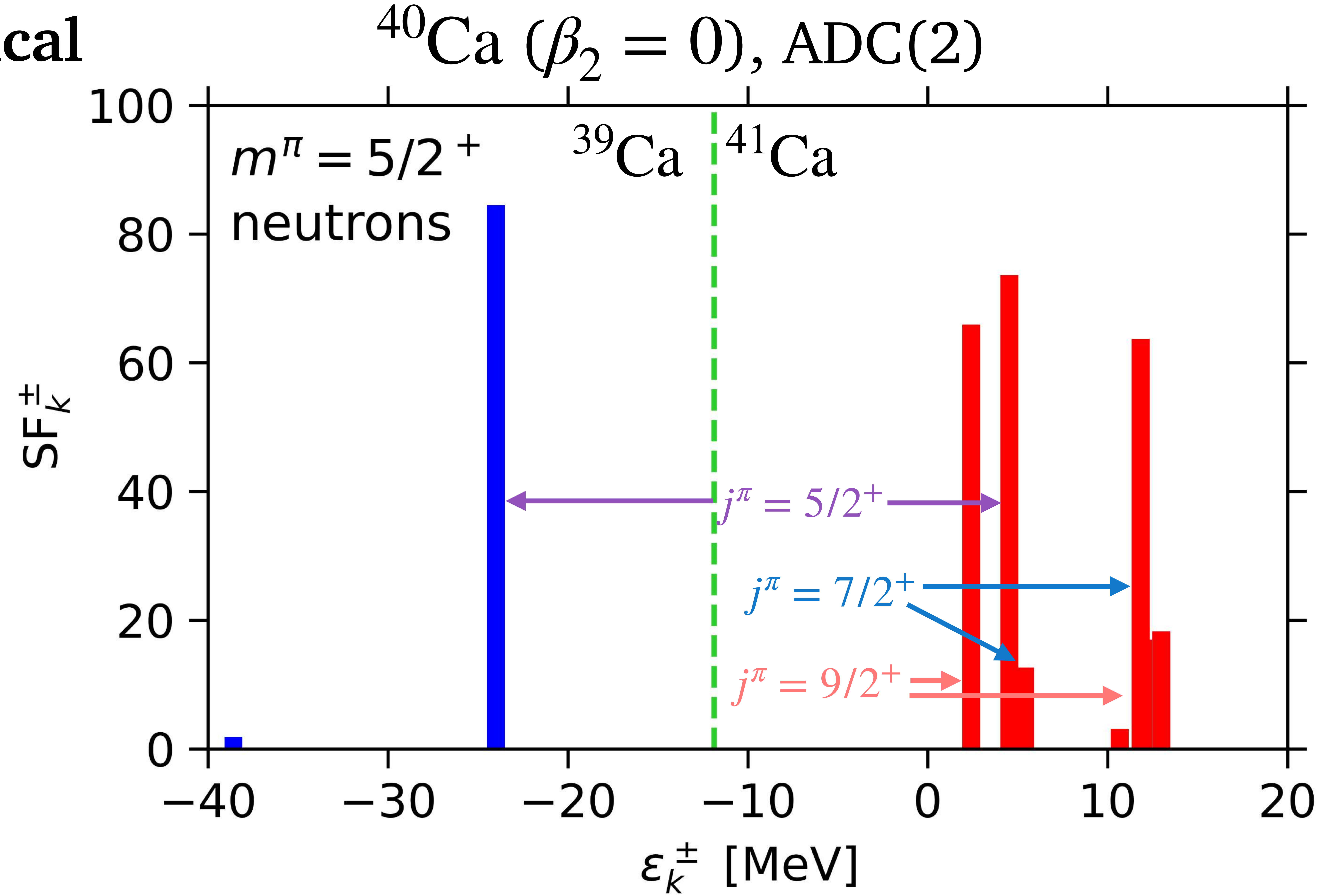
spherical



[Scalesi *et al.* n°2]

dDSCGF(2) results - Spectroscopic Amplitudes

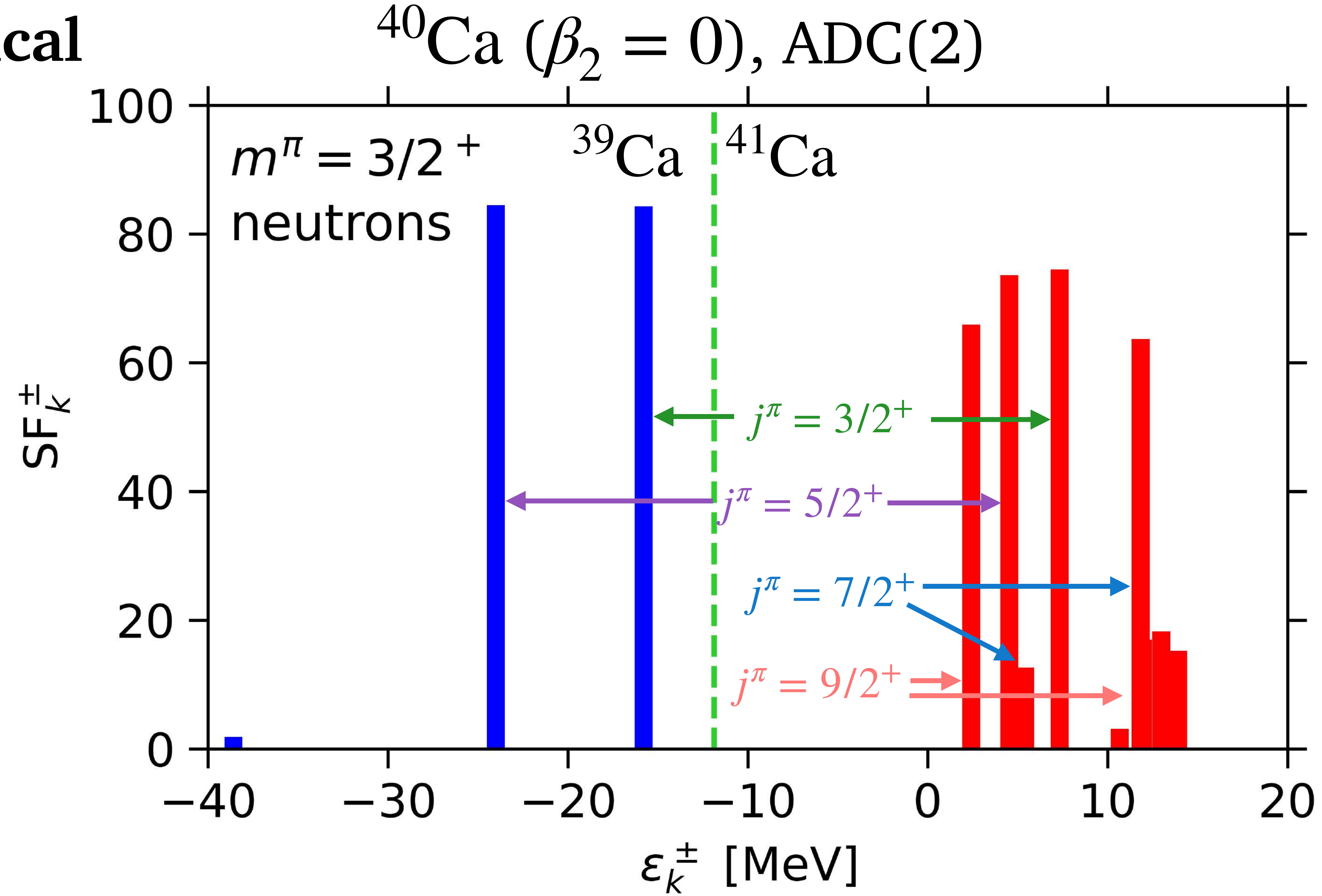
spherical



[Scalesi *et al.* n°2]

dDSCGF(2) results - Spectroscopic Amplitudes

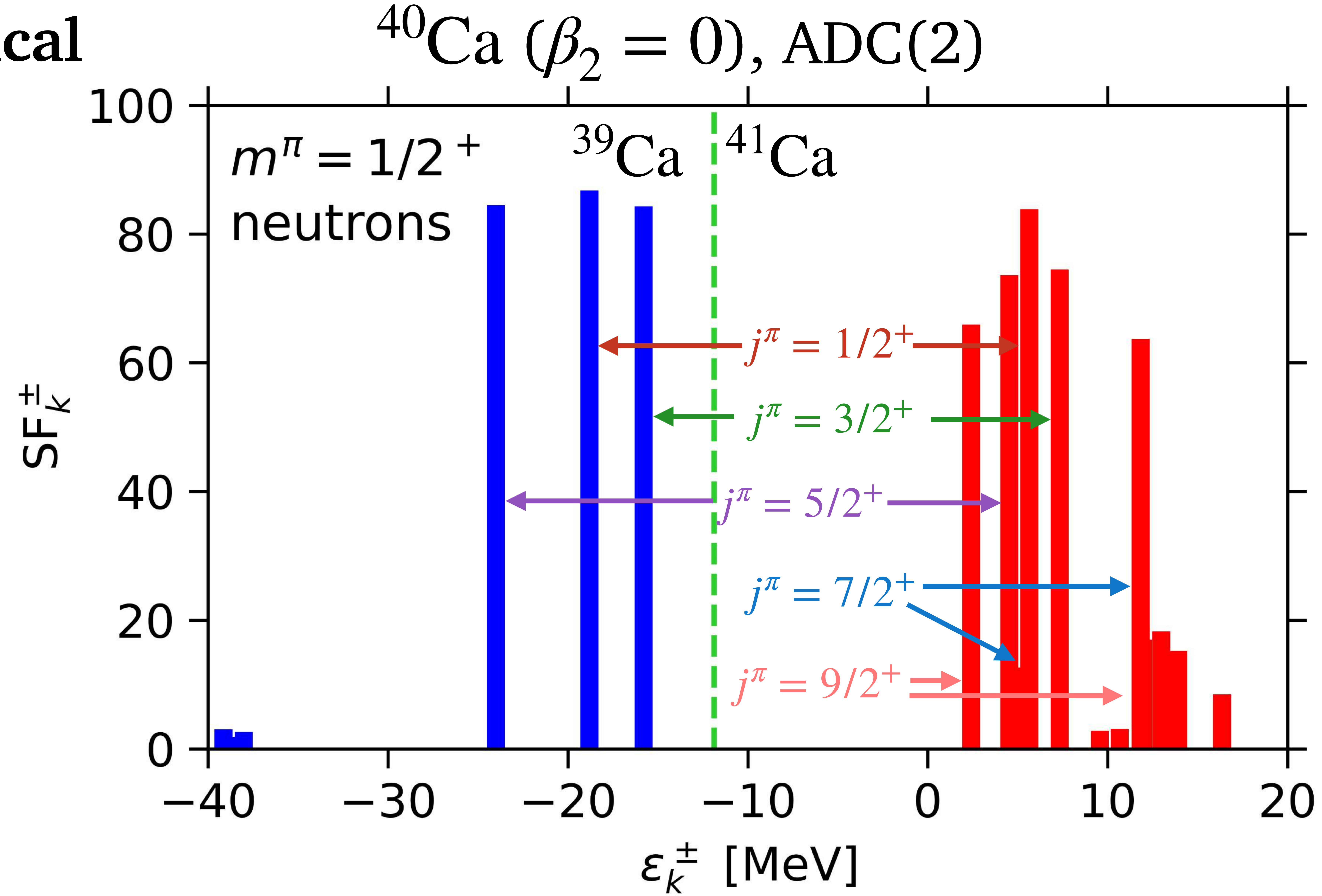
spherical



[Scalesi *et al.* n°2]

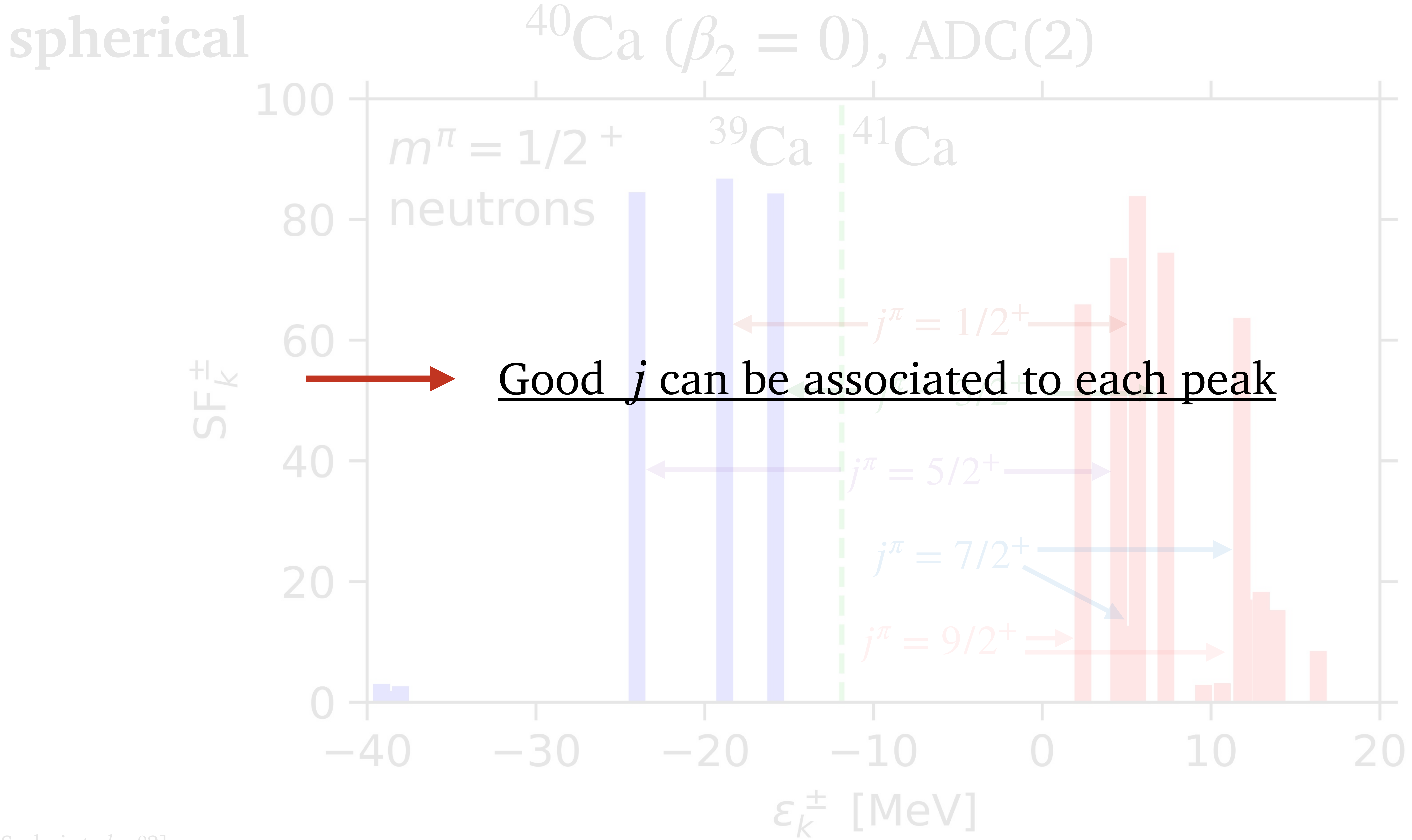
dDSCGF(2) results - Spectroscopic Amplitudes

spherical



[Scalesi *et al.* n°2]

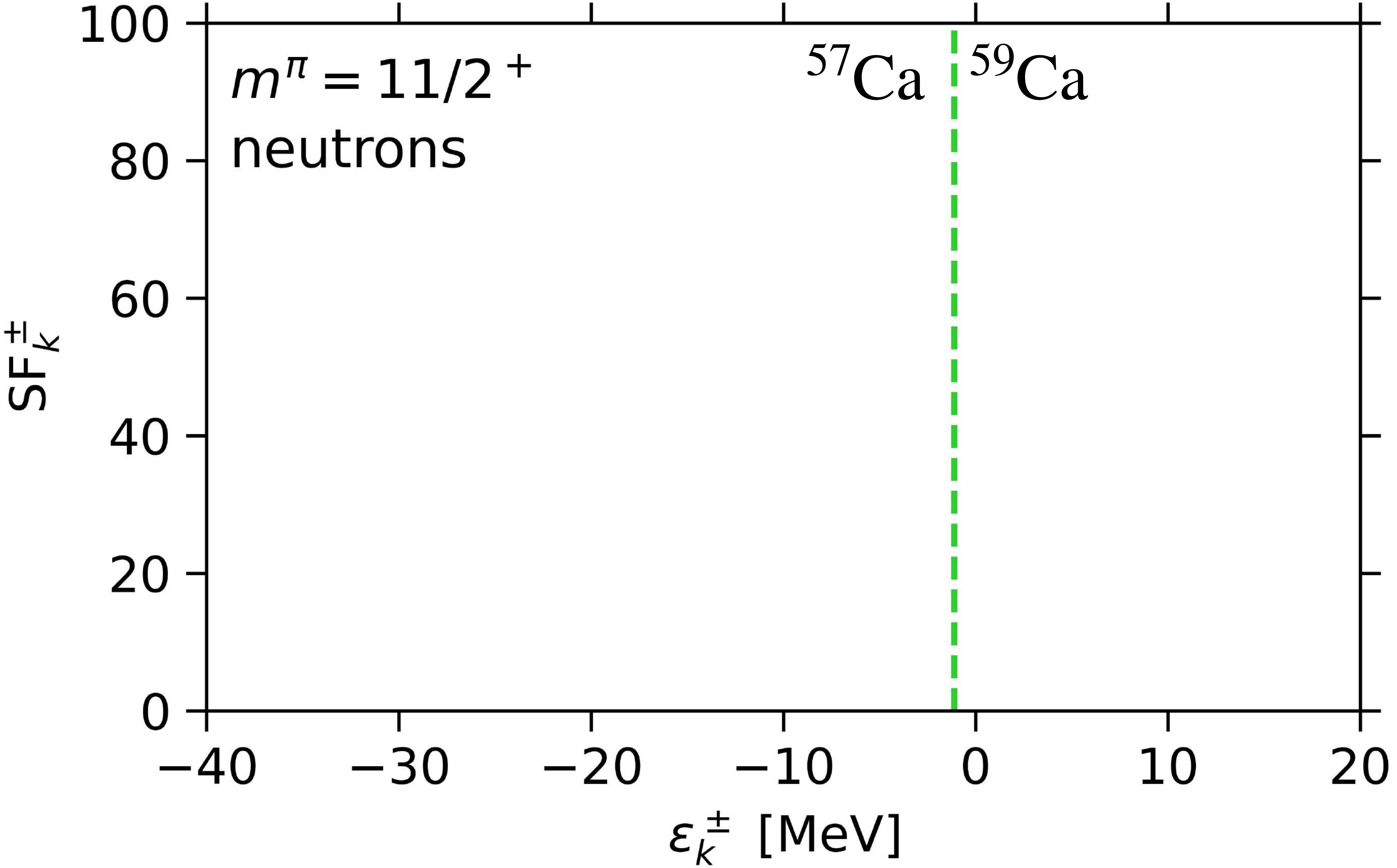
dDSCGF(2) results - Spectroscopic Amplitudes



Good j can be associated to each peak

[Scalesi *et al.* n°2]

weakly deformed ^{58}Ca ($\beta_2 = -0.03$), ADC(2)



[Scalesi *et al.* n°2]

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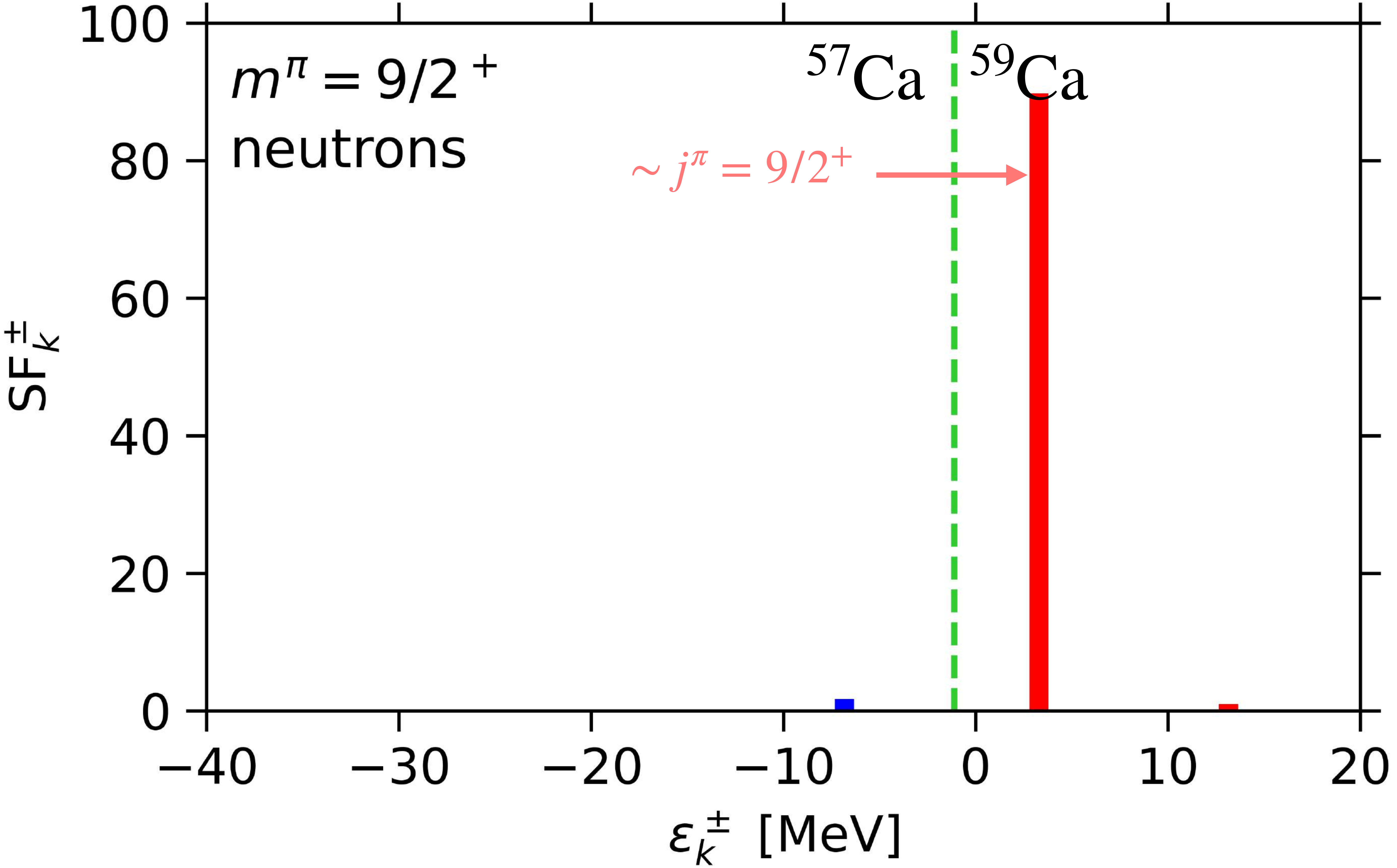
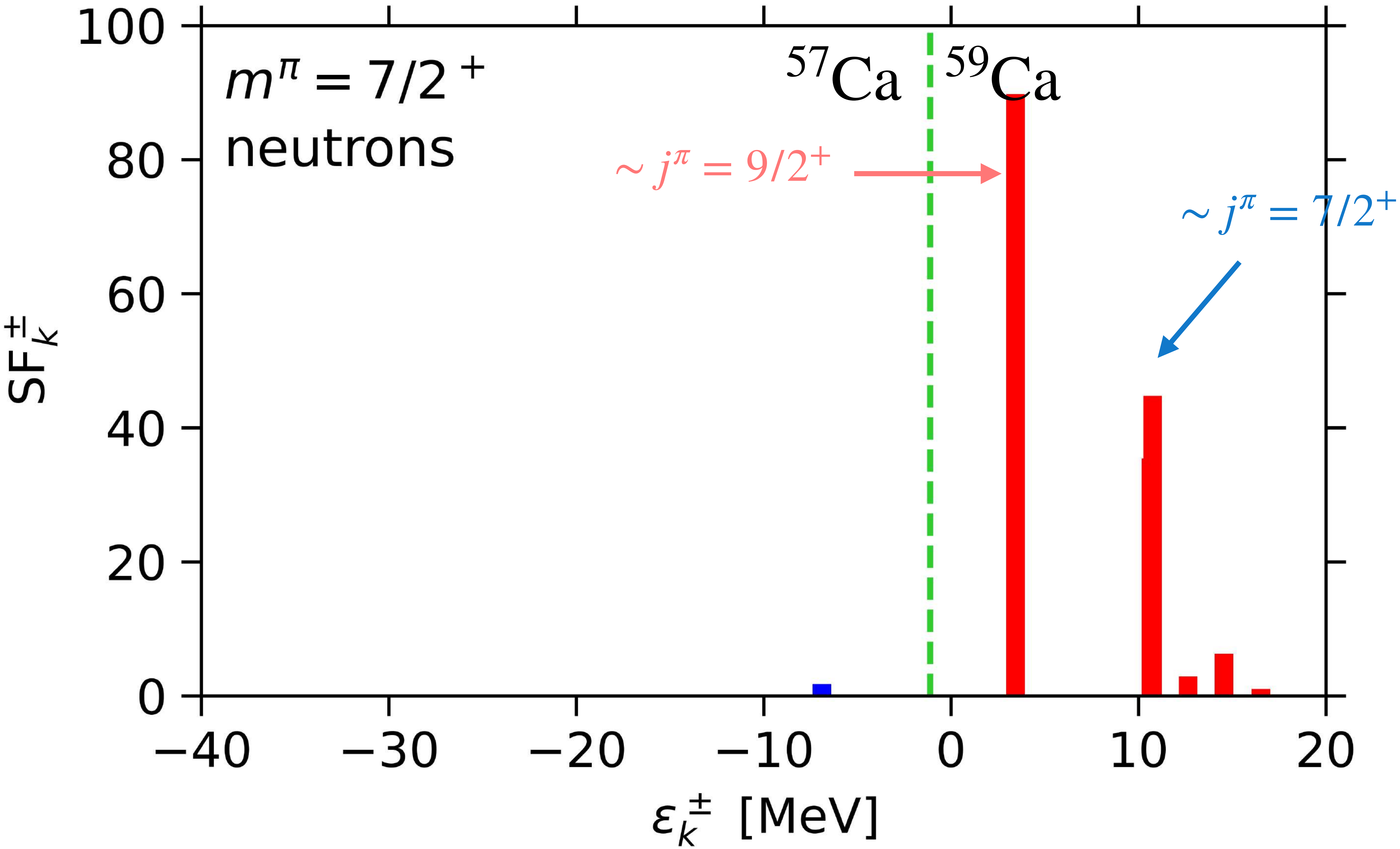


[Scalesi *et al.* n°2]

dDSCGF(2) results - Spectroscopic Amplitudes

weakly deformed $^{58}\mathrm{Ca}\ (\beta_2 = -0.03)$, ADC(2)



[Scalesi *et al.* n°2]

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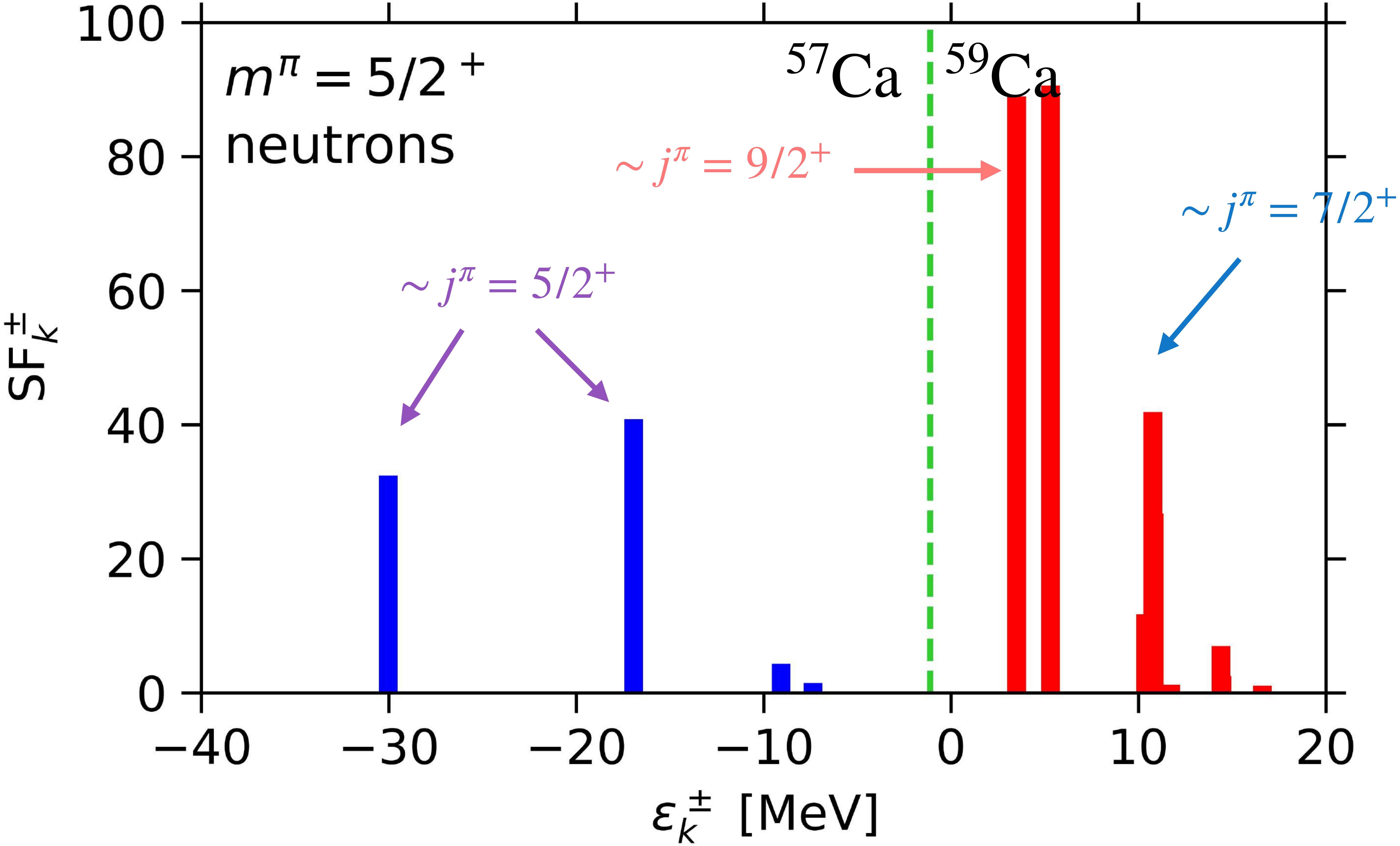

[Scalesi *et al.* n°2]

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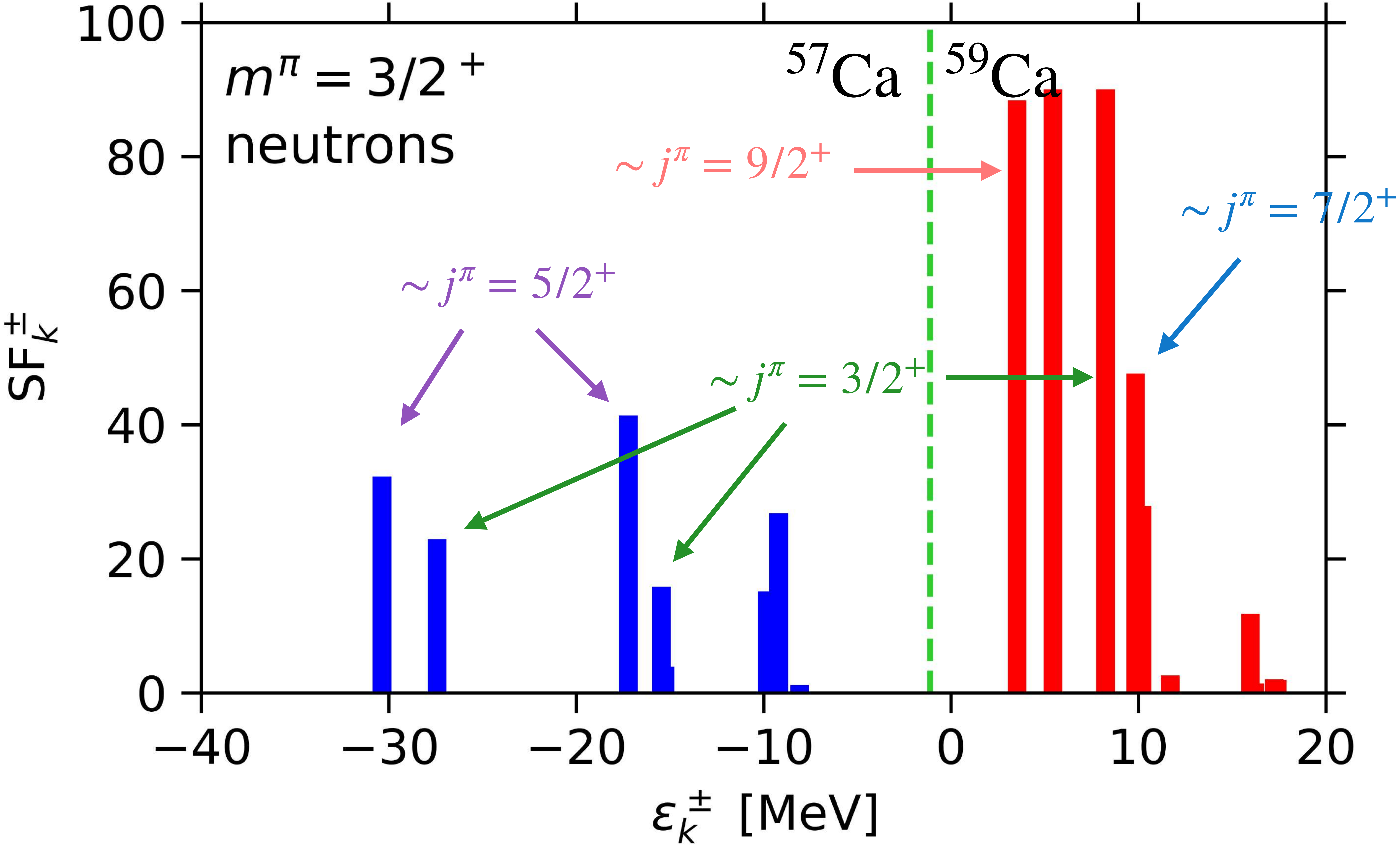

[Scalesi *et al.* n°2]

dDSCGF(2) results - Spectroscopic Amplitudes

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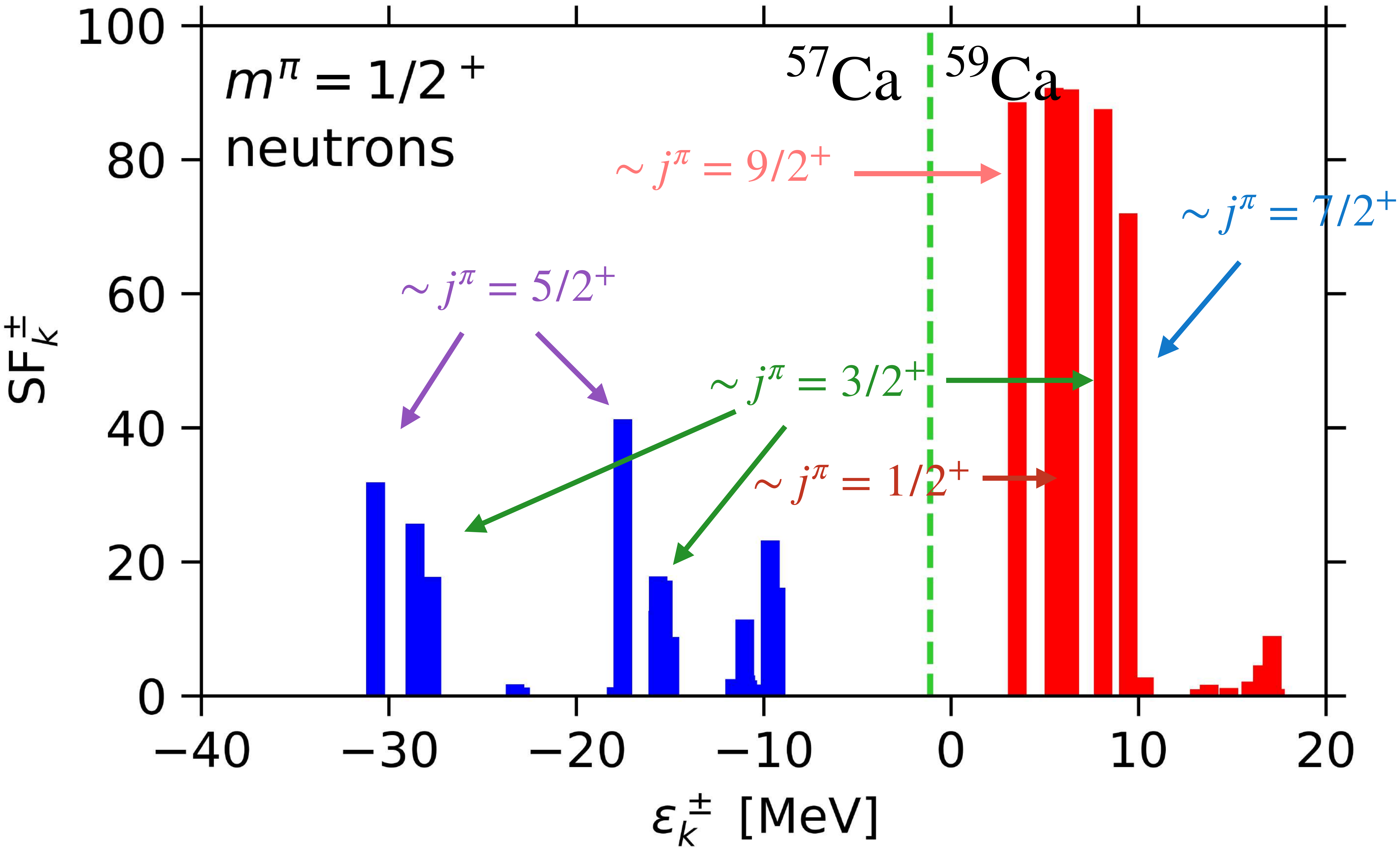
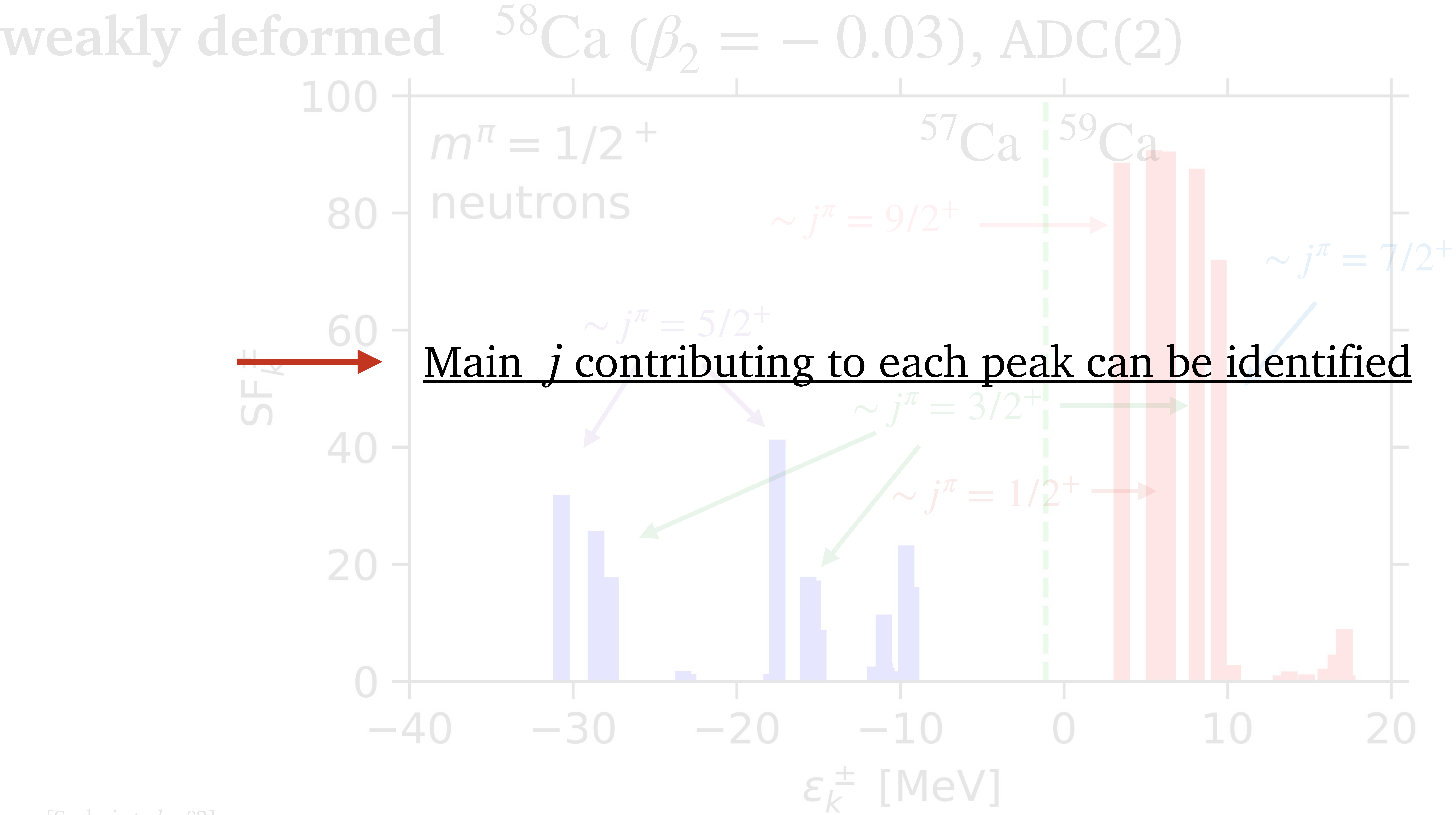


[Scalesi *et al.* n°2]

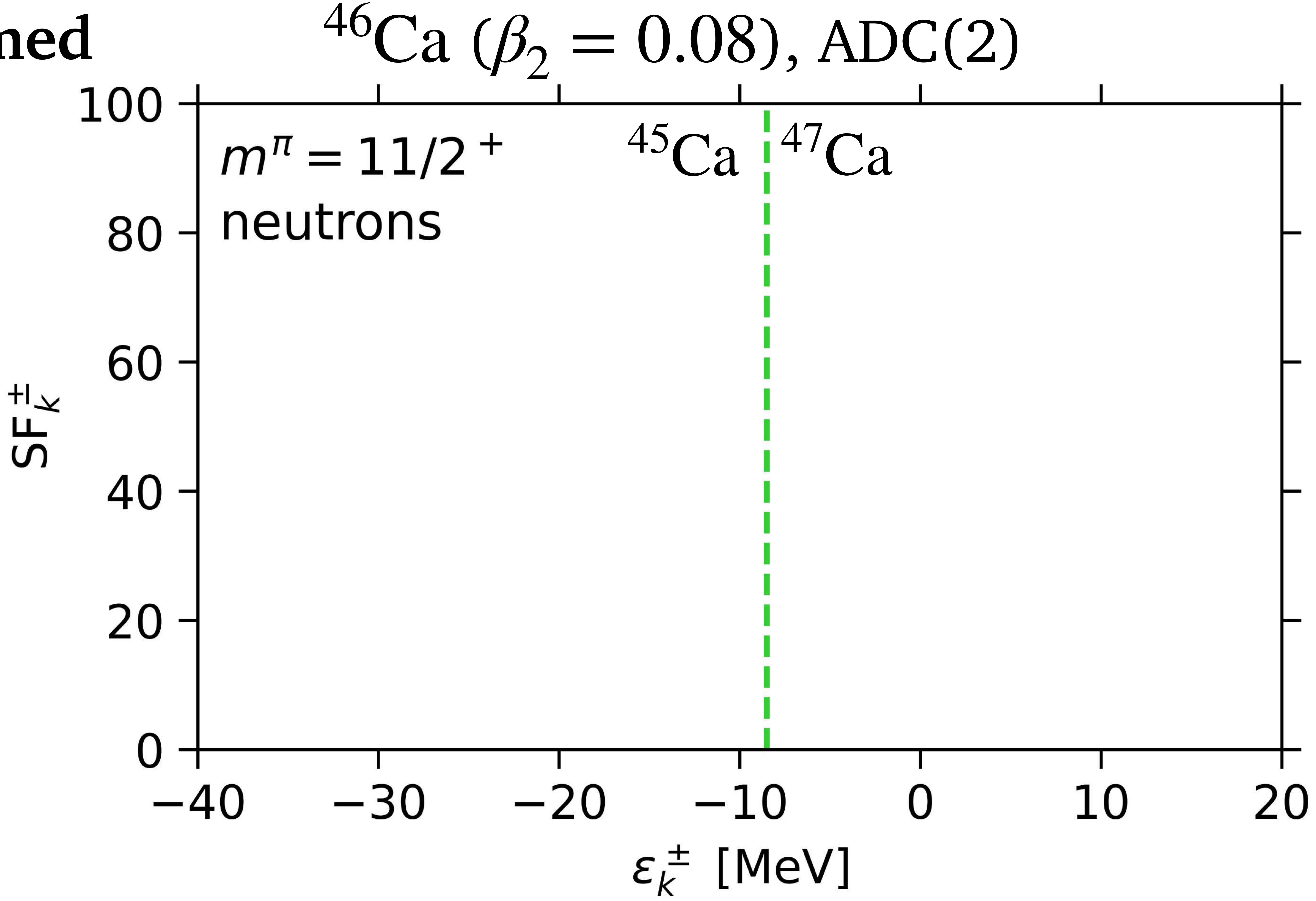
dDSCGF(2) results - Spectroscopic Amplitudes



Main j contributing to each peak can be identified

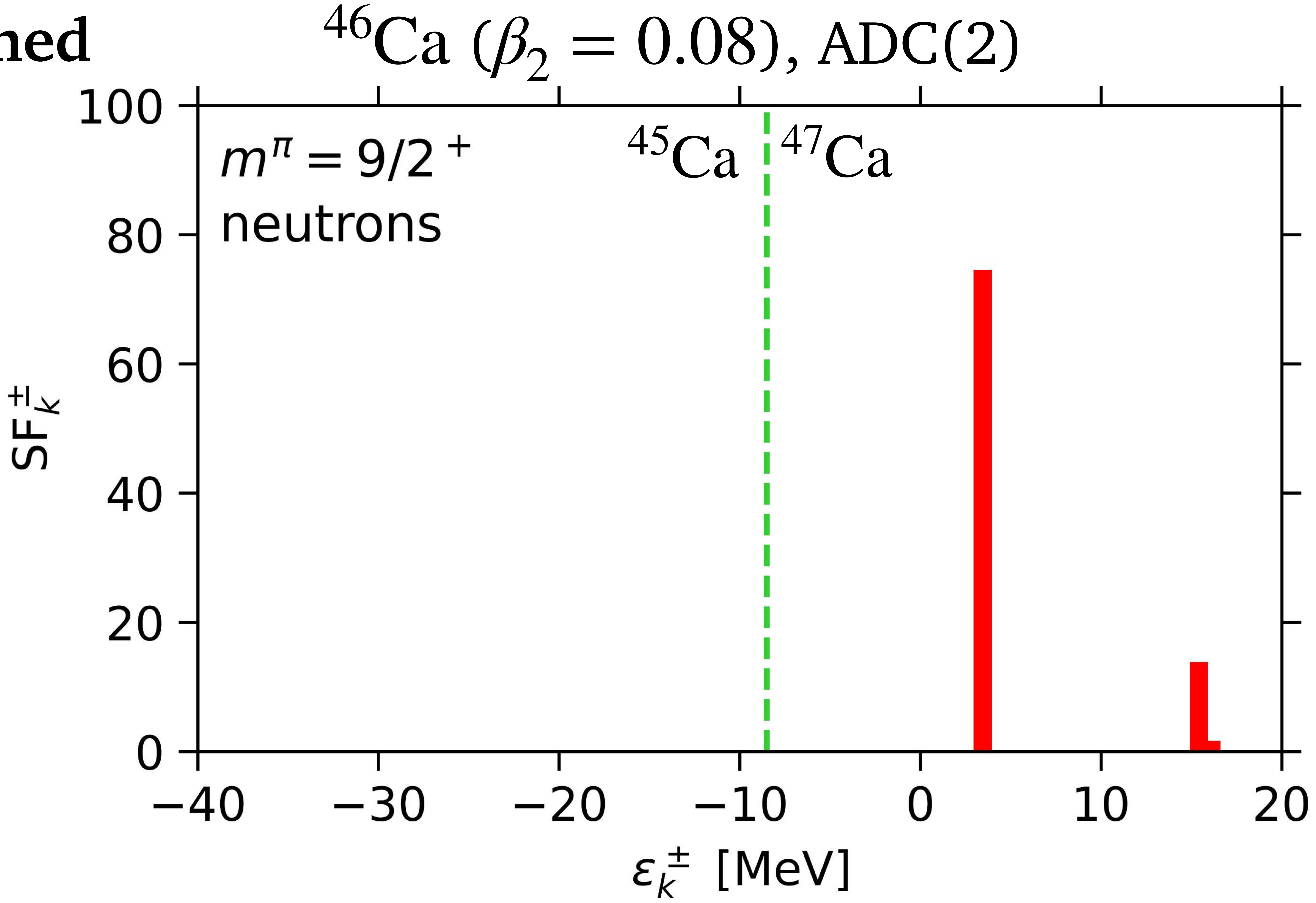
[Scalesi *et al.* n°2]

deformed



[Scalesi *et al.* n°2]

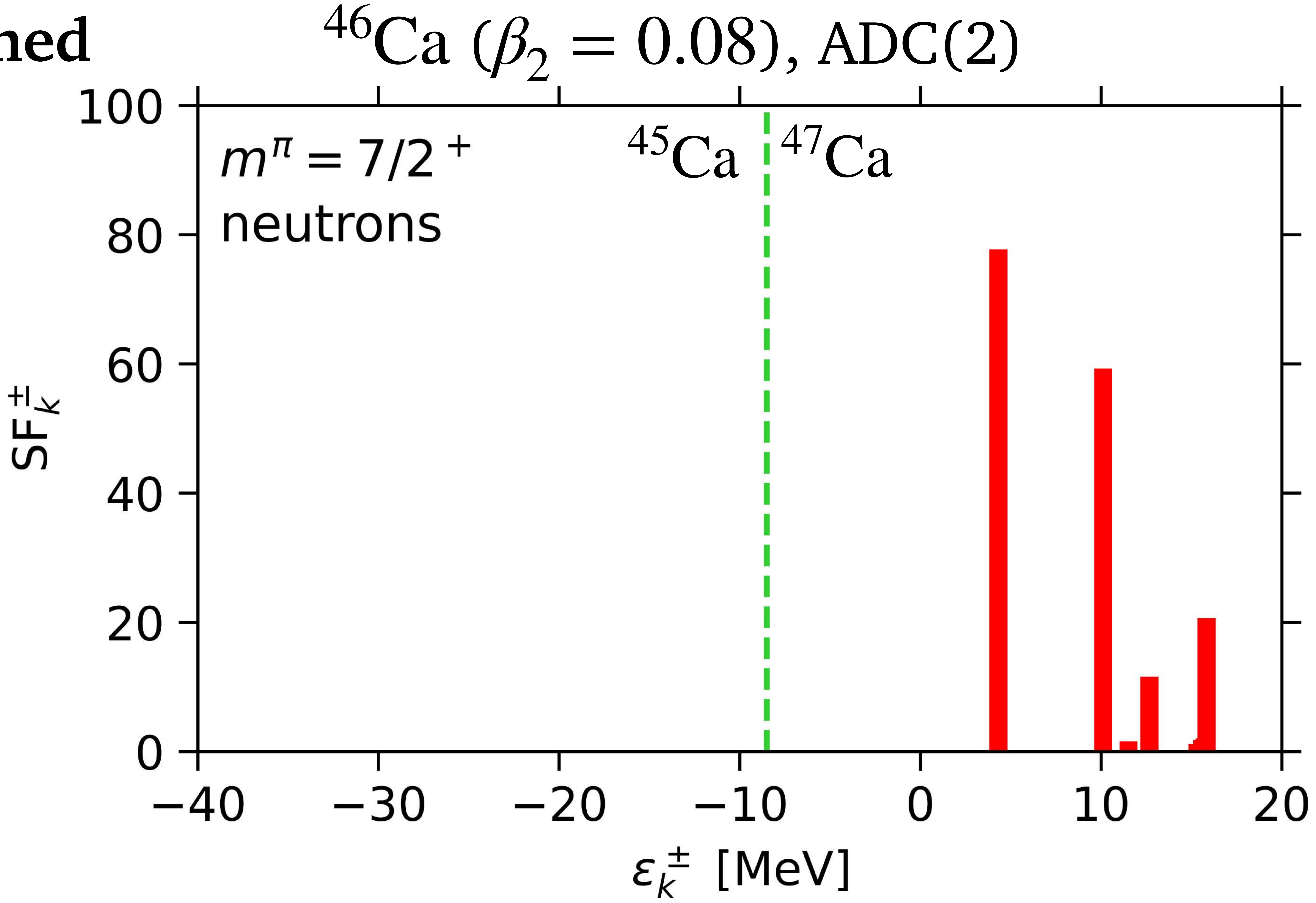
deformed



[Scalesi *et al.* n°2]

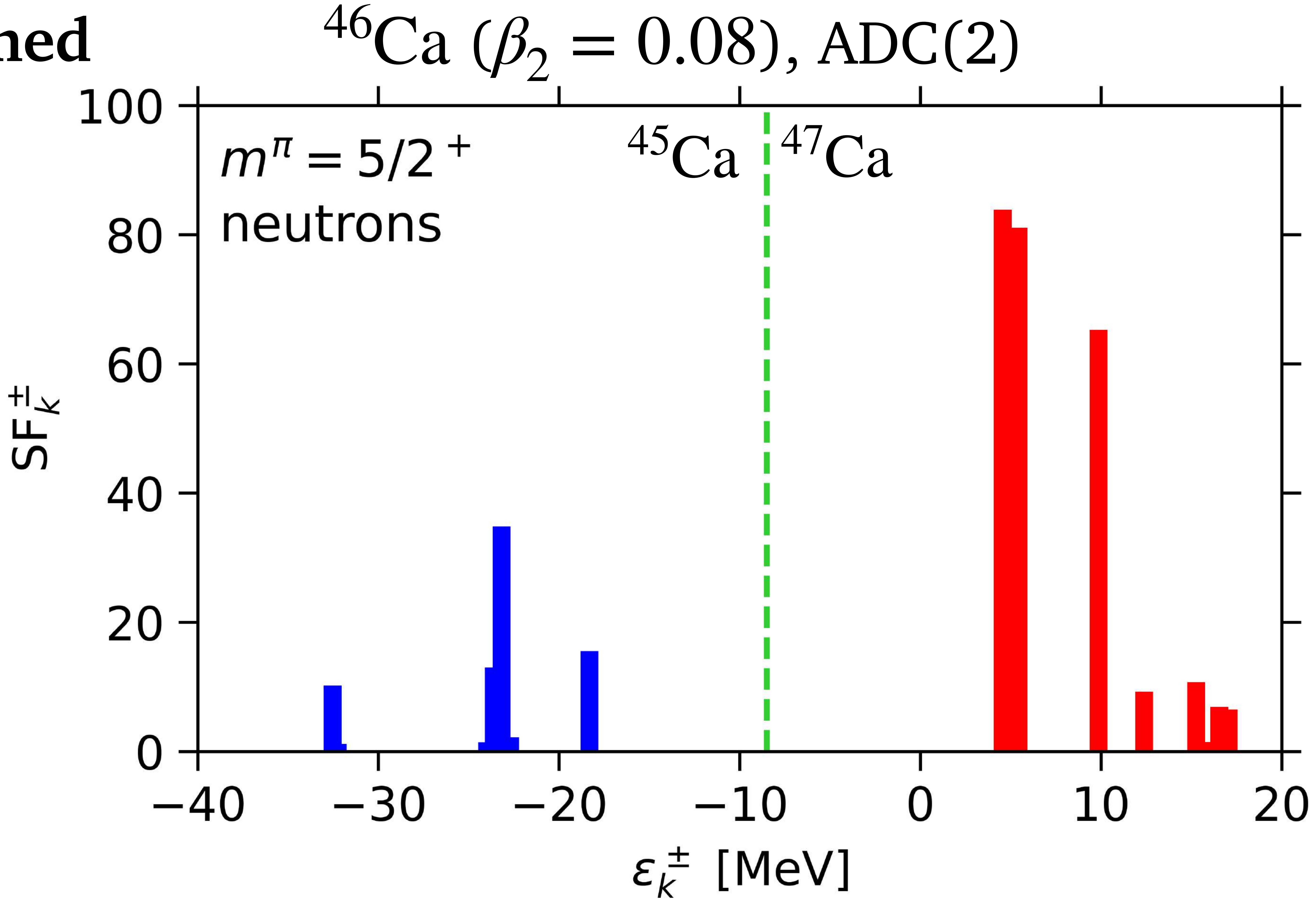
dDSCGF(2) results - Spectroscopic Amplitudes

deformed



[Scalesi *et al.* n°2]

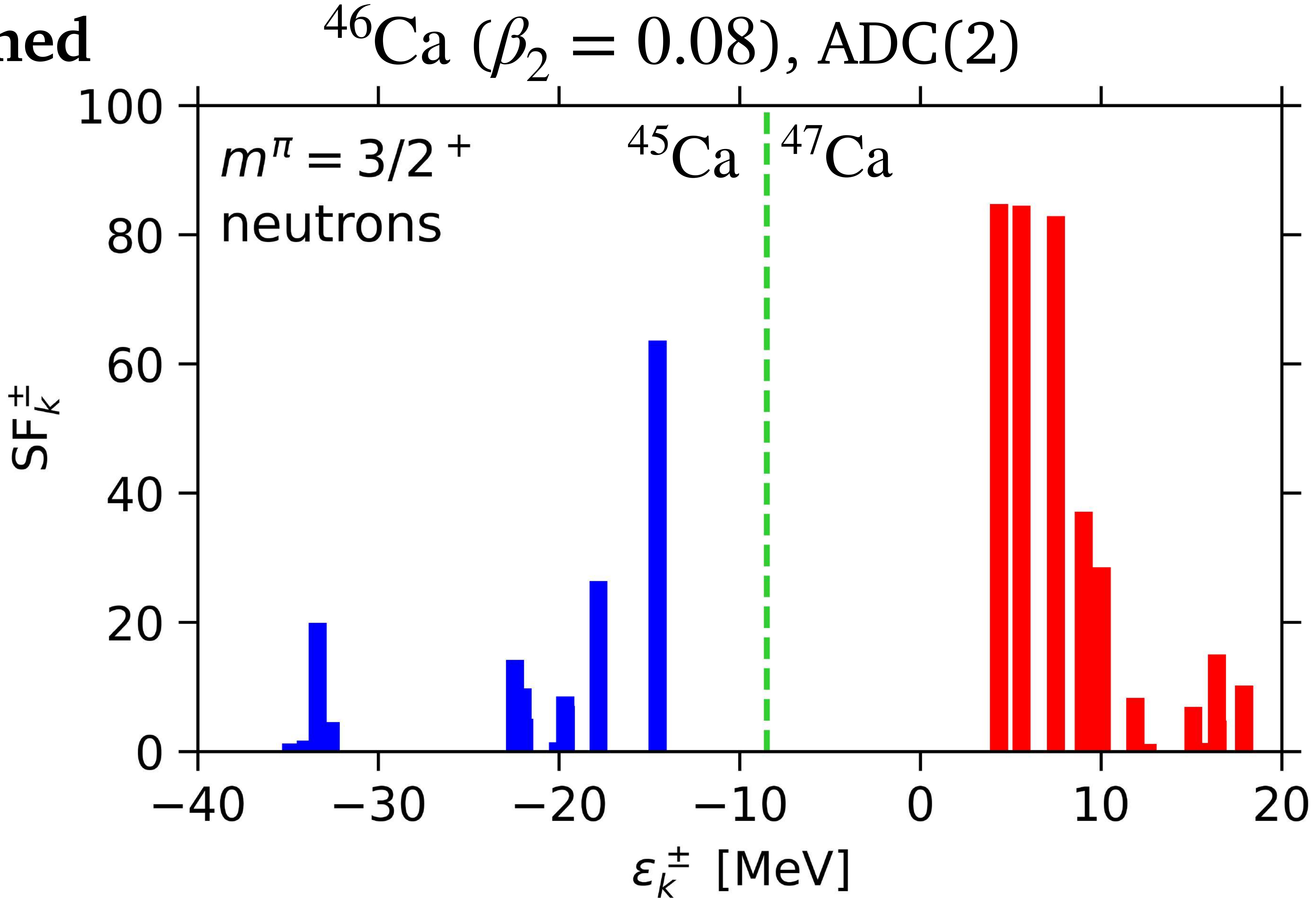
deformed



[Scalesi *et al.* n°2]

dDSCGF(2) results - Spectroscopic Amplitudes

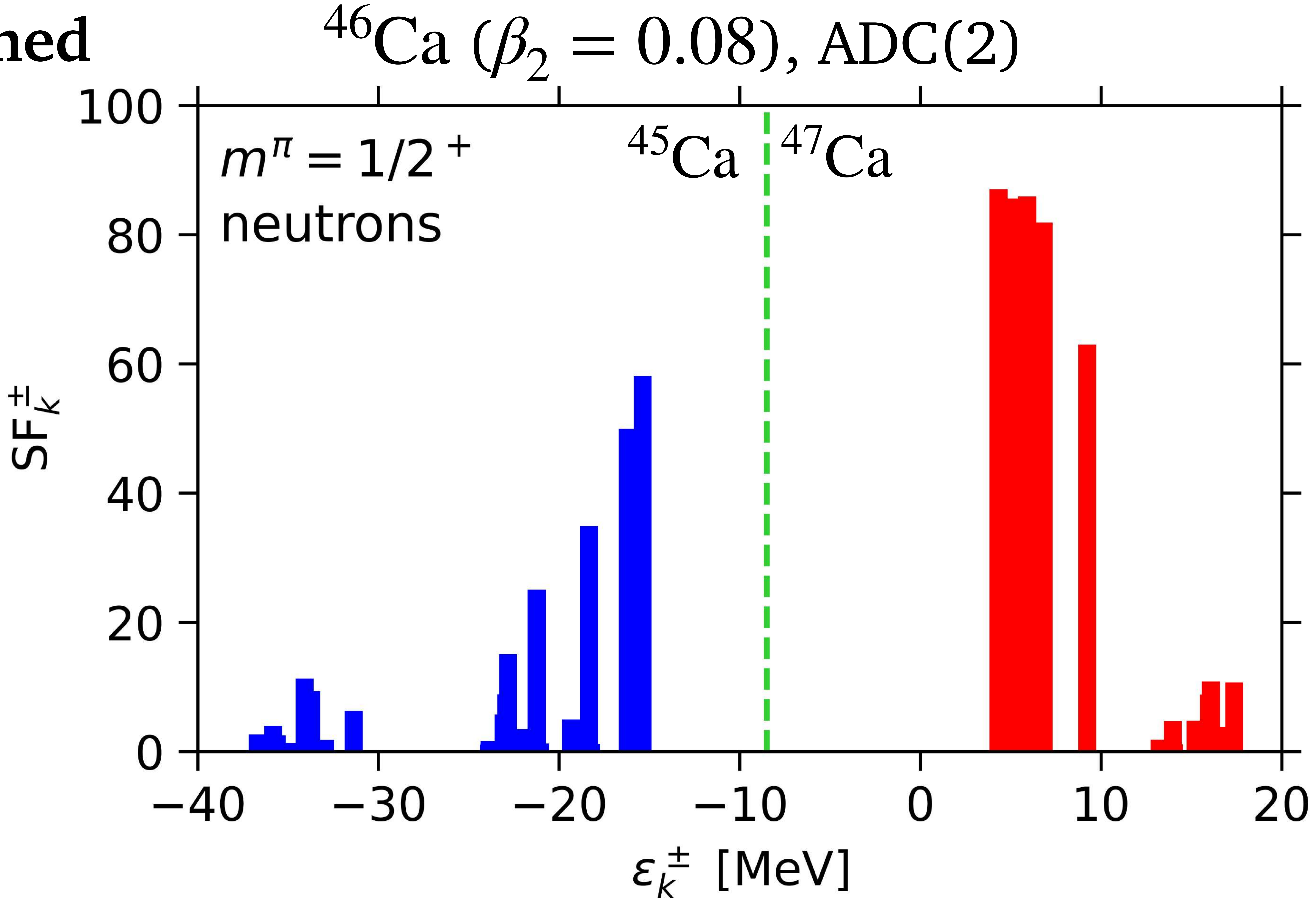
deformed



[Scalesi *et al.* n°2]

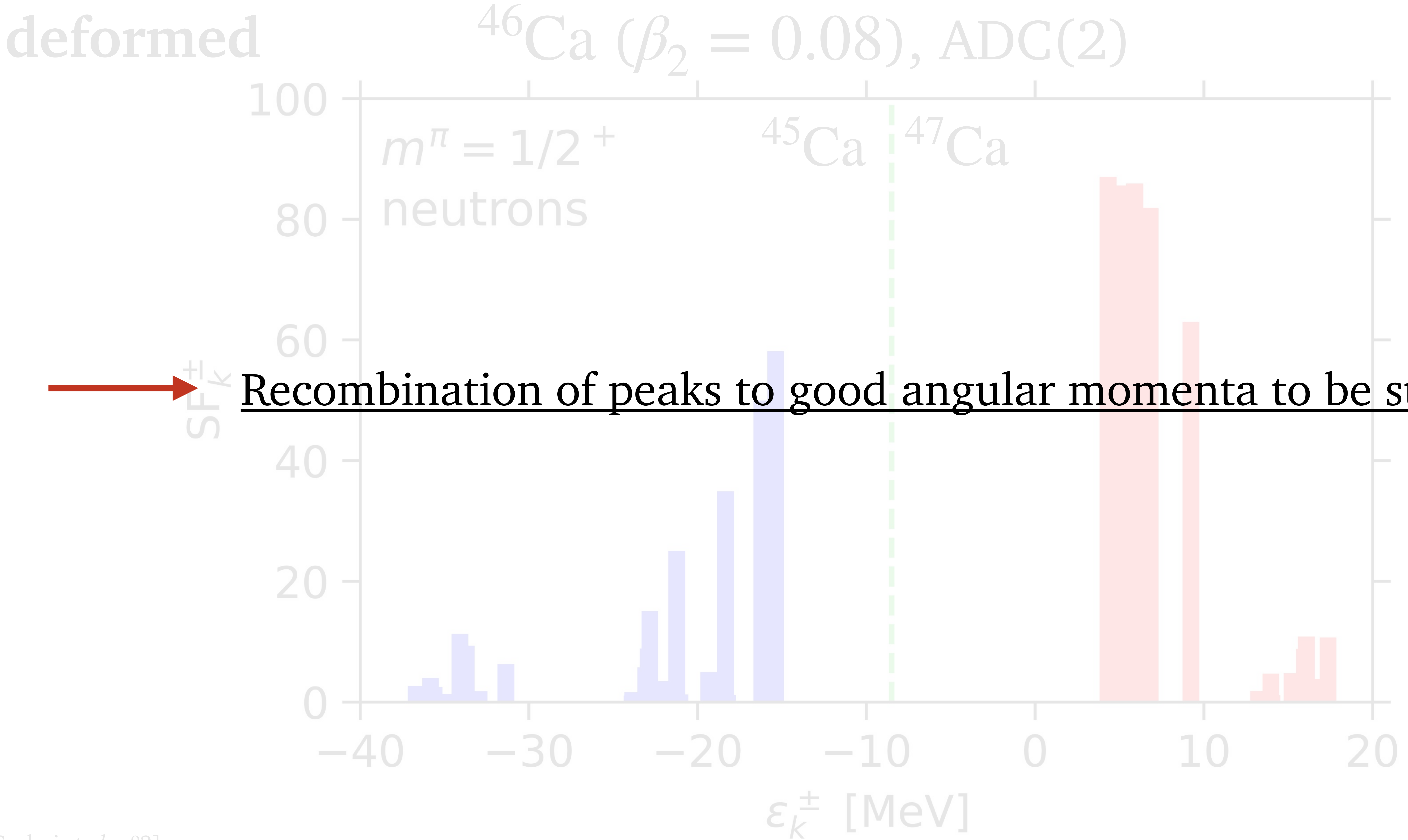
dDSCGF(2) results - Spectroscopic Amplitudes

deformed



[Scalesi *et al.* n°2]

dDSCGF(2) results - Spectroscopic Amplitudes



→ <u>Recombination of peaks to good angular momenta to be studied!</u>

[Scalesi *et al.* n°2]

Cost of deformation in *ab initio* methods

- **Different scalings:**

$N!$ N^p 2^N

NCSM

CI

CC

MBPT

SCGF

Montecarlo

Cost of deformation in *ab initio* methods

$\cancel{N!}$ N^p $\cancel{2^N}$

N

e_{max} \ Symmetry	Spherical (N^S)	Full (N)
0	1	2
1	3	8
2	6	20
3	10	40
4	15	70
5	21	112
6	28	168
7	36	240
8	45	330
9	55	440
10	66	572
11	78	728
12	91	910
13	105	1120
14	120	1360
15	136	1632

- **m-scheme** (needed for deformed calculations)
- Natural Orbitals (**NAT**)
- Importance Truncation (**IT**)

p

Truncation scheme	Scaling
(B)MBPT(2)	N^5
(B)MBPT(3)	N^6
(B)MBPT(4)	N^7
(B)CCSD	N^6
(B)CCSDT	N^8
IMSRG(2)	N^6
ADC(3)	N^6

- Greater cost for **non-perturbative** methods
- **BMBPT(2)** has the most gentle scaling

Deformed Natural Orbitals

- Main objective: reduce the cost of an expensive calculation
- How it can be done: via an **auxiliary cheaper calculation**

[Tichai *et al.* 2018]
[Hoppe *et al.* 2021]
[Scalesi *et al.* n°3]

V^{HO}_{abcd} (e_{max})

$\tilde{e}_{max} < e_{max}$

Cheap beyond mean-field calculation (dBMBPT)

Mean-field calculation (dHFB)

Expensive beyond mean-field calculation (**dDSCGF**)

ρ^{def}_{ab}

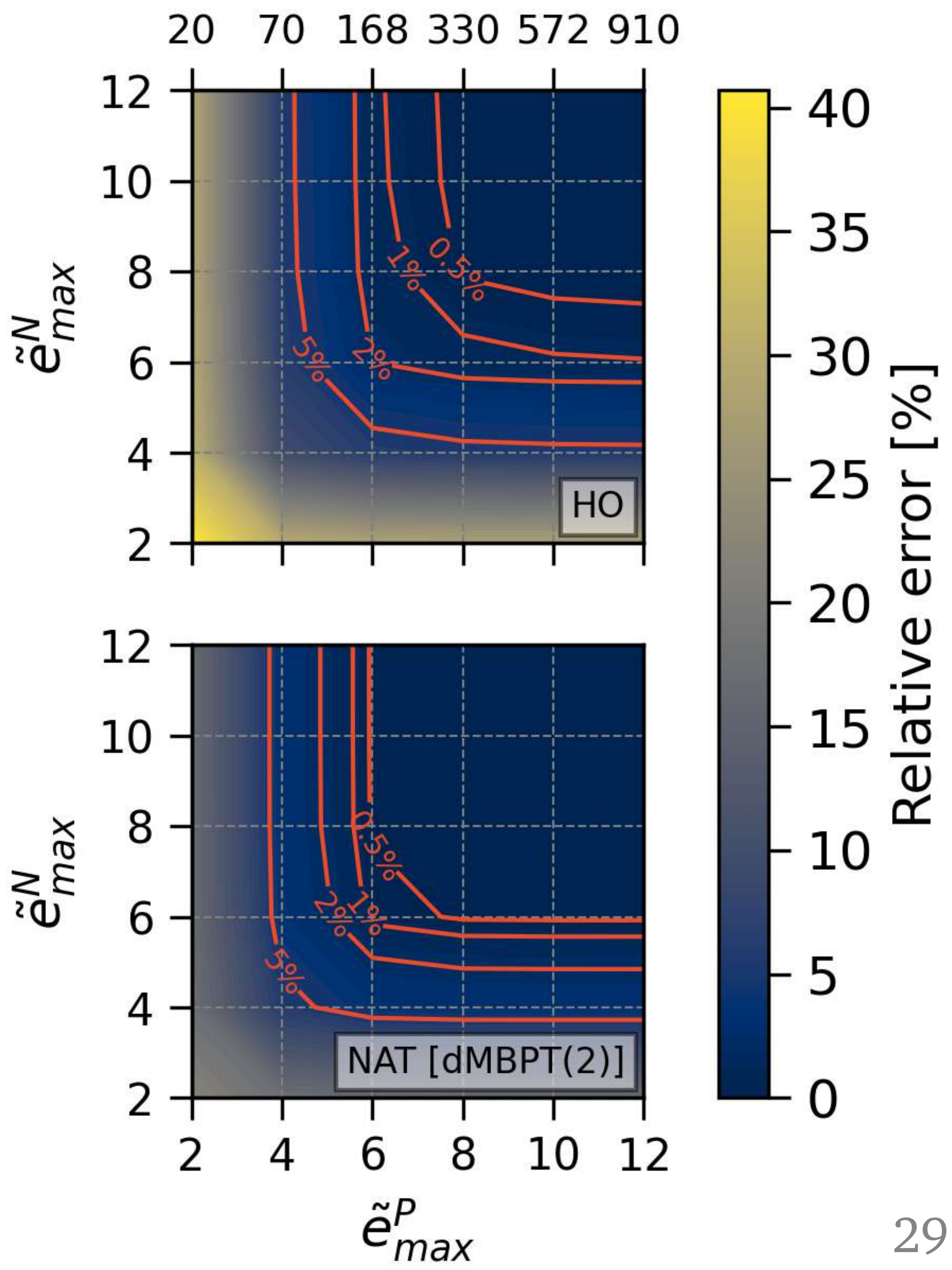
V^{NAT}_{abcd} (e_{max})

truncation

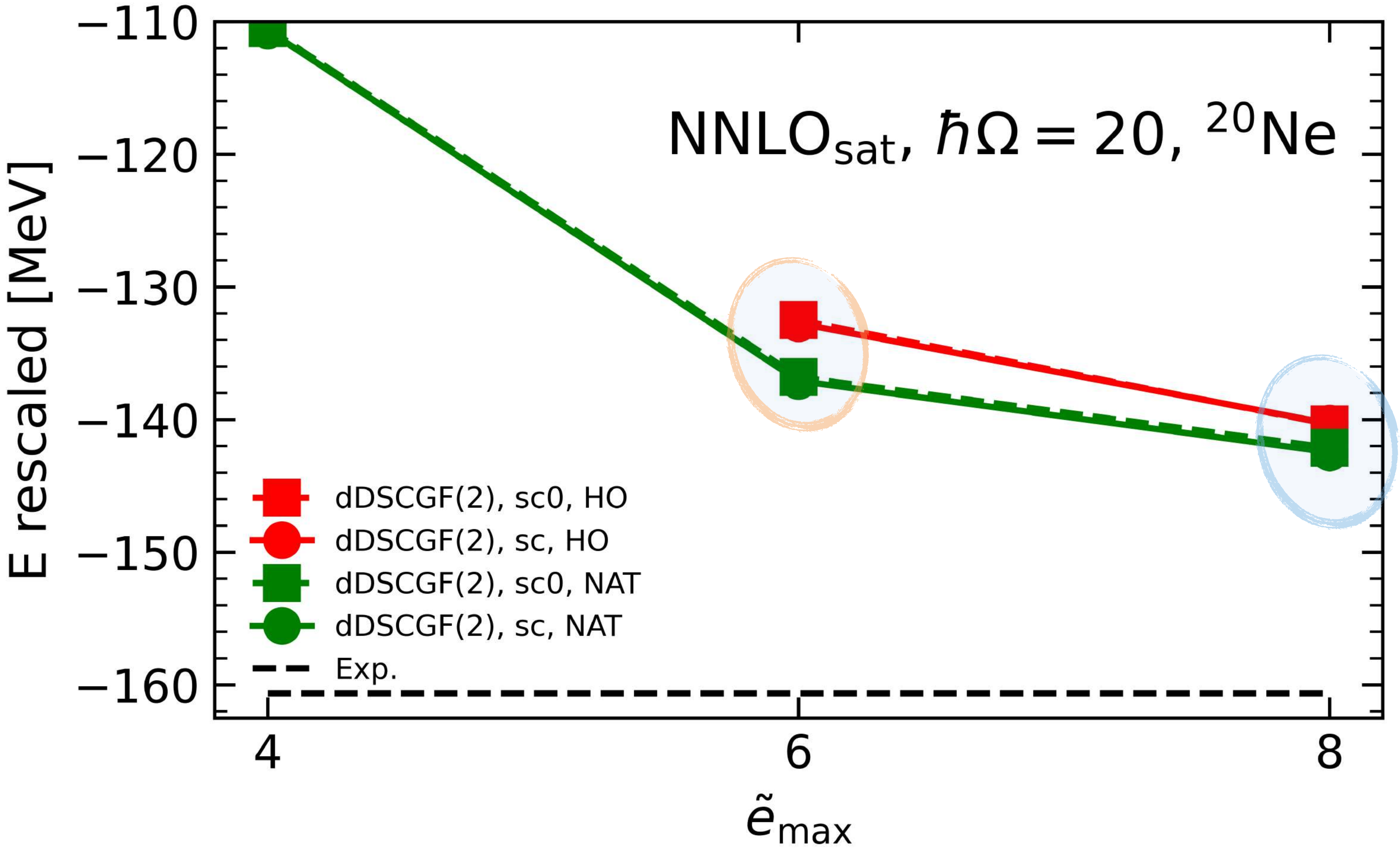
V^{NAT}_{abcd} ($\tilde{e}_{max}$)

^{20}Ne

EM 1.8/2.0



Deformed Natural Orbitals: application to dDSCGF(2)



Dyson formalism → **wrong part. num.** A

- Problem when looking to small diff.
- **Naïve rescaling** of energy based on A

↓

Clear separation between HO and NAT

⟶ $\tilde{e}_{max} = 6$ → 4.3 MeV gain

⟶ $\tilde{e}_{max} = 8$ → 2.0 MeV gain

[Scalesi *et al.* n°3]

Deformed Natural Orbitals: application to dDSCGF(2)

$\tilde{e}_{max}$	time* [h]
2	0.001
4	0.002
6	0.042
8	0.650
10	4.550
12	22.130

*104 OpenMP processors

Dyson formalism → **wrong part. num.** A

- Problem when looking to small diff.
- **Naïve rescaling** of energy based on A

↓

Clear separation between HO and NAT

⟶ $\tilde{e}_{max} = 6$ → 4.3 MeV gain

⟶ $\tilde{e}_{max} = 8$ → 2.0 MeV gain

[Scalesi *et al.* n°3]

Conclusions and future perspectives

Conclusions:

- It is a good strategy to set up methods **breaking $SU(2)$** and **not $U(1)$**
- **Correlations** captured by dDSCGF bring visible results on observables w.r.t. dBMBPT2 and sGSCGF
- **Deformed Natural Orbitals** can help to lighten the cost of beyond mean-field calculations

Future perspectives:

- Combine NAT with Importance truncation (**IT**) and tensor factorization techniques (**TF**)
- Formulations of proper **particle adjustment** in Dyson SCGF formalism
- Associate **Spectroscopic distribution** with good angular momentum
- Beyond ADC(2): extended ADC(2) and **ADC(3)** $\longrightarrow$ Numerical optimization code (MPI)
- dDSCGF with **good angular momentum** $\rightarrow$ Symmetry Restoration (yet to be formulated) / MR-SCGF†

[Porro *et al.* 2021] [Frosini, Duguet, Tamagno 2024] [Sokolov *et al.* 2018]