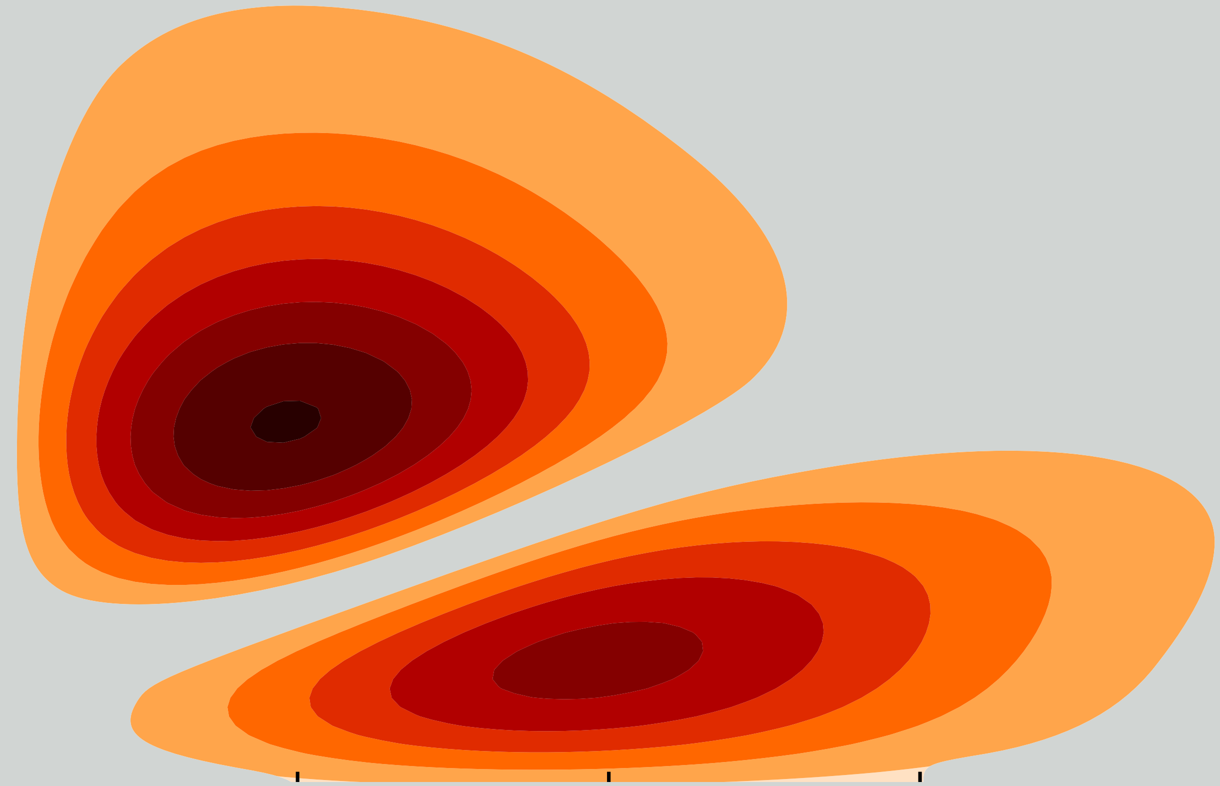

LARGE-SCALE DIAGONALIZATION, BETA-DECAY, AND LOW-MOMENTUM SCALES OF FINITE NUCLEI

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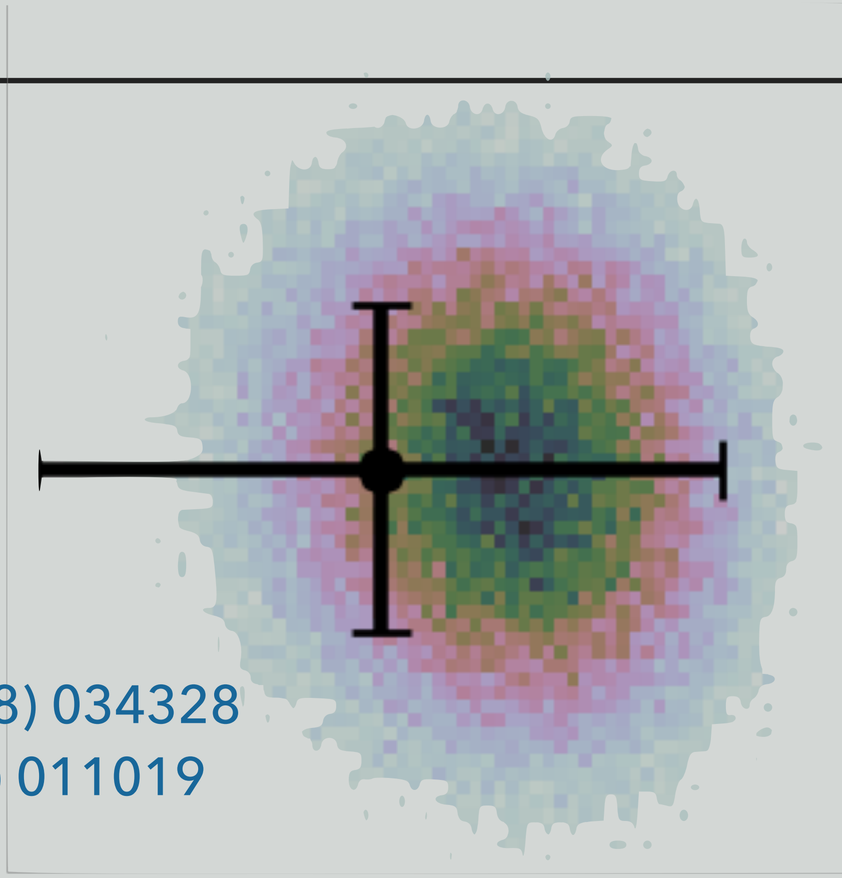
Department of Physics, Chalmers University of Technology, Sweden

ECT* workshop: *"Precise beta decay calculations for searches for new physics"*, April 8–12, 2019

Outline

- **Part 1:**
  The nuclear many-body problem and uncertainties
  - Interactions and many-body solvers
  - Convergence and limitations for the ab initio No-Core Shell Model

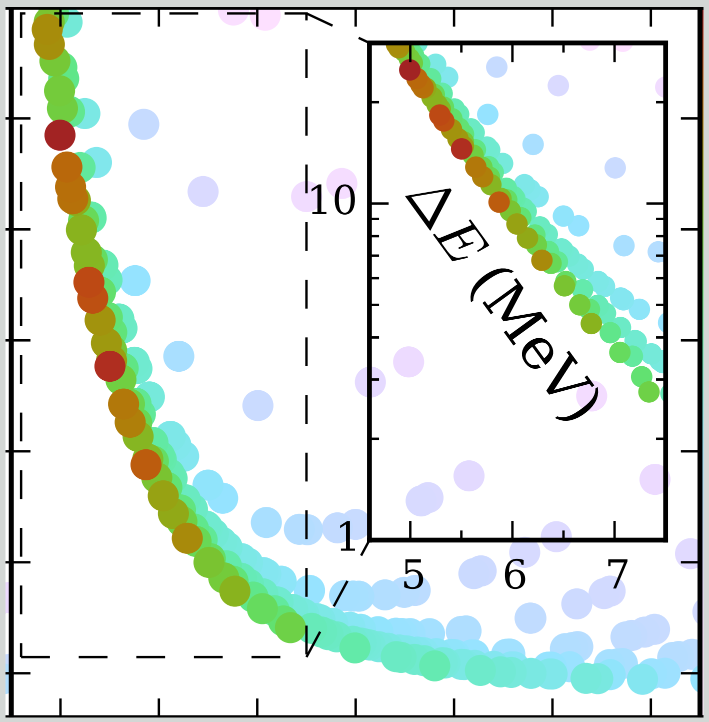


Phys. Rev. C 97 (2018) 034328
Phys. Rev. X 6 (2016) 011019
PPNP 69 (2013) 131

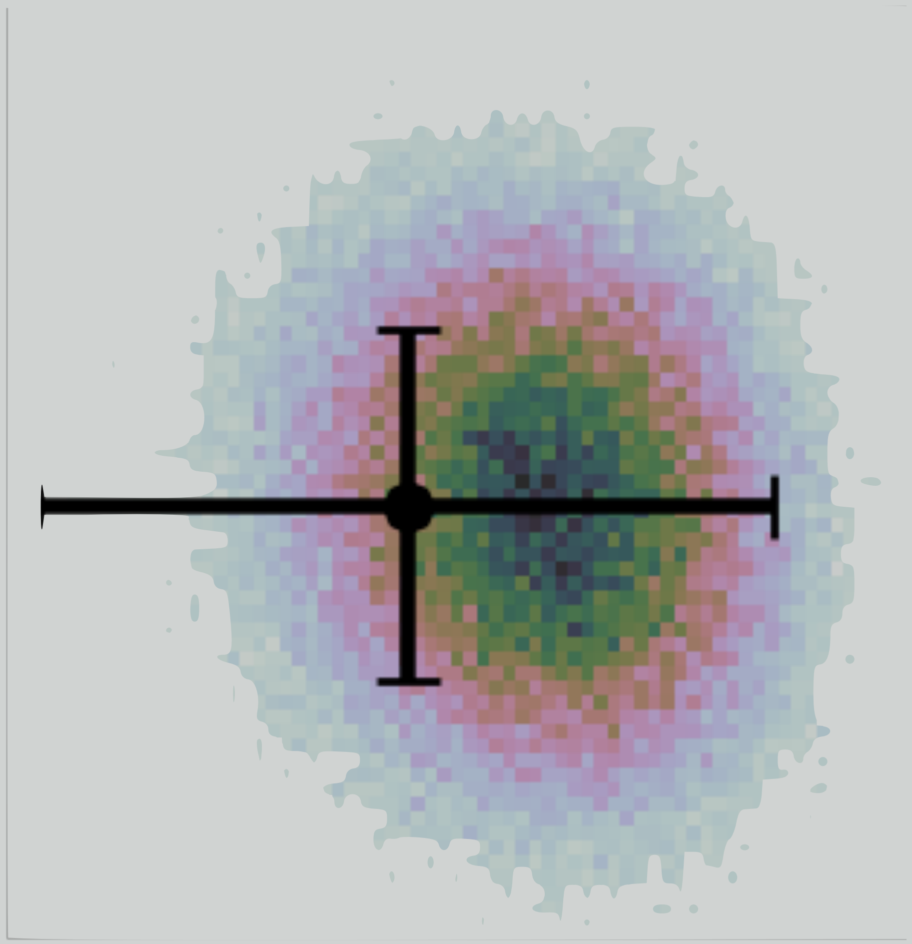
- **Part 2:**
  Selected (preliminary) results

Unpublished

- **Part 3:**
  Many-body systems in finite oscillator spaces
  - IR extrapolations at fixed UV cutoff
  - Low-momentum scales of finite nuclei



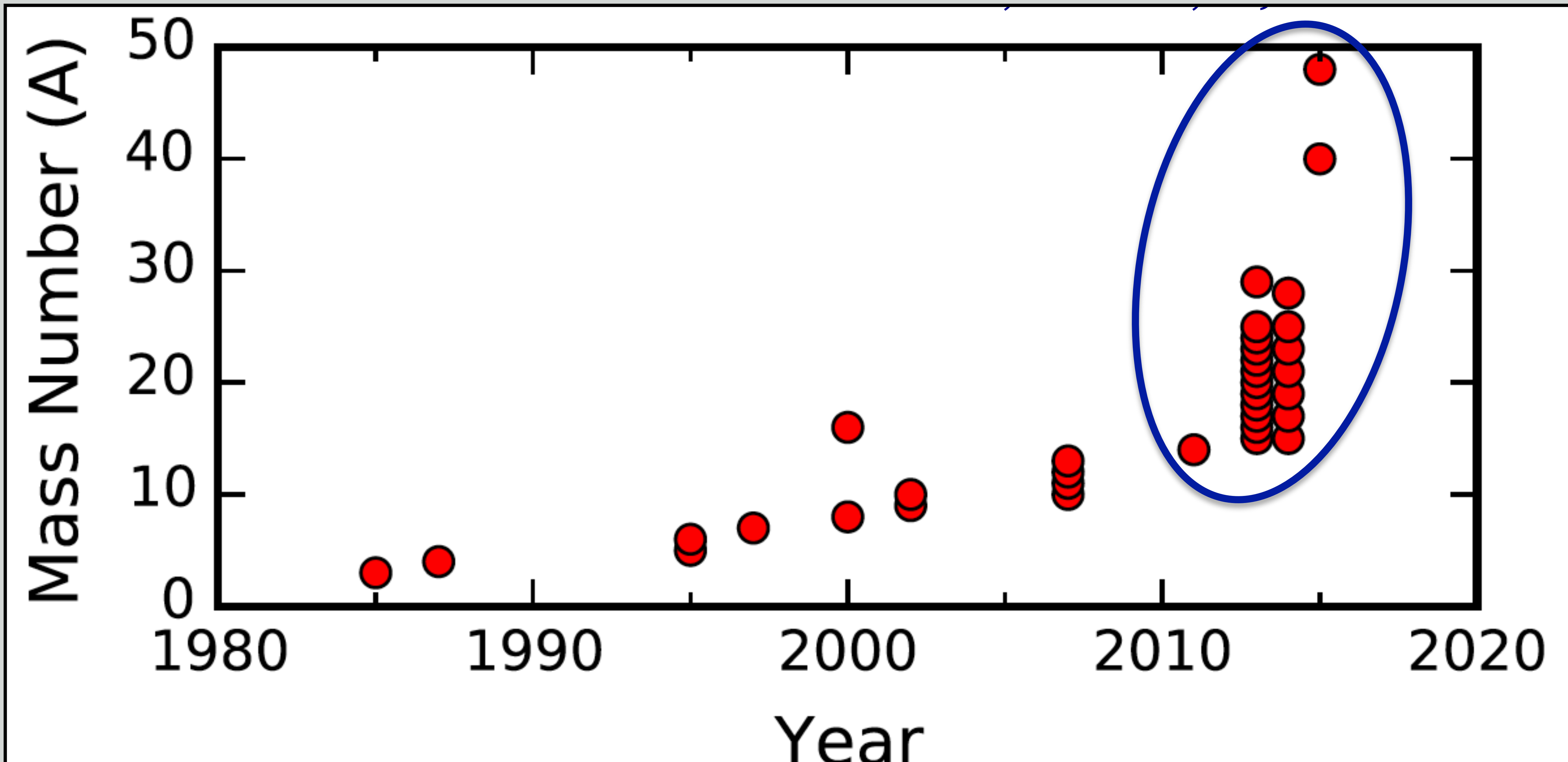
Phys. Rev. C 91, (2015) 061301R
Phys. Rev. C 97, (2018) 034328



Part 1: The nuclear many-body problem and uncertainties

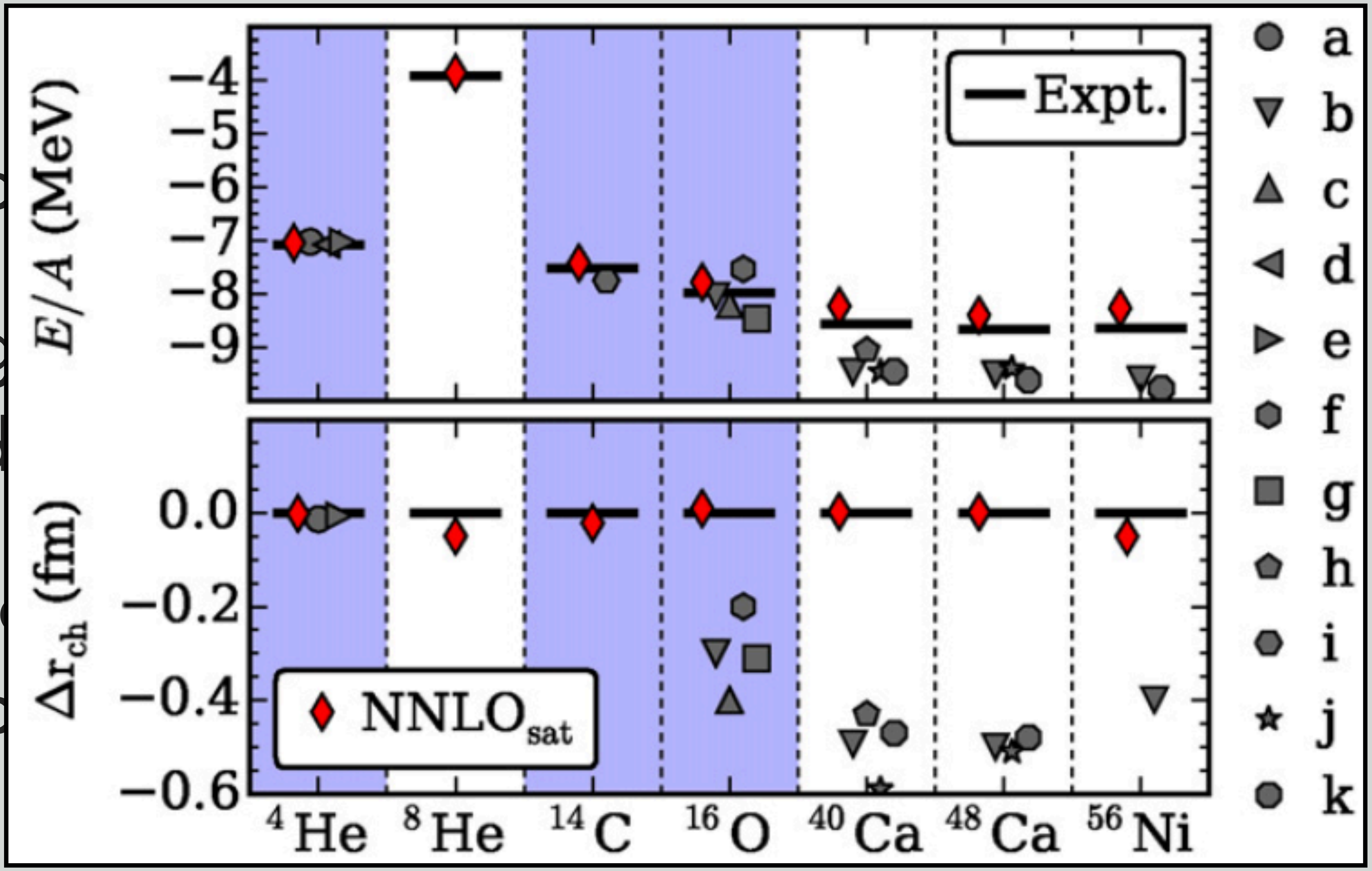
SUMMARY — PART 1A

- Many-body methods with polynomial scaling (CC, IMSRG, SCGF) reach calcium and nickel regions, and even beyond…



SUMMARY — PART 1A

- Many-body methods with polynomial scaling (CC, IMSRG, SCGF) reach calcium and nickel regions, and even beyond…
- Computational capabilities exceed accuracy of available interactions.
- New generation o
  - different fitting
    intermediate d
- Goal: Credible pr
  ab initio nuclear p

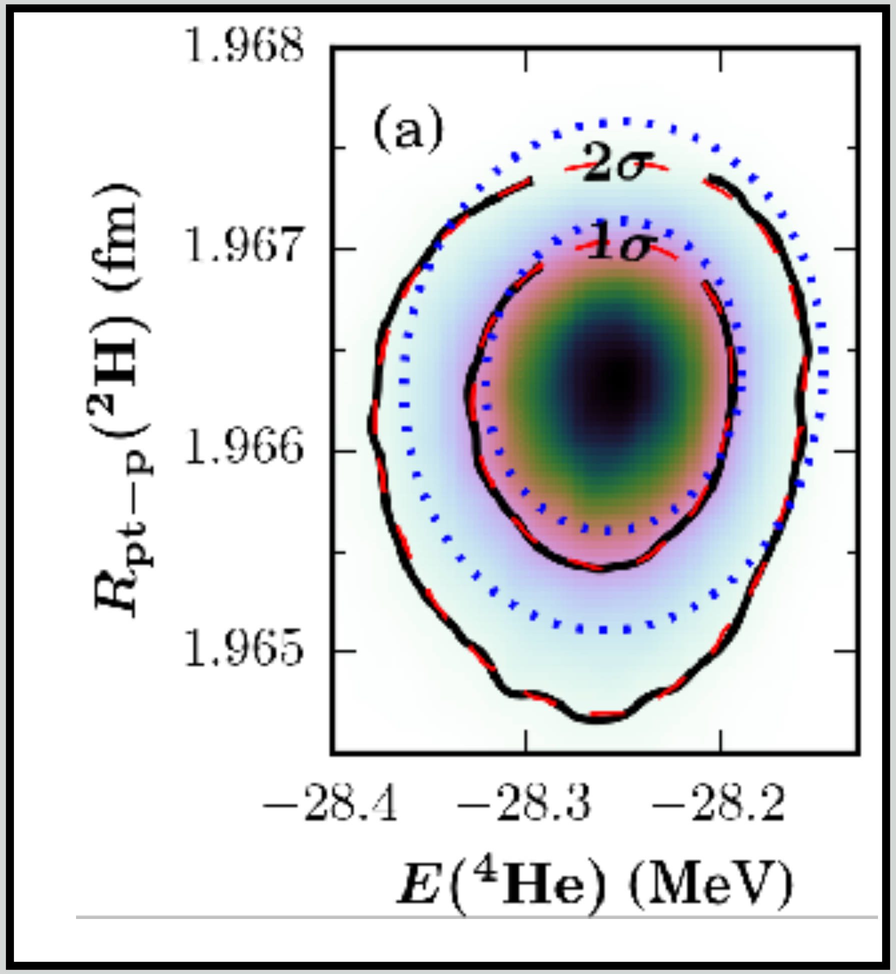


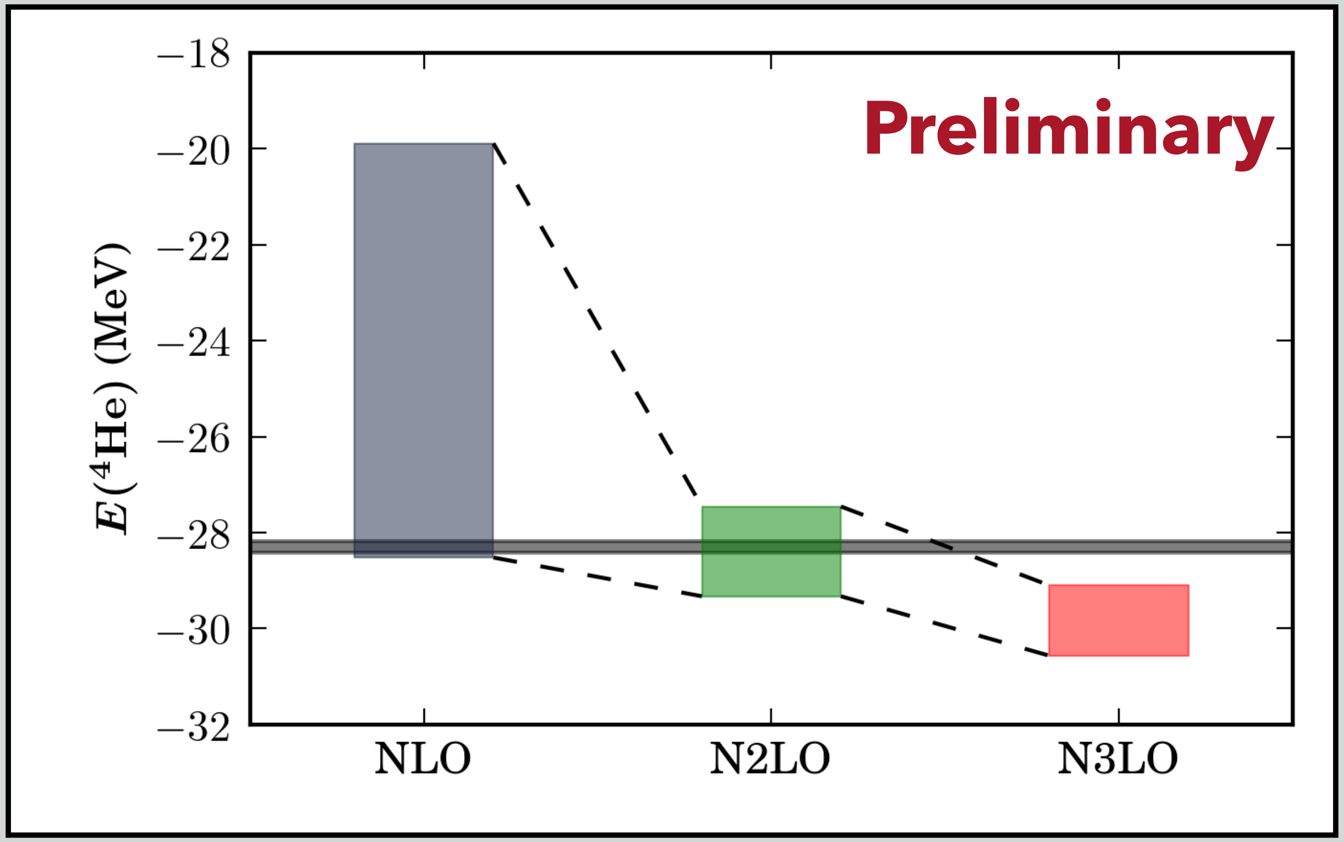
SUMMARY — PART 1A

- Many-body methods with polynomial scaling (CC, IMSRG, SCGF) reach calcium and nickel regions, and even beyond…
- Computational capabilities exceed accuracy of available interactions.
- New generation of nuclear interactions:
  - different fitting strategies (saturation point); including intermediate delta particle; revisit power counting.
- Goal: Credible program for uncertainty quantification in ab initio nuclear physics

QUANTIFIED THEORETICAL UNCERTAINTIES

- **Statistical:** parametric uncertainties (should be done also for phenomenological models).
- **Systematic**: method (many-body solver) and numerical uncertainty.
- **Systematic**: physics model uncertainty.





Phys. Rev. X 6 (2016) 011019

Part 1b:
Ab initio No-Core Shell Model

The no-core shell model

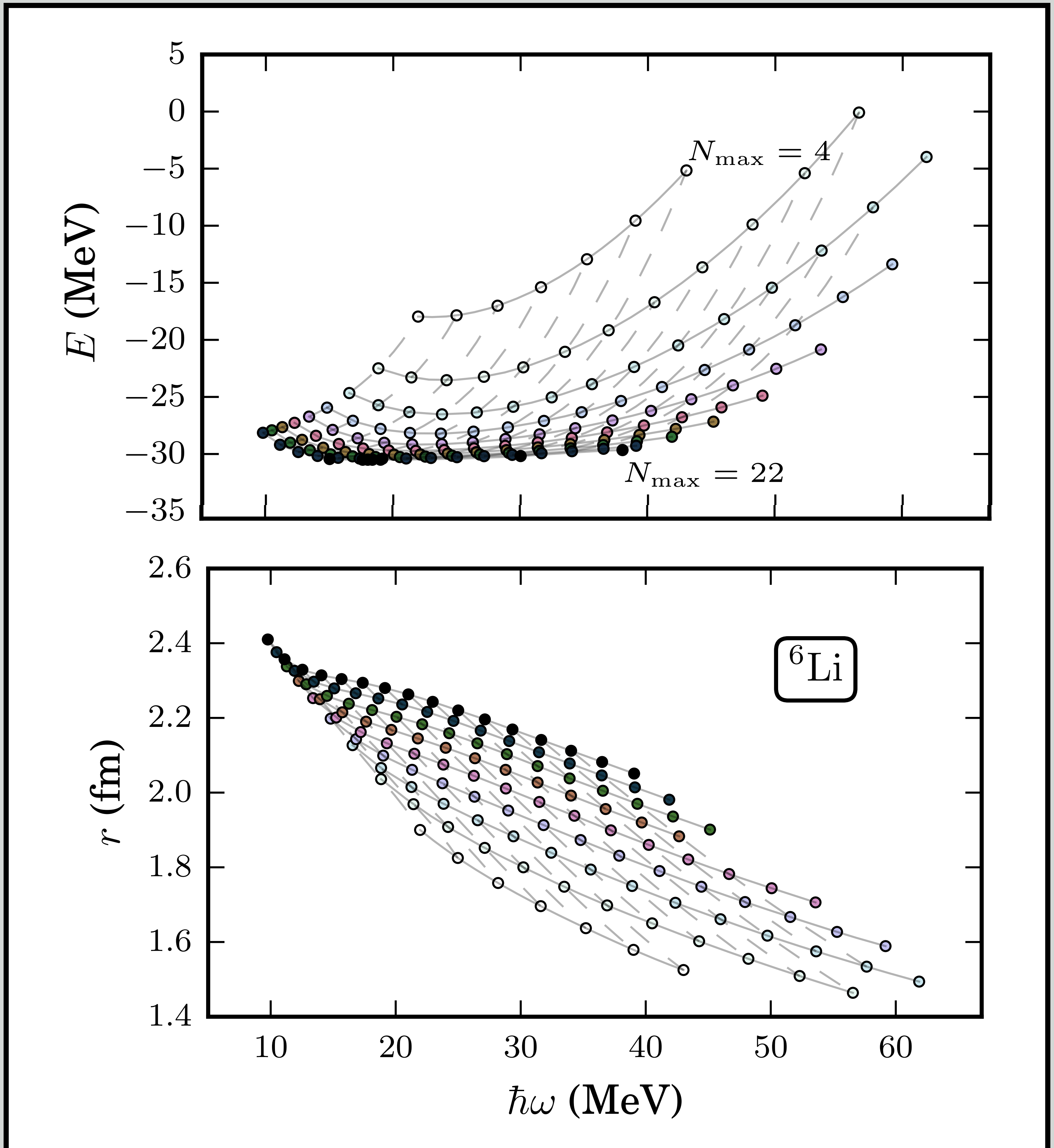
- Many-body Schrödinger equation
  - A-nucleon wave function;
  - Non-relativistic, point nucleons
- Hamiltonian:

$$H_A = \frac{1}{A}\sum_{i<j}^{A}\frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j}^{A} V_{NN,ij} + \sum_{i<j<k}^{A} V_{NNN,ijk}$$

- Many-body basis: Slater determinants composed of harmonic oscillator single-particle states
- Respects translational invariance and includes full antisymmetrization

P. Navråtil et al, PPNP 69 (2013) 131

The no-core shell model

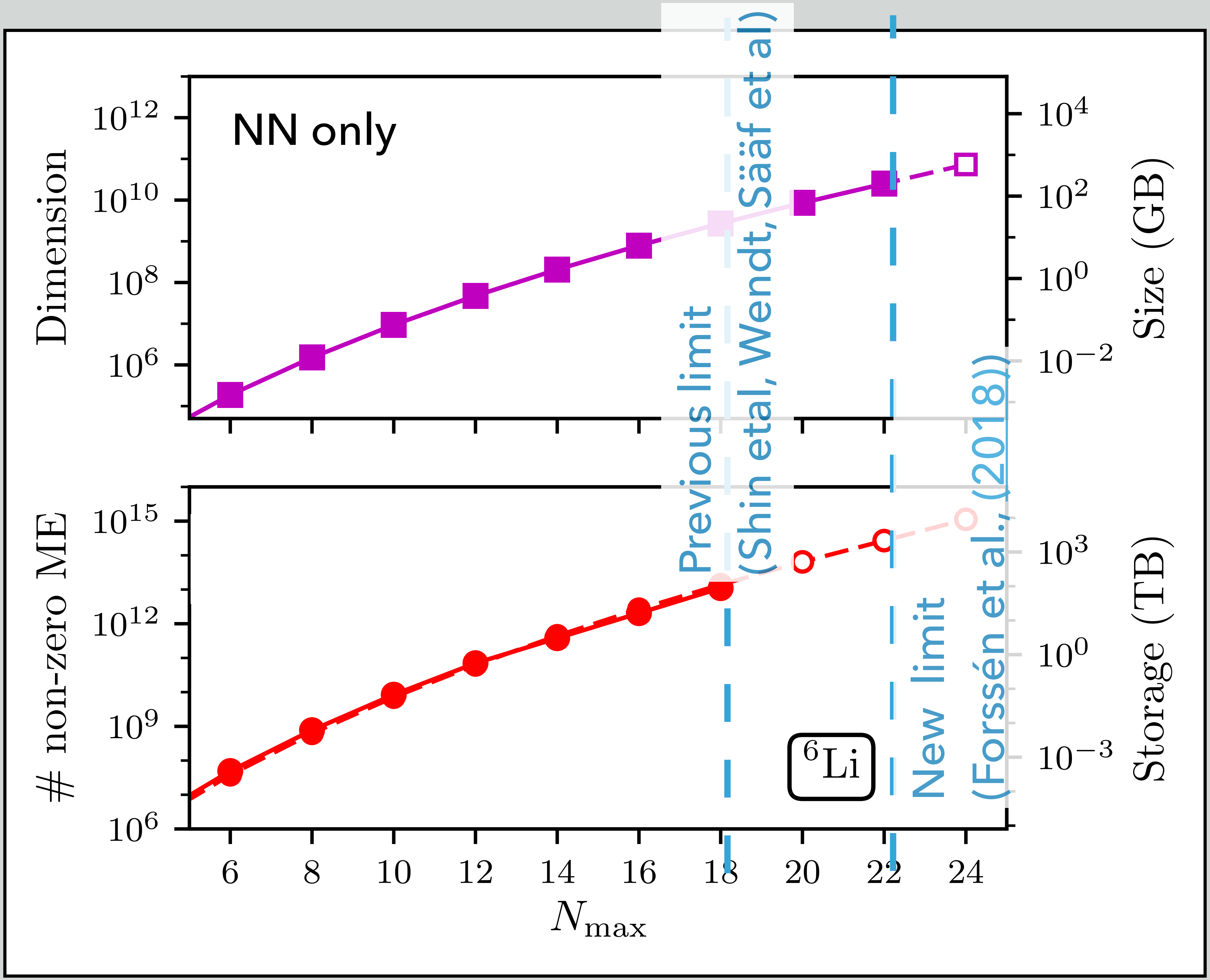


Bare interactions used (here NNLOopt).

Model space parameters: N_{max} and HO frequency.

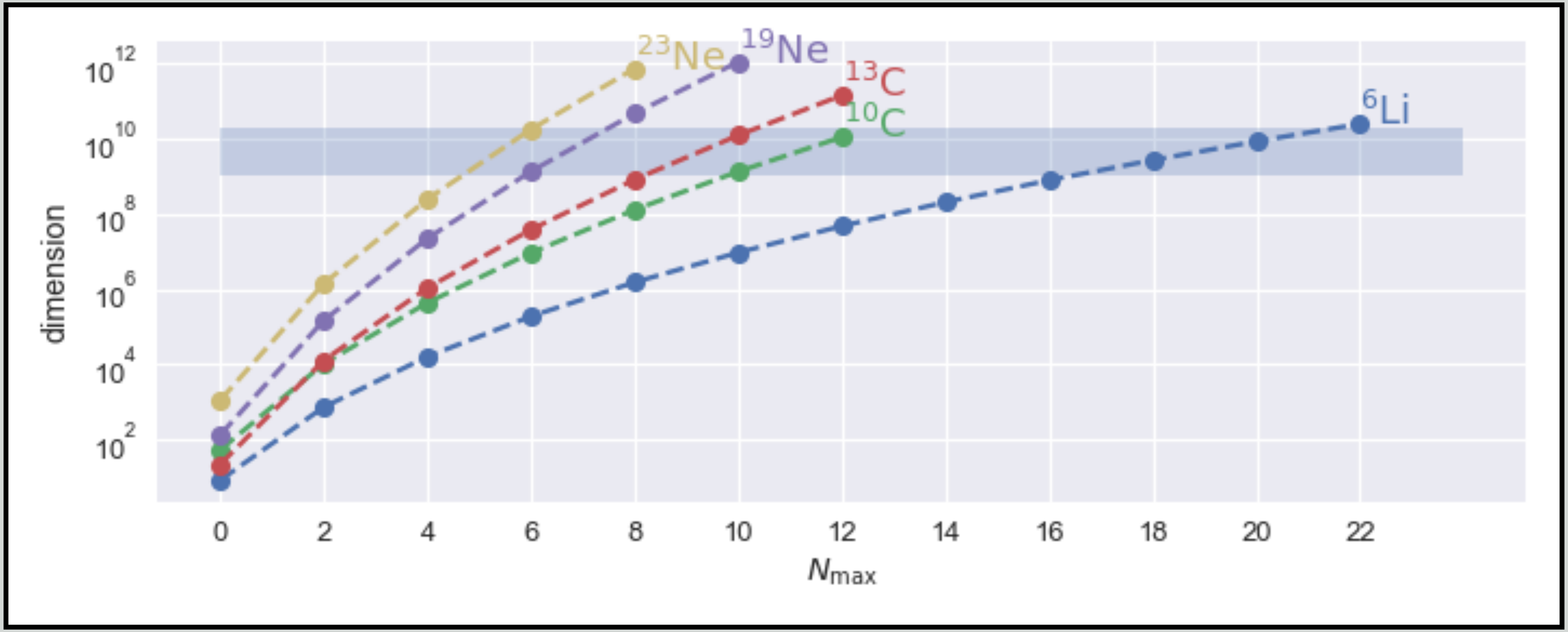
Convergence pattern needs to be understood (part 3).

The NCSM curse of dimensionality – explicit matrix storage

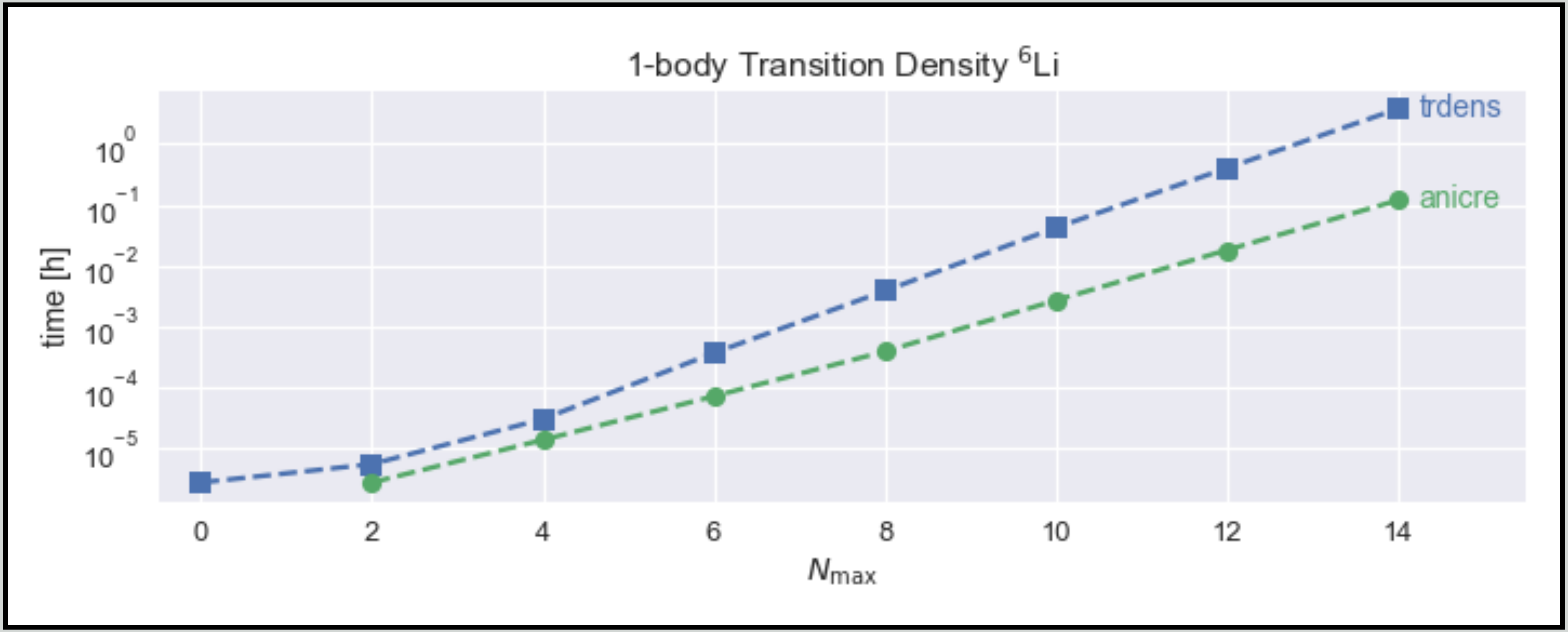


Phys. Rev. C 97 (2018) 034328

Dimensions: p- and sd-shell



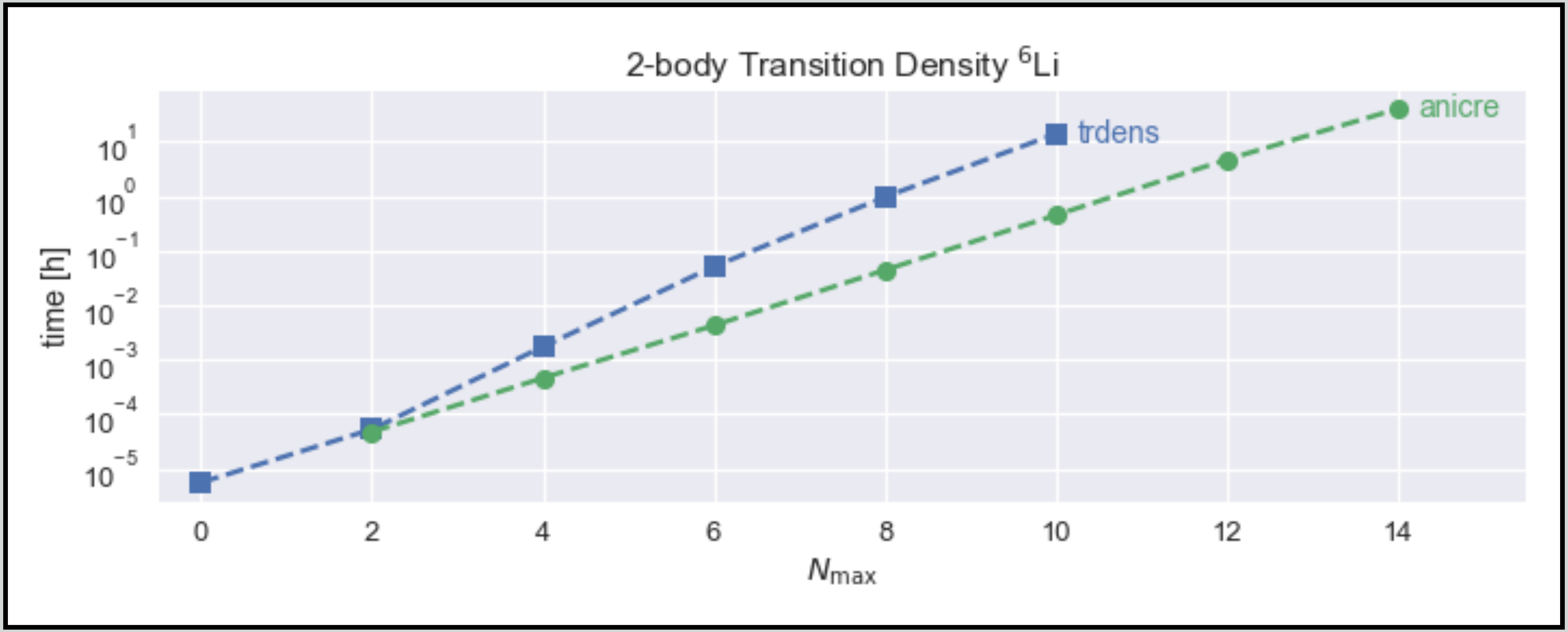
Transition densities



$$\left(\xi_f J_f \parallel T_\lambda \parallel \xi_i J_i\right) = \hat{\lambda}^{-1} \sum \left(a \parallel T_\lambda \parallel b\right) \left(\xi_f J_f \left\| \left[a_a^\dagger a_b\right]_\lambda \right\| \xi_i J_i\right)$$

TRDENS: Phys. Rev. C 70 (2004) 014317
ANICRE: D. Sääf, PhD thesis (2015)

Transition densities

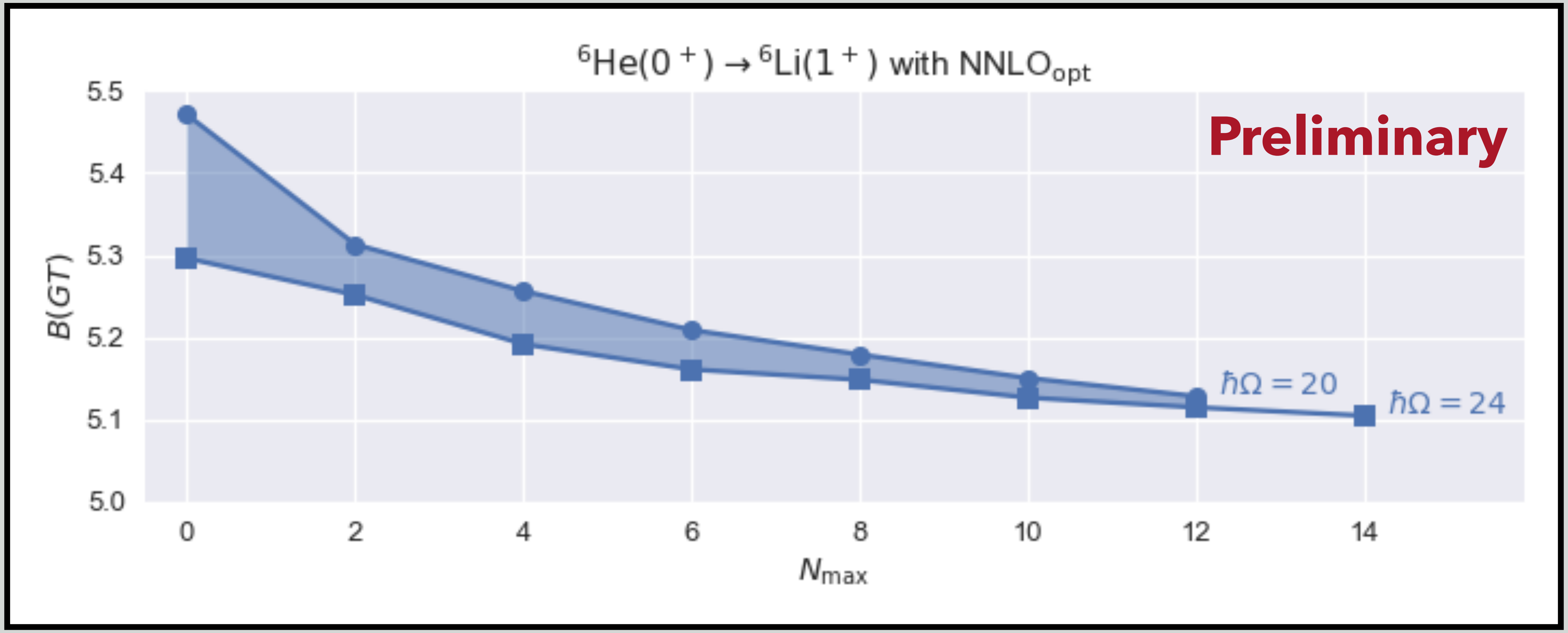


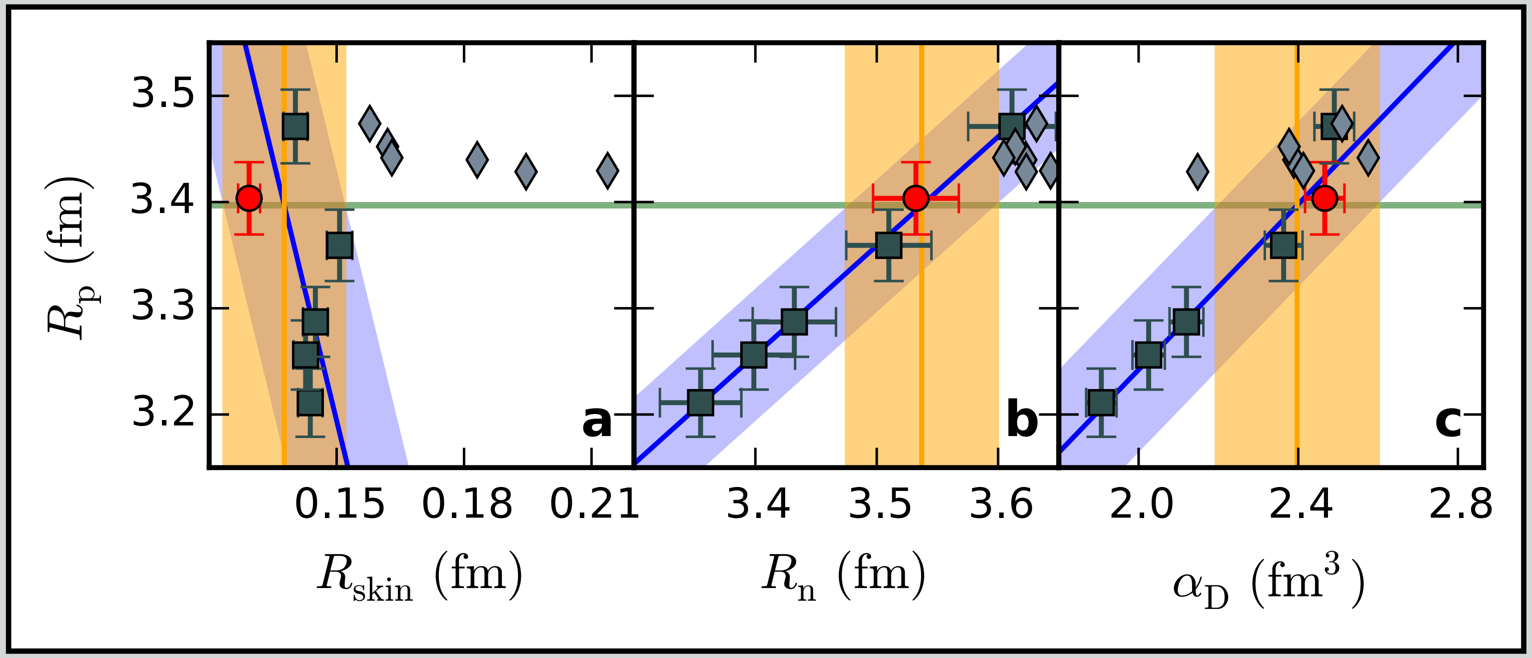
$$\left(\xi_f J_f \,\|\, T_\lambda \,\|\, \xi_i J_i\right) = \hat{\lambda}^{-1} \sum \left(a, b \,\|\, T_\lambda \,\|\, c, d\right) \left(\xi_f J_f \,\middle\|\, \left[a_a^\dagger a_b^\dagger a_c a_d\right]_\lambda \,\middle\|\, \xi_i J_i\right)$$

TRDENS: Phys. Rev. C 70 (2004) 014317
ANICRE: D. Sääf, PhD thesis (2015)

Part 2:
Selected (preliminary) results

A=6 Gamow-Teller transition (IA)





Possibly employ correlation studies to constrain prediction.

A=19 Gamow-Teller transition

N_{max}	B(GT) $^{6}He(0^{+}) \rightarrow {}^{6}Li(1^{+})$ $\hbar\Omega$=24 MeV	B(GT) $^{19}Ne(1/2^{+}) \rightarrow {}^{19}F(1/2^{+})$ $\hbar\Omega$=28 MeV
2	5.251	2.013
4	5.191	2.059
...	...	
14	5.104	

Preliminary

Dark matter scattering off nuclei

Rate of nuclear scattering events in direct detection experiments:

$$\frac{\mathrm{d}\mathcal{R}}{\mathrm{d}q^2} = \frac{\rho_\chi}{m_A m_\chi} \int \mathrm{d}^3\vec{v}\, f(\vec{v} + \vec{v}_e)\, v \frac{\mathrm{d}\sigma}{\mathrm{d}q^2}$$

- astrophysics $\longrightarrow m_\chi,\ \rho_\chi,\ f$ - dark matter mass, density, velocity distributions
- particle and nuclear physics $\longrightarrow \frac{\mathrm{d}\sigma}{\mathrm{d}q^2}$

Scattering cross section:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}q^2} = \frac{1}{(2J+1)v^2} \sum_{\tau,\tau'} \left[\sum_{\ell=M,\Sigma',\Sigma''} R_\ell^{\tau\tau'} W_\ell^{\tau\tau'} + \frac{q^2}{m_N^2} \sum_{\substack{\ell=\Phi'',\Phi'' M,\\ \tilde{\Phi}',\Delta,\Delta\Sigma'}} R_\ell^{\tau\tau'} W_\ell^{\tau\tau'} \right]$$

- dark matter response functions $R_m^{\tau\tau'}\left(v_T^{\perp 2}, \frac{q^2}{m_N^2}, c_i^\tau c_j^{\tau'} \right)$
- nuclear response functions $W_\ell^{\tau\tau'}(q^2)$

Uncertainties?

- ρ_χ: $\pm 30\%$, $f(\vec{v})$: $\pm$? (important only for light DM), $W_l^{\tau\tau'}$: $\pm$?

Non-relativistic EFT and nuclear response functions

- nuclear response functions:

$$W_{AB}^{\tau\tau'}(q^2) = \sum_{L\leq 2J} \langle J, T, M_T \| \hat{A}_{L;\tau}(q) \| J, T, M_T \rangle \langle J, T, M_T \| \hat{B}_{L;\tau'}(q) \| J, T, M_T \rangle$$

  - $\hat{A}_{L;\tau}$, $\hat{B}_{L;\tau}$ – nuclear response operators:

$$M_{LM;\tau}(q) = \sum_{i=1}^{A} M_{LM}(q\boldsymbol{\rho}_i)\, t_{(i)}^{\tau}, \quad \Sigma'_{LM;\tau}(q) = -\mathrm{i} \sum_{i=1}^{A} \left[\frac{1}{q} \overleftrightarrow{\nabla}_{\boldsymbol{\rho}_i} \times \mathbf{M}_{LL}^{M}(q\boldsymbol{\rho}_i) \right] \cdot \vec{\sigma}_{(i)} t_{(i)}^{\tau},$$

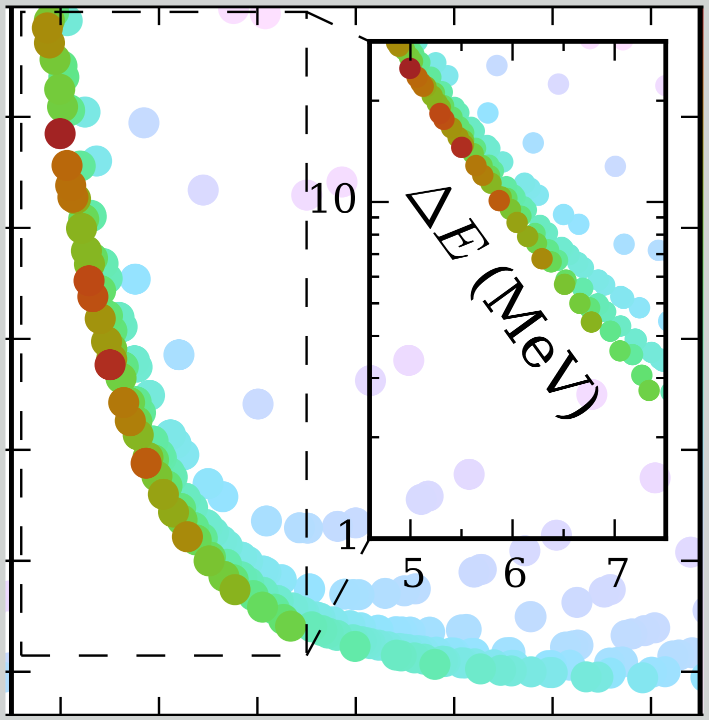
$$\Sigma''_{LM;\tau}(q) = \sum_{i=1}^{A} \left[\frac{1}{q} \overleftrightarrow{\nabla}_{\boldsymbol{\rho}_i} M_{LM}(q\boldsymbol{\rho}_i) \right] \cdot \vec{\sigma}_{(i)} t_{(i)}^{\tau}, \quad \Delta_{LM;\tau}(q) = \sum_{i=1}^{A} \mathbf{M}_{LL}^{M}(q\boldsymbol{\rho}_i) \cdot \frac{1}{q} \overleftrightarrow{\nabla}_{\boldsymbol{\rho}_i} t_{(i)}^{\tau},$$

$$\tilde{\Phi}'_{LM;\tau}(q) = \sum_{i=1}^{A} \left[\left(\frac{1}{q} \overleftrightarrow{\nabla}_{\boldsymbol{\rho}_i} \times \mathbf{M}_{LL}^{M}(q\boldsymbol{\rho}_i) \right) \cdot \left(\vec{\sigma}_{(i)} \times \frac{1}{q} \overleftrightarrow{\nabla}_{\boldsymbol{\rho}_i} \right) + \frac{1}{2} \mathbf{M}_{LL}^{M}(q\boldsymbol{\rho}_i) \cdot \vec{\sigma}_{(i)} \right] t_{(i)}^{\tau},$$

$$\Phi''_{LM;\tau}(q) = \mathrm{i} \sum_{i=1}^{A} \left(\frac{1}{q} \overleftrightarrow{\nabla}_{\boldsymbol{\rho}_i} M_{LM}(q\boldsymbol{\rho}_i) \right) \cdot \left(\vec{\sigma}_{(i)} \times \frac{1}{q} \overleftrightarrow{\nabla}_{\boldsymbol{\rho}_i} \right) t_{(i)}^{\tau}$$

  - nuclear ground-state wave functions $|J, T, M_T\rangle$ calculated within (no-core) shell model

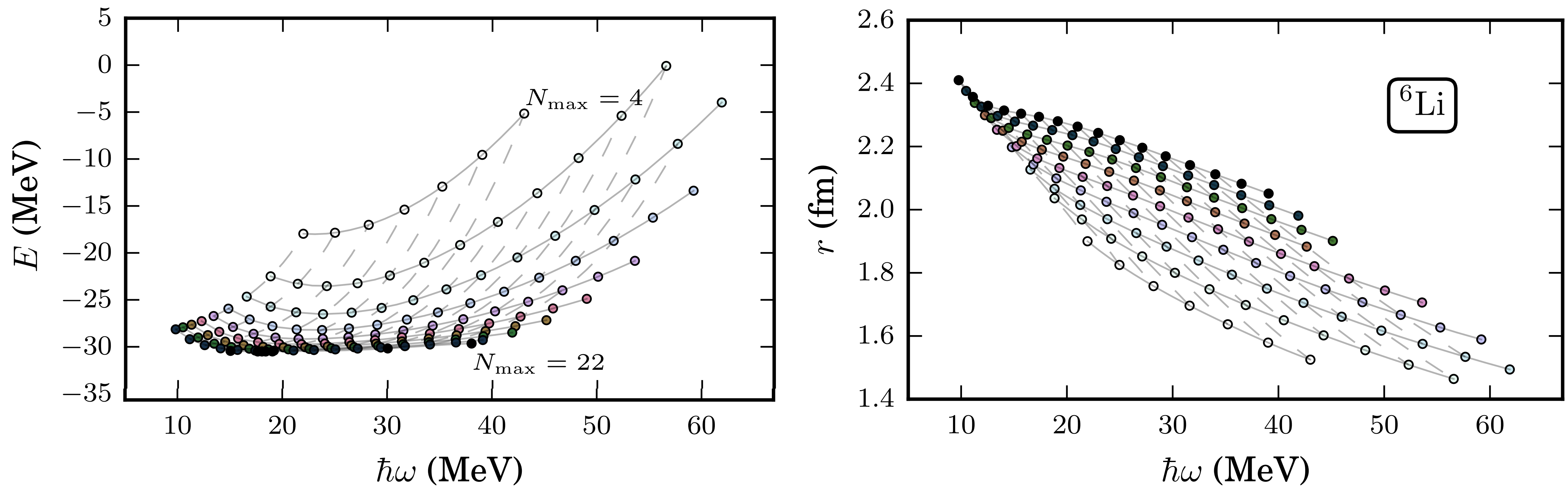
D. Gazda, R. Catena, CF: Phys. Rev. D 95 (2017) 103011



Part 3: Many-body systems in finite oscillator spaces

6-Li ground-state observables

NN interaction: NNLOopt (Ekström et al, 2013)



- From N_{max}=20 to 22 the variational minimum changes by < 90 keV.
- However, mostly we will be restricted to smaller model spaces.
- Convergence behaviour of radius?

Convergence in finite oscillator spaces

- What is the equivalent of Lüscher's formula for the harmonic oscillator basis?
  [Lüscher, Comm. Math. Phys. 104, 177 (1986)]

- Convergence in momentum space (UV) and in position space (IR) needed
  [Stetcu et al. (2007); Coon et al. (2012); Furnstahl et al. (2012, 2015); König et al. (2014)]

- Choose regime (N, $\hbar\omega$) with negligible UV corrections.
- The infrared error term is universal for short range Hamiltonians.

- It can be systematically corrected and resembles error from putting system into an infinite well.

$$E(L) = E_\infty + Ae^{-2k_\infty L} + \mathcal{O}(e^{-4k_\infty L})$$

$$\langle r^2\rangle_L \approx \langle r^2\rangle_\infty [1 - (c_0\beta^3 + c_1\beta + c_2)e^{-\beta}]$$

What (precisely) is the IR scale L?

Key idea: compute eigenvalues of kinetic energy and compare with *corresponding* (hyper)spherical cavity to find L.

What is the corresponding cavity?

Single particle	A particles (product space)	A particles in No-core shell model
Diagonalize $T_{kin}=p^2$	Diagonalize A-body T_{kin}	Diagonalize A-body T_{kin}
3D spherical cavity	A fermions in 3D cavity	3(A-1) hyper-radial cavity

$$L_2 = \sqrt{2(N+3/2+2)}b$$

$$L_{\rm eff} = \left(\frac{\sum_{nl} \nu_{nl} a_{l,n}^2}{\sum_{nl} \nu_{nl} \kappa_{l,n}^2}\right)^{1/2}$$

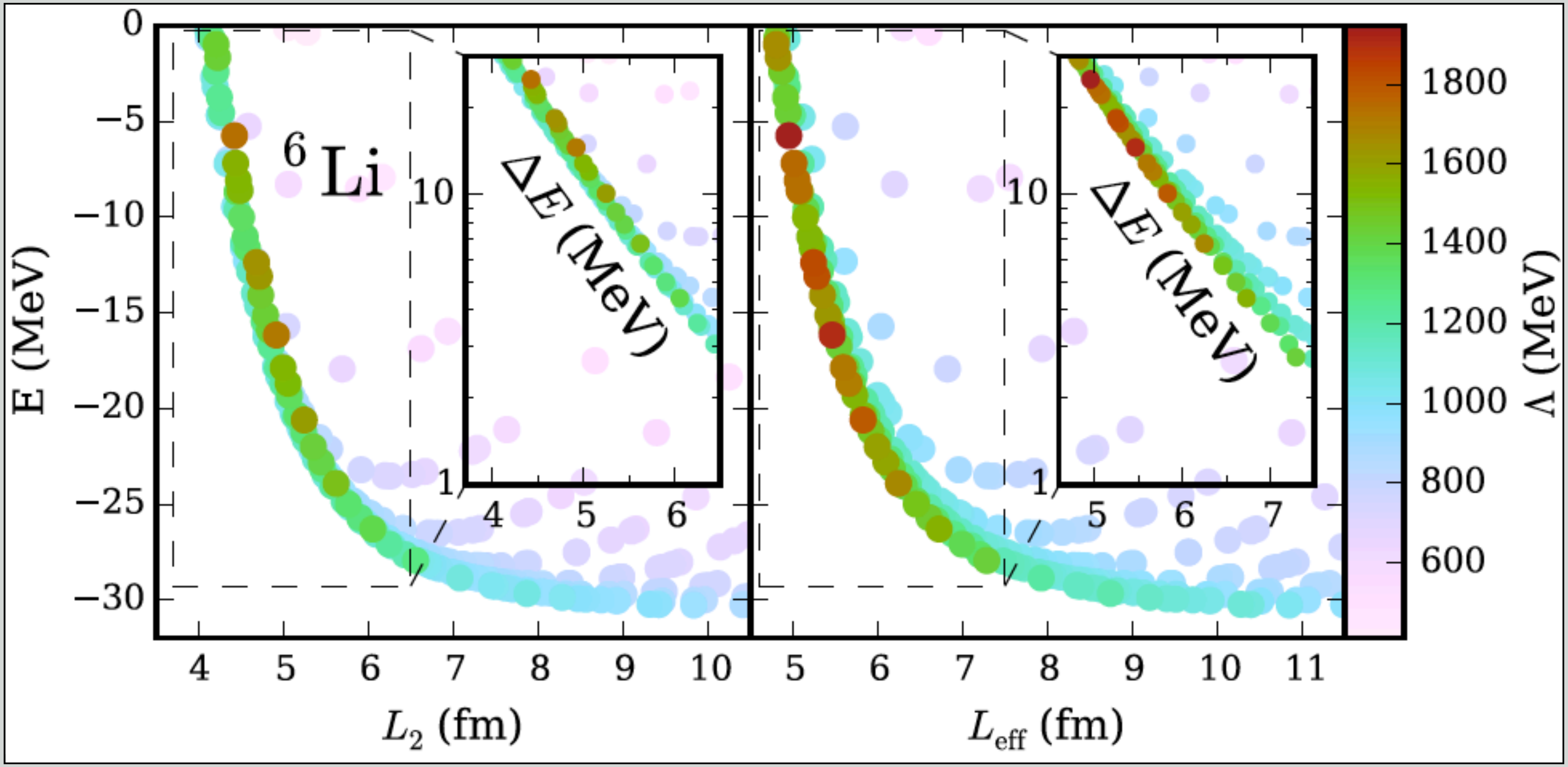
$$L_{\rm eff} = b\frac{X_{1,\mathcal{L}}}{\sqrt{T_{1,\mathcal{L}}(N_{\rm max}^{\rm tot})}}$$

More, Ekström, Furnstahl, Hagen, Papenbrock, PRC 87, 044326 (2013)

Furnstahl, Hagen, Papenbrock, Wendt, J. Phys. G 42, 034032 (2015)

Wendt, Forssén, Papenbrock, Sääf, PRC 91, 061301(R) (2015)

IR length in NCSM spaces



Diagonalize kinetic energy in 3(A-1) dimensional harmonic oscillator; seek lowest antisymmetric state and equate to hyperspherical cavity with radius Leff.

Wendt et al. (2015)

A practical approach to IR extrapolations

- In practice it is often challenging to fulfill:
  1. ... being UV converged
  2. ... reaching asymptotically large values of $k_\infty L$
- Moreover, we lack a physical interpretation of k_∞ for many-body systems.

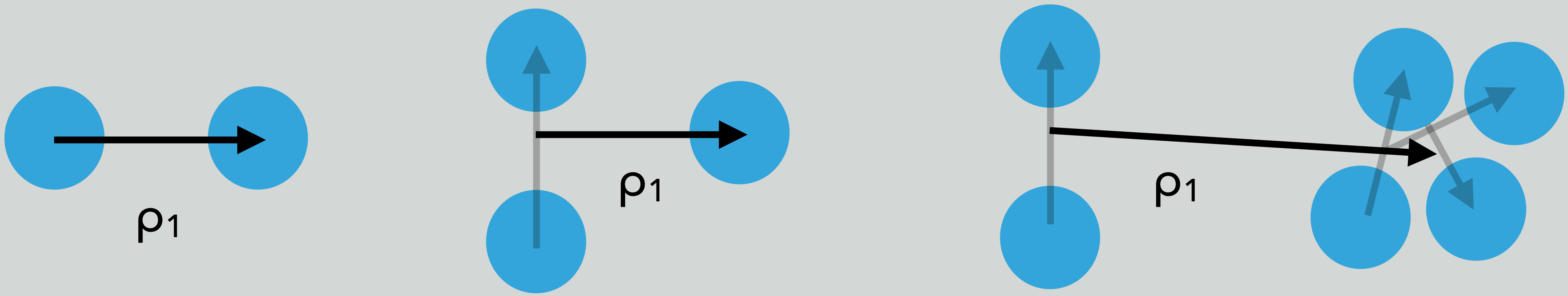
A practical approach to IR extrapolations

- Perform instead the extrapolation at a fixed (not necessarily UV converged) value of Λ
- The LO IR extrapolation becomes

$$E(L,\Lambda) = E_\infty(\Lambda) + a(\Lambda)\exp\left[-2k_\infty(\Lambda)L\right]$$

- Previous work on UV corrections [eg. Furnstahl et al. 2012] just represents a special case of this general formula.
- We treat $E_\infty(\Lambda)$, $a(\Lambda)$, $k_\infty(\Lambda)$ as fit parameters; and include also an estimated NLO correction as a weighting factor.

Hyperradial well, explains low-momentum scale



d=p+n $\quad$ ^{3}H=d+n $\quad$ ^{6}Li=d+^{4}He

NCSM: hyper-radial well

$$\vec{\rho}^{\,2} = \sum_{j=1}^{A-1} \vec{\rho}_j^{\,2}.$$

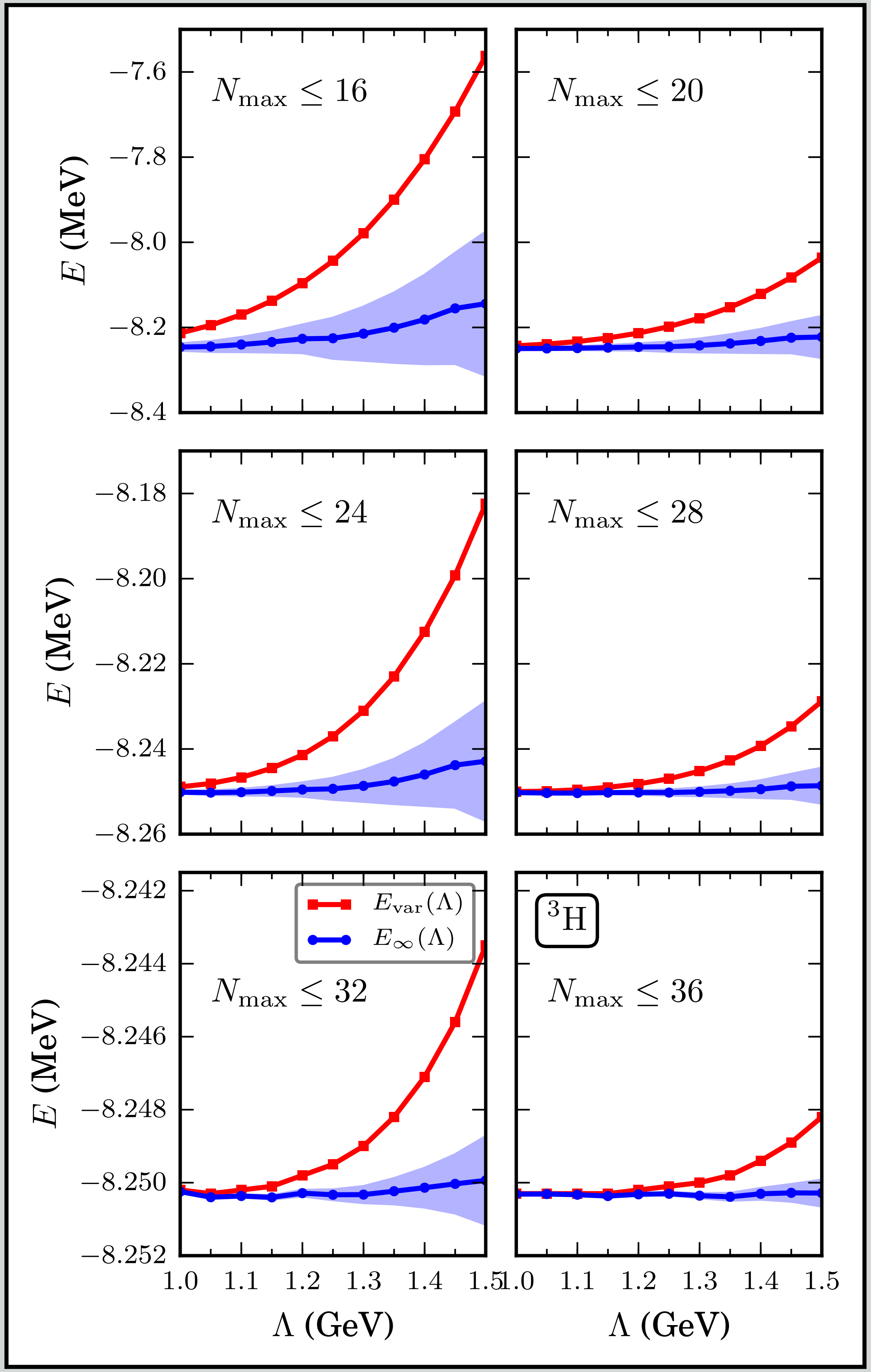
$$e^{-k_1|\vec{\rho}_1|}$$

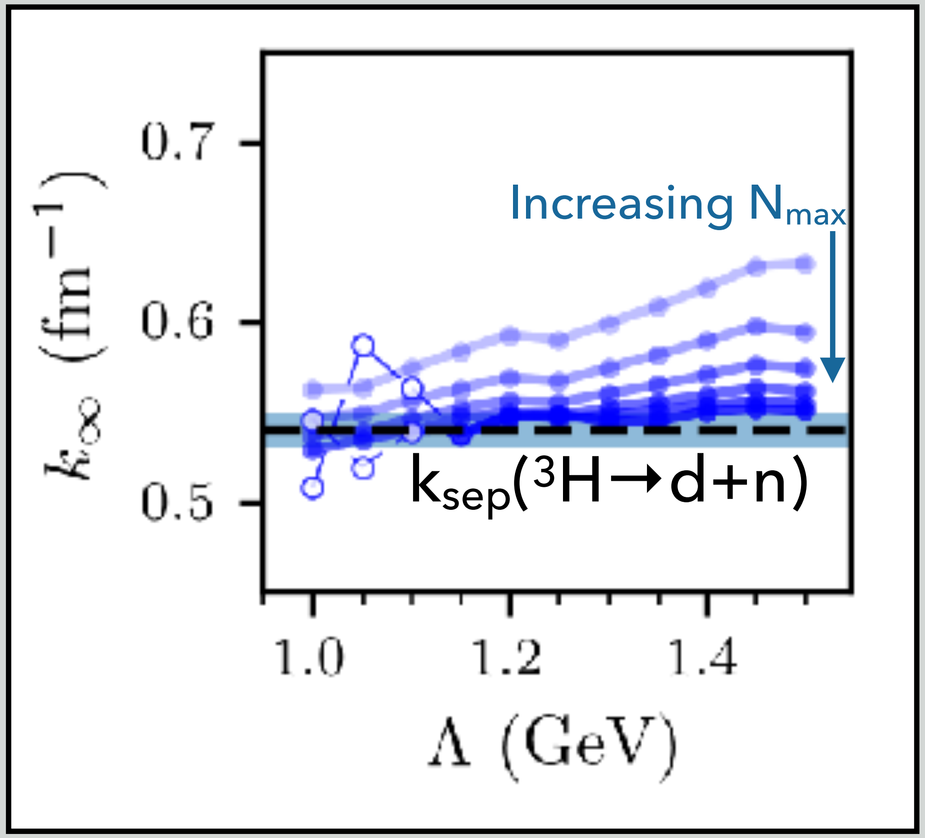
Separation energy for lowest threshold

$$S = \frac{\hbar^2 k_\infty^2}{2m}$$

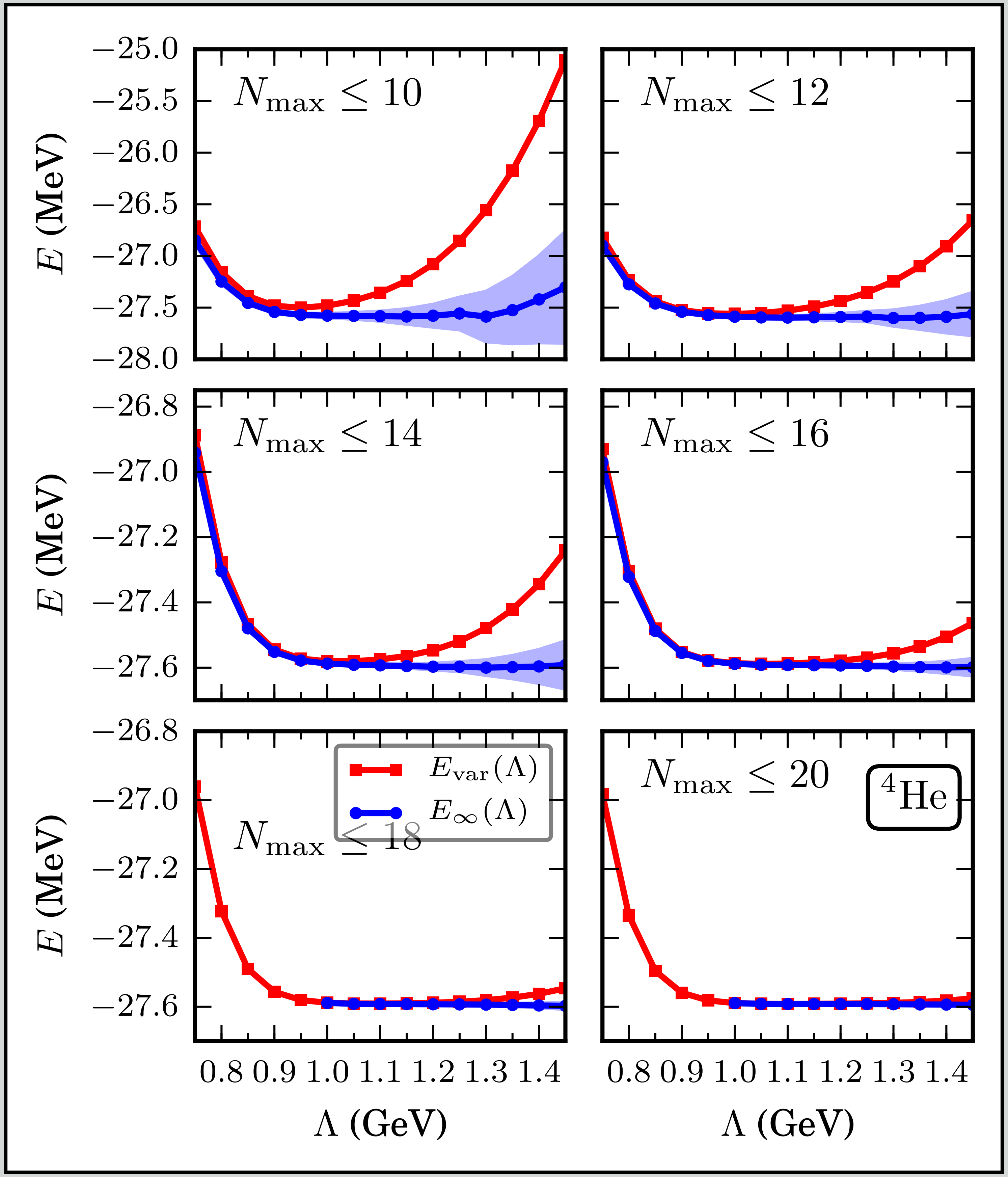
See also König and Lee, arXiv:1701.00279 for volume dependence of N-Body Bound States in lattice calculations.

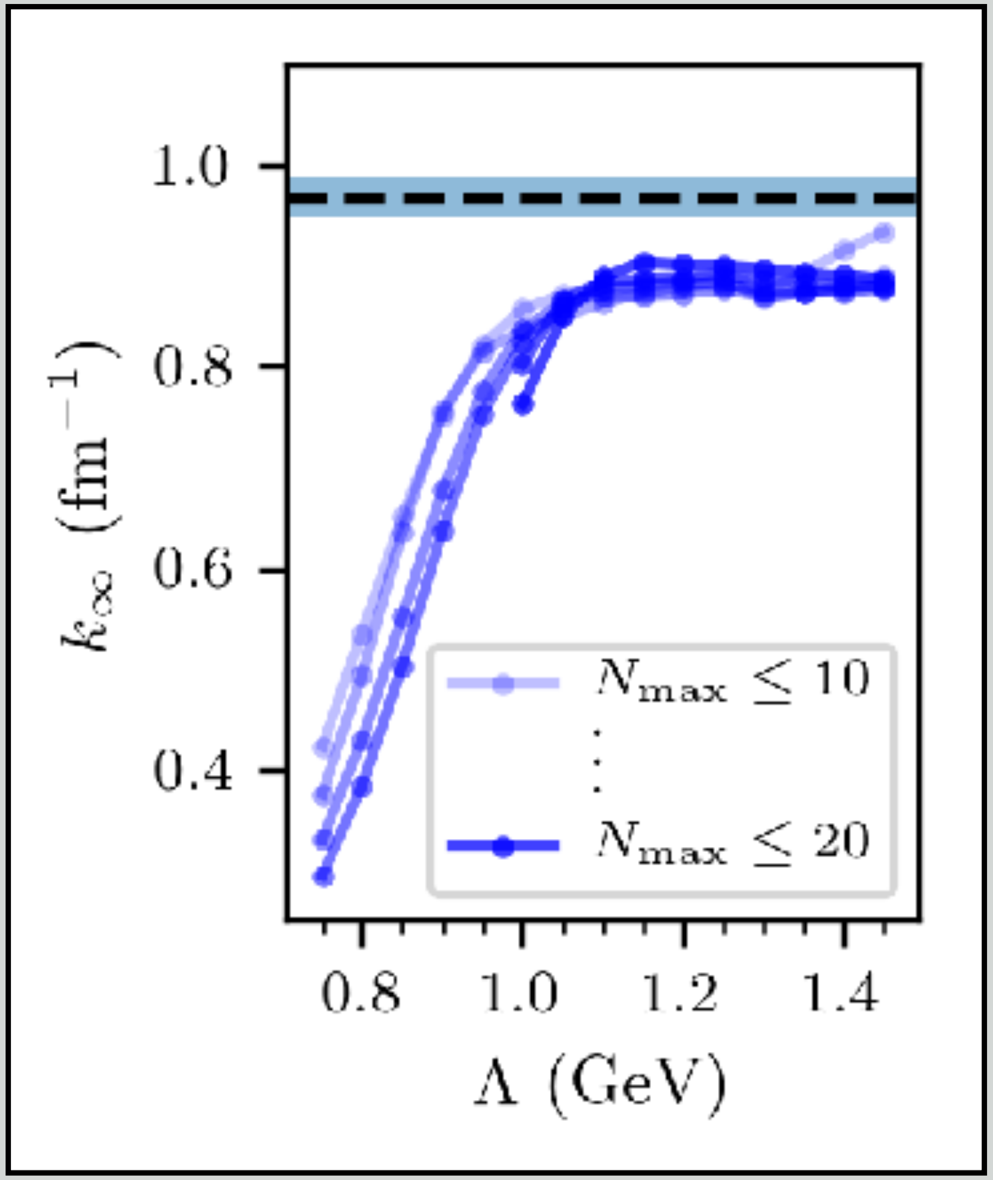
Results: A=3 — ground-state energy



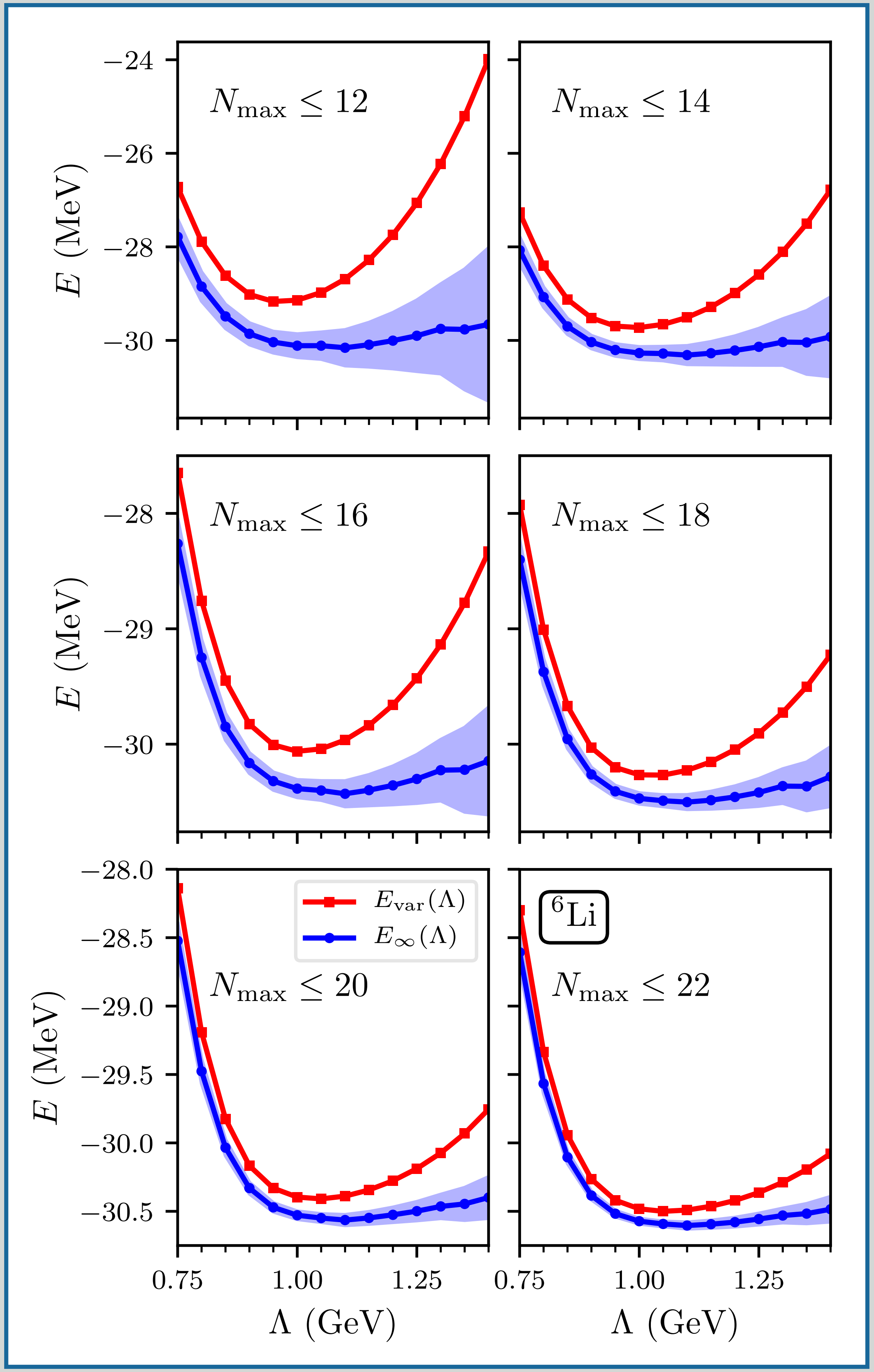


Results: A=4 — ground-state energy





Results: ^{6}Li — ground-state energy

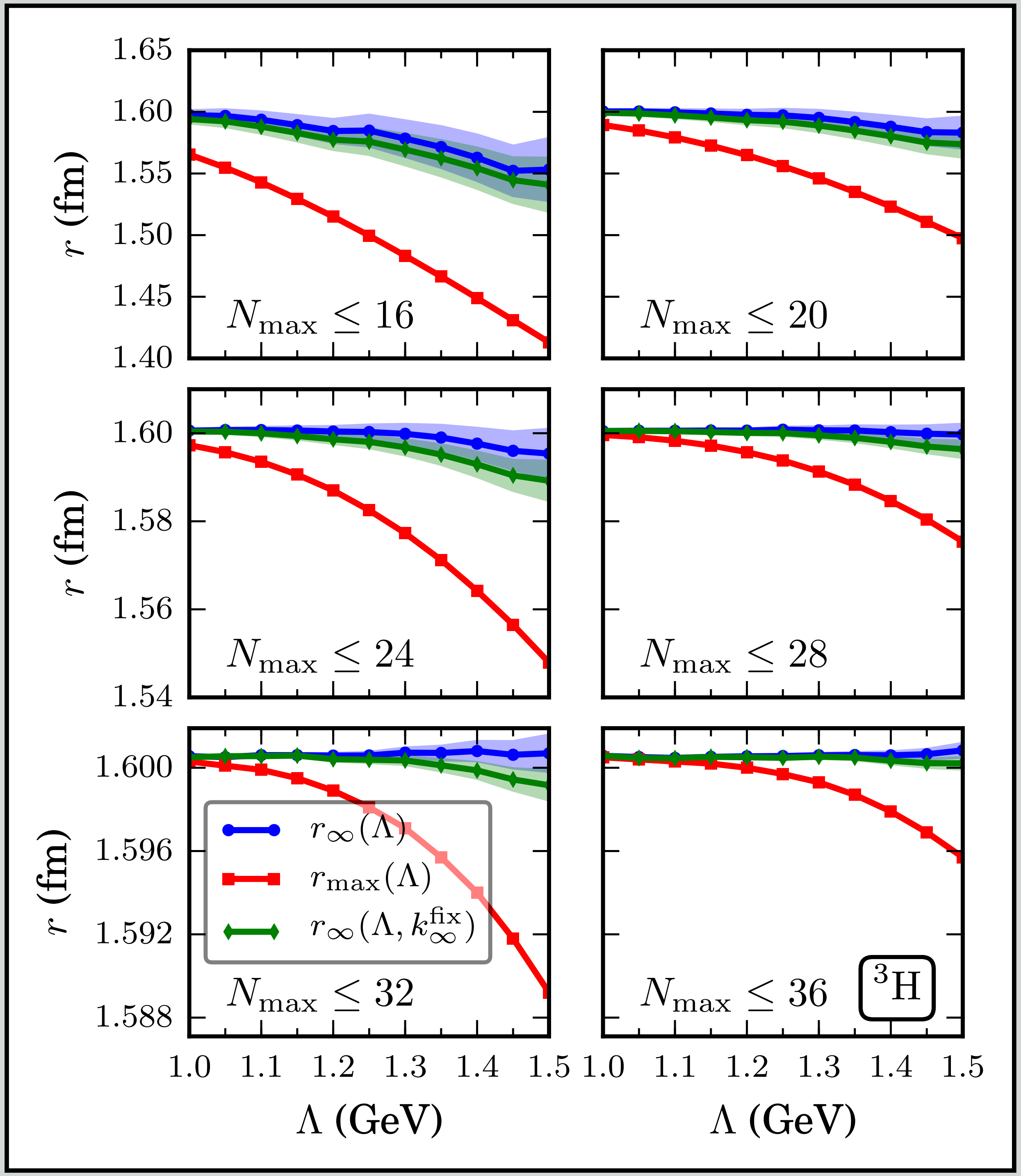


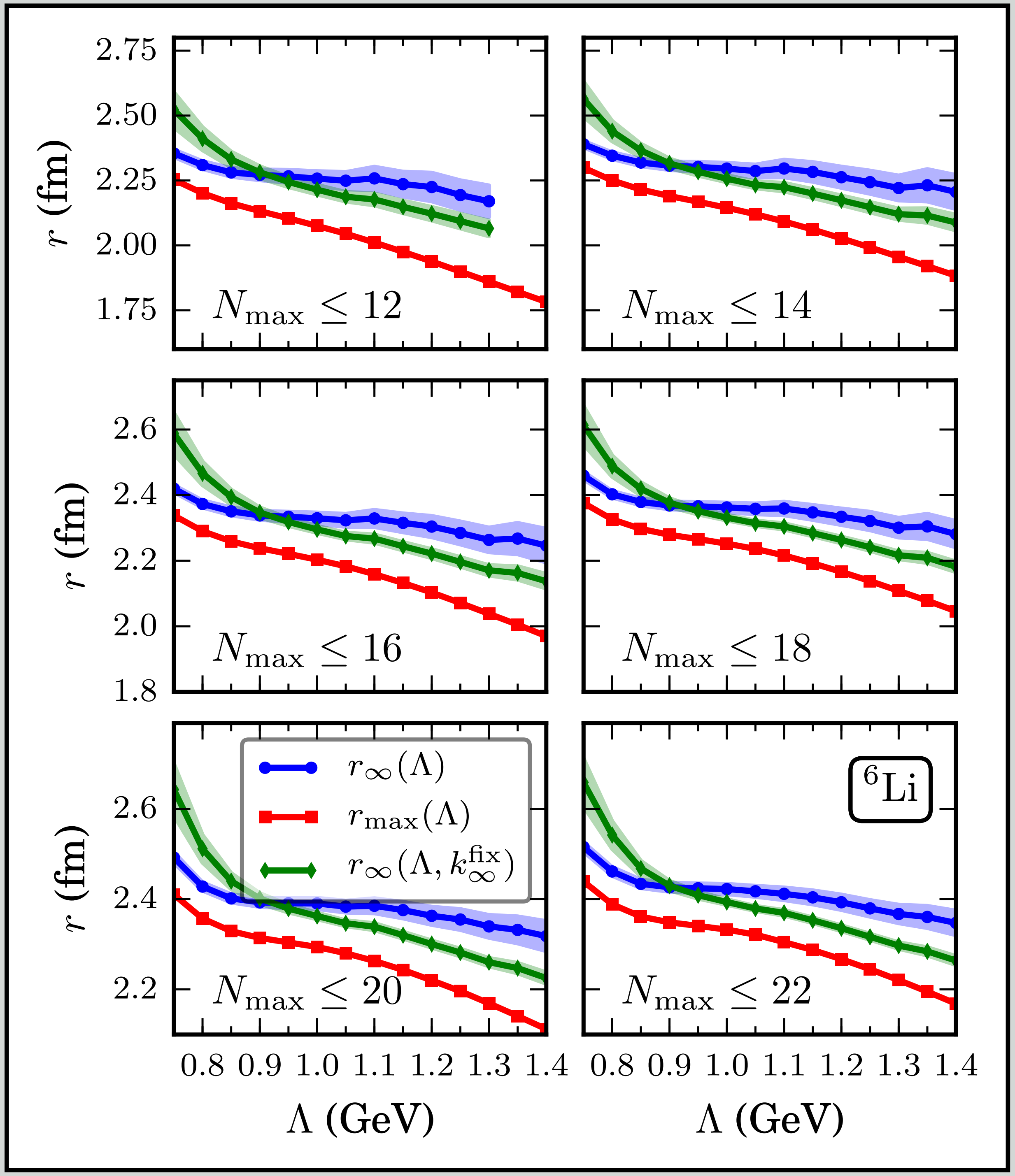
From extrapolation

From extracted threshold

Nucleus	Channel	k_∞	k_{sep}
^{3}H	d+n	0.54(1)	0.54(1)
^{3}He	d+p	0.51(2)	0.51(1)
^{4}He	^{3}H+p	0.84(5)	0.97(3)
^{6}Li	^{4}He+d	0.44(5)	0.19(8)

Results: ^{3}H, ^{6}Li — point-proton radii





Acknowledgments

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