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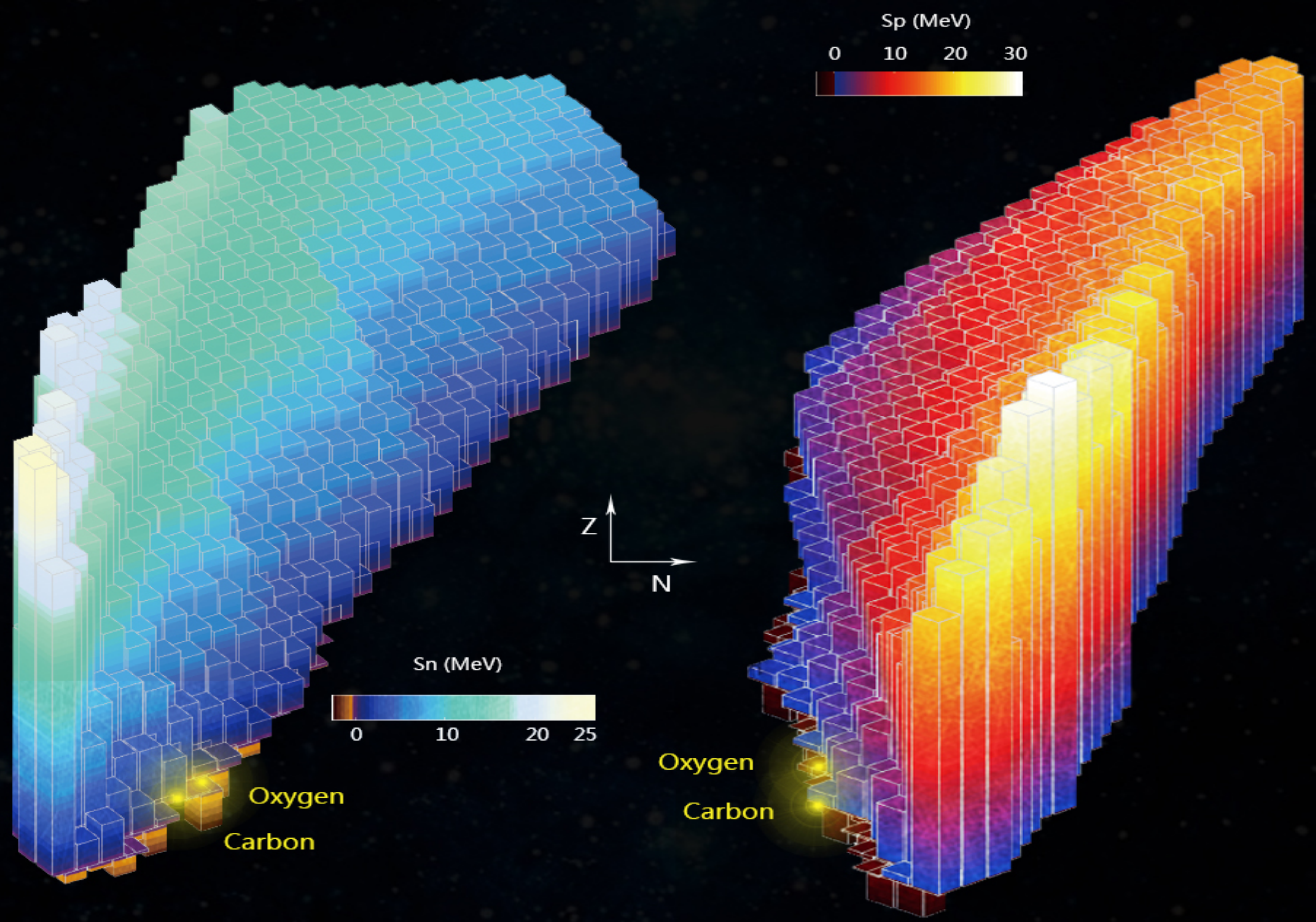
Arthur B. McDonald
Canadian Astroparticle Physics Research Institute

2nd Joint Canada-APCTP Meeting on Nuclear Theory

In-medium similarity renormalization group with resonance and continuum



Bai-Shan Hu (胡柏山)
Aug 9, 2022
@ TRIUMF

Outline

I. What is IMSRG?

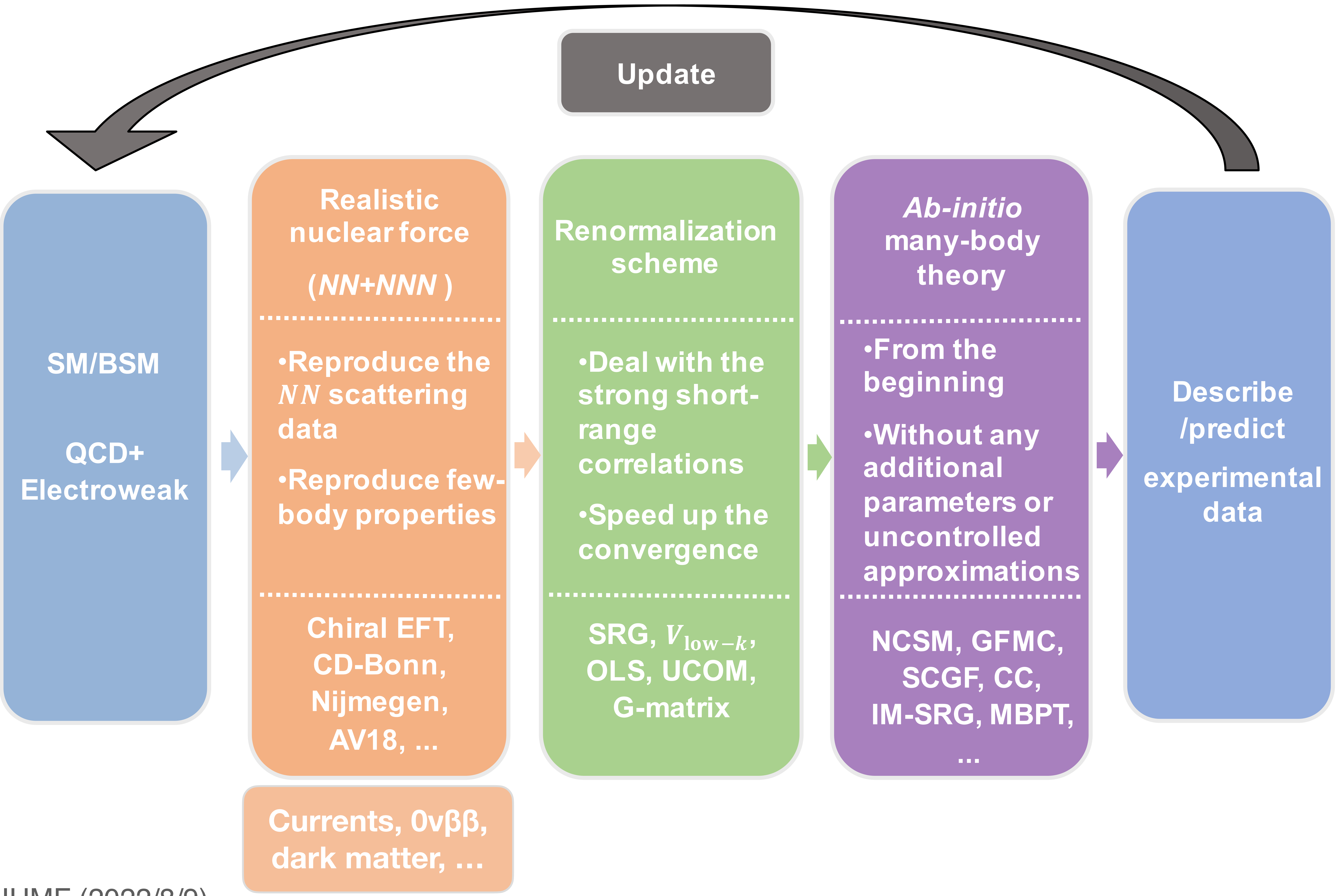
II. Why continuum?

III. How to include continuum into IMSRG

- resonance
- halo

IV. Summary

Workflow of *ab-initio* nuclear calculation



Similarity Renormalization Group

drive the Hamiltonian towards a band- or block-diagonal form via continuous unitary transformation

$$U(s) \cdot U^{\dagger}(s) = U(s) \cdot U^{-1}(s) = 1$$

$$H(s) = U(s) H(0) U^{\dagger}(s)$$

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$

$$\eta(s) = \frac{dU(s)}{s} U^{\dagger}(s) = -\eta^{\dagger}(s)$$

$$O(s) = U(s) O U^{\dagger}(s)$$

- **Developed by Glazek and Wilson and by Wegner around in 1993**

  S. D. Glazek and K. G. Wilson, Phys. Rev. D 48, 5863 (1993)
  F. Wegner, Ann. Phys. (Leipzig) 3, 77 (1994)

- **Soften nucleon-nucleon interaction from 2007**

  S.K. Bogner, R.J. Furnstahl, R.J. Perry, Phys. Rev. C 75, 061001 (2007)
  H. Hergert and R. Roth, Phys. Rev. C 75, 051001(R) (2007)

- **In-medium SRG as a nuclear many-body method**

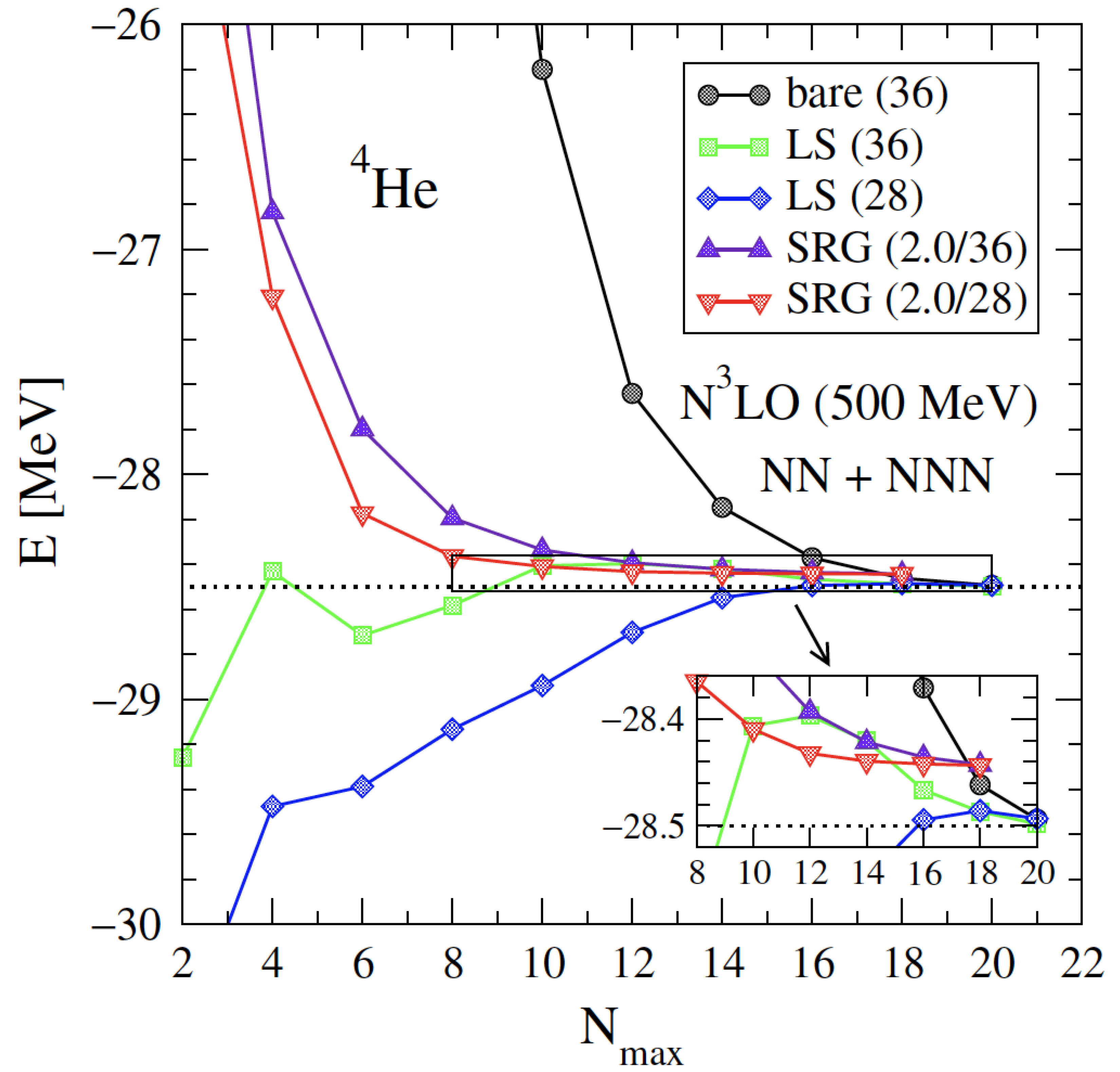
  Tsukiyama, S. K. Bogner, and A. Schwenk, PRL106, 222502 (2011); PRC85, 061304(R) (2012)
  H. Hergert, *et al.*, PRL**110**, 242501 (2013)
  S.R. Stroberg, *et al.*, Phys. Rev. Lett. 118, 032502 (2017)

SRG: soften nuclear interaction

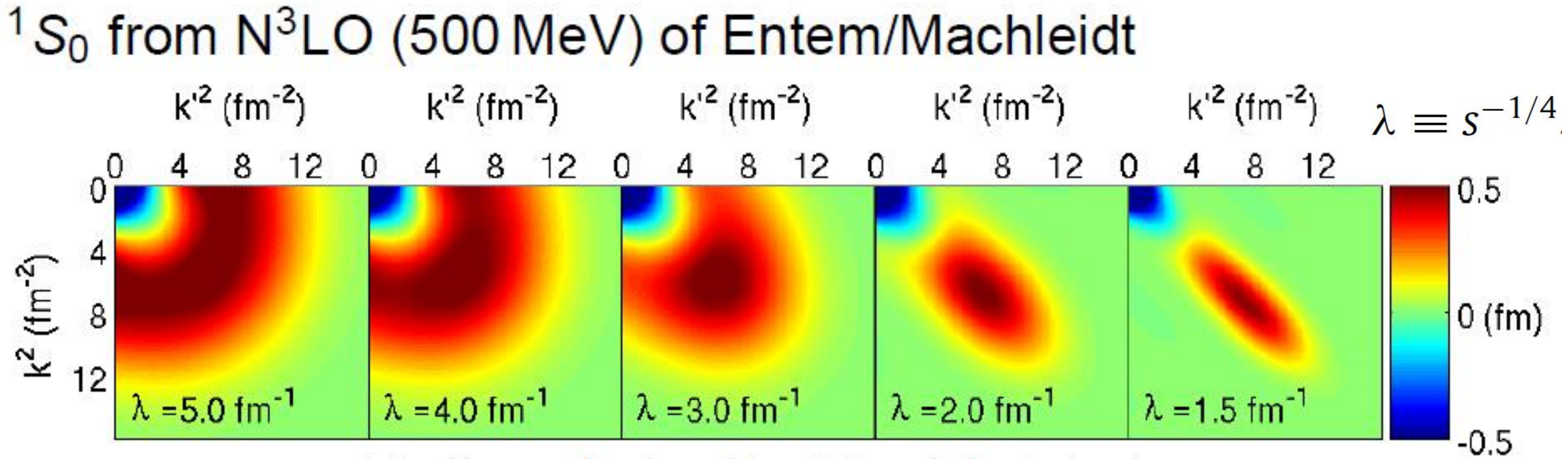
$$H(s=0) = T_{\text{rel}} + V \qquad \eta(s) = [T_{\text{rel}}, H(s)]$$

$$\frac{dH(s)}{ds} = [\eta(s), H(s)] \qquad \frac{dH(s)}{ds} = \left[[T_{\text{rel}}, H(s)], H(s)\right]$$

$$\frac{dV_s(k,k')}{ds} = -\left(k^2 - k'^2\right)^2 V_s(k,k') + \frac{2}{\pi}\int_0^\infty q^2 dq \left(k^2 + k'^2 - 2q^2\right) V_s(k,q) V_s(q,k')$$



E. D. Jurgenson, P. Navrátil, and R. J. Furnstahl, PRL**103**, 082501 (2009)



http://www.physics.ohio-state.edu/~ntg/srg/

In-Medium SRG (IM-SRG)

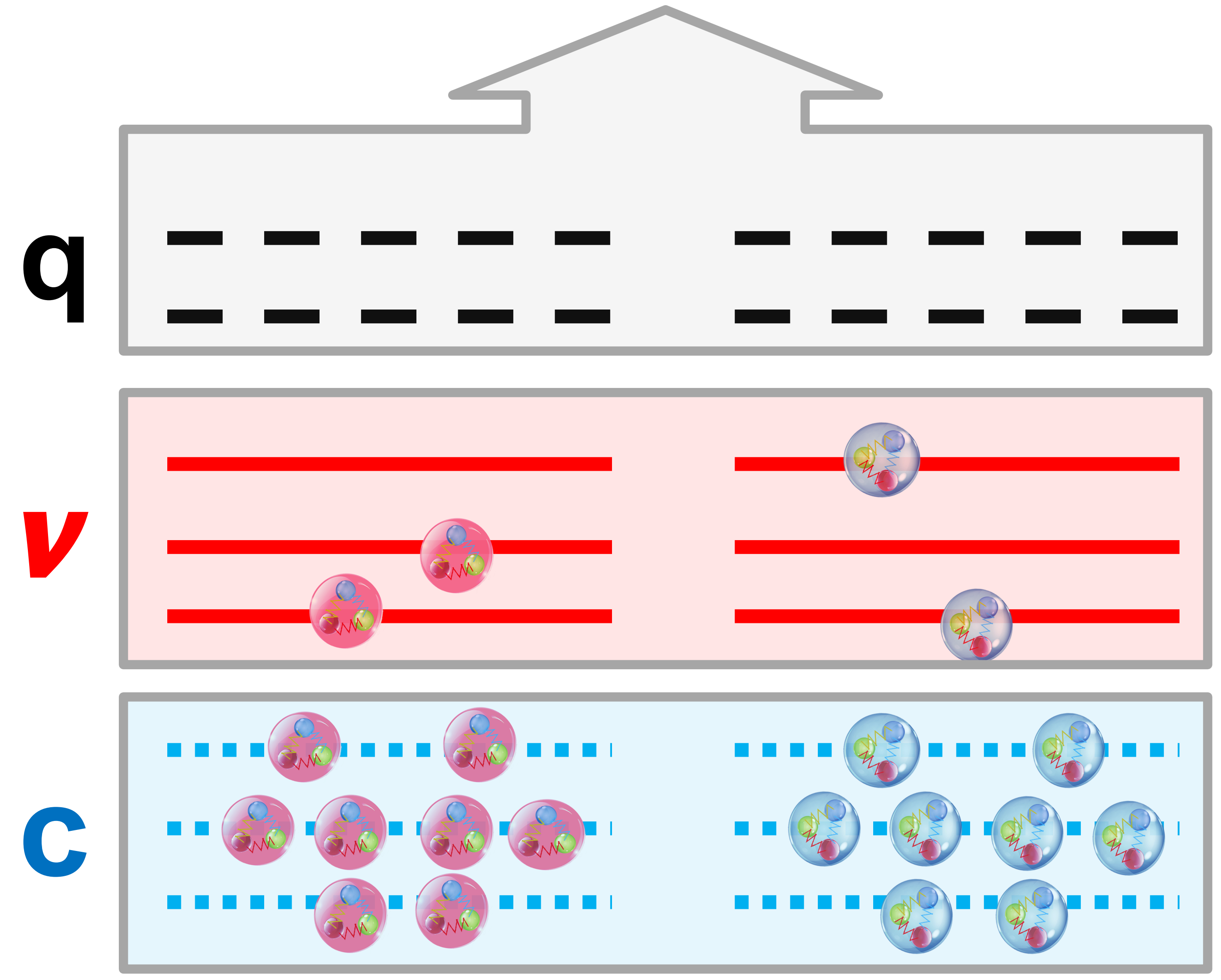
- ***H* is normal ordered with a finite-density reference state:**

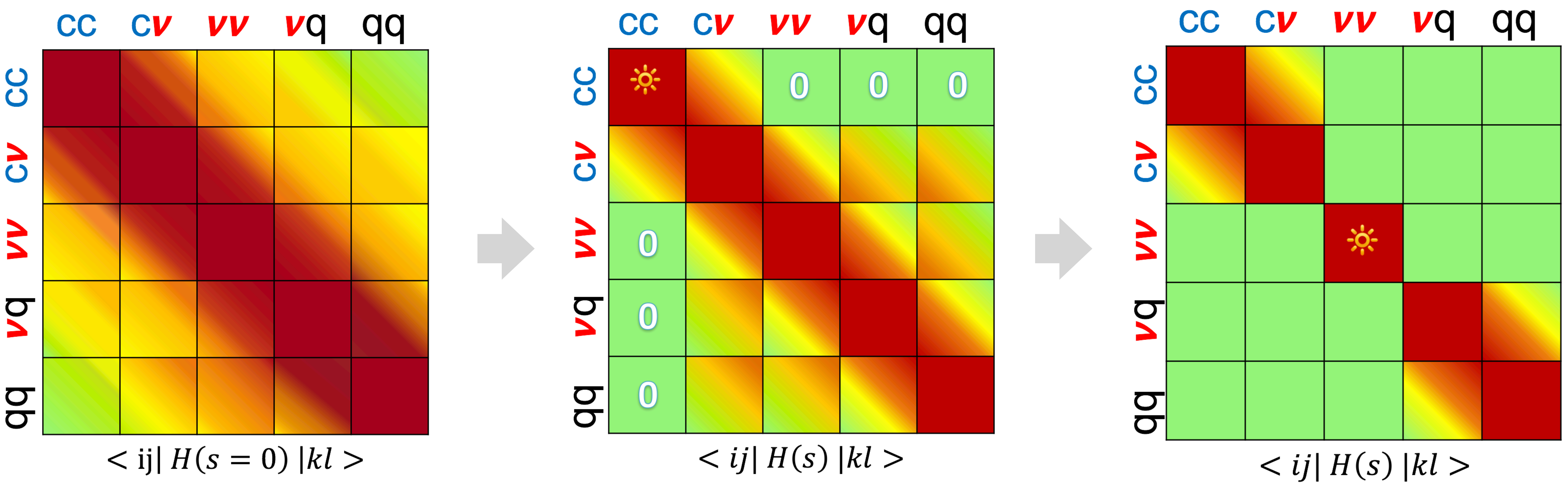
$$H = E_0 + \sum_{ij} f_{ij}\{a_i^\dagger a_j\} + \frac{1}{4}\sum_{ijkl}\Gamma_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36}\sum_{ijklmn} W_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

- **Generator:**

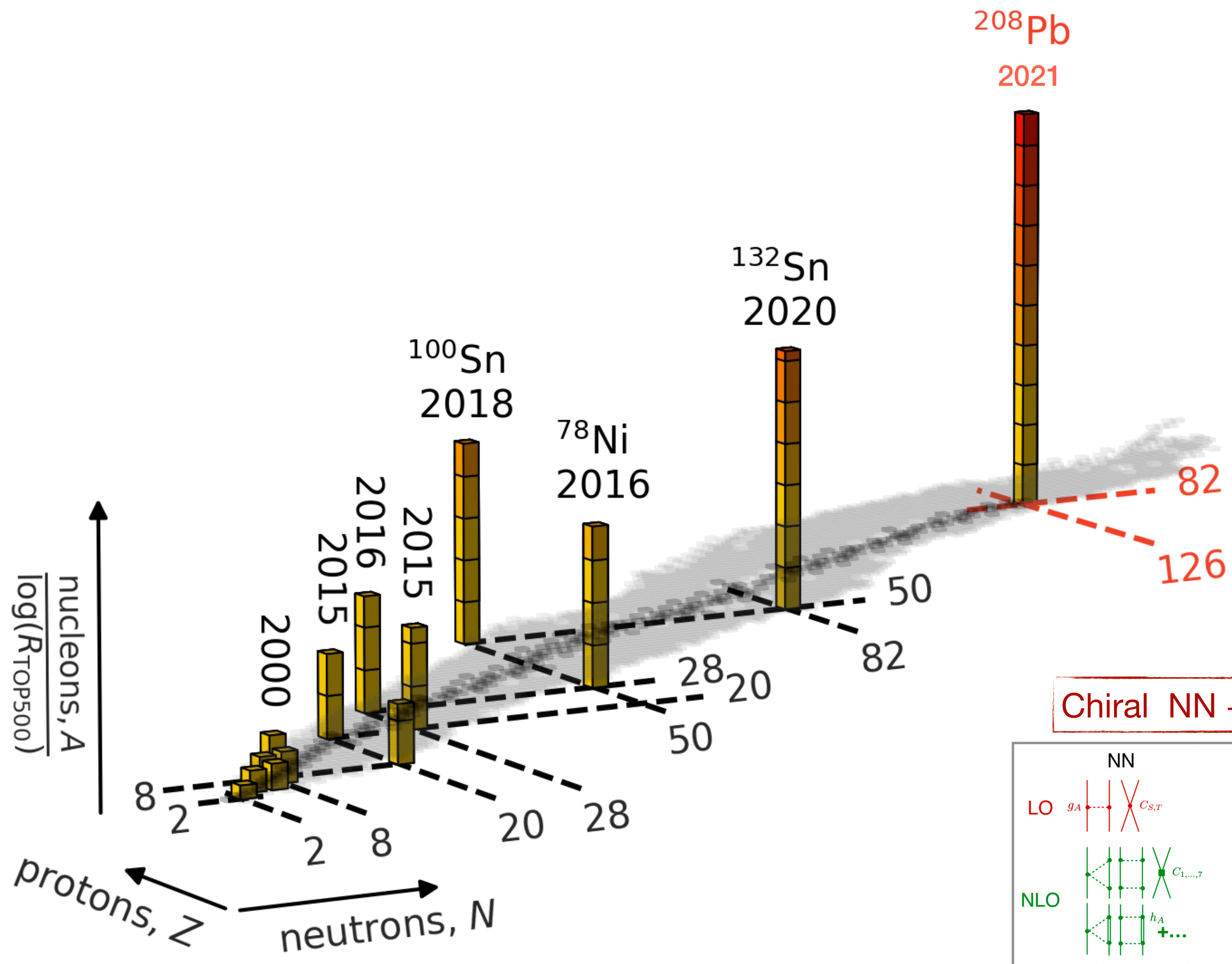
e.g.,

$$\eta(s) \equiv \sum_{ph}\frac{f_{ph}(s)}{\Delta_{ph}(s)}\{a_p^\dagger a_h\} + \sum_{pp'hh'}\frac{\Gamma_{pp'hh'}(s)}{\Delta_{pp'hh'}(s)}\{a_p^\dagger a_{p'}^\dagger a_{h'} a_h\} - H.c.$$

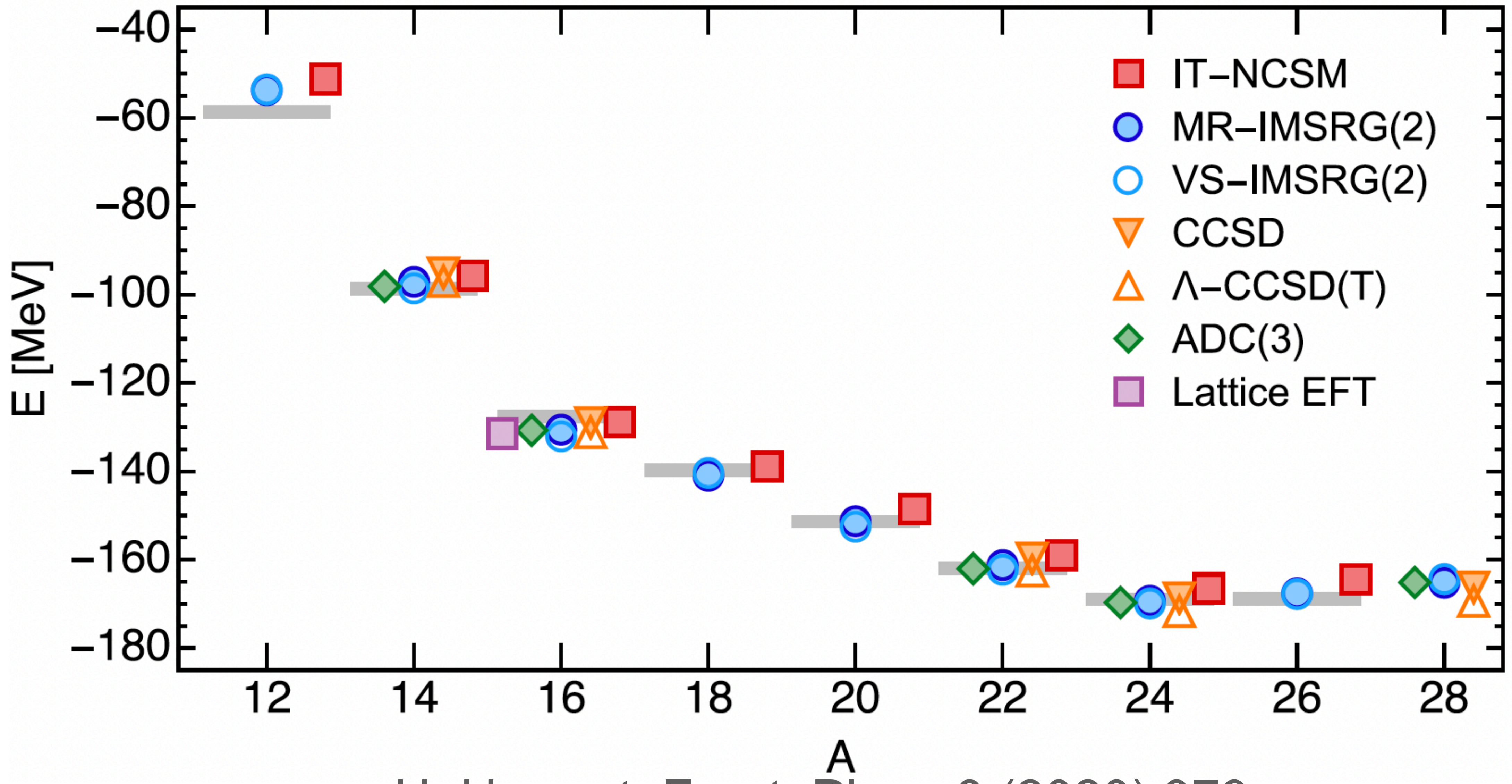




Ab initio results for ^{208}Pb region

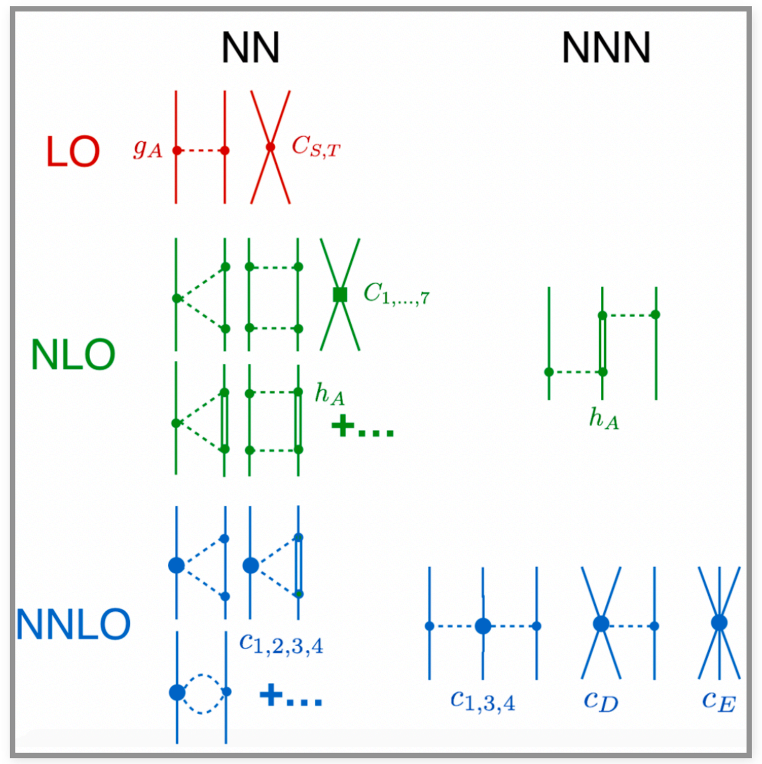


Precision of different methods: 1~2%



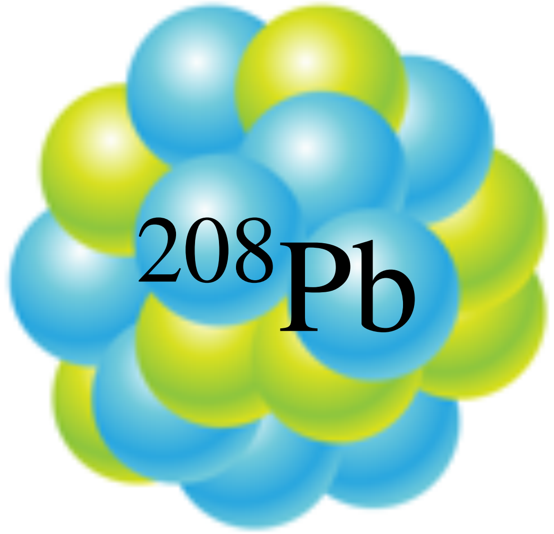
H. Hergert, Front. Phys. 8 (2020) 379

Chiral NN + 3N

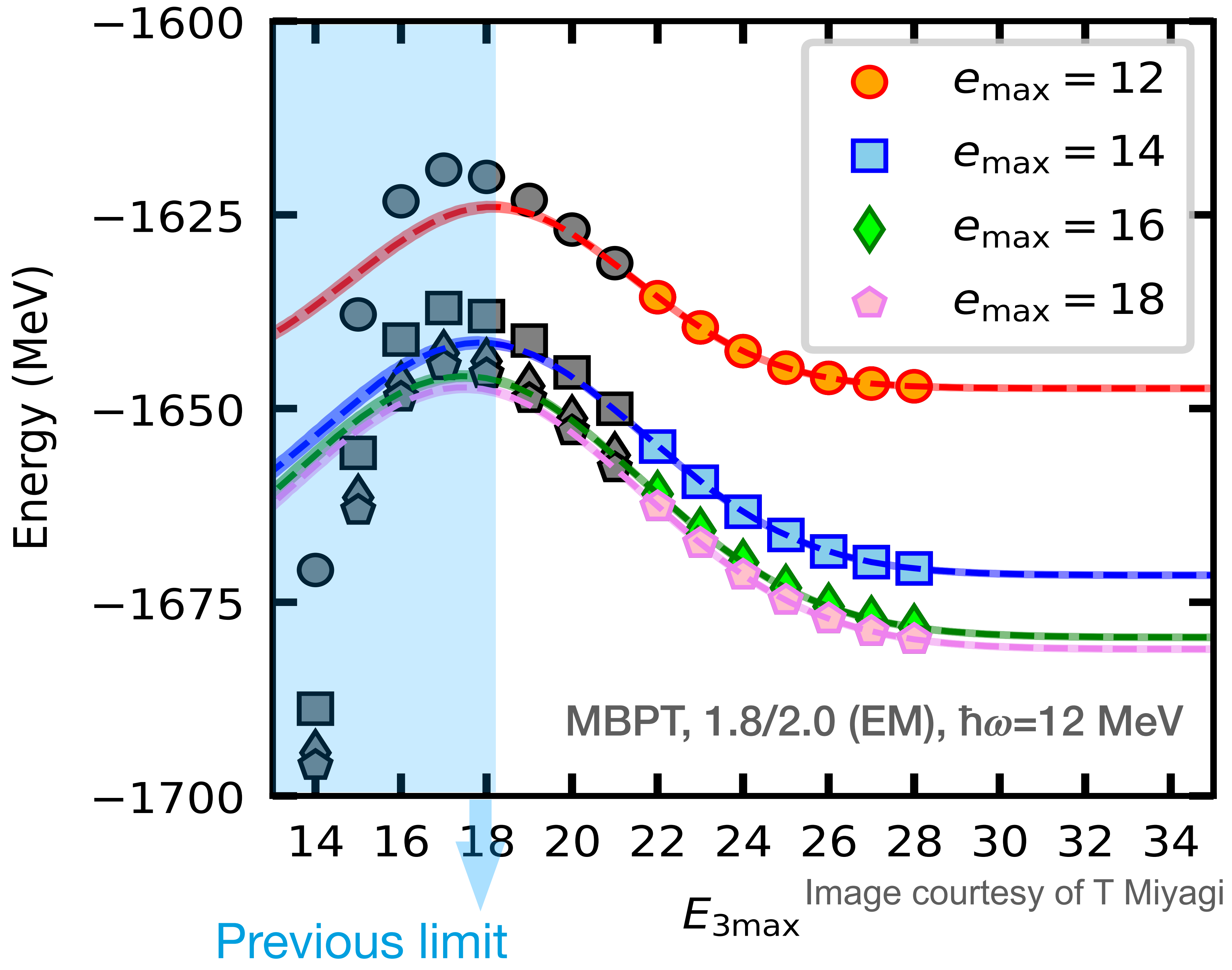


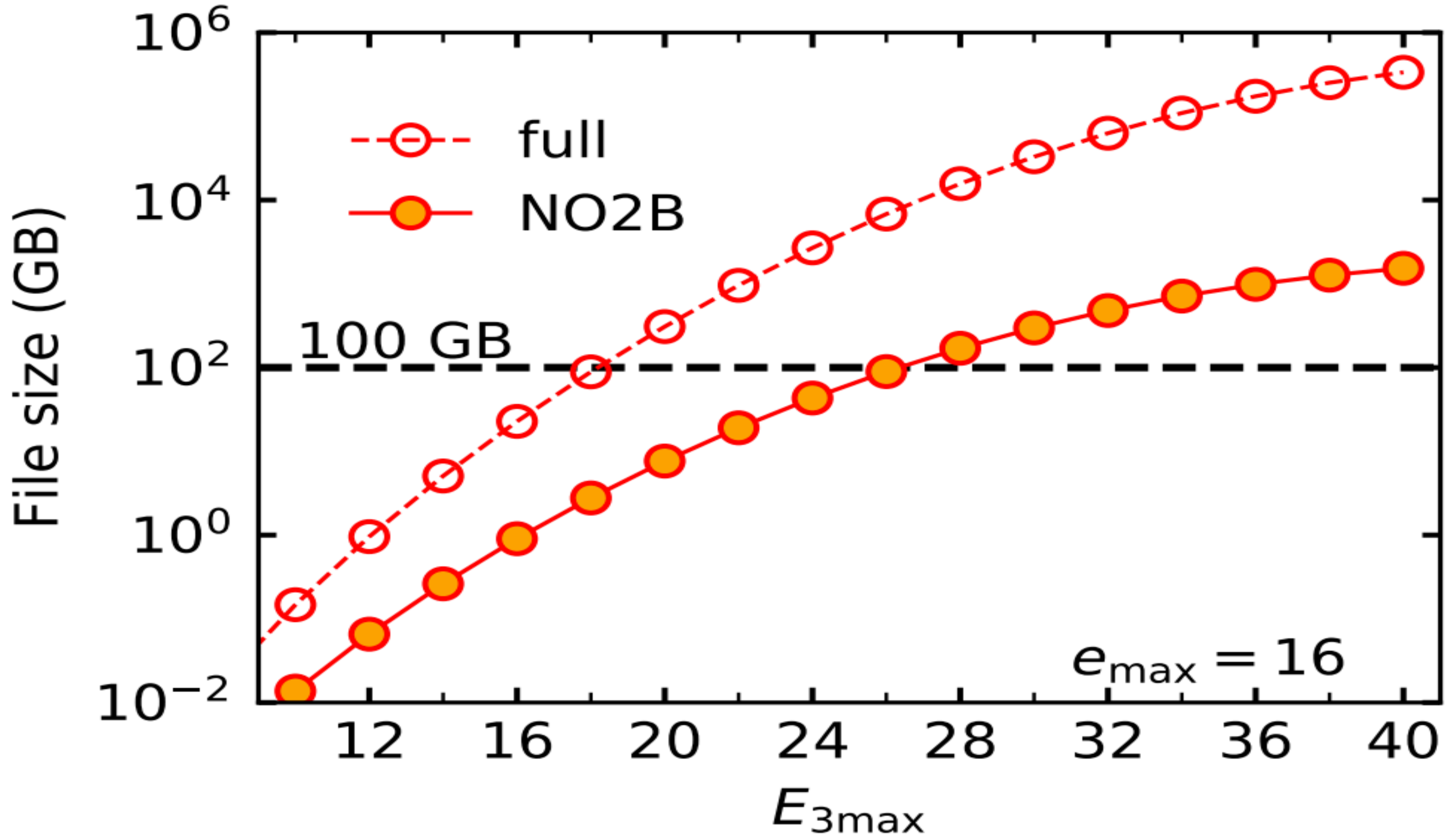
History matching
Emulator technology
Statistical tools

New 3N storage scheme
IMSRG, CC

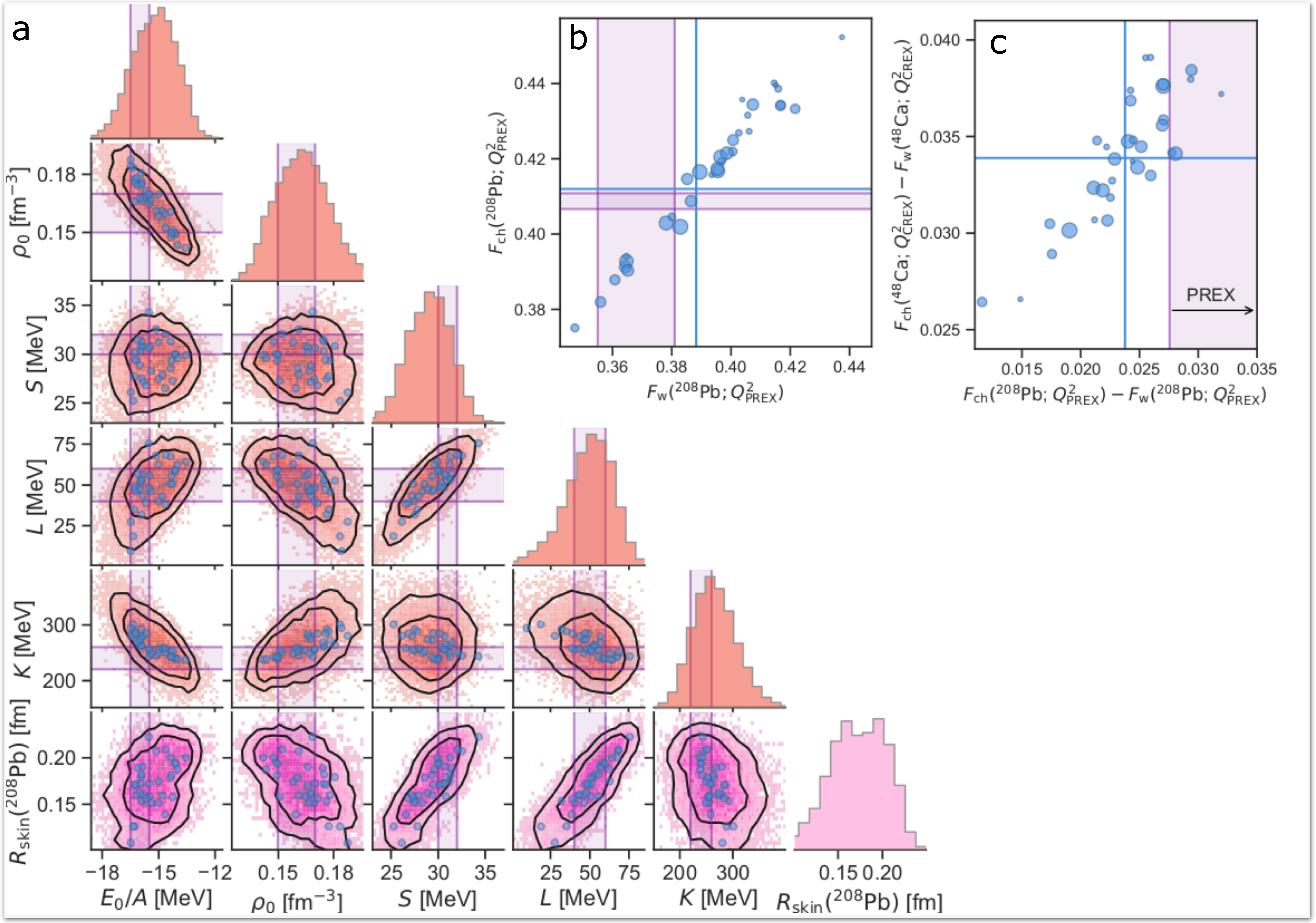


Ab initio calculation of ^{208}Pb



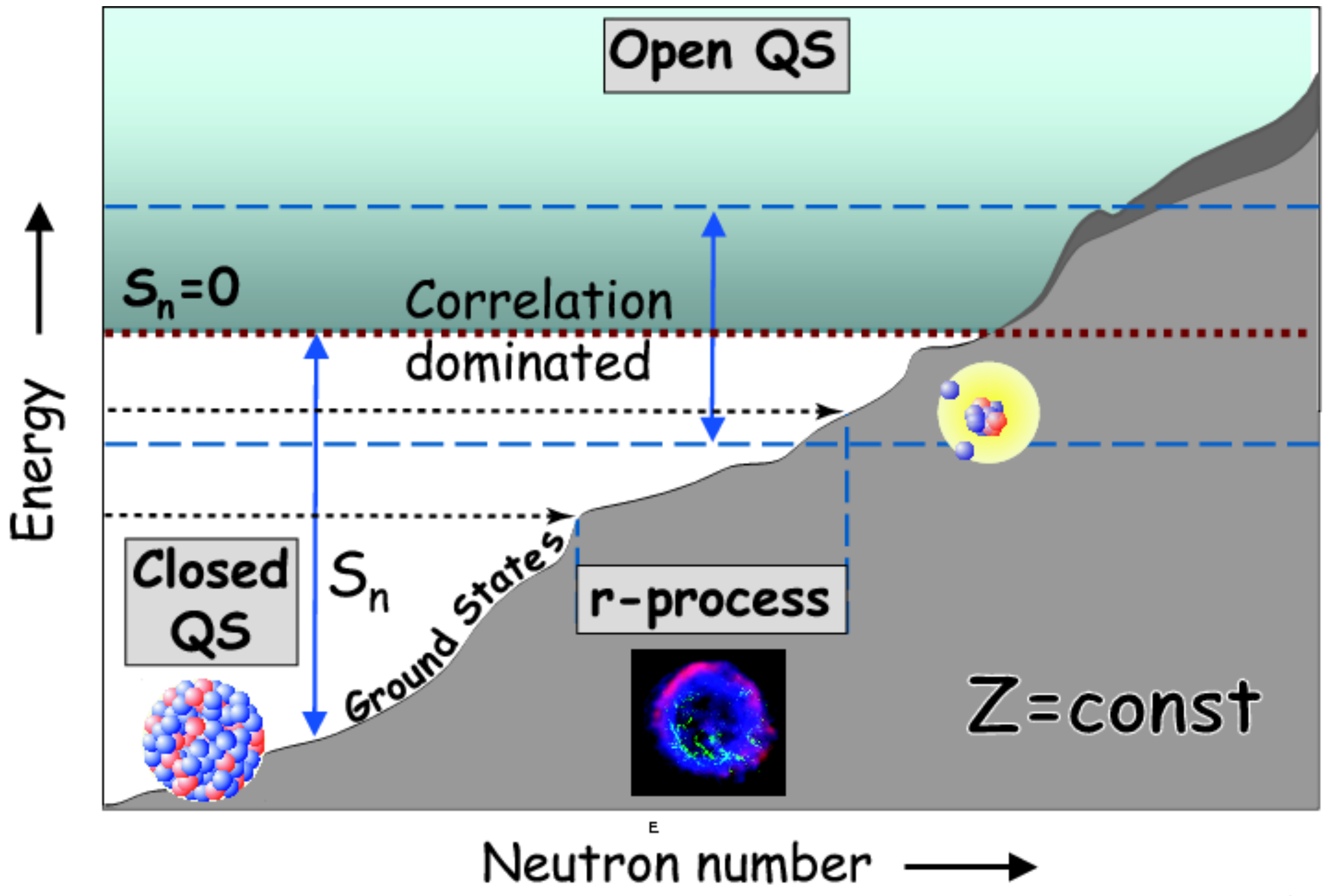


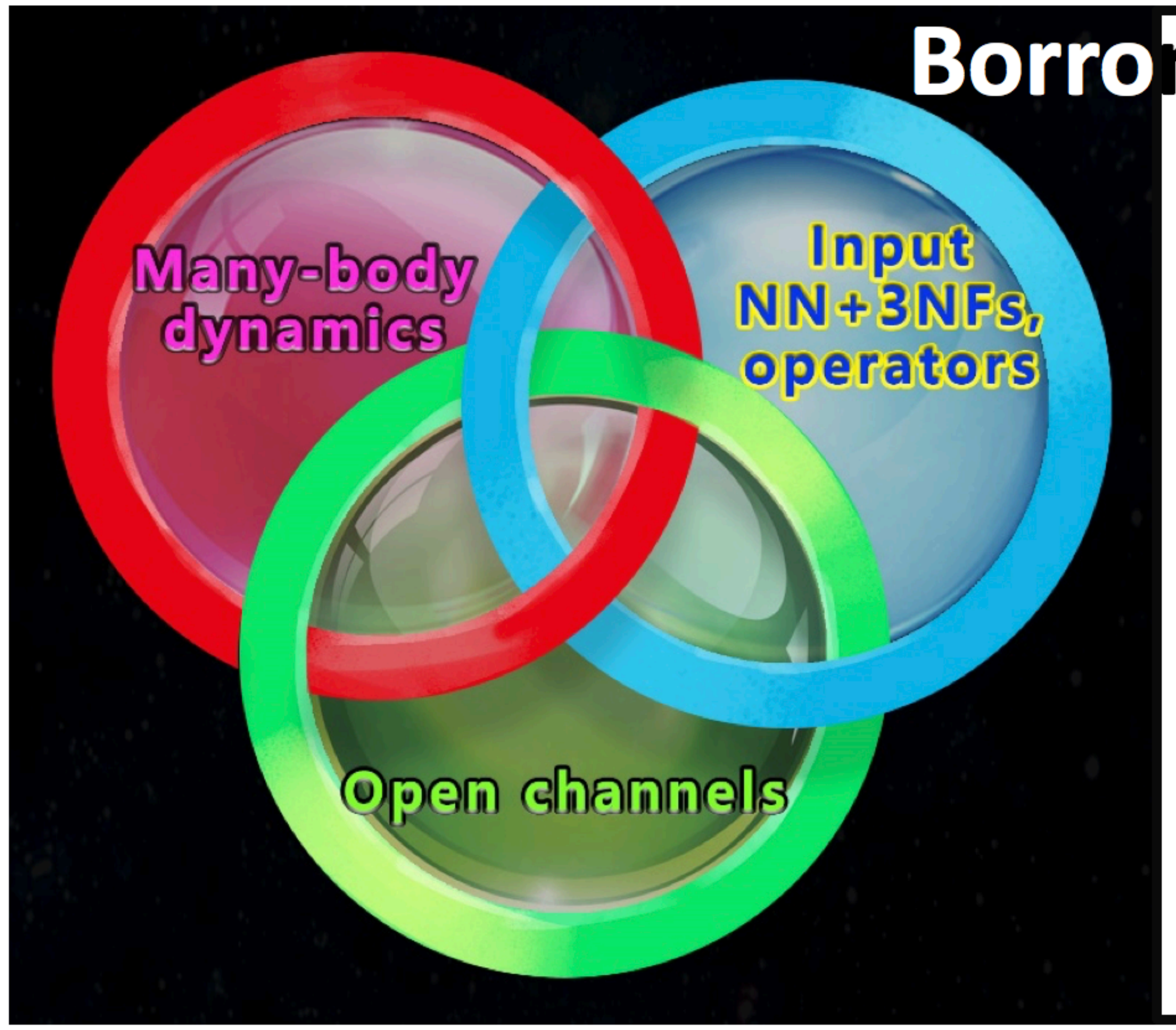
T Miyagi, *et al.*, PRC105 (2022) 014302



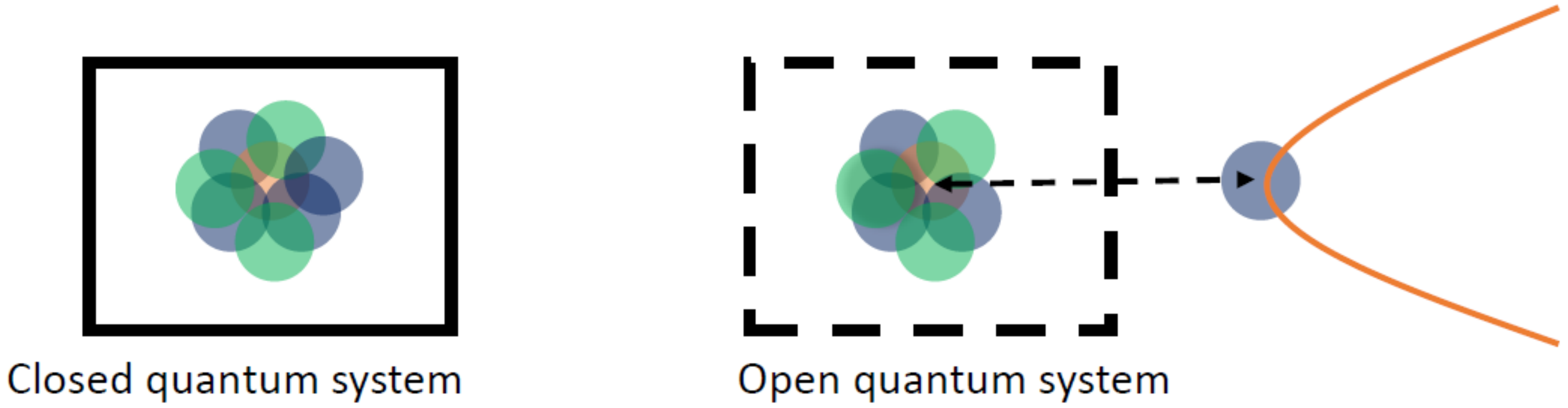
BS Hu, WG Jiang, T Miyagi, ZH Sun, *et al.*, Nat. Phys. (2022), in press.
arXiv:2112.01125v1 (2021)

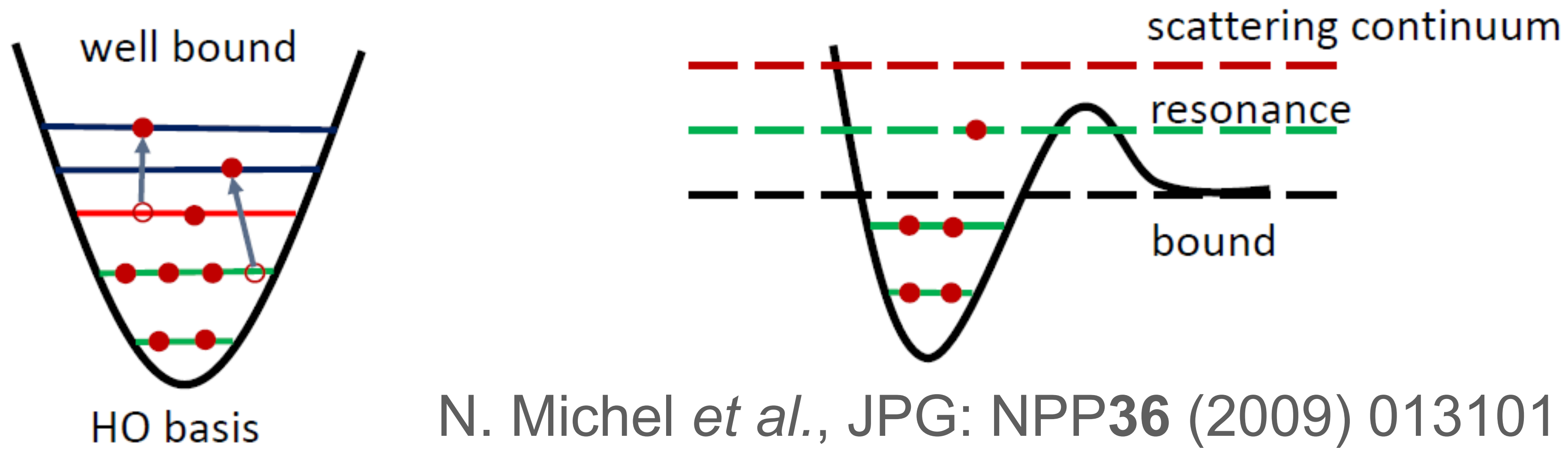
Nucleus as an open quantum system





- Neutron/Proton-rich nuclei
- Clustering
- New magic number
- Halo structure
- Genuine intrinsic resonance

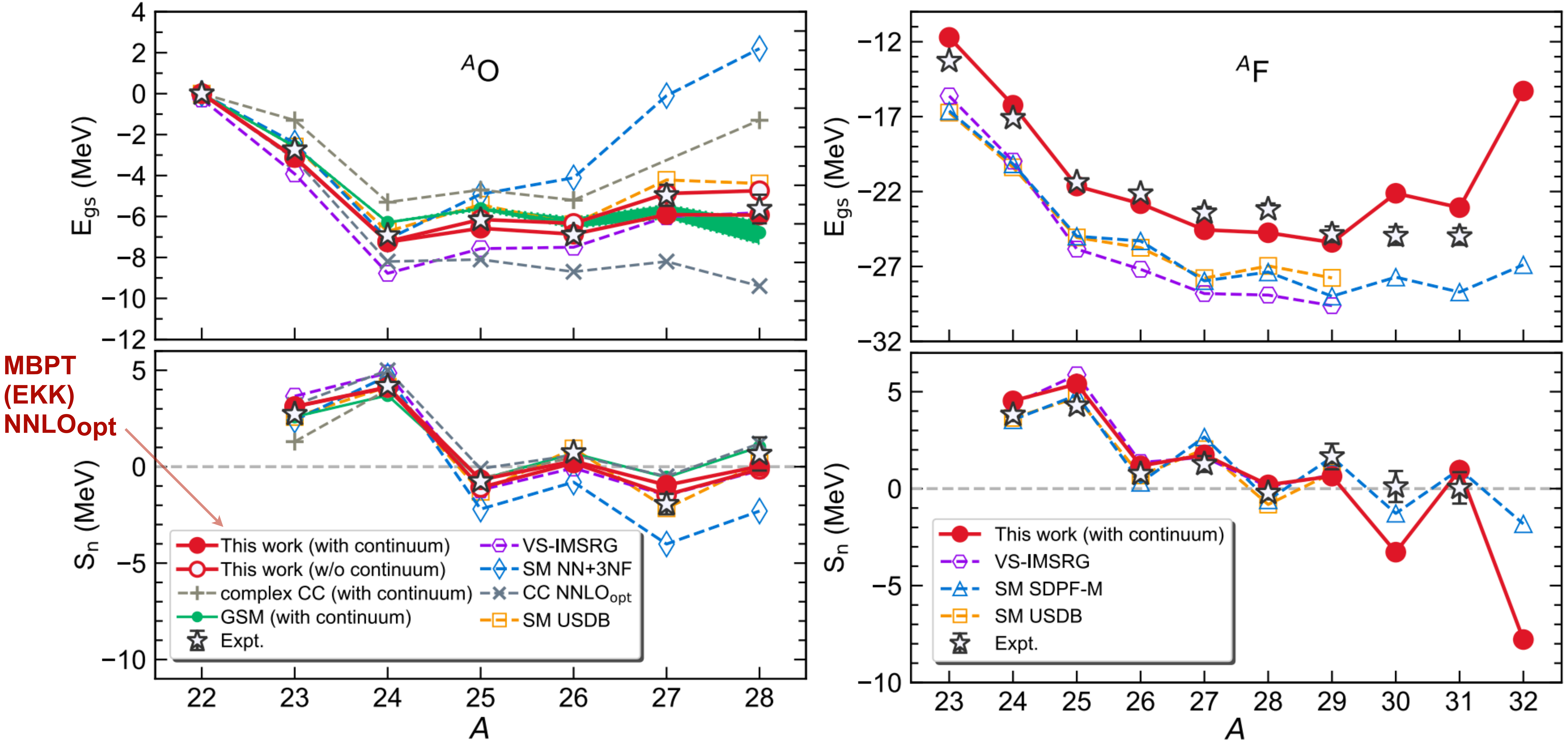




N. Michel *et al.*, JPG: NPP**36** (2009) 013101

- **Bound, resonant and scattering states may be strongly coupled**
- **Need *ab initio* nuclear theory including the continuum**

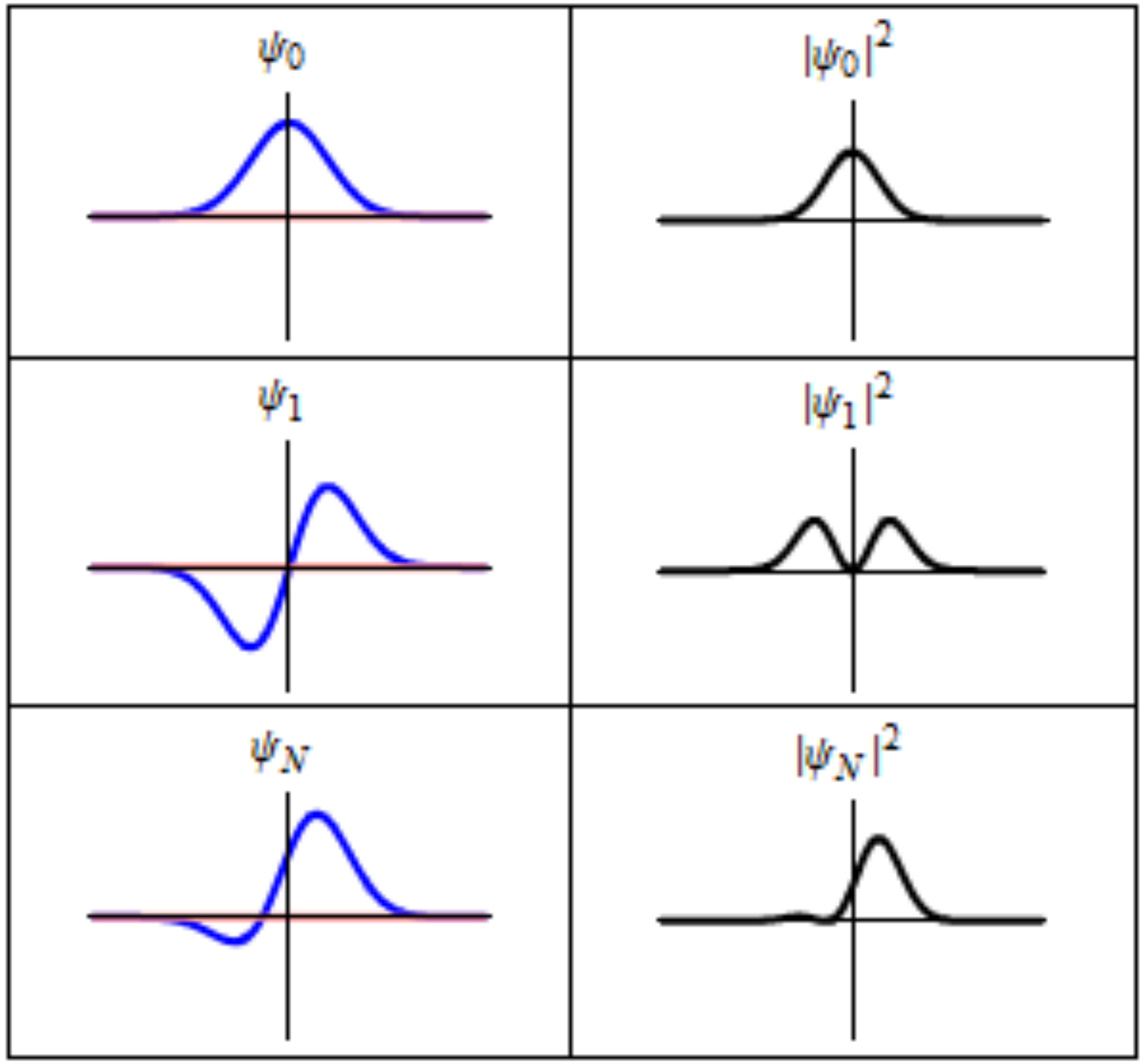
Why consider the continuum effect?



BSHu, Q. Wu, et al., PLB **802** (2020) 135206; arXiv:2001.02832

Resonances

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle$$



From Wikipedia

Time-independent:

$$H|\psi\rangle = E|\psi\rangle \qquad \psi(t,\boldsymbol{r}) = \exp\left(-\frac{iE}{\hbar}t\right)\psi(0,\boldsymbol{r})$$

probability at ***r*** is unchanged over time

Complex energy: $E = E_0 - i\frac{\Gamma}{2}$

$$|\psi(t,\boldsymbol{r})|^2 = \left|\exp\left(-\frac{iE_0}{\hbar}t\right)\exp\left(-\frac{\Gamma}{2\hbar}t\right)\psi(0,\boldsymbol{r})\right|^2$$

$$= \exp\left(-\frac{\Gamma}{\hbar}t\right)|\psi(0,\boldsymbol{r})|^2$$

Describe a resonance decaying exponentially with half-life $t_{1/2}=\hbar\ln 2/\Gamma$

Gamow-Berggren basis

- **The wave function of a resonance with a peak at energy e_0 and a width γ**

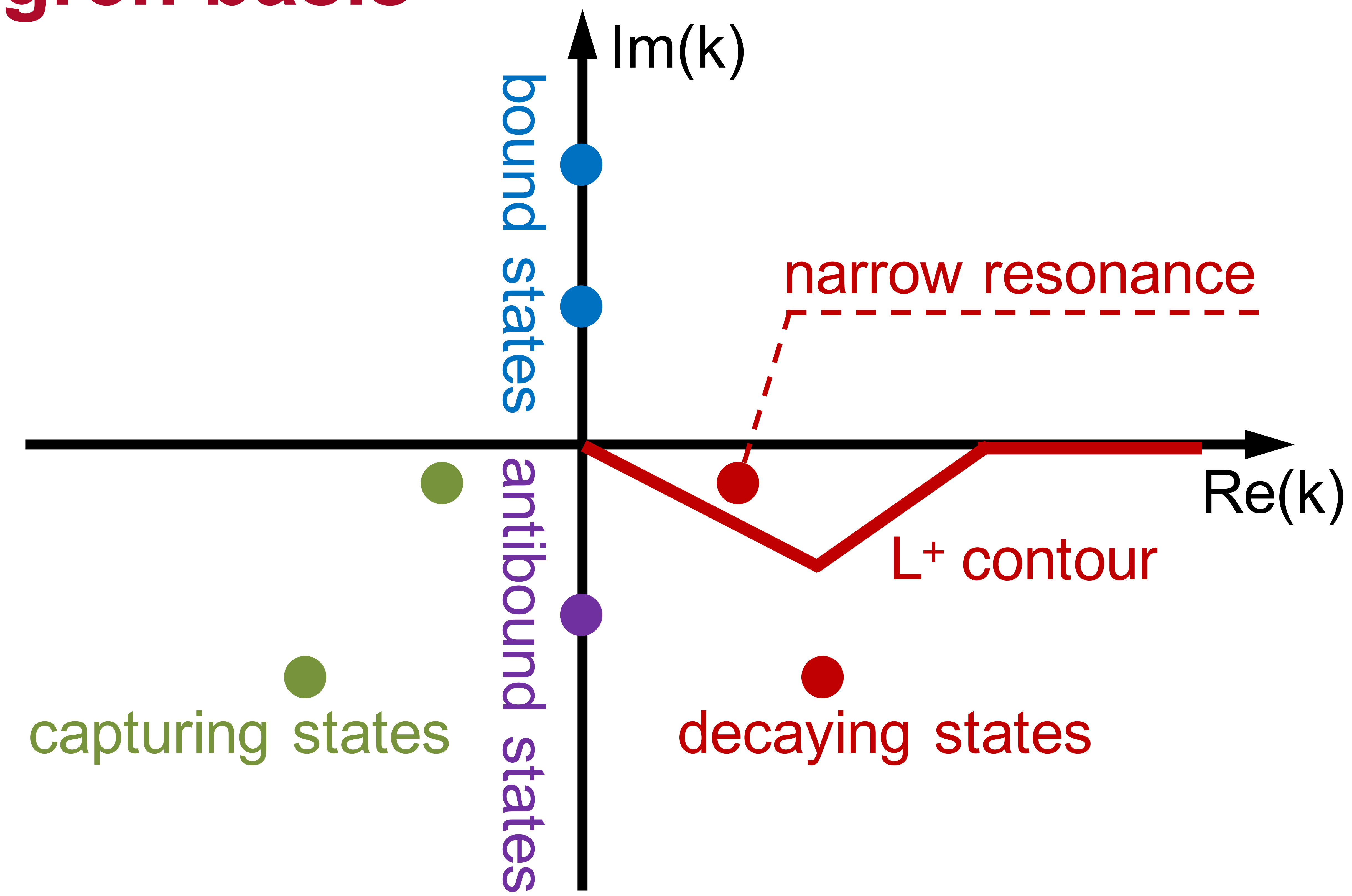
$$\Phi(e,\mathbf{r}) = \sqrt{\frac{\gamma/2}{\pi\left[\left(e-e_0\right)^2+(\gamma/2)^2\right]}}\,\Psi(\mathbf{r})$$

- **Through Fourier transformation, we obtain time evolution of the resonance**

$$\Phi(t,\mathbf{r}) = \Psi(\mathbf{r})e^{-i\tilde{e}t/\hbar} \qquad \boxed{\tilde{e}_n = \frac{\hbar^2 k_n^2}{2m} = e_n - i\frac{\gamma_n}{2}} \qquad t_{1/2} = \frac{\hbar ln2}{\gamma}$$

Gamow state: complex energy

G. Gamow, Z. Phys.51 (1928) 204



Berggren basis in complex-*k* plane, describing bound, resonance and scattering on equal footing

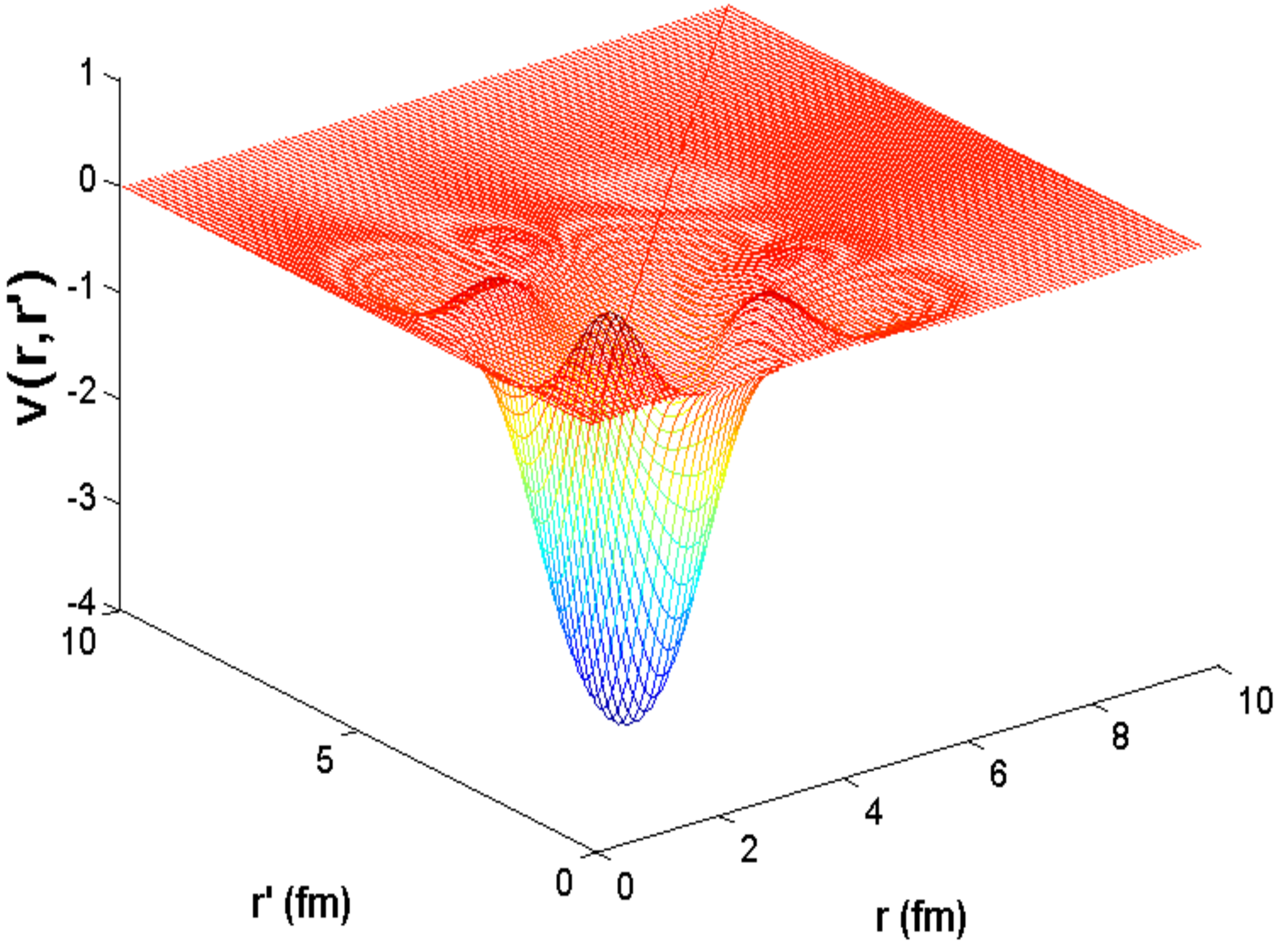
T. Berggren, Nucl. Phys. A109 (1968) 265

Orthogonality and completeness:

$$\delta(r-r') = \sum_n u_n(\tilde{e}_n, r)u_n\left(\tilde{e}_n, r'\right) + \int_{L^+} d\tilde{e}\, u(\tilde{e}, r)u\left(\tilde{e}, r'\right)$$

bound, resonance — **scattering (discretized)**

Gamow Hartree-Fock



Step❶: Solve the HF equations in HO representation

$$H_{\mathrm{int}} = \sum_{i=1}^{A}\left(1-\frac{1}{A}\right)\frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j}^{A}\left(V_{NN,ij} - \frac{\vec{p}_i\cdot\vec{p}_j}{mA}\right) + \sum_{i<j<k}^{A} V_{NNN,ijk}$$

Step❷: Extract the non-local HF potential *υ(r,r')*

$$h_{ij}^{\mathrm{HF}} = \langle i|t|j\rangle + \langle i|v|j\rangle = \langle i|t|j\rangle + \sum_{k=1}^{A}\langle ik|V|jk\rangle$$

Step❸: Obtain the radial wave function *u(r)/r* in complex-*k* plane

$$\tilde{e}_n = \frac{\hbar^2 k_n^2}{2m} = e_n - i\frac{\gamma_n}{2}$$

G. Gamow, Z. Phys.51 (1928) 204

$$u''(r) = \left[\frac{l(l+1)}{r^2} + v^{(\mathrm{loc})}(r) - k^2\right]u(r) + \int_0^{+\infty} v^{(\mathrm{non-loc})}(r,r')\,u(r')\,dr'$$

$$\begin{cases} u(\tilde{e},r) \sim C_0 r^{l+1} & r\to 0 \\ u(\tilde{e},r) \sim C^+H_{l\eta}^+(kr) + C^-H_{l\eta}^-(kr) & r\to+\infty \end{cases}$$

Resonance: outgoing

$$u_n(\tilde{e}_n, r) \sim O_l(k_n r) \sim e^{ik_n r}$$

exterior complex scaling

$$\int_0^{+\infty} u(\tilde{e},r)^2 dr = \int_0^R u(\tilde{e},r)^2 dr + \left(C^+\right)^2\int_R^{+\infty} H_{l\eta}^+(kr)^2 dr$$

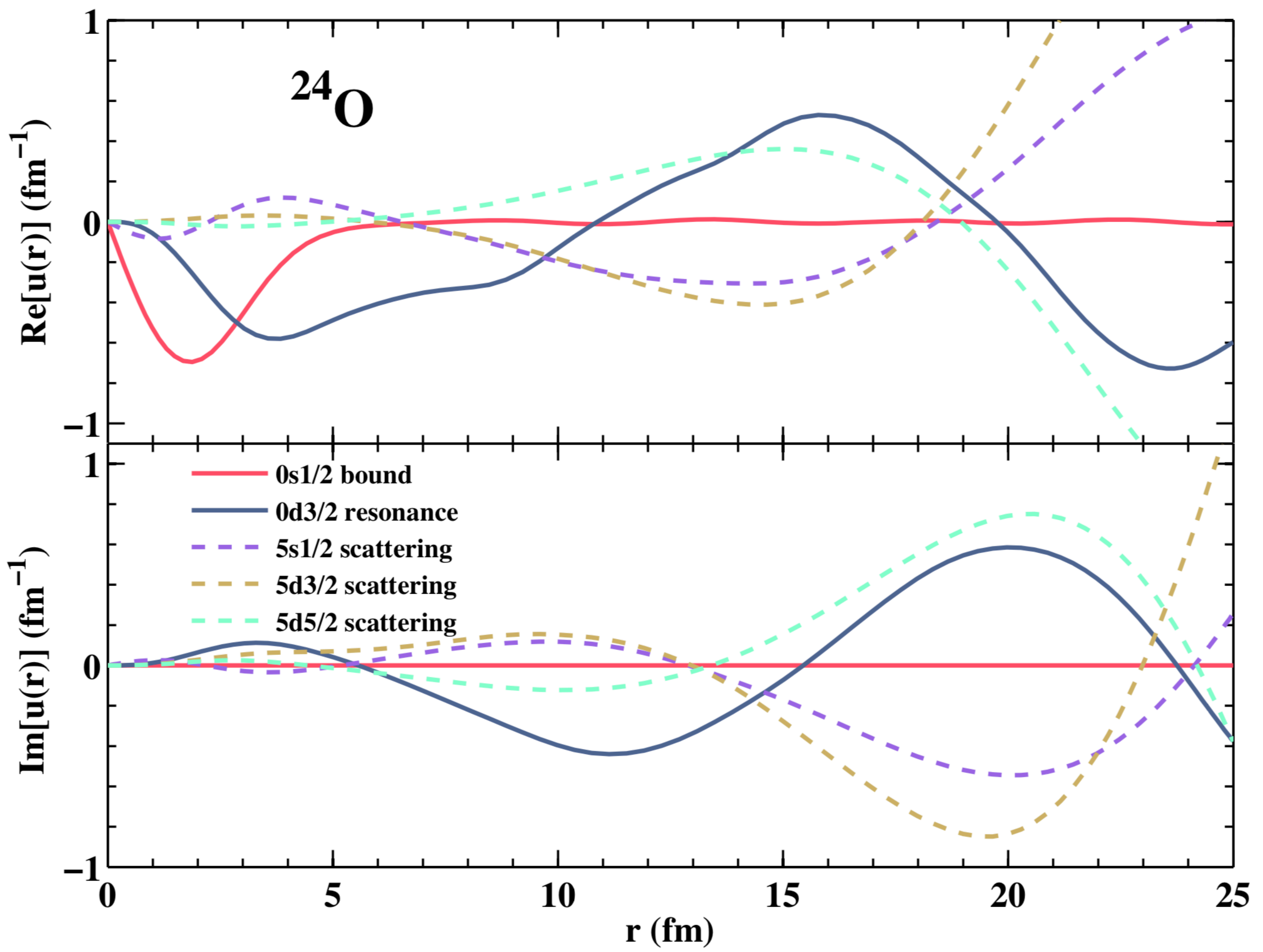
$$= \int_0^R u(\tilde{e},r)^2 dr + \left(C^+\right)^2\int_0^{+\infty} H_{l\eta}^+\left(kR + kxe^{i\theta}\right)^2 e^{i\theta}dx$$

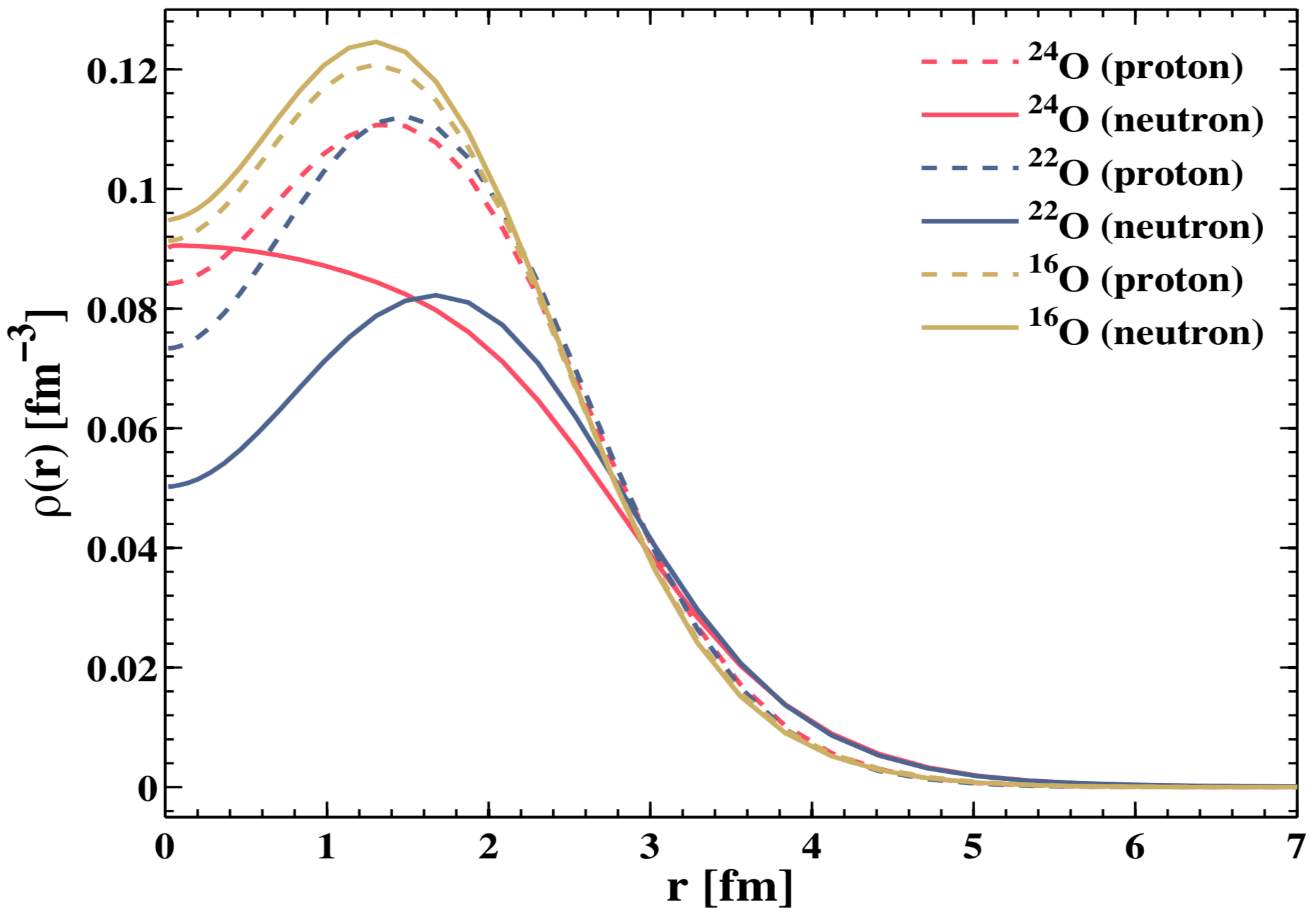
Results of GHF

sp energies

	^{16}O		^{22}O		^{24}O		^{28}O	
	Re(E)	Im(E)	Re(E)	Im(E)	Re(E)	Im(E)	Re(E)	Im(E) MeV
$0s_{1/2}$	−48.858	0.000	−57.720	0.000	−59.313	0.000	−55.076	0.000
$0p_{3/2}$	−22.735	0.000	−27.729	0.000	−28.132	0.000	−28.101	0.000
$0p_{1/2}$	−13.863	0.000	−23.501	0.000	−22.669	0.000	−21.674	0.000
$0d_{5/2}$	–	–	− 3.251	0.000	−3.993	0.000	−6.687	0.000
$1s_{1/2}$	–	–	− 0.964	0.000	−2.374	0.000	−3.978	0.000
$0d_{3/2}$	–	–	3.014	−0.626	2.312	−0.368	1.088	−0.081

sp resonance





NCSM
CC
GFMC
IM-SRG

Included continuum coupling

NCSMC, SS-HORSE
complex CC
GFMC
???

IM-SRG with resonance and continuum

- Include continuum degree of freedom into IM-SRG via Gamow-Berggren ensemble (Gamow Hartree-Fock)
- Extend the continuous unitary transformation (Hermitian) to the orthogonal transformation (complex symmetric)
- Describe bound, resonance and continuum states in a unified framework
- Combine with resonating group method (RGM) for nuclear reactions

IMSRG framework

IMSRG Hermitian (HO/HF basis)	$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$	Gamow IMSRG Complex symmetric (Berggren basis)
$\langle a \| H \| b \rangle = \langle b \| H \| a \rangle^*$ $H(s) = U(s)H(0)U^\dagger(s)$ $U(s) \cdot U^\dagger(s) = U(s) \cdot U^{-1}(s) = 1$ $\eta(s) = \frac{dU(s)}{s} U^\dagger(s) = -\eta^\dagger(s)$	$H(s) = U(s)HU^{-1}(s)$ $O(s) = U(s)OU^{-1}(s)$	$\langle \tilde{\alpha} \| H \| \beta \rangle = \langle \tilde{\beta} \| H \| \alpha \rangle^* = \langle \beta \| H \| \tilde{\alpha} \rangle$ $H(s) = U(s)H(0)U^T(s)$ $U(s) \cdot U^T(s) = U(s) \cdot U^{-1}(s) = 1$ $\eta(s) = \frac{dU(s)}{s} U^T(s) = -\eta^T(s)$

Magnus expansion:

T.D. Morris, N.M. Parzuchowski, and S.K. Bogner, PRC**92** (2015) 034331

$$U(s) = e^{\Omega(s)}$$

$$\frac{d\Omega(s)}{ds} = \eta(s) + \frac{1}{2}[\Omega(s), \eta(s)] + \frac{1}{12}[\Omega(s), [\Omega(s), \eta(s)]] + \cdots$$

$$H(s) = e^{\Omega(s)} H e^{-\Omega(s)} = H + [\Omega(s), H] + \frac{1}{2}[\Omega(s), [\Omega(s), H]] + \cdots$$

$$O(s) = e^{\Omega(s)} O e^{-\Omega(s)} = O + [\Omega(s), O] + \frac{1}{2}[\Omega(s), [\Omega(s), O]] + \cdots$$

e.g., White generator η:

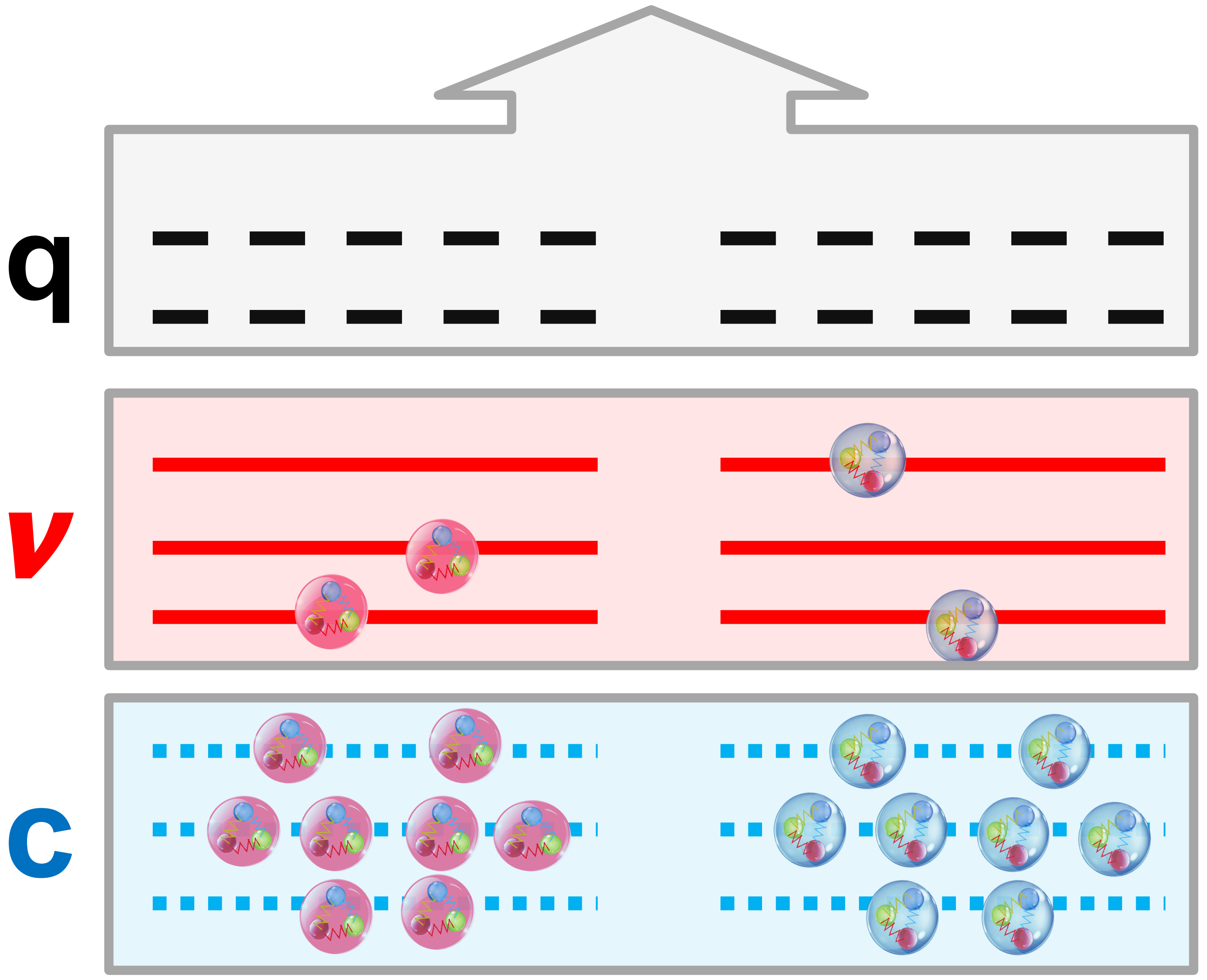
$$\eta_{12} = \frac{f_{12}}{f_{11} - f_{22} + \Gamma_{1212}}$$

$$\eta_{1234} = \frac{\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234}}$$

$$A_{1234} = \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}$$

Perform all calculations at two-body level — IMSRG(2)

$$H = E_0 + \sum_{ij} f_{ij} \left\{ a_i^\dagger a_j \right\} + \frac{1}{4} \sum_{ijkl} \Gamma_{ijkl} \left\{ a_i^\dagger a_j^\dagger a_l a_k \right\} + \frac{1}{36} \sum_{\substack{ijk\\lmn}} W_{ijklmn} \left\{ a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l \right\}$$

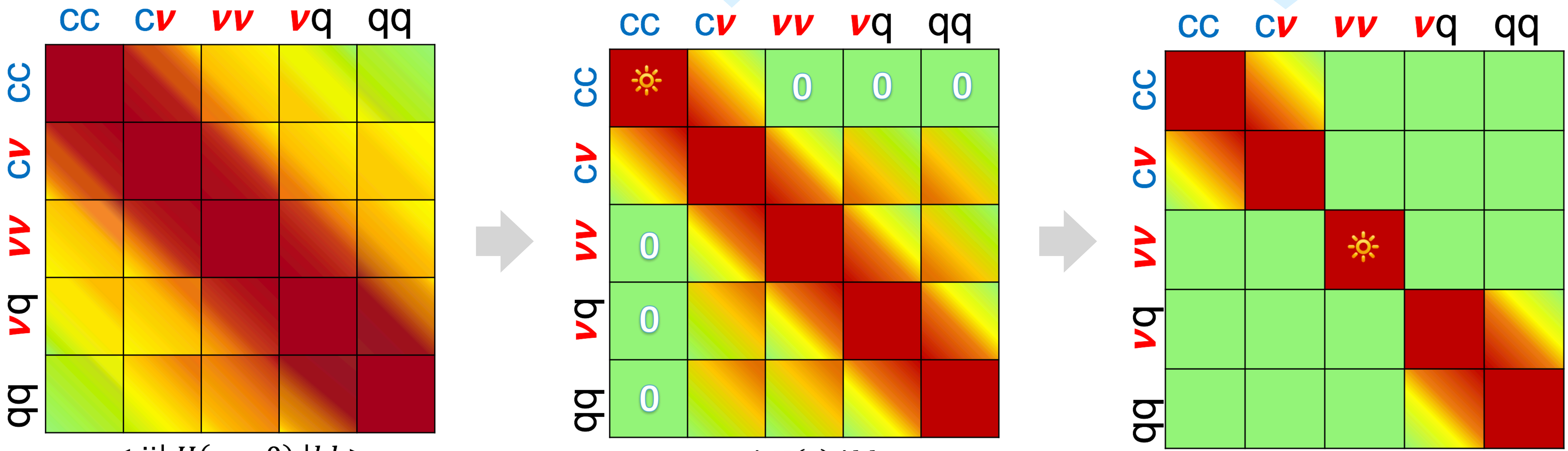


EOM-IMSRG closed-shell nuclei

$$H^{\text{od}} \equiv \langle v|H|c\rangle + \langle q|H|c\rangle + \langle vv|H|cc\rangle + \langle qv|H|cc\rangle + \langle qq|H|cc\rangle$$

VS-IMSRG shell-model effective interaction

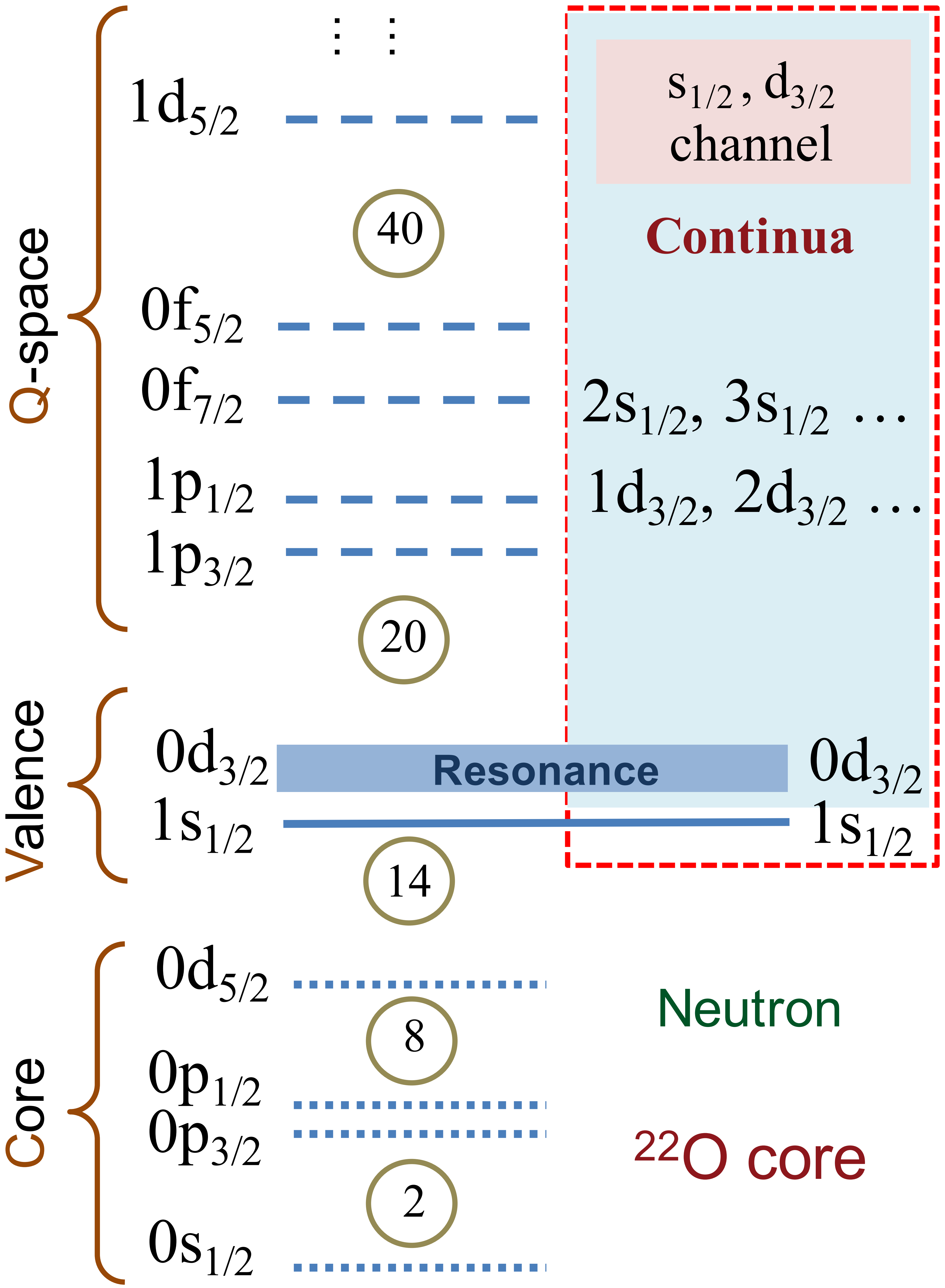
$$H^{\text{od}} \equiv \langle v|H|c\rangle + \langle q|H|c\rangle + \langle q|H|v\rangle + \langle vv|H|cc\rangle + \langle qv|H|cc\rangle + \langle qq|H|cc\rangle + \langle vv|H|vc\rangle + \langle qv|H|vc\rangle + \langle qq|H|vc\rangle + \langle qv|H|vv\rangle + \langle qq|H|vv\rangle$$



$< ij|\, H(s=0)\, |kl >$ → $< ij|\, H(s)\, |kl >$ → $< ij|\, H(s)\, |kl >$

Difficulties caused by continuum states

< vv | H^od | vq > !!!



$$H(s) = e^{\eta(s)} H e^{-\eta(s)} = H + [\eta(s), H] + \frac{1}{2}[\eta(s), [\eta(s), H]] + \cdots$$

$$\left\langle v \left| \eta^{\text{White}} \right| q \right\rangle = \frac{\langle v | H^{od} | q \rangle}{\langle v | H^{d} | v \rangle - \langle q | H^{d} | q \rangle}$$

< v | H^d | v > close to < q | H^d | q > : generates high-order terms in the transformation of H

$$\theta = \frac{1}{2} \tan^{-1}[2a/(E_l - E_r)]. \qquad (10)$$

magnitude. Note that the degenerate case $E_l = E_r$ is nonsingular, generating an angle of $\pm\pi/4$ (either angle can be chosen). Such a large transformation angle should be avoided if possible, however, since it generates high-order terms in the transformation of H.

S.R. White, J. Chem. Phys. 117 (2002) 7472

IMSRG(3) or …

Similar to many-multi-shells effective interaction

❶

$$\left\langle v \left| \eta^{\text{White}} \right| q \right\rangle = \frac{\langle v | H^{od} | q \rangle}{\langle v | H^d | v \rangle - \langle q | H^d | q \rangle}$$

$$\left\langle v \left| \eta^{\text{White}} \right| q \right\rangle = \frac{\langle v | H^{od} | q \rangle}{\langle v | H^d | v \rangle - \langle q | H^d | q \rangle + \Delta}$$

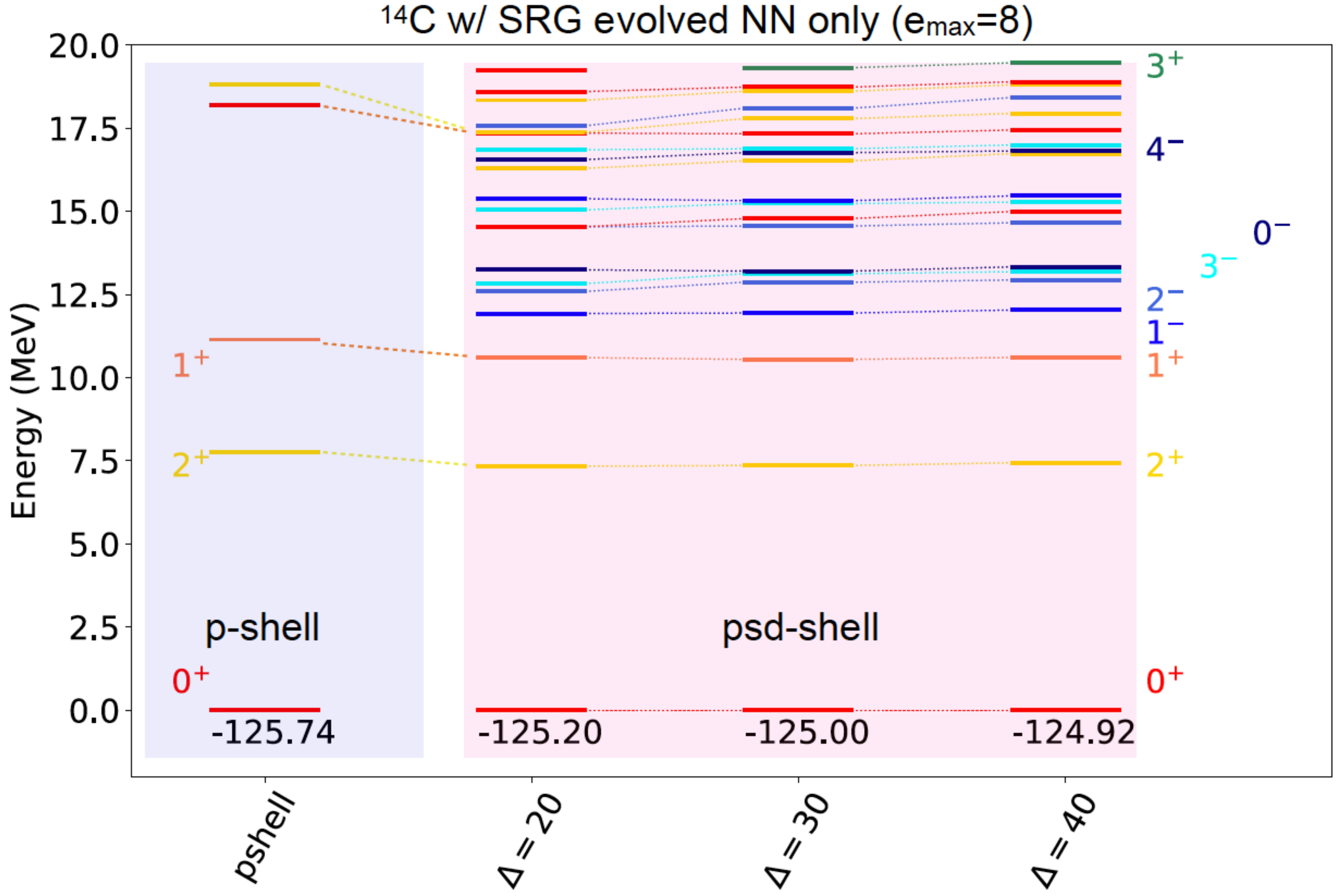
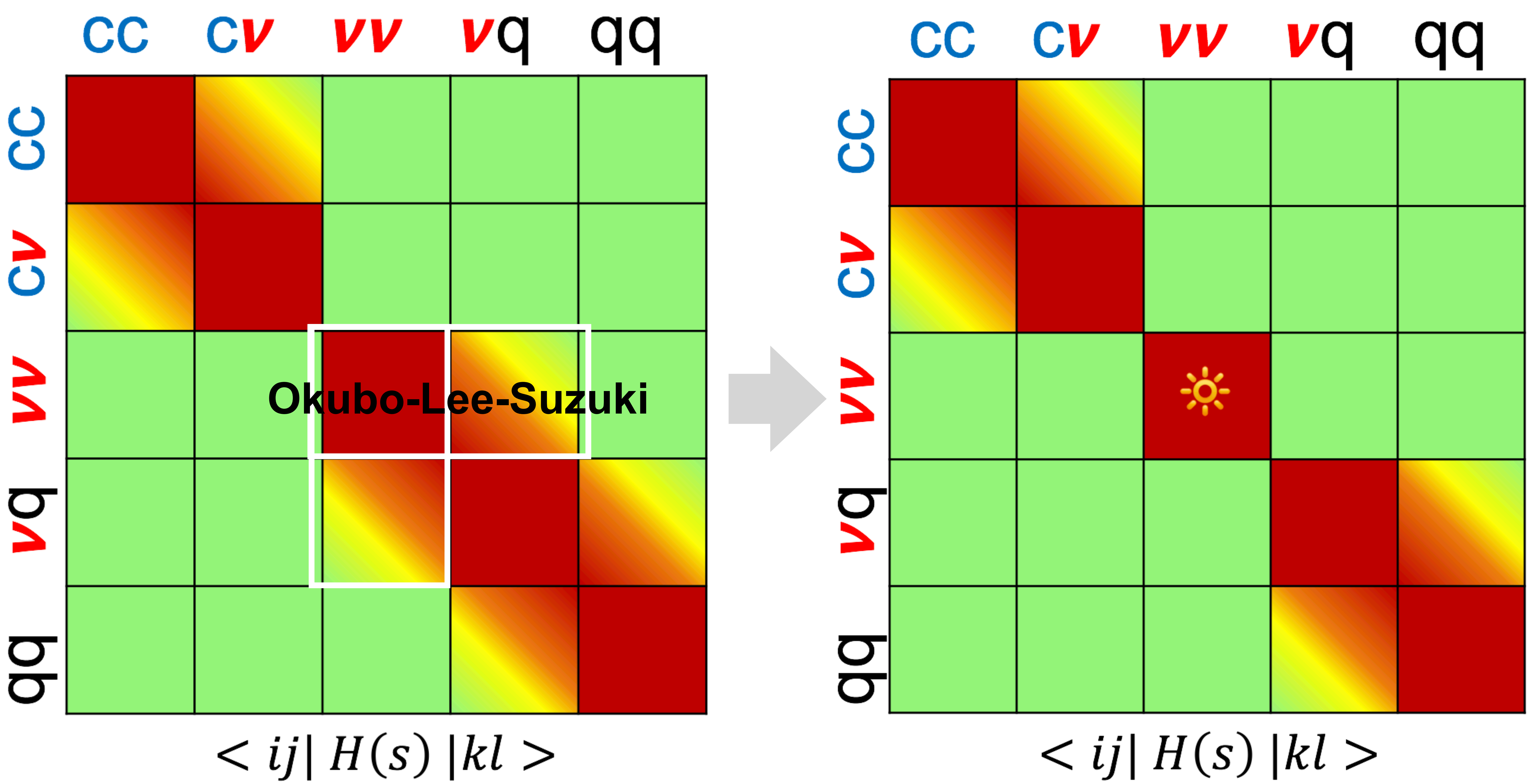


Figure credit: T. Miyagi

❷

Use Okubo-Lee-Suzuki to decouple *vv* from *v*q



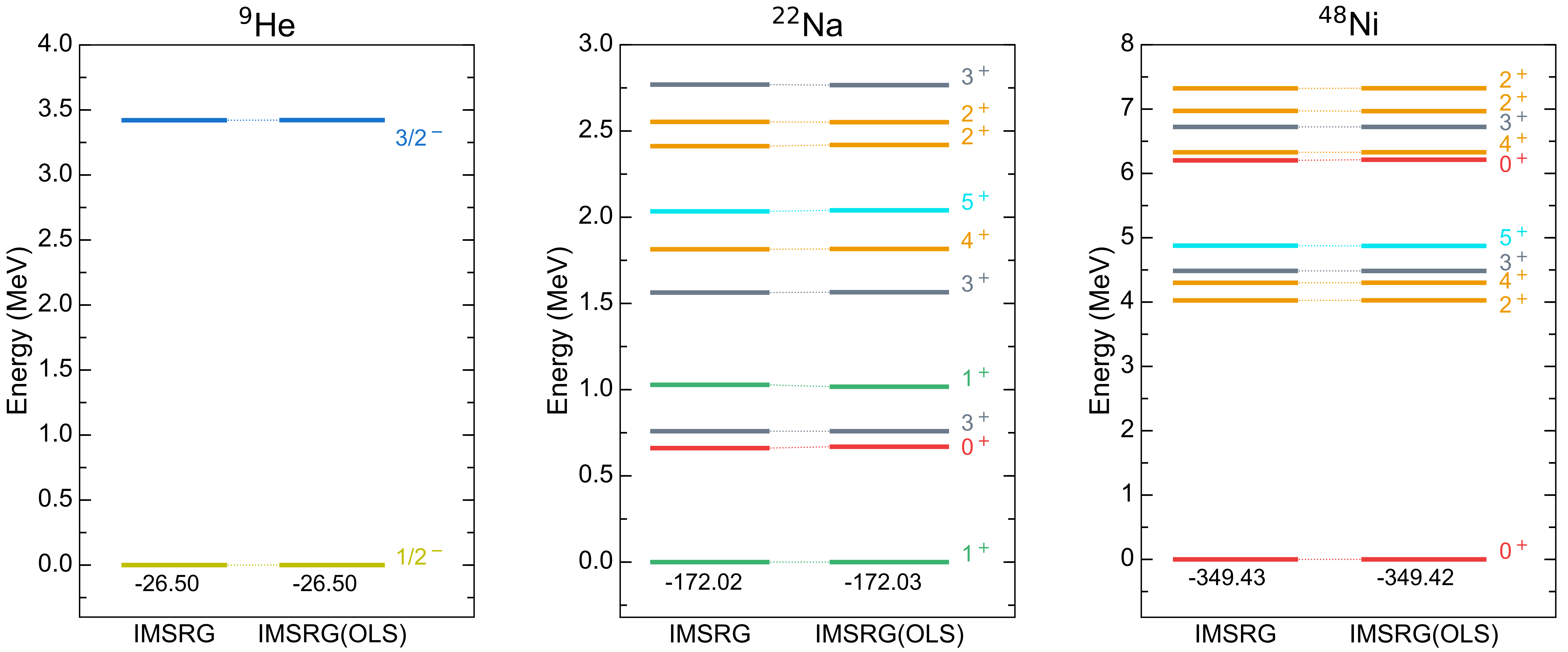
$$\omega = Q\omega P \qquad \langle \alpha_Q | \omega | \alpha_P \rangle = \sum_{k \in \kappa} \langle \alpha_Q | k \rangle \langle \tilde{k} | \alpha_P \rangle$$

$$\bar{H}_{\text{eff}} = [P(1+\omega^T\omega)P]^{-1/2}(P + P\omega^T Q)H(P + Q\omega P)[P(1+\omega^T\omega)P]^{-1/2}$$

VS-IMSRG with OLS

EM1.8/2.0(NN + 3N), emax = 12, e3max = 16, $\hbar\omega$ = 16 MeV

Using ensemble normal ordering (ENO)
Without continuum

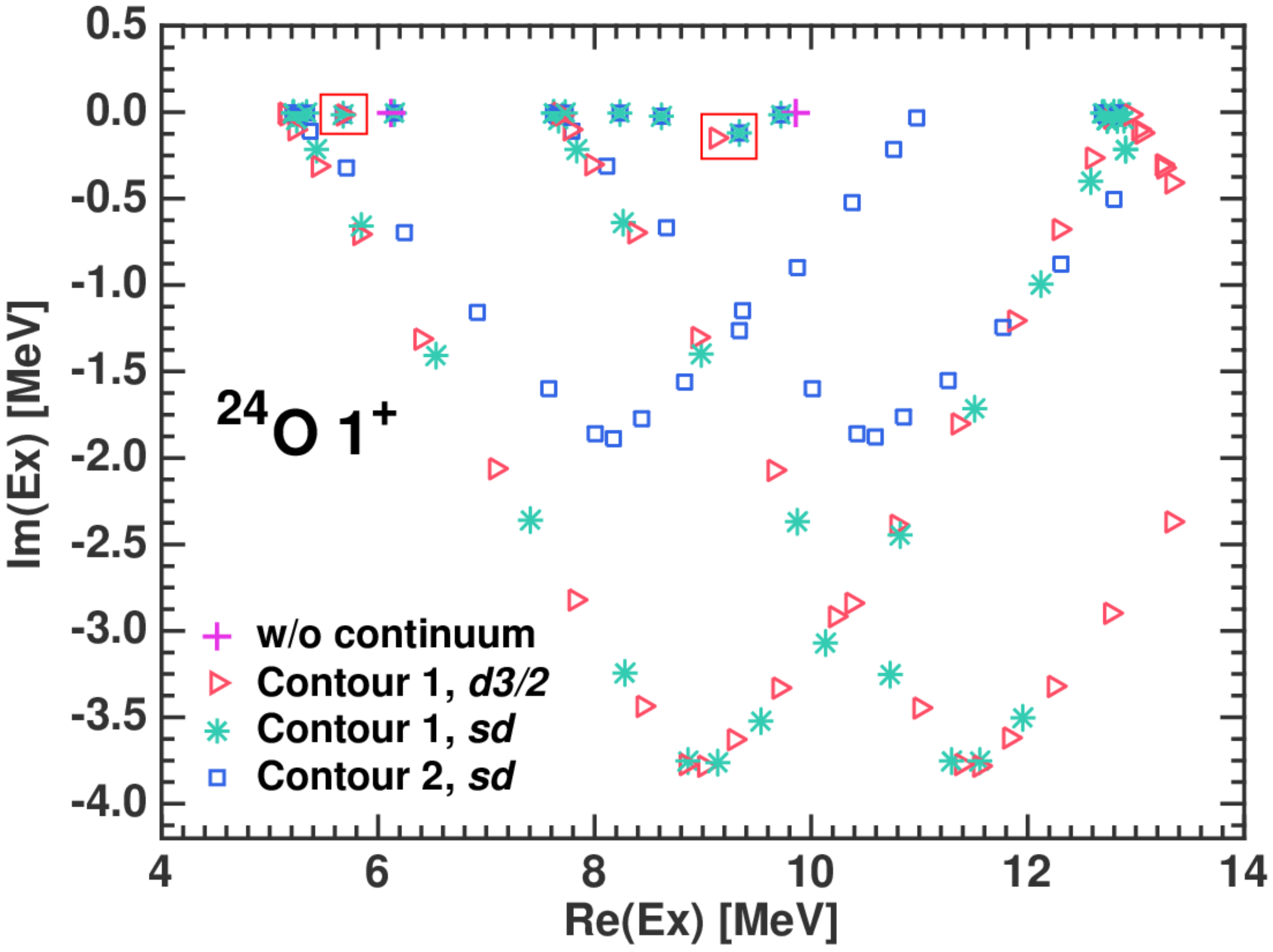


BS Hu, et al., In preparation (2022)

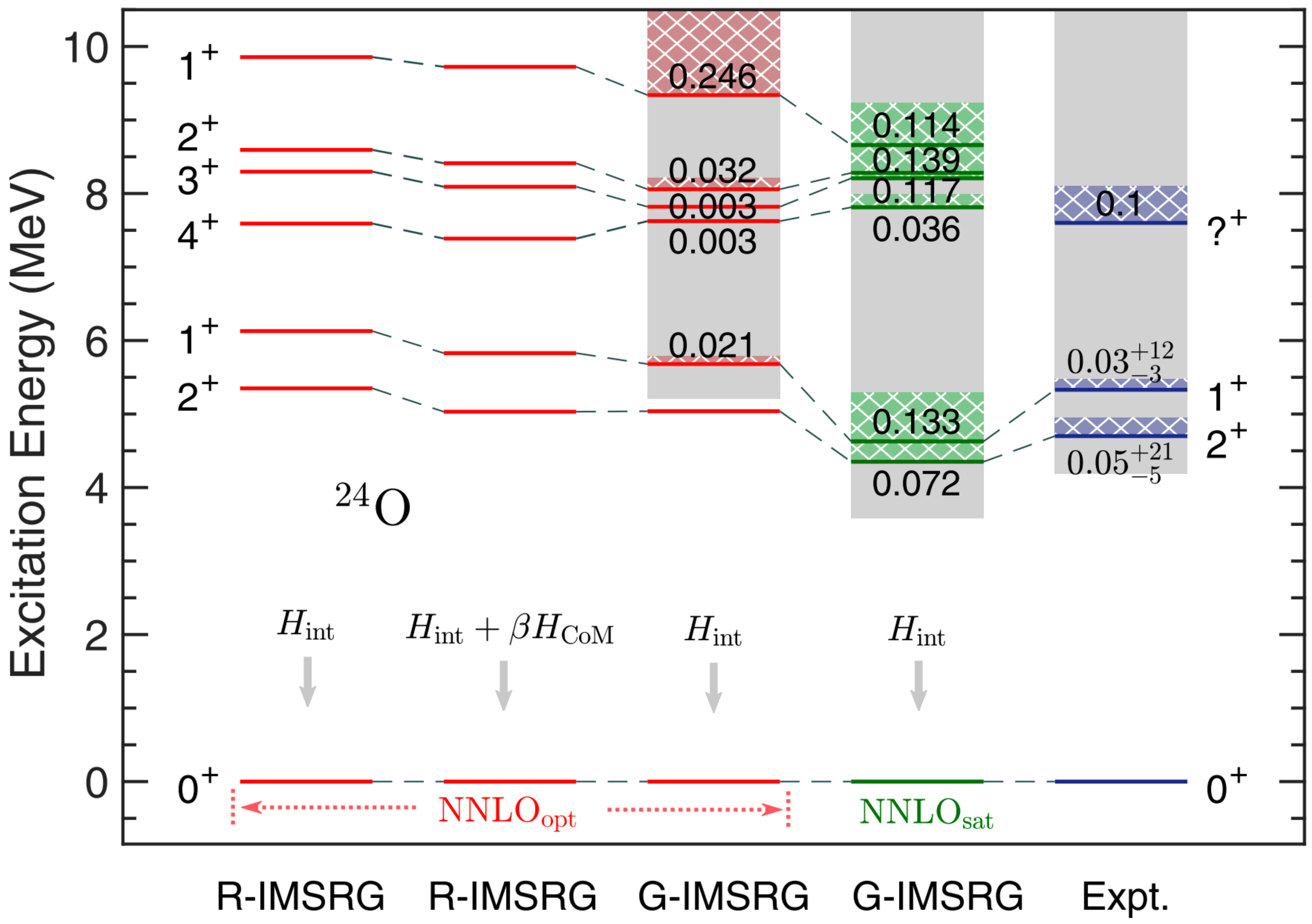
Gamow EOM-IMSRG results

BSHu, Q. Wu, et al., PRC **99** (2019) 061302(R); arXiv:1906.10539

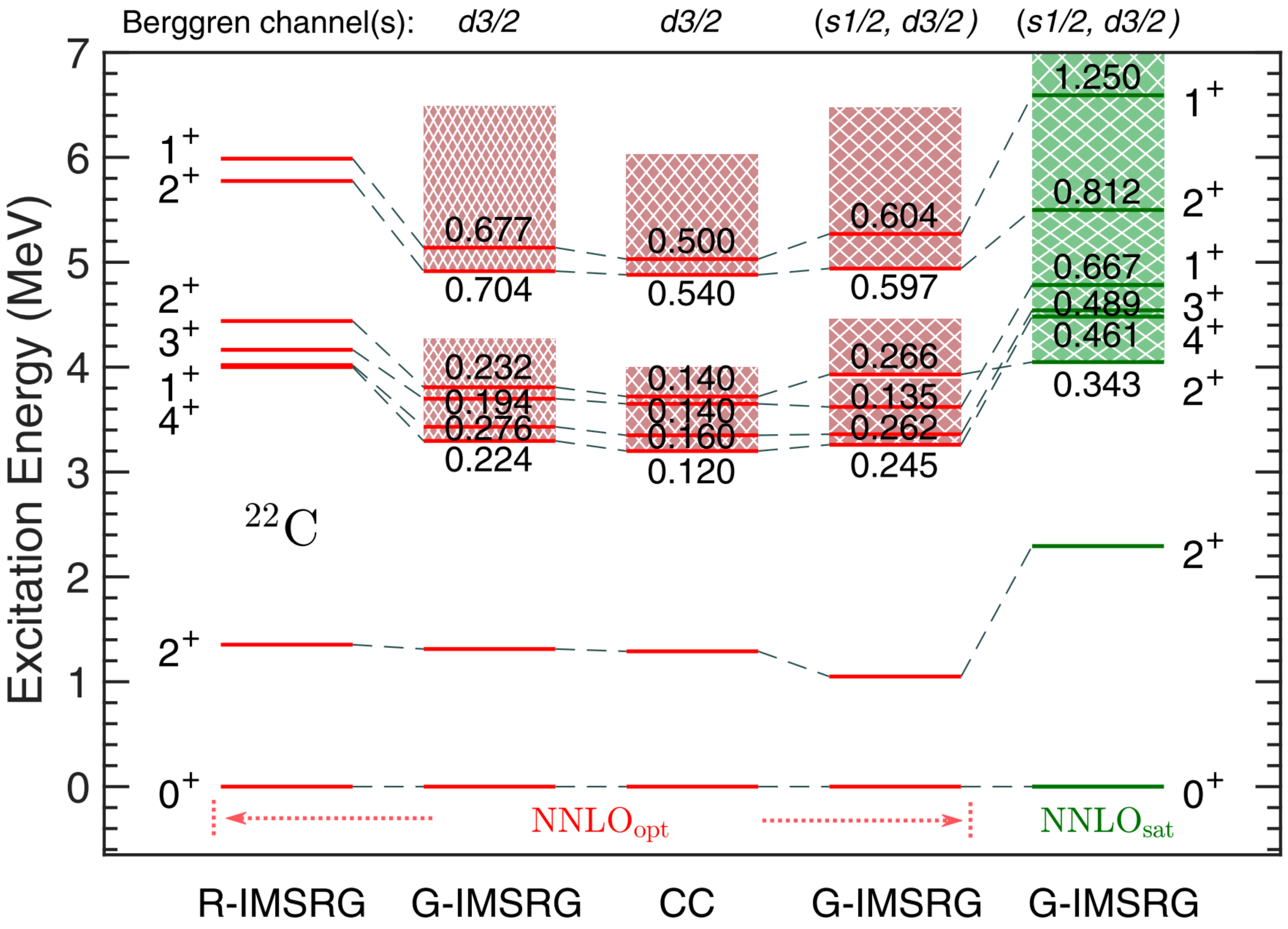
Convergence against different contour and discretization number



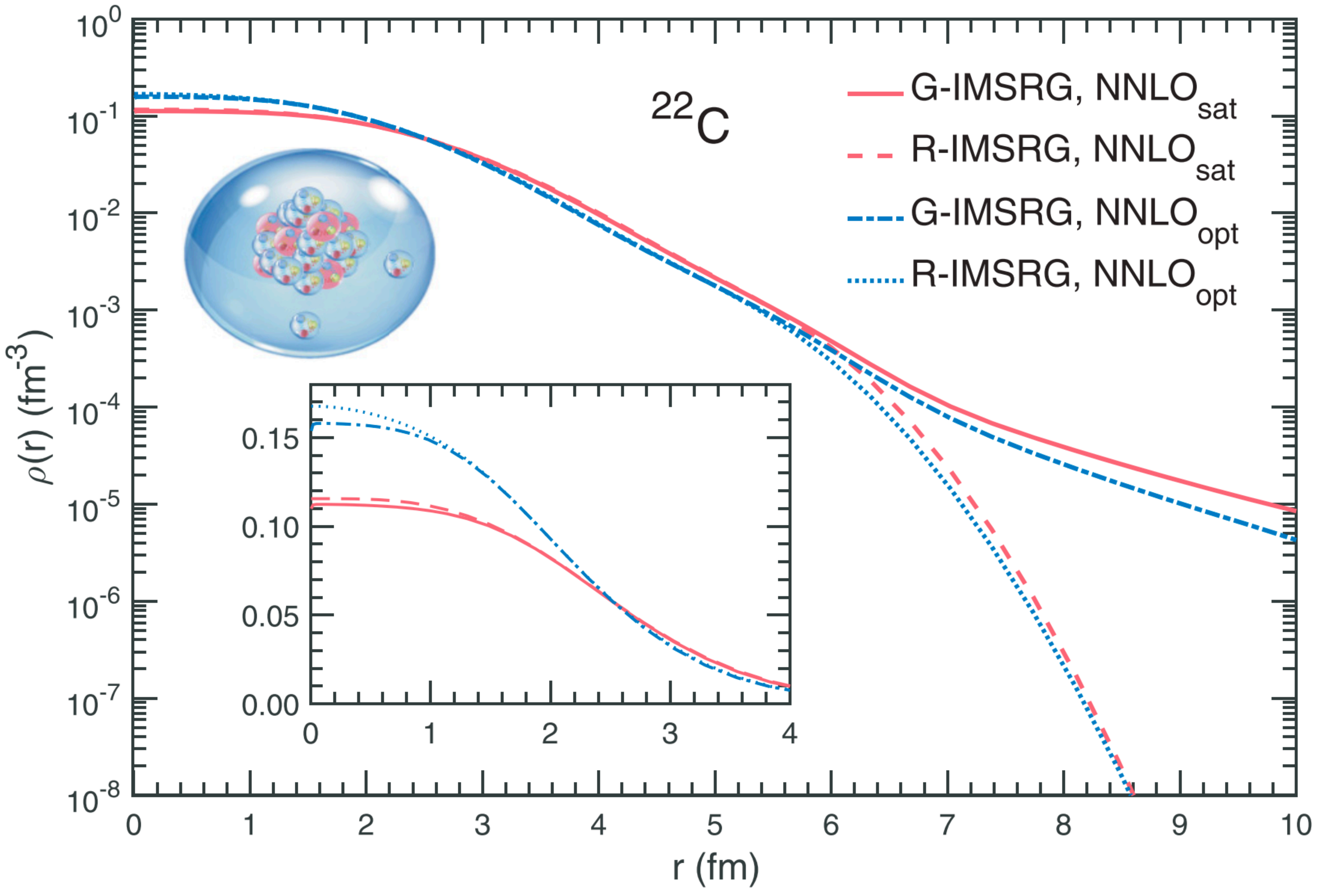
Center-of-mass spurious excitation



EOM-IMSRG for Borromean ^{22}C



BSHu, Q. Wu, et al., PRC **99** (2019) 061302(R); arXiv:1906.10539



NNLO$_{sat}$	R-IMSRG	G-IMSRG cont. *s*, *d* waves	Expt. Estimated
matter radius (fm)	2.98	3.14	3.44 ± 0. 08❶ 3.38 ± 0.10❷

❶: Y. Togano *et al.*, PLB**761** (2016) 412

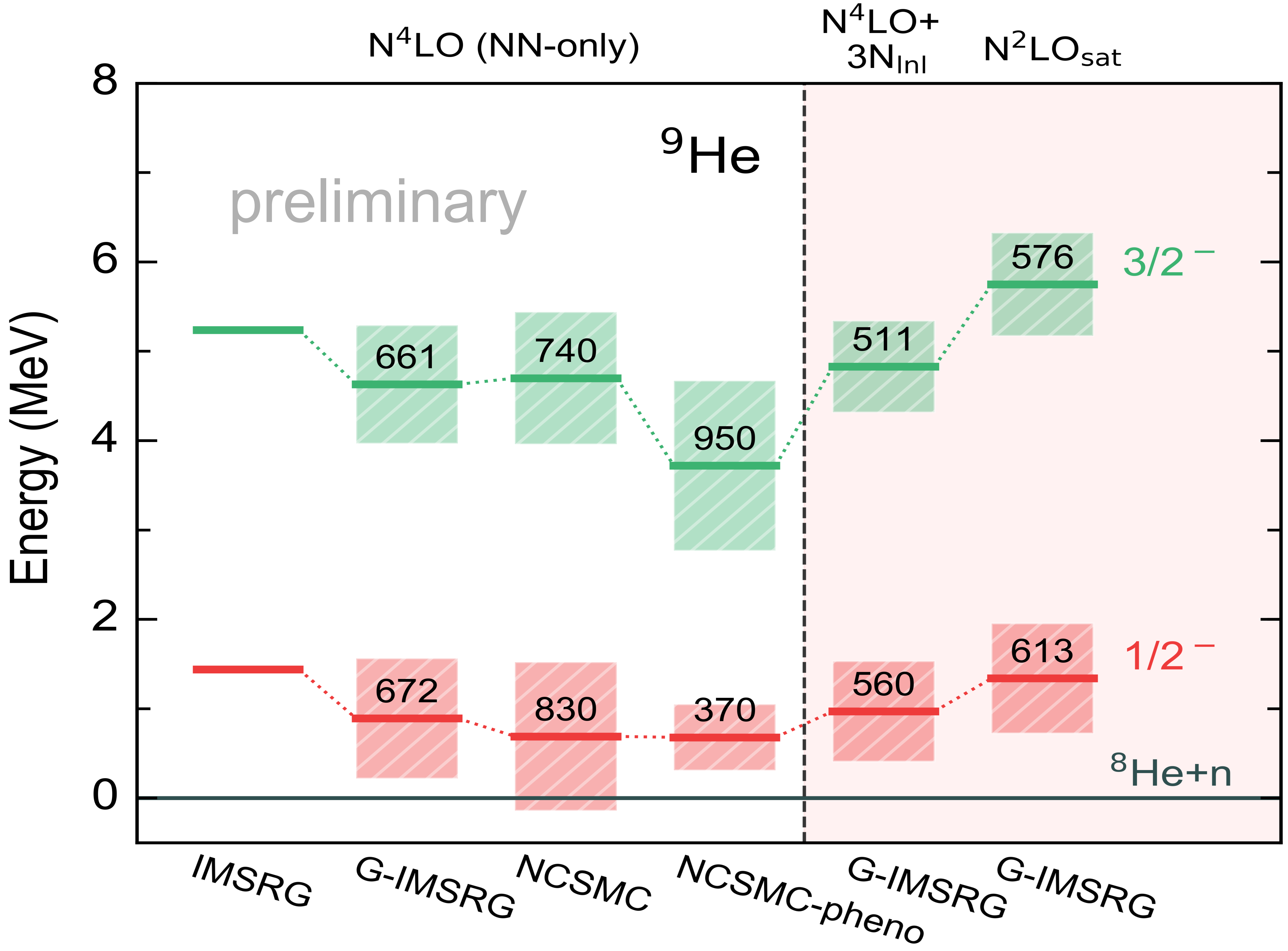
❷: T. Nagahisa and W. Horiuchi, PRC**97** (2018) 054614

Benchmark with NCSMC

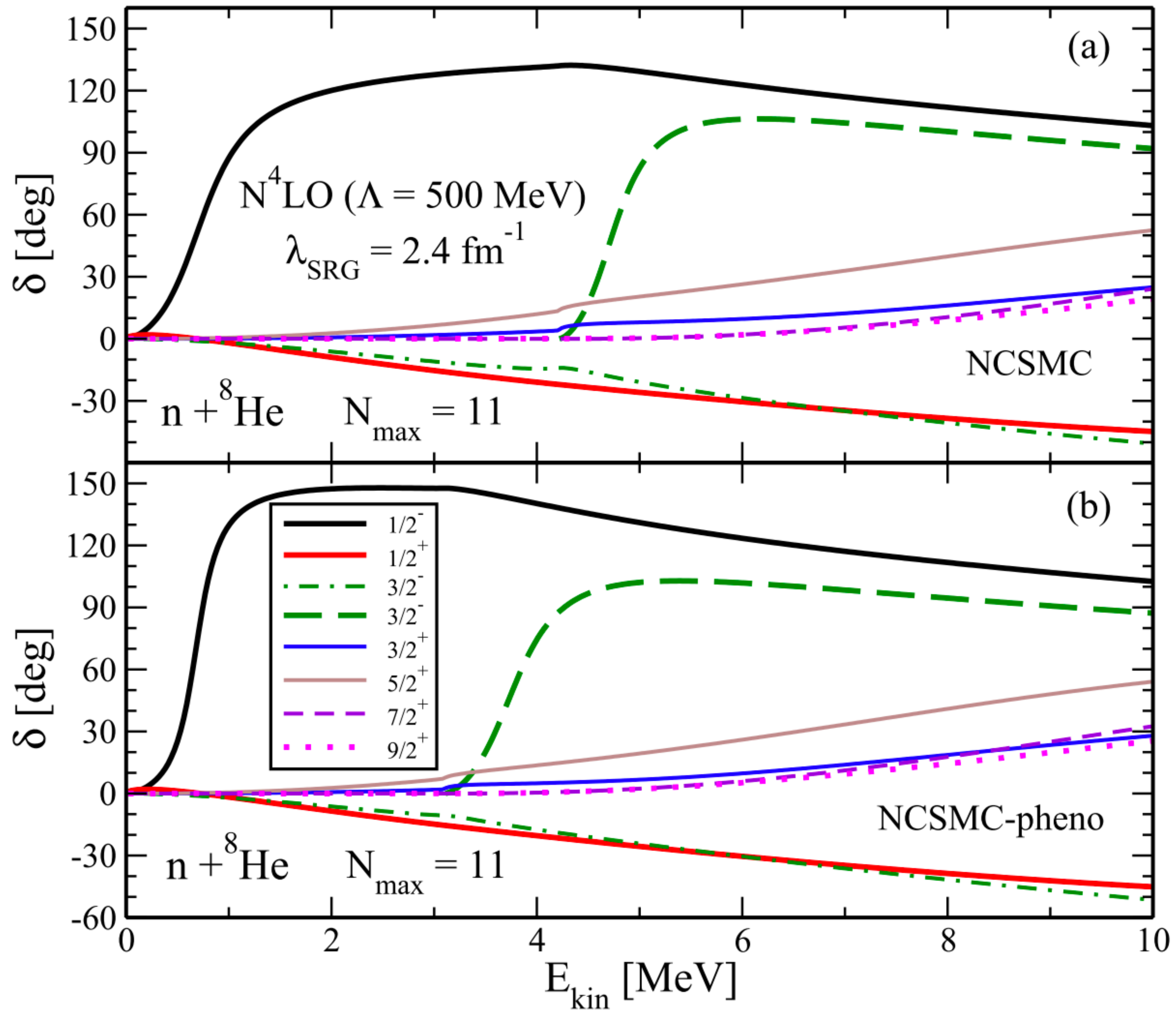
Core: ^{4}He

Valence space: neutron $p_{1/2}$, $p_{3/2}$ resonances and $s_{1/2}$, $p_{1/2}$, $p_{3/2}$, $d_{5/2}$ continua

$$N^4LO(500),\ \lambda_{SRG} = 2.4\ \text{fm}^{-1},\ \hbar\Omega = 20\ \text{MeV}$$



$E_{g.s.}$ (MeV)	^{4}He	^{6}He	^{8}He
IMSRG(ENO)	−28.50	−28.25	−29.47
NCSM	−28.36	−28.94(20)	−30.23(30)
Expt.	−28.30	−29.27	−31.41



M. Vorabbi, A. Calci, P. Navrátil, *et al.*, PRC**97**, 034314 (2018)

N=20 isotones: proton rich

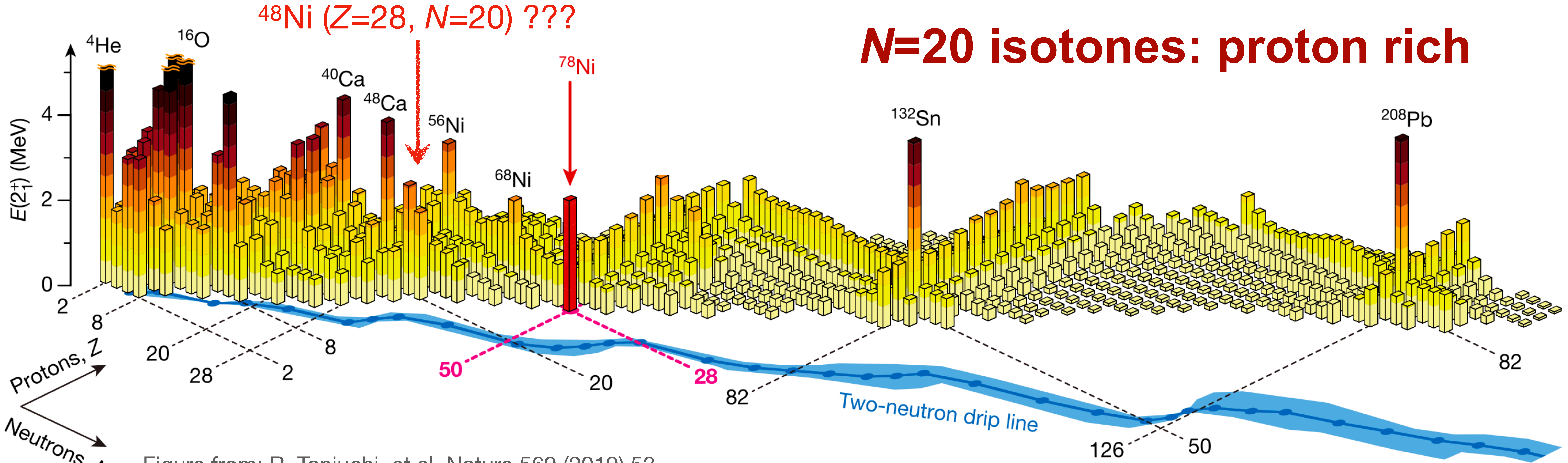
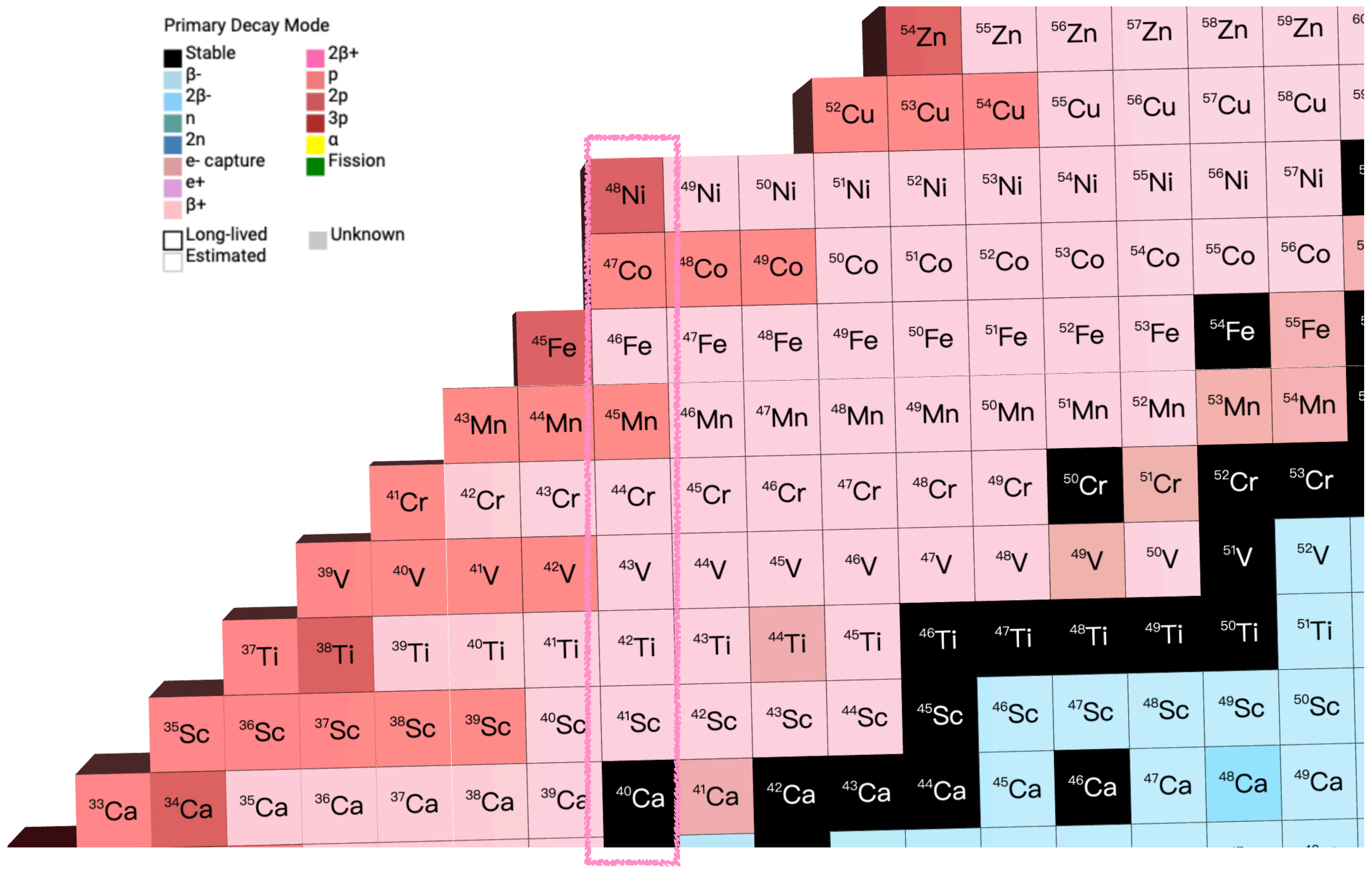
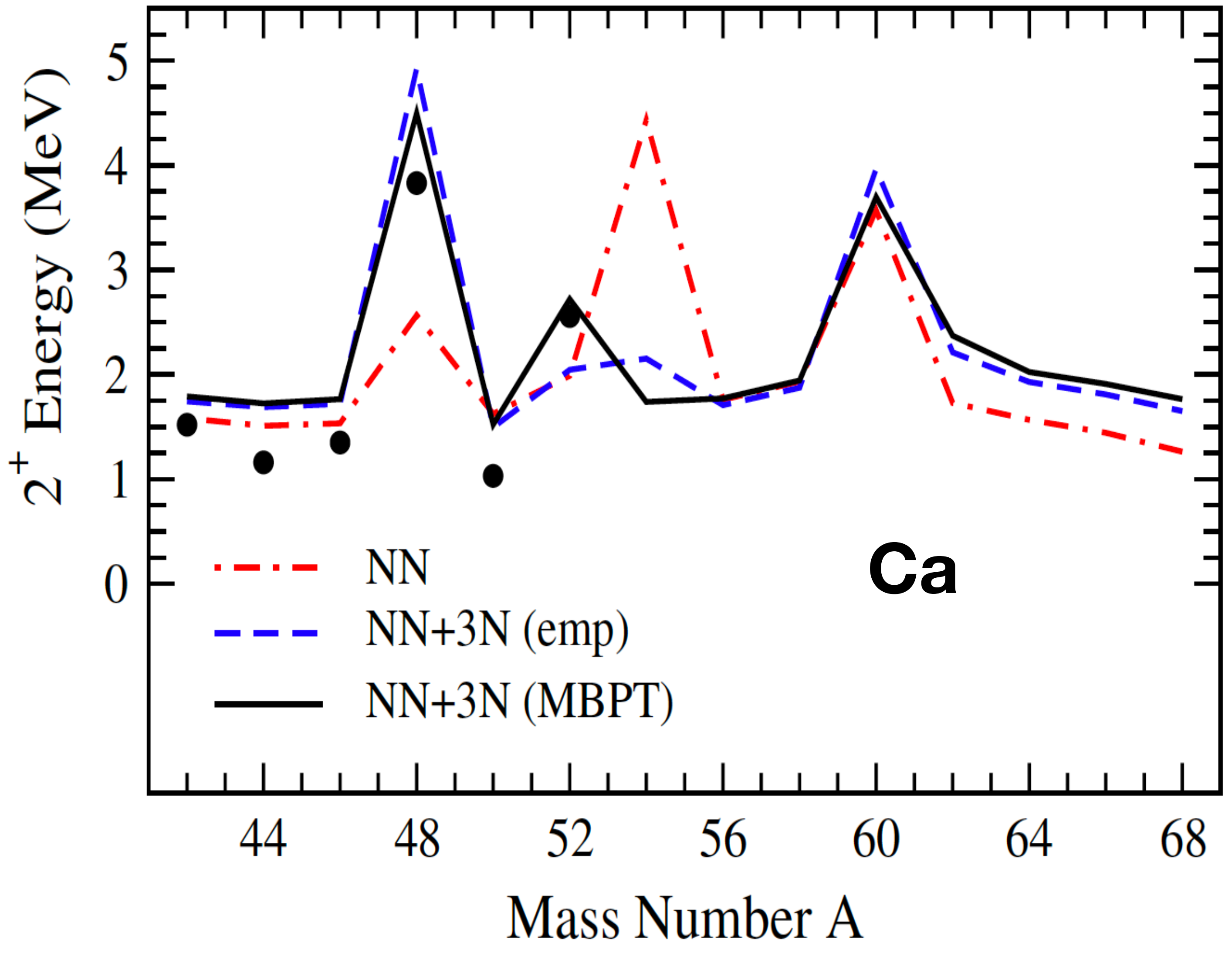


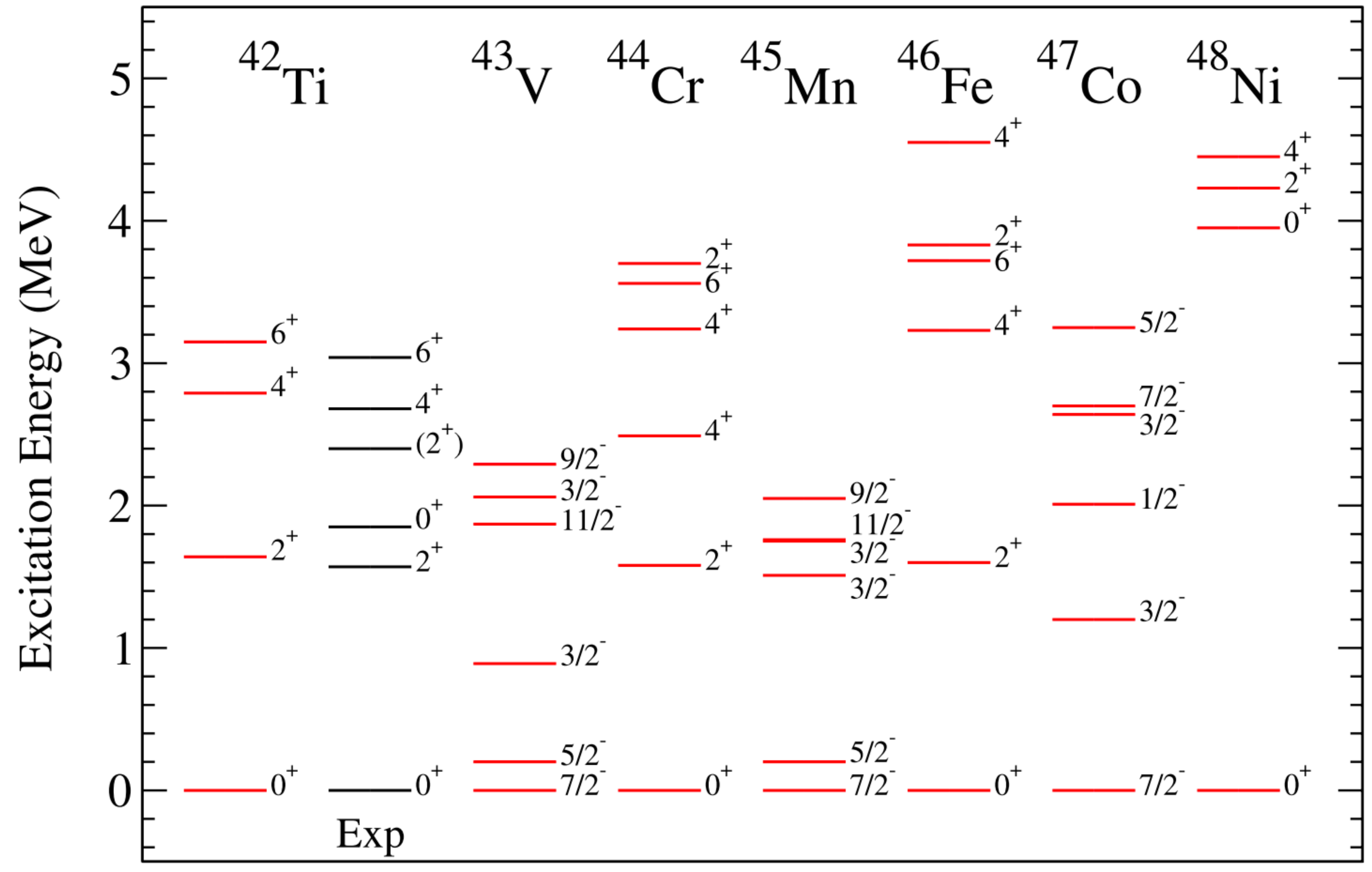
Figure from: R. Taniuchi, et al, Nature 569 (2019) 53



MBPT (NN+3NF)

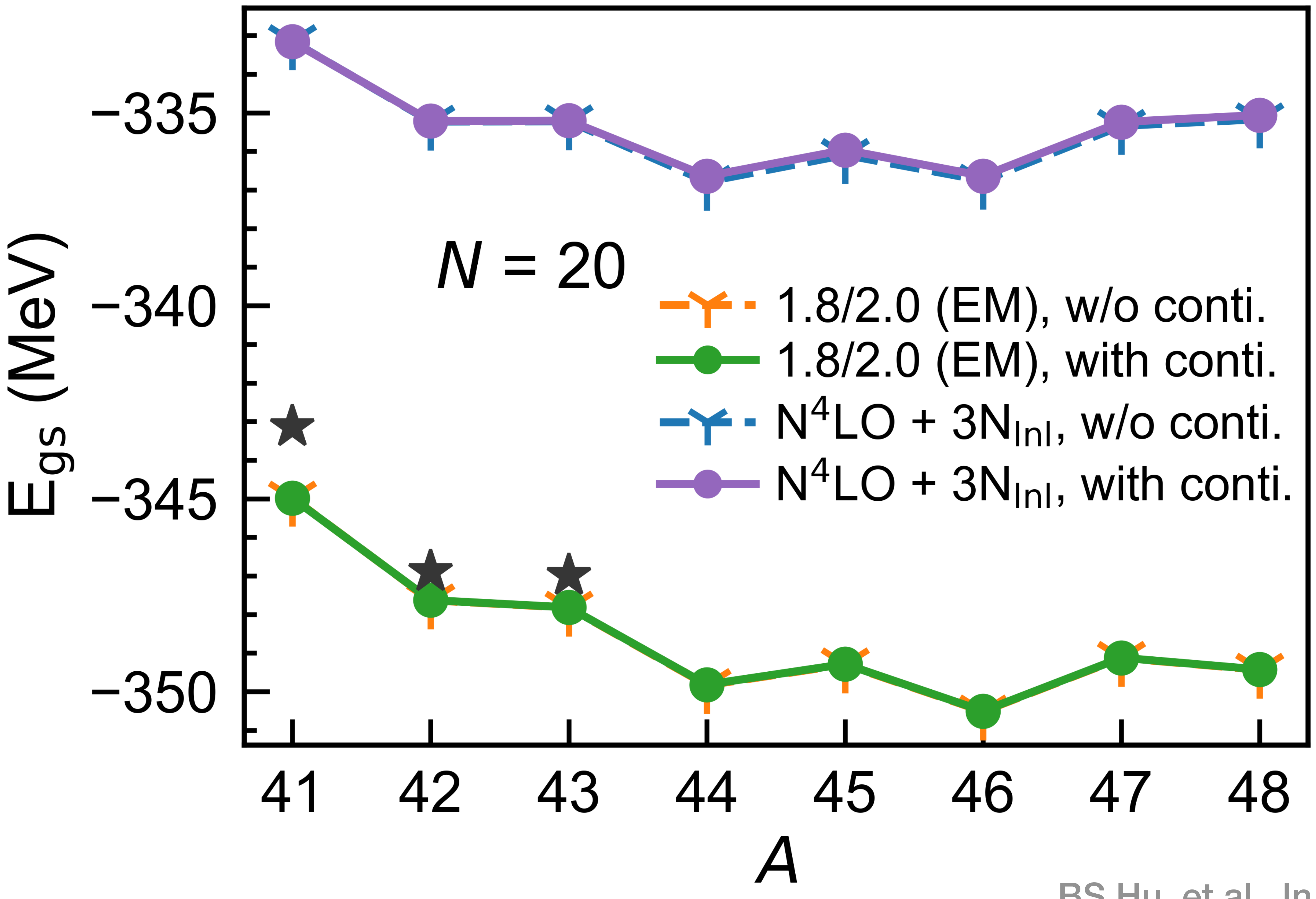


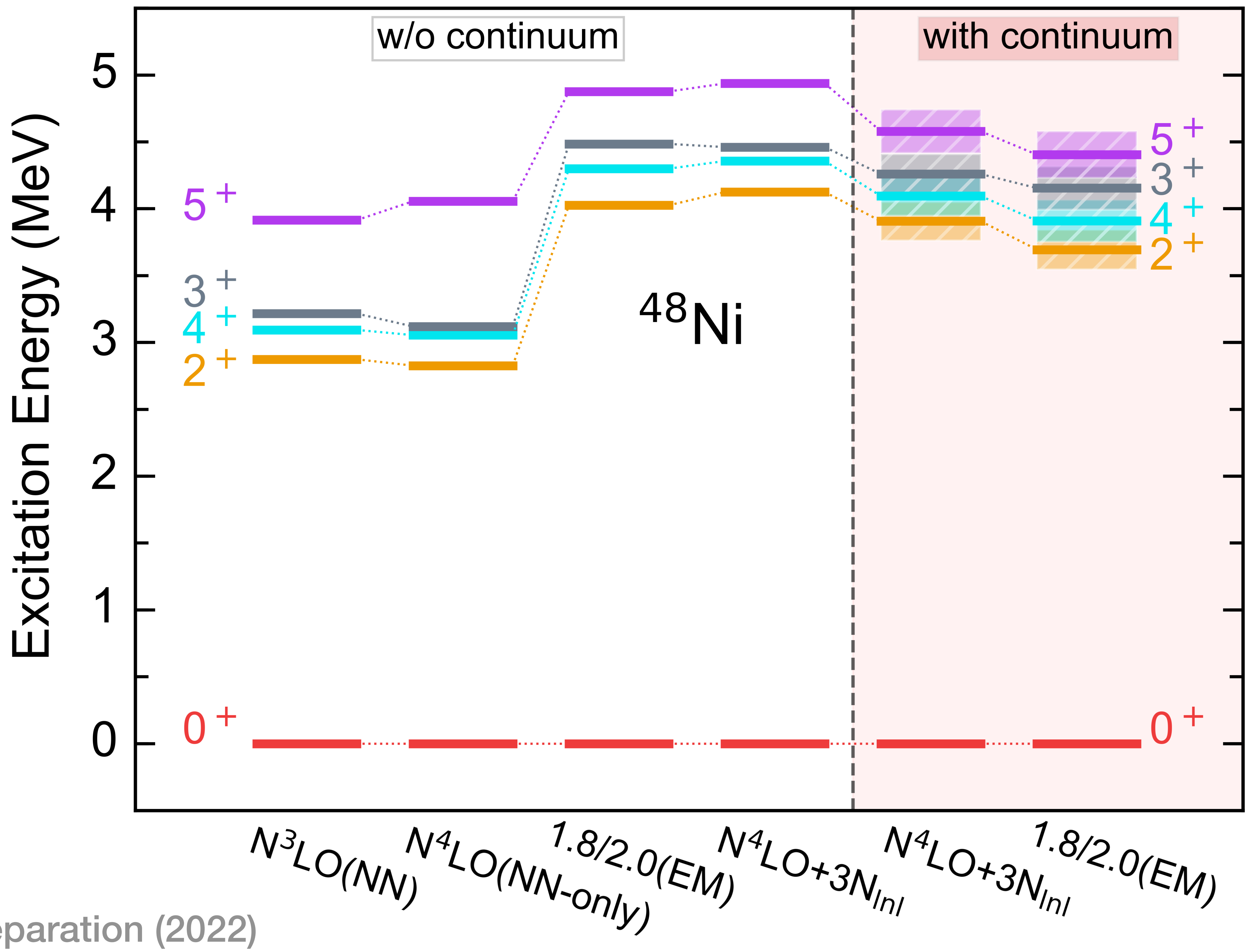
J. Holt, et al, JPG:NPP 40 (2013) 075105



J. Holt, J. Menéndez and A. Schwenk, PRL110 (2013) 022502

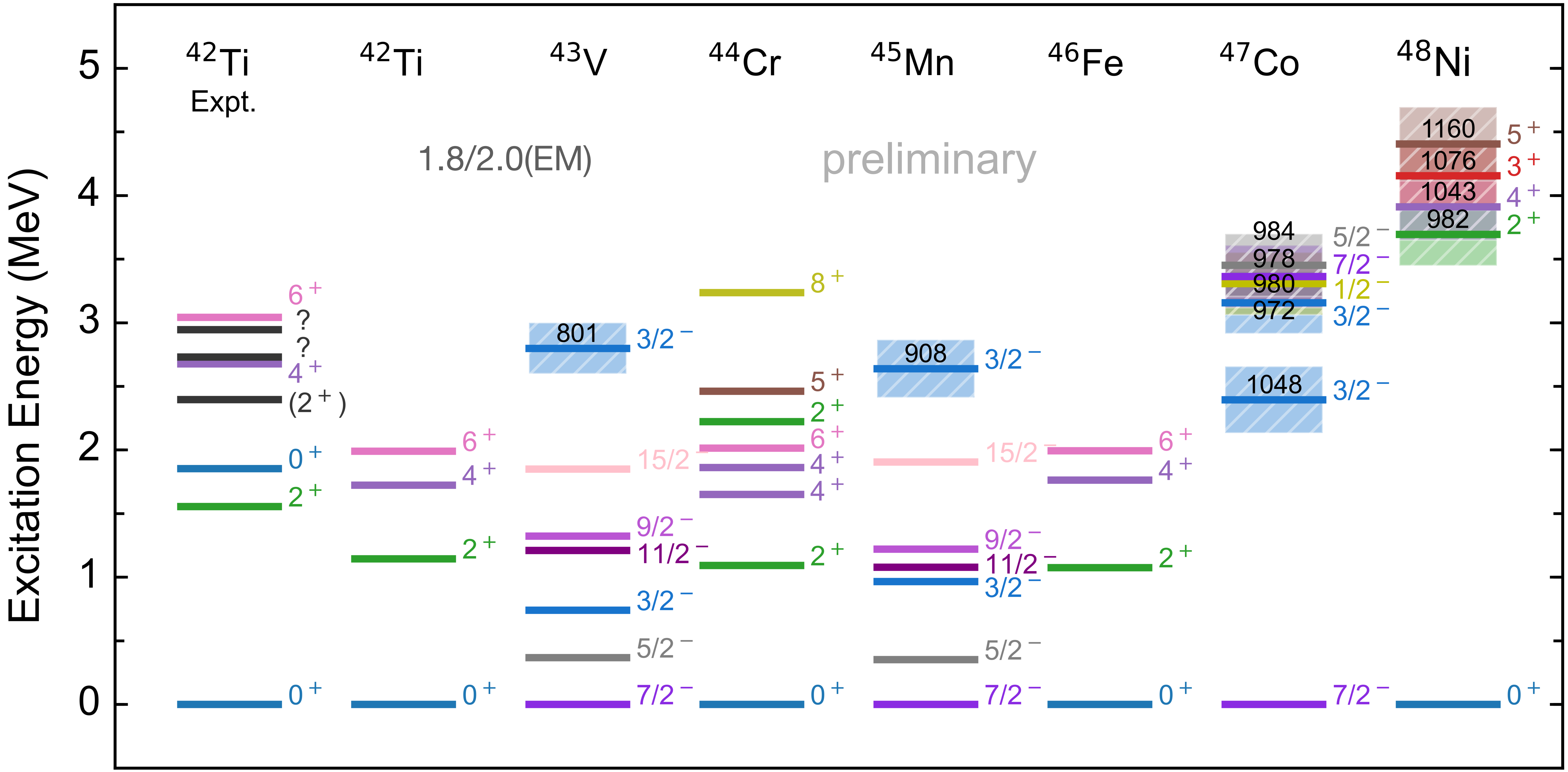
Gamow VS-IMSRG results



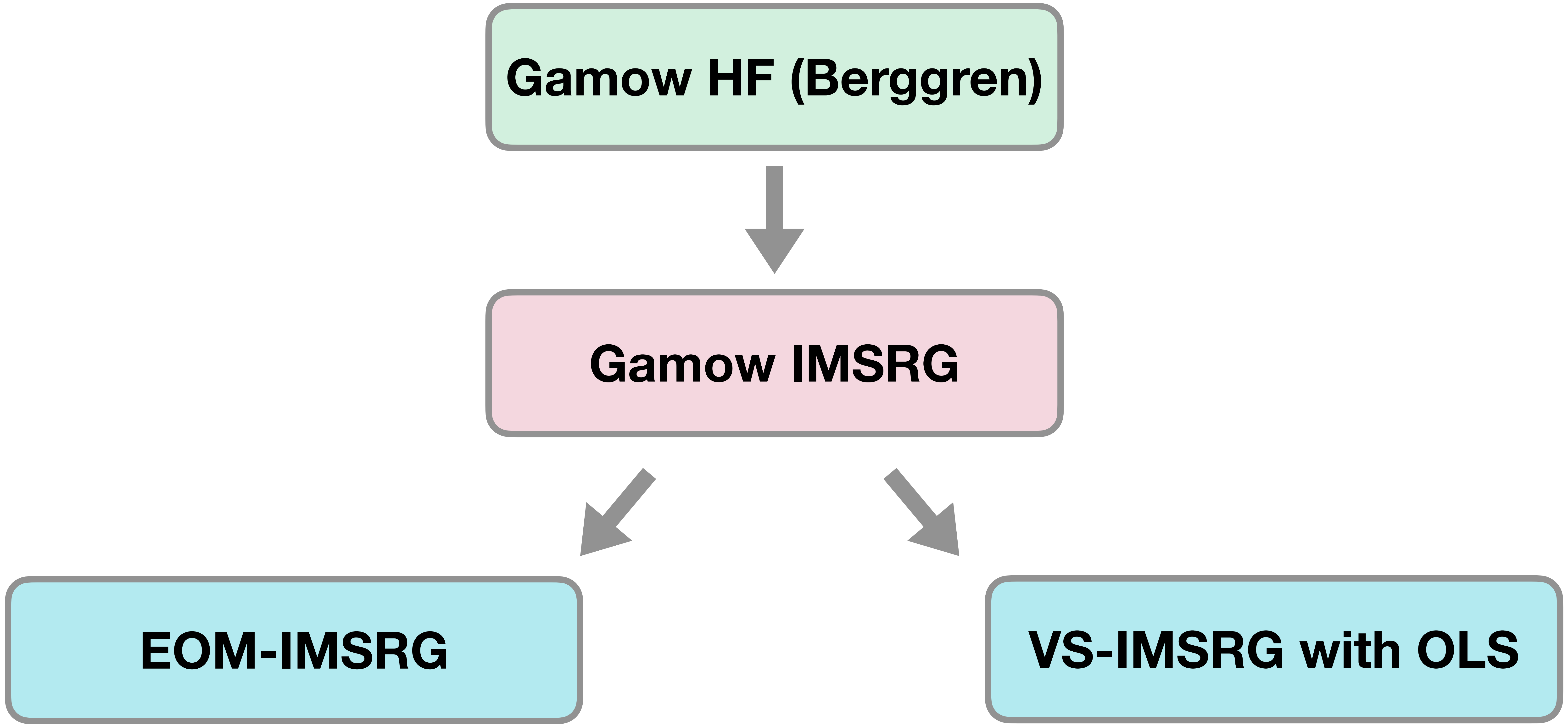


BS Hu, et al., In preparation (2022)

Gamow VS-IMSRG results



Summary



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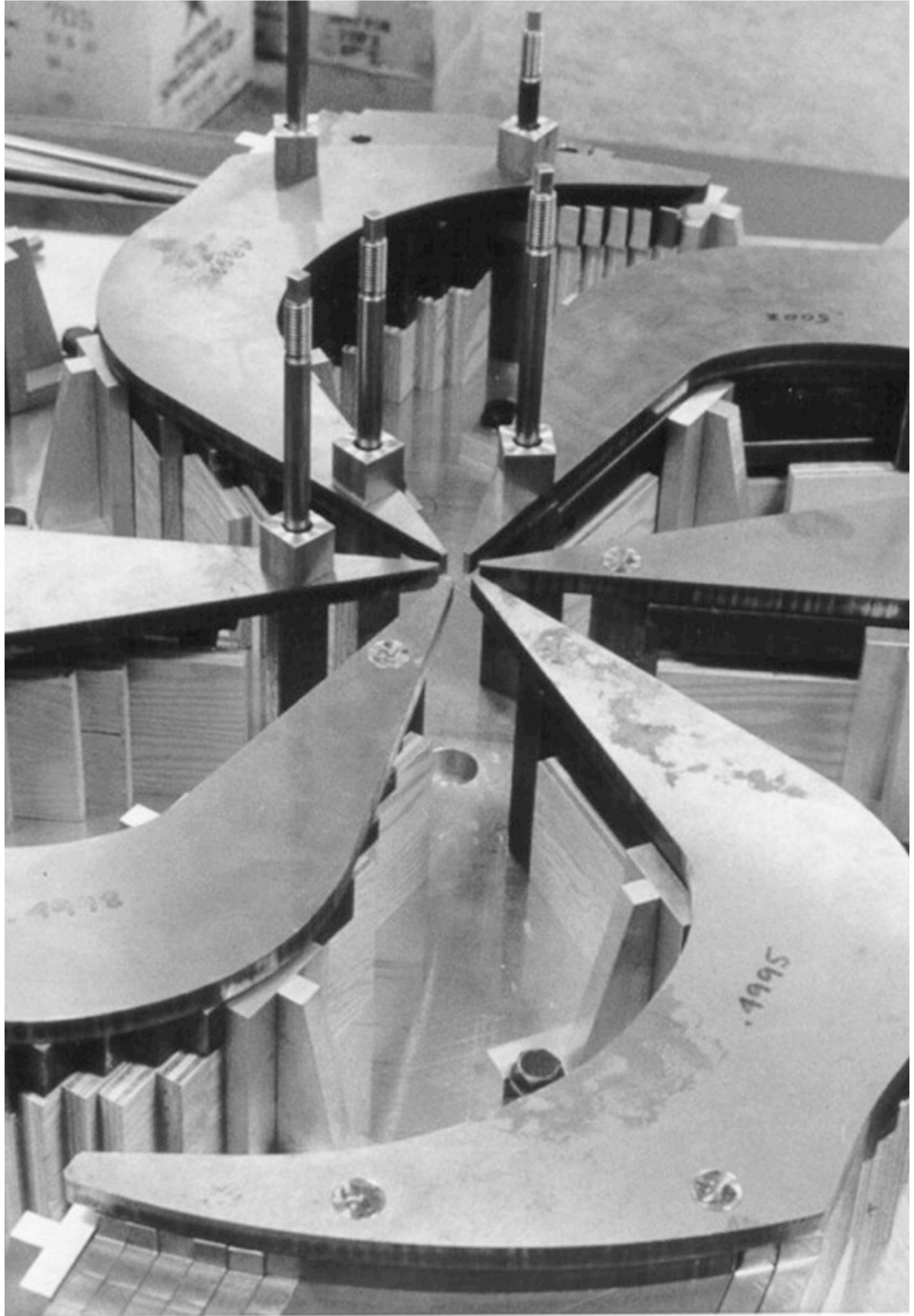
Thank you
Merci



Discovery, accelerated