Ab initio no-core shell model study of lighter nuclei with realistic NN interactions*

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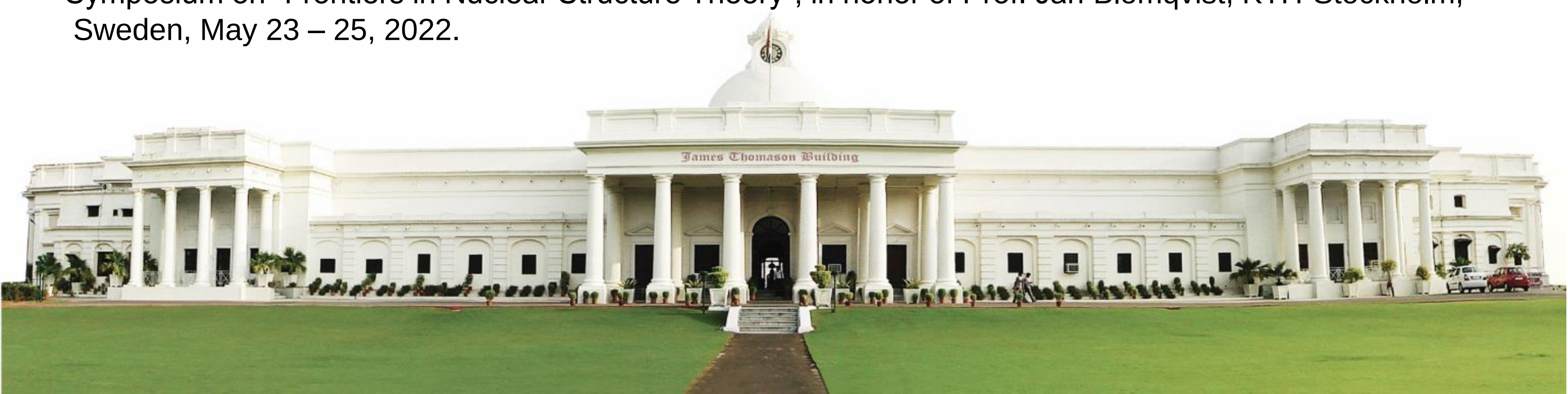
Symposium on "Frontiers in Nuclear Structure Theory", in honor of Prof. Jan Blomqvist, KTH-Stockholm, Sweden, May 23 – 25, 2022.



Outline:

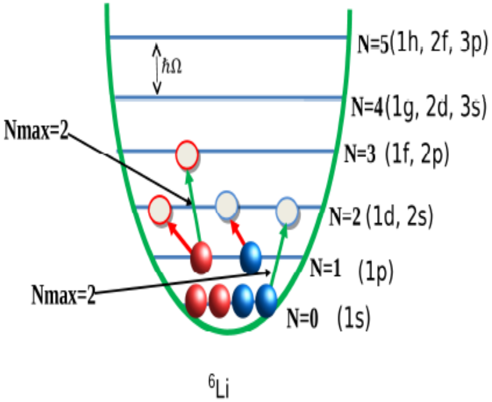
A. Why ab-initio?

B. Ab initio results for lighter nuclei

No core shell model results for O and F chain

No core shell model results for B, C, Ne and N chain

C. Conclusions



Why ab initio ?

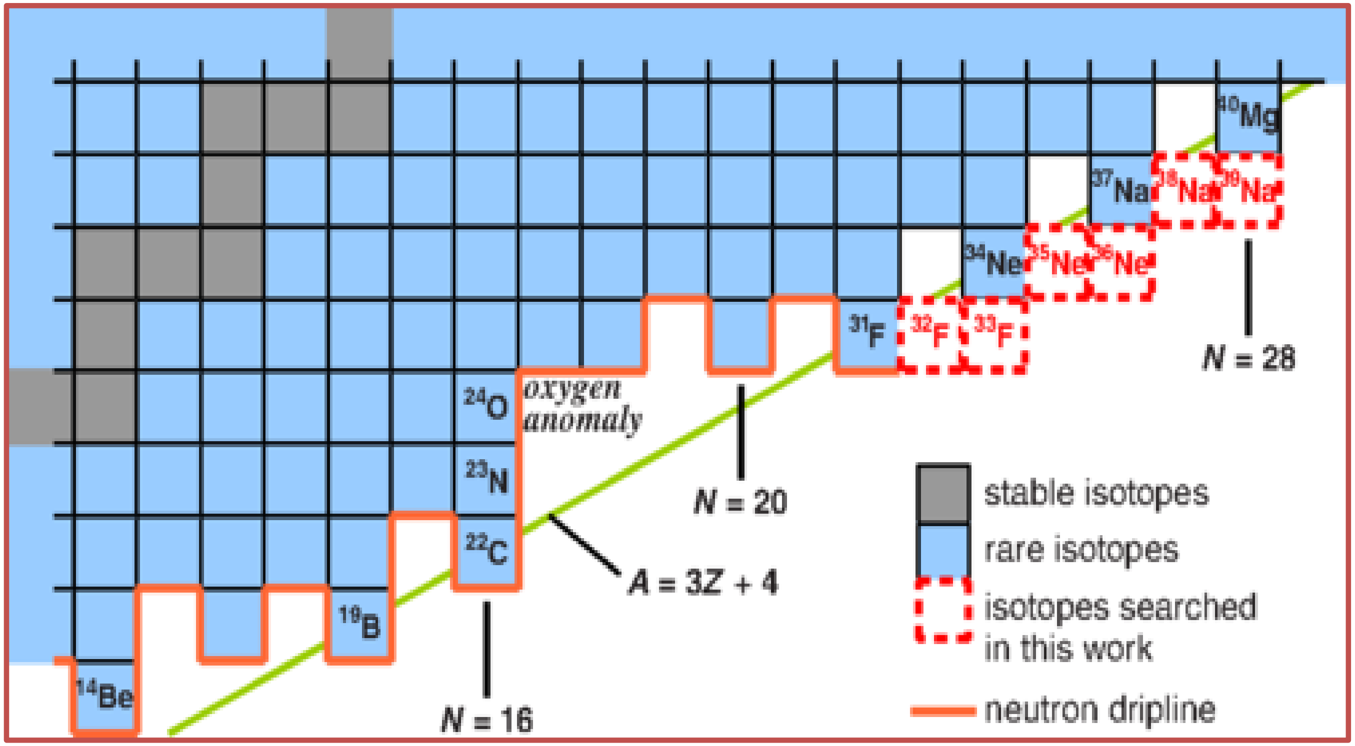
Recent Experimental results of exotic nuclei from RIKEN

Location of drip line !!!

Drip line of O was confirmed 20 yrs ago !!!

Location of the Neutron Drip line at Fluorine and Neon
D.S. Ahn et al., Phys. Rev. Lett. 123, 212501 (2019)

This work confirmed that ^{31}F and ^{34}Ne are the heaviest bound isotopes of fluorine and neon, respectively.



More details about drip line: N. Tsunoda, T. Otsuka et al., Nature 587, 66 (2020).

Ab Initio Theory

$$H|\Psi> = E|\Psi>$$

Different types of realistic NN interactions for NCSM

Based on Meson Exchange:

- **Argonne potentials**
  Local potential – av8', av18
- **Bonn potential**
  Non-local, Charge dependent-CDB2K
- **INOY- Inside Non Local Outside Yukawa tail.**

Based on χEFT (Chiral effective field theory) :

Potentials are guided by QCD, softer potentials.

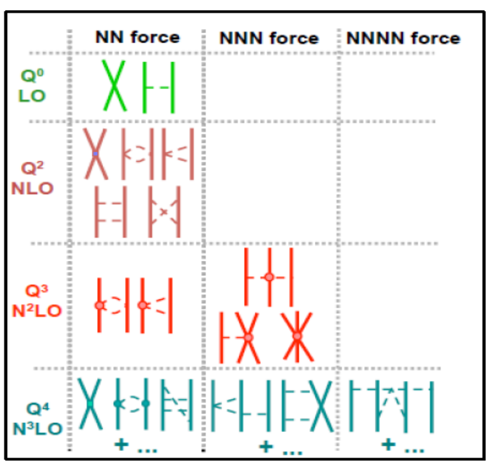
- **N^2LO (Next-to-next leading order)**
- **N^3LO (Next-to-next-to-next leading order)**

Modern Many-Body Methods

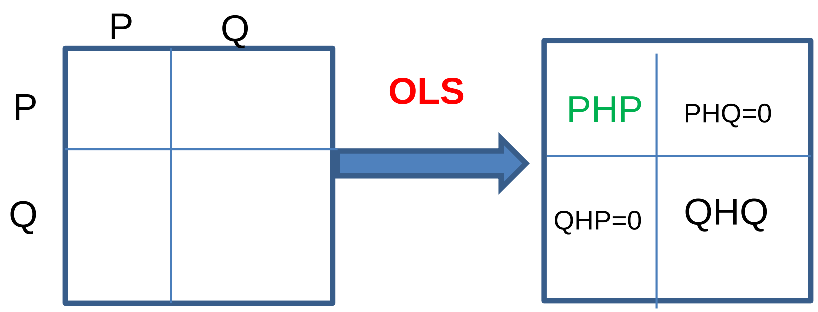
- **No Core Shell Model**
- **Green Function Monte Carlo**
- **Many-Body Perturbation Theory**
- **….**

NCSM with core:

- **Coupled Cluster Theory (CCEI)**
- **In Medium Similarity Renormalization Group (IM-SRG)**



When we use interactions (AV18,CDB2K, INOY etc.) that generate strong short range correlation, we get a problem with convergence. So, we need a normalization procedure that softens the interaction.



Unitary transformation:

$$H_{eff} = Pe^{-S}He^{S}P$$

Where anti-Hermitian operator

$$S = \operatorname{arctanh}(\omega - \omega^{+})$$

NCSM with Core

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PHYSICAL REVIEW C **94**, 064306 (2016)

Spectroscopic factor strengths using *ab initio* approaches

P. C. Srivastava* and Vikas Kumar
Department of Physics, Indian Institute of Technology, Roorkee 247 667, India

PHYSICAL REVIEW C **96**, 024316 (2017)

First-principles results for electromagnetic properties of *sd* shell nuclei

Archana Saxena* and Praveen C. Srivastava†
Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247 667, India

PHYSICAL REVIEW C **97**, 024310 (2018)

***Ab initio* calculations of Gamow-Teller strengths in the *sd* shell**

Archana Saxena,[1,*] Praveen C. Srivastava,[1,†] and Toshio Suzuki[2,3,‡]
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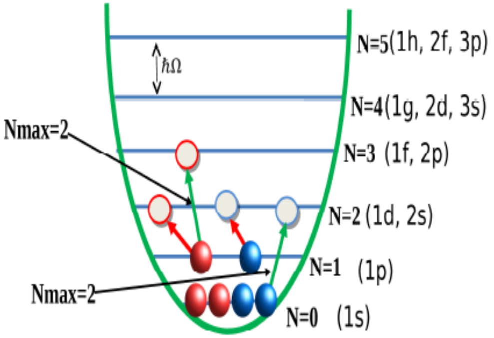
[2]*Department of Physics, College of Humanities and Sciences, Nihon Univerity, Sakurajosui 3, Setagaya-ku, Tokyo 156-8550, Japan*
[3]*National Astronomical Observatory of Japan, Osawa 2, Mitaka, Tokyo 181-8588, Japan*

PHYSICAL REVIEW C **101**, 064304 (2020)

Second-forbidden nonunique β^- decays of ^{24}Na and ^{36}Cl assessed by the nuclear shell model

Anil Kumar,[1,*] Praveen C. Srivastava,[1,†] Joel Kostensalo,[2,‡] and Jouni Suhonen[2,§]
[1]*Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247 667, India*
[2]*University of Jyvaskyla, Department of Physics, P.O. Box 35 (YFL), FI-40014, University of Jyvaskyla, Finland*

No Core Shell Model



^{6}Li

The starting Hamiltonian

$$H_A = T_{rel} + V = \frac{1}{A}\sum_{i<j}^{A}\frac{(\vec{p_i} - \vec{p_j})^2}{2m} + \sum_{i<j}^{A} V_{NN,ij} + \cdots \ldots$$

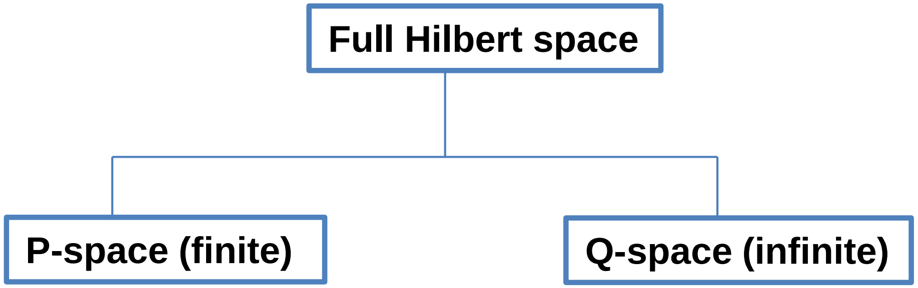
Relative kinetic energy **Two nucleon interaction (including Coulomb part)**

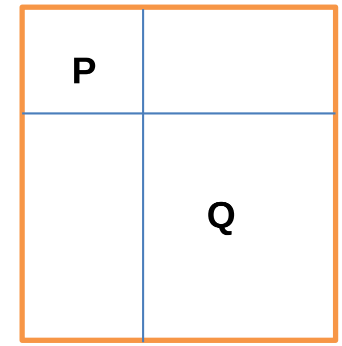
We add H.O. center-of-mass term

$$H_{CM} = T_{CM} + U_{CM}\,, \qquad where \;\; U_{CM} = \frac{1}{2}\, Am\,\Omega^2\,\vec{R}^2\,, \qquad \vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r_i}$$

$$H_A^{\Omega} = H_A + H_{CM} = \sum_{i=1}^{A} h_i + \sum_{i<j}^{A} V_{i,j}^{\Omega,A} = \sum_{i=1}^{A}\left[\frac{\vec{p_i}^2}{2m} + \frac{1}{2}m\Omega^2\vec{r_i}^2\right] + \sum_{i<j}^{A}\left[V_{NN,ij} - \frac{1}{2A}m\Omega^2(\vec{r_i} - \vec{r_j})^2\right]$$

Addition of the HO Hamiltonian does not affect the system properties





P + **Q** =1

P-space projection operator **Q-space projection operator**

Effective shell model Hamiltonian:

$$H^{\Omega}_{A,eff} = P\left\{\sum_{i<j}^{A}\left[\frac{\vec{p}_i^2}{2m} + \frac{1}{2}m\Omega^2\vec{r}_i^2\right] + \sum_{i<j}^{A}\left[V^{NN}_{ij} - \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2\right]_{\mathrm{eff}}\right\}P.$$

Finally, we subtract the C.M. Hamiltonian Hc.m. and include the Lawson projection term to shift the spurious C.M. excitations.

$$H^{\Omega}_{A,eff} = P\left\{\sum_{i<j}^{A}\left[\frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2\right] + \sum_{i<j}^{A}\left[V^{NN}_{ij} - \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2\right]_{\mathrm{eff}} + \underbrace{\beta\left(H_{\mathrm{c.m.}} - \frac{3}{2}\hbar\Omega\right)}_{\text{Lawson term}}\right\}P.$$

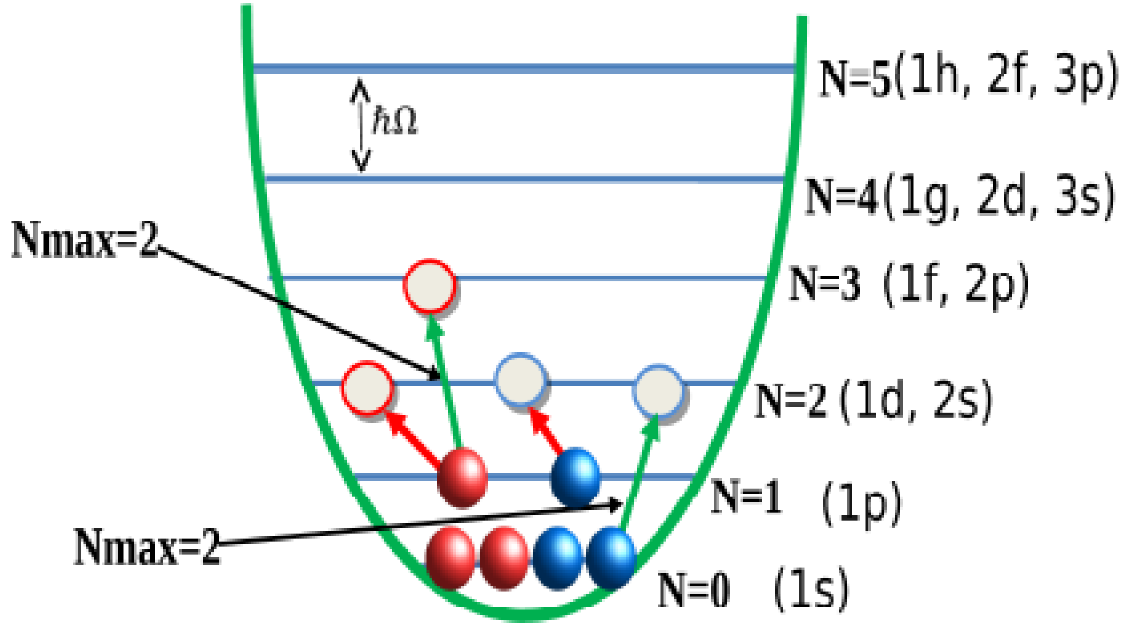
Review: B. R. Barrett, P. Navrátil and J. P. Vary, Prog. Part. Nucl. Phys. 69, 131 (2013)

In NCSM, all nucleons are treated as active, which means there is no assumption of an inert core.

In NCSM calculations, there are two variational parameters: harmonic oscillator (HO) frequency (Ω) and truncation parameter Nmax.

Nmax

Maximum number of HO quanta in many-body HO basis space above the unperturbed A-nucleons configuration.



Positive Parity (Natural Parity) >>> Nmax=0,2,4…

Negative Parity (Unnatural Parity) >>> Nmax=1,3,5…

^{6}Li

No Core Shell Model

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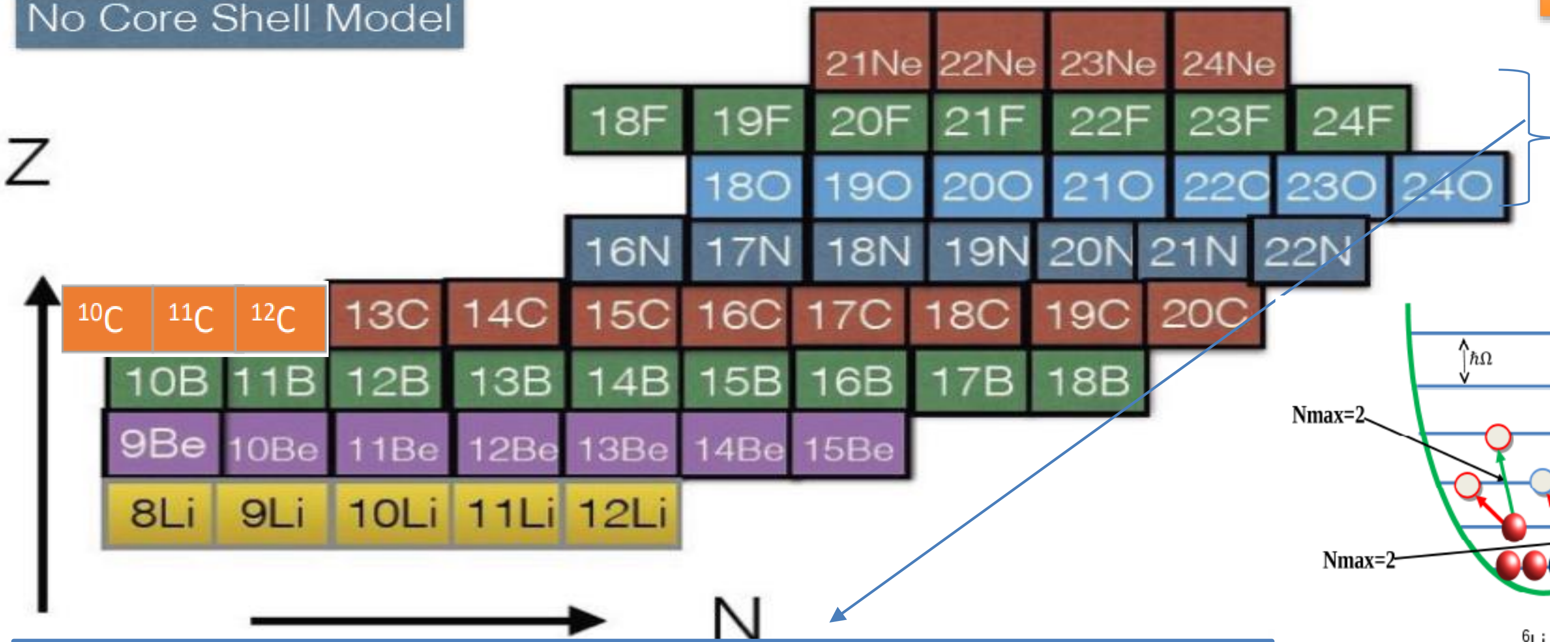

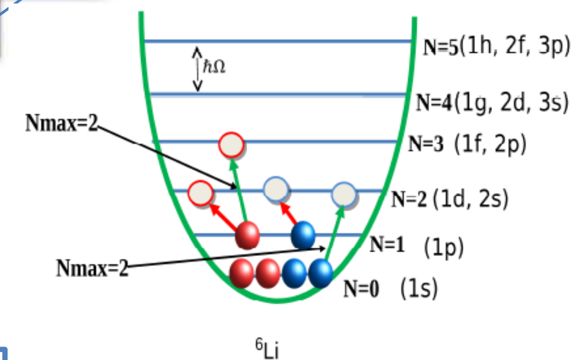

Ab initio no-core shell model study of $^{18-23}$O and $^{18-24}$F isotopes

Archana Saxena[1] and Praveen C Srivastava[2,1]

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Journal of Physics G: Nuclear and Particle Physics, Volume 47, Number 5

Citation Archana Saxena and Praveen C Srivastava 2020 *J. Phys. G: Nucl. Part. Phys.* **47** 055113

PHYSICAL REVIEW C **102**, 044309 (2020)

***Ab initio* no-core shell model study of $^{10-14}$B isotopes with realistic *NN* interactions**

Priyanka Choudhary,[1,*] Praveen C. Srivastava,[1,†] and Petr Navrátil[2,‡]

[1]*Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, India*

[2]*TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada*

***Ab initio* no-core shell model description of $^{10-14}$C isotopes**

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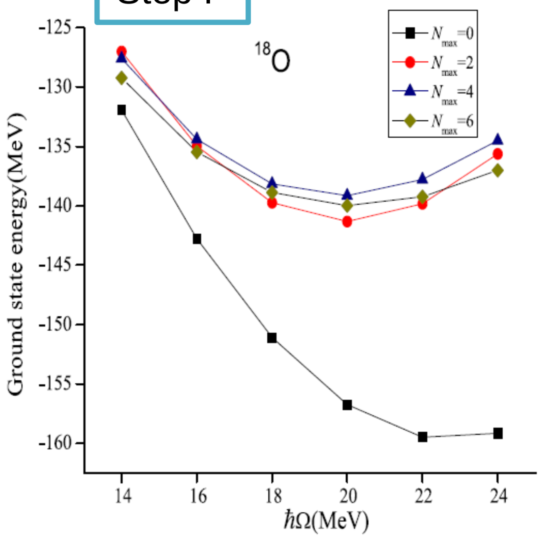
[2]*University of Victoria, 3800 Finnerty Road, Vicotria, British Columbia V8P 5C2, Canada*

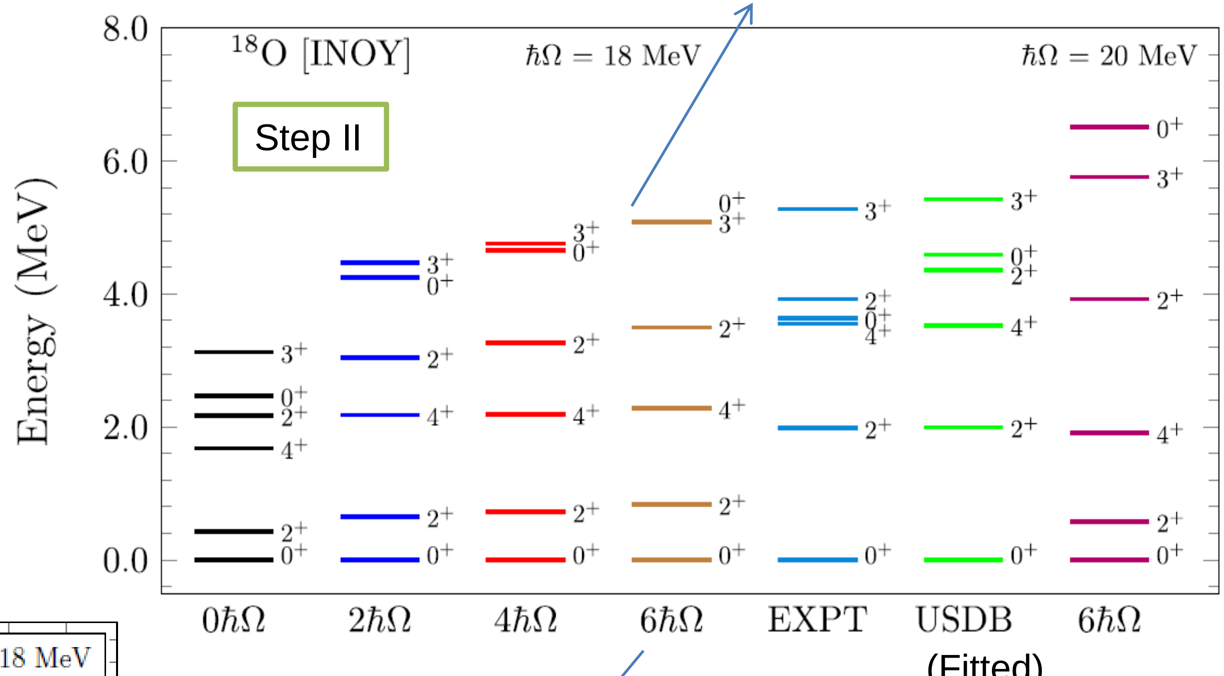
[3]*TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada*

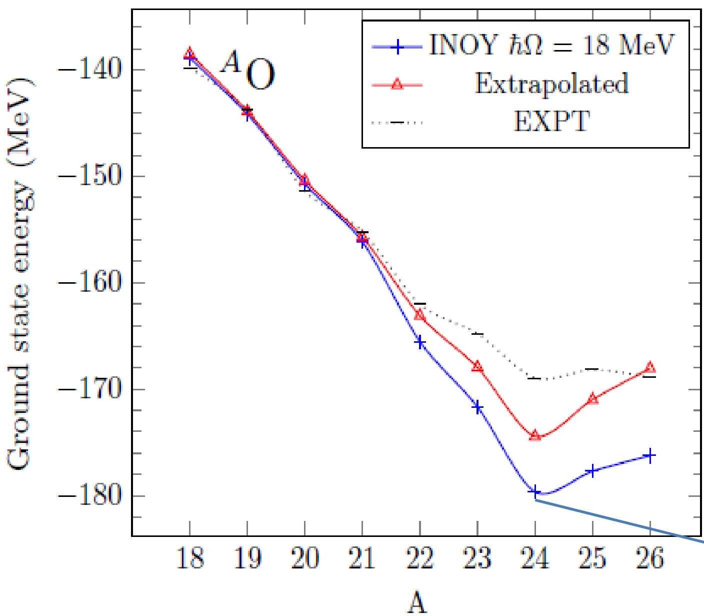
No Core Shell Model Study of $^{18-23}O$ and $^{18-24}F$ isotopes

First time such heavy calculations are done !

Step I



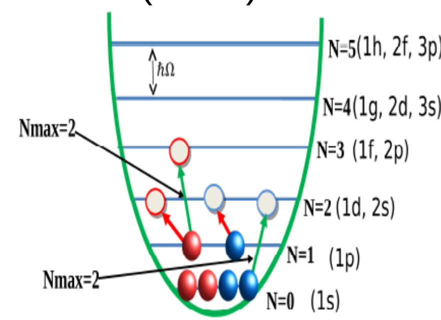




Matrix size (N X N)

Nmax	6	3.40×10^8
Nmax	8	1.22×10^{10}

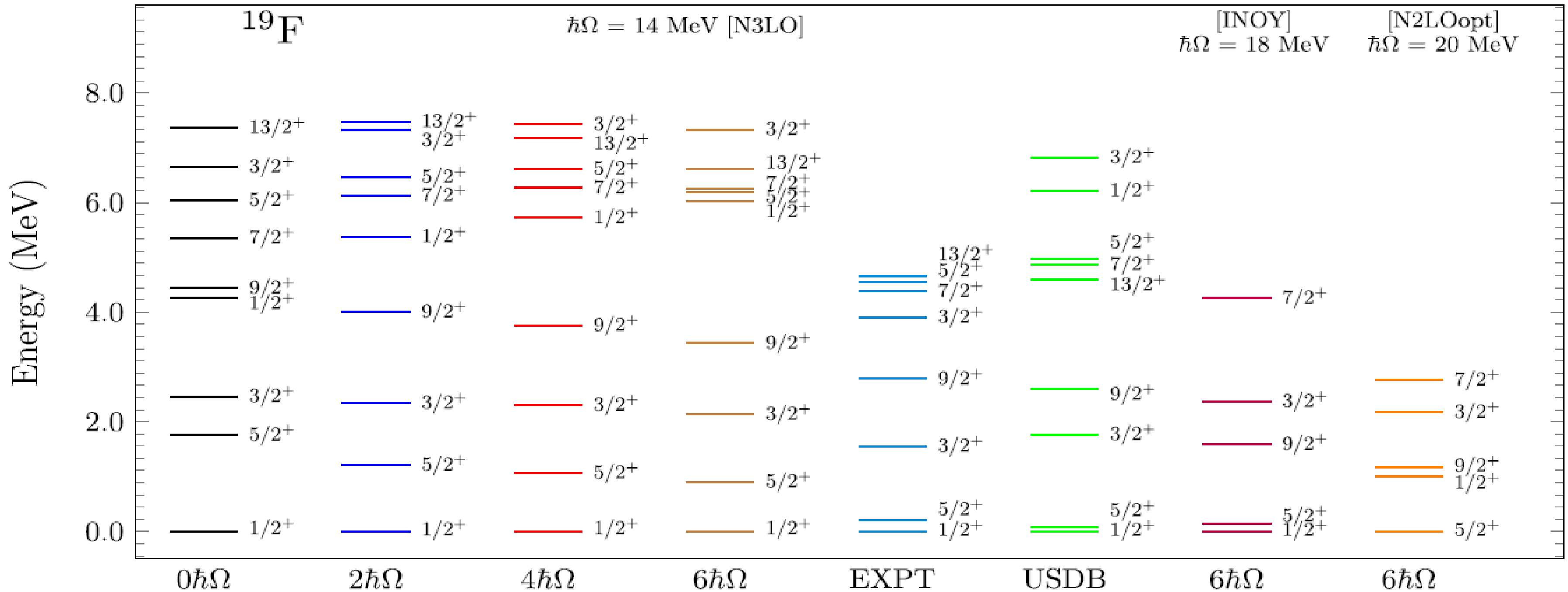
12 Days for Nmax = 6

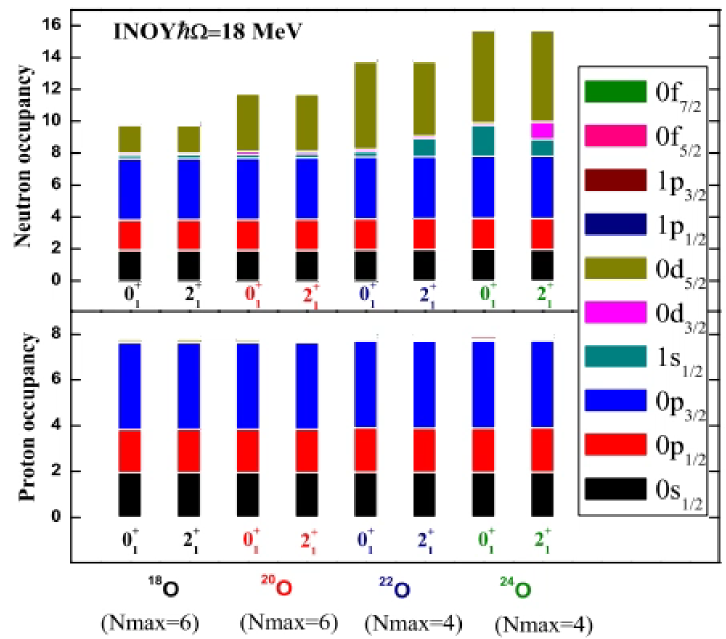


We need large RAM and 10-TB HDD to perform no core shell model calculations

Not possible with fitted interaction

A. Saxena and P.C. Srivastava, J. Phys. G: Nucl. Part. Phys. 47, 055113 (2020)





A. Saxena and P.C. Srivastava, J. Phys. G: Nucl. Part. Phys. 47, 055113 (2020)

Ab-initio no-core shell model study of $^{10-14}\mathrm{B}$ isotopes with realistic NN interactions

VOLUME 88, NUMBER 15 PHYSICAL REVIEW LETTERS 15 APRIL 2002

Ab Initio Shell Model Calculations with Three-Body Effective Interactions for _p_-Shell Nuclei

Petr Navrátil and W. Erich Ormand
Lawrence Livermore National Laboratory, L-414, P.O. Box 808, Livermore, California 94551

..Contrary to the experimental observation of 3+, when the AV8' potential is used, indicating the need for true three-body forces.

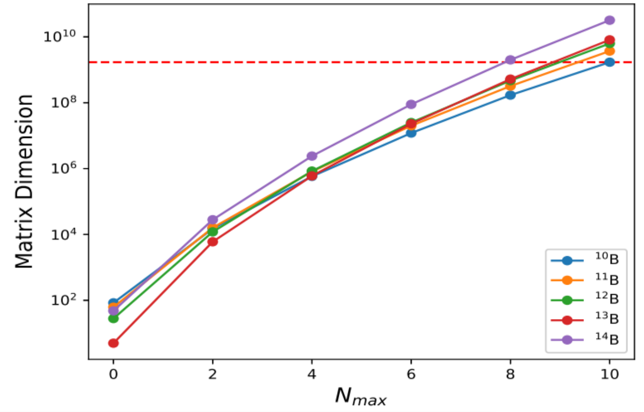
PHYSICAL REVIEW C **102**, 044309 (2020)

Ab initio no-core shell model study of $^{10-14}$B isotopes with realistic _NN_ interactions

Priyanka Choudhary[1,*] Praveen C. Srivastava[1,†] and Petr Navrátil[2,‡]
[1]*Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, India*
[2]*TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada*

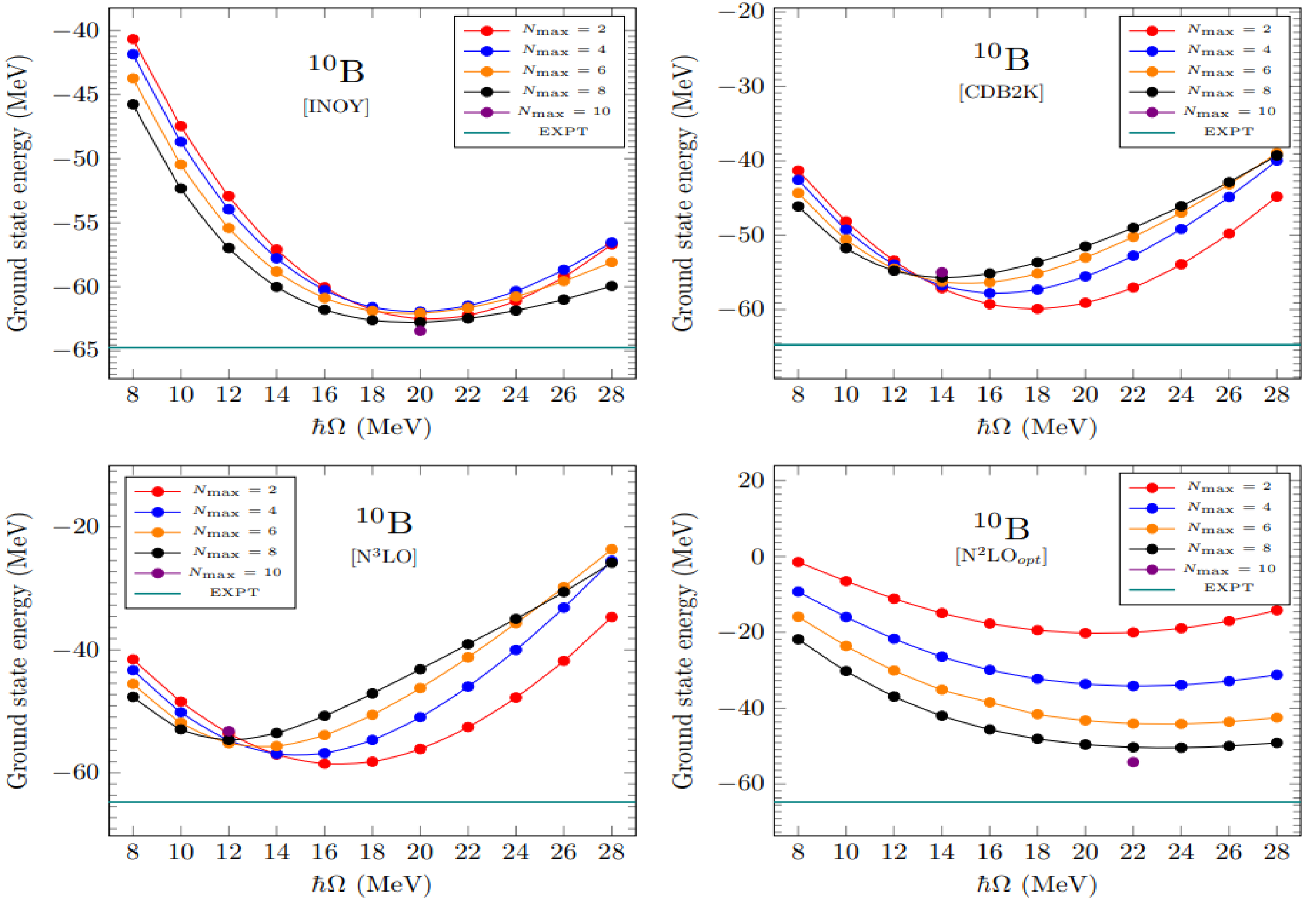
Dimension for B chain:

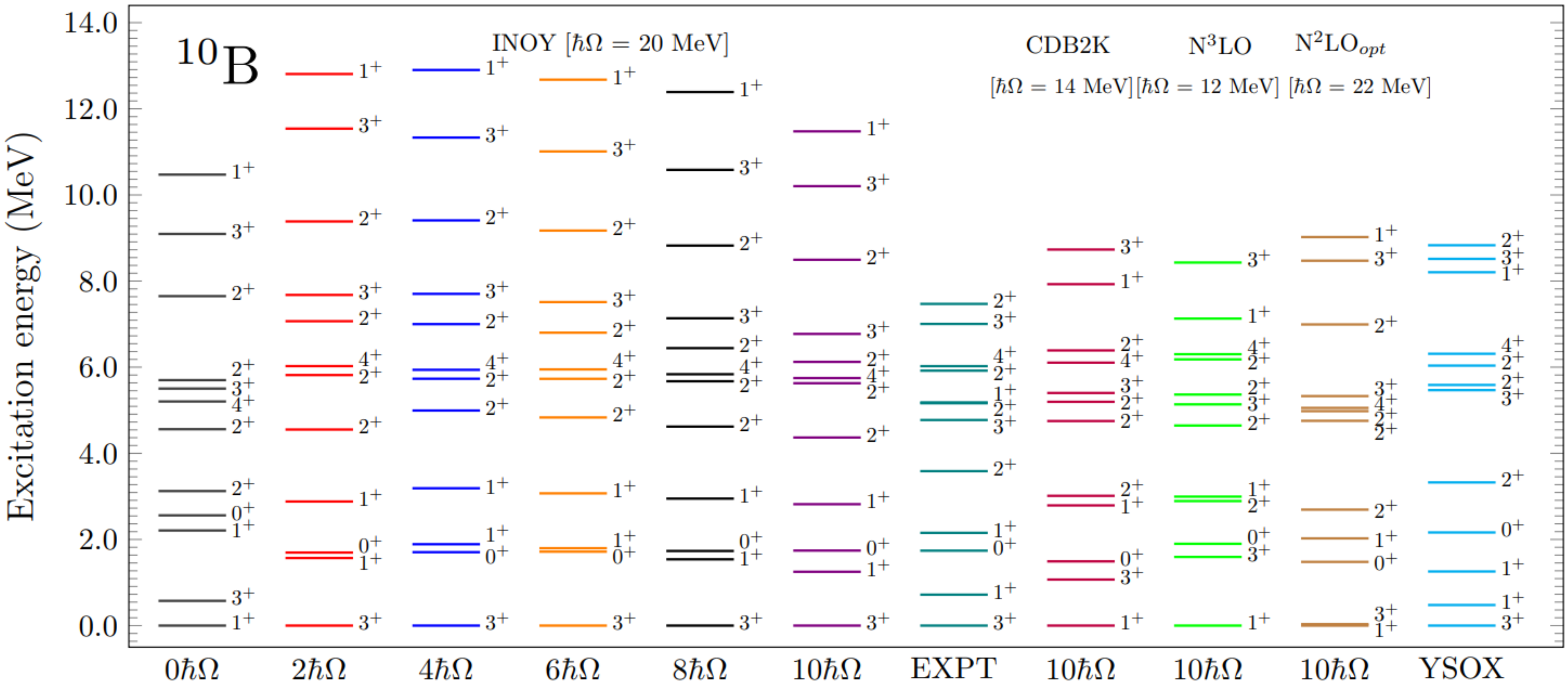
N_{max}	^{10}B	^{11}B	^{12}B	^{13}B	^{14}B
0	84	62	28	5	48
2	1.5×10^4	1.6×10^4	1.2×10^4	6.0×10^3	2.8×10^4
4	5.8×10^5	8.1×10^5	8.4×10^5	6.0×10^5	2.4×10^6
6	1.2×10^7	2.0×10^7	2.5×10^7	2.3×10^7	8.9×10^7
8	1.7×10^8	3.2×10^8	4.7×10^8	5.2×10^8	2.0×10^9
10	1.7×10^9	3.7×10^9	6.3×10^9	8.1×10^9	3.2×10^{10}



Maximum basis sizes up to which we reached is Nmax = 10 for ^{10}B, Namx=8 for ^{11,12,13}B and Nmax=6 for ^{14}B with m-scheme dimensions up to 1.7 billion.

Ground state energy of ^{10}B:

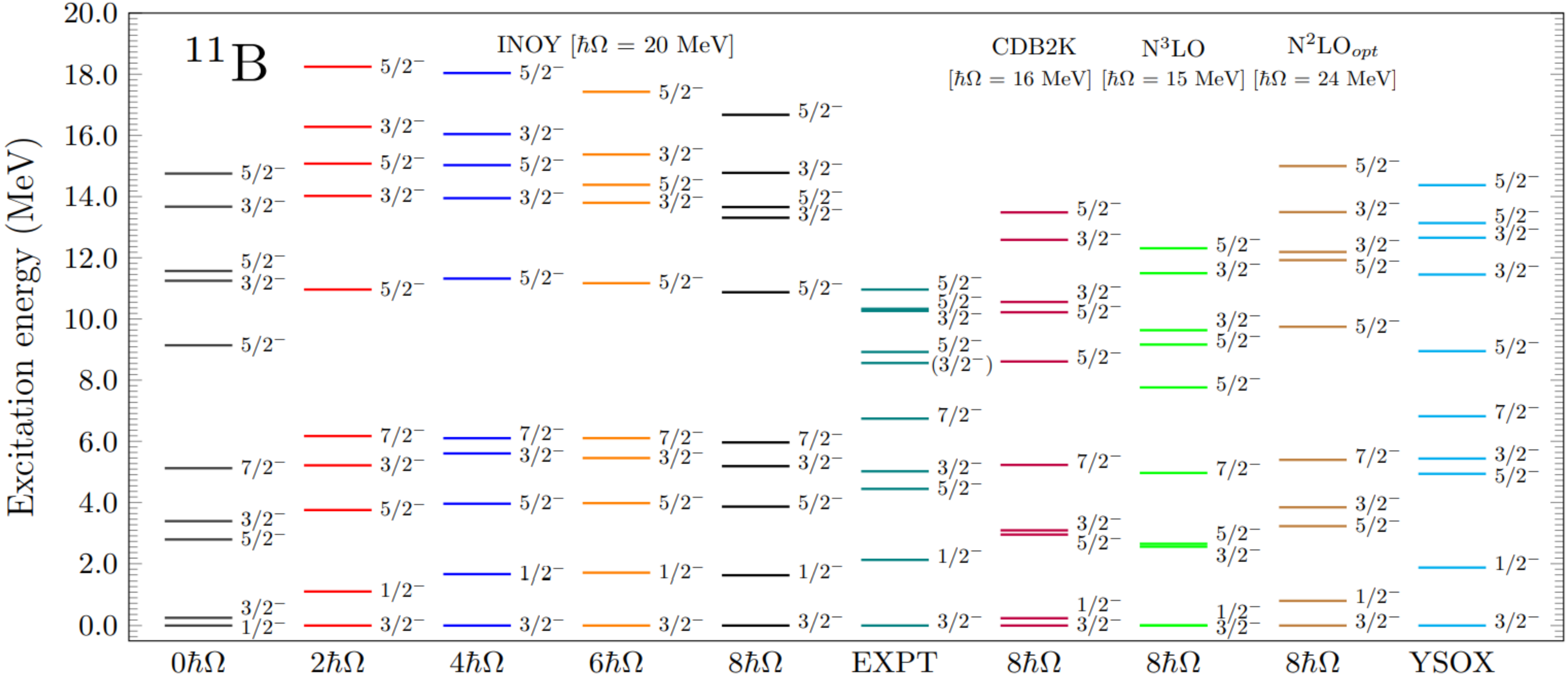




- Reproduces the correct g.s. 3^+ with the INOY interaction. INOY is a two-body interaction but also has the effect of three-body forces via short range and nonlocal character.

- Unable to reproduce the correct g.s. as 3^+ with the CDB2K, N3LO and N2LO_opt interactions.

P. Choudhary, P.C. Srivastava and P. Navratil, Phys. Rev. C 102, 044309 (2020)



- ❑ **Reproduces the correct g.s. with all four interactions using NCSM.**

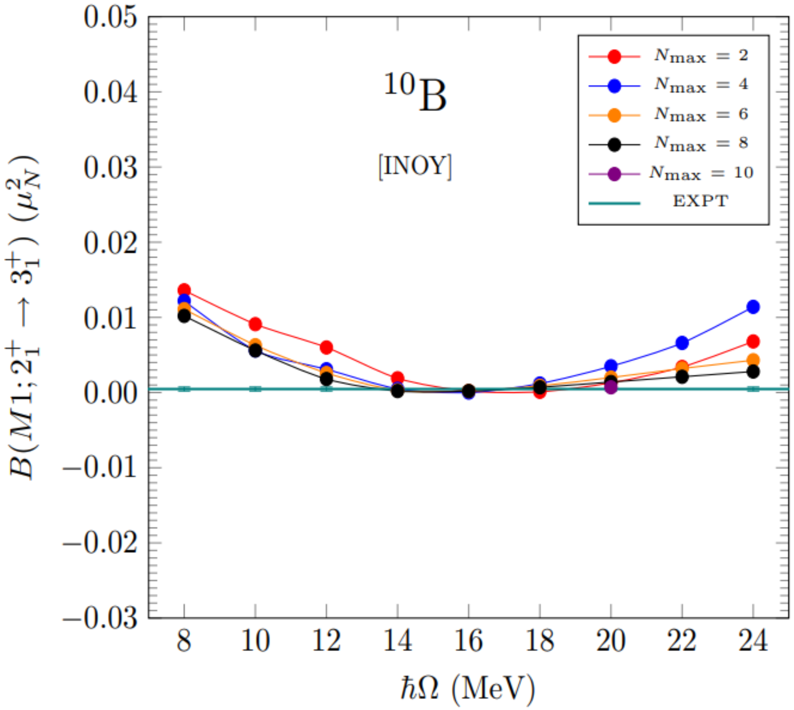
- ❑ **We get correct excited states up to ~ 7 MeV with all interactions except the N3LO.**

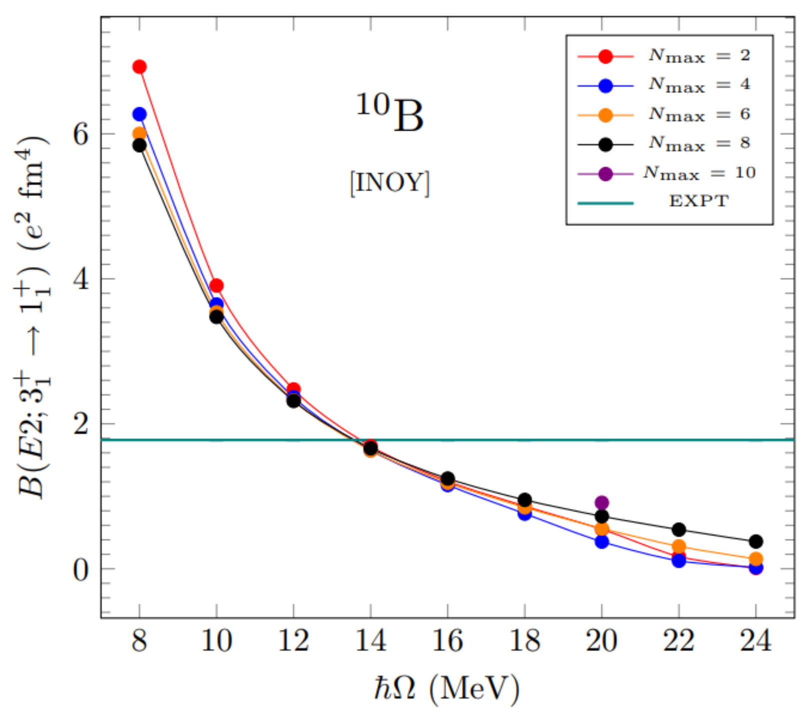
- ❑ **For N3LO interaction, $3/2^-$ and $1/2^-$ states are almost degenerate, while the INOY gives a splitting close to the experiment. This splitting depends on the strength of the spin-orbit interaction, which is The apparently largest for INOY interaction.**

Electromagnetic properties of boron isotopes

^{10}B	Expt.	INOY	CDB2K	N^3LO	N^2LO_{opt}	YSOX
$Q(3^+)$	0.0845(2)	0.061	0.071	0.077	0.067	0.073
$\mu(3^+)$	1.8004636(8)	1.836	1.852	1.856	1.838	1.806
$E_{g.s.}(3^+)$	−64.751	−63.433	−54.979	−53.225	−54.181	−65.144
$B(E2; 3_1^+ \rightarrow 1_1^+)$	1.777(9)	0.911	2.091	2.686	1.482	0.757
$B(M1; 2_1^+ \rightarrow 3_1^+)$	0.00047(27)	0.0007	0.002	0.003	0.0001	0.004
^{11}B	Expt.	INOY	CDB2K	N^3LO	N^2LO_{opt}	YSOX
$Q(3/2^-)$	0.04059(10)	0.027	0.030	0.031	0.029	0.043
$\mu(3/2^-)$	2.688378(1)	2.371	2.537	2.622	2.366	2.501
$E_{g.s.}(3/2^-)$	−76.205	−74.926	−66.034	−62.915	−59.993	−76.686
$B(E2; 7/2_1^- \rightarrow 3/2_1^-)$	1.83(44)	0.814	1.258	1.478	1.032	3.118
$B(M1; 3/2_1^- \rightarrow 1/2_1^-)$	0.519(18)	0.708	0.976	1.051	0.766	0.835
^{12}B	Expt.	INOY	CDB2K	N^3LO	N^2LO_{opt}	YSOX
$Q(1^+)$	0.0132(3)	0.009	0.009	0.010	0.010	0.014
$\mu(1^+)$	1.003(1)	0.561	0.134	0.022	0.282	0.737
$E_{g.s.}(1^+)$	−79.575	−78.304	−69.350	−68.062	−61.226	−79.264
$B(M1; 1_1^+ \rightarrow 0_1^+)$	NA	0.047	0.078	0.086	0.066	0.026
$B(M1; 2_1^+ \rightarrow 1_1^+)$	0.251(36)	0.125	0.197	0.339	0.170	0.204
^{13}B	Expt.	INOY	CDB2K	N^3LO	N^2LO_{opt}	YSOX
$Q(3/2^-)$	0.0365(8)	0.025	0.029	0.031	0.028	0.042
$\mu(3/2^-)$	3.1778(5)	2.844	2.815	2.830	2.781	2.959
$E_{g.s.}(3/2^-)$	−84.454	−85.205	−75.856	−74.716	−65.624	−84.185
$B(E2; 5/2_1^- \rightarrow 1/2_1^-)$	NA	1.800	2.281	2.721	1.990	0.787
$B(M1; 3/2_1^- \rightarrow 1/2_1^-)$	NA	0.984	1.035	1.065	0.982	0.729
^{14}B	Expt.	INOY	CDB2K	N^3LO	N^2LO_{opt}	YSOX
$Q(2^-)$	0.0297(8)	0.016	0.025	0.025	0.004	0.026
$\mu(2^-)$	1.185(5)	0.778	0.926	0.914	0.550	0.614
$E_{g.s.}(2^-)$	−85.422	−82.002	−76.929	−77.549	−51.413	−84.454
$B(M1; 2_1^- \rightarrow 1_1^-)$	NA	2.579	2.457	2.436	2.755	2.656

Transition strengths of ^{10}B





- **The convergence of the $B(M_1; 2_1^+ \to 3_1^+)$result is obtained at smaller $\hbar\Omega$ and lower Nmax.**
- **B(E2) value varies even for the larger value of the Nmax parameter.**

  - **Magnetic dipole moments converge quickly and accurately since they have no "r" dependence.**
  - **Quadrupole moment Q converges slowly because of its " r^2 " dependence.**
  - **Hence, Q is much more difficult to compute because of the huge model spaces required in order to convergence and also obtain the correct result.**

Observables dependence on A:

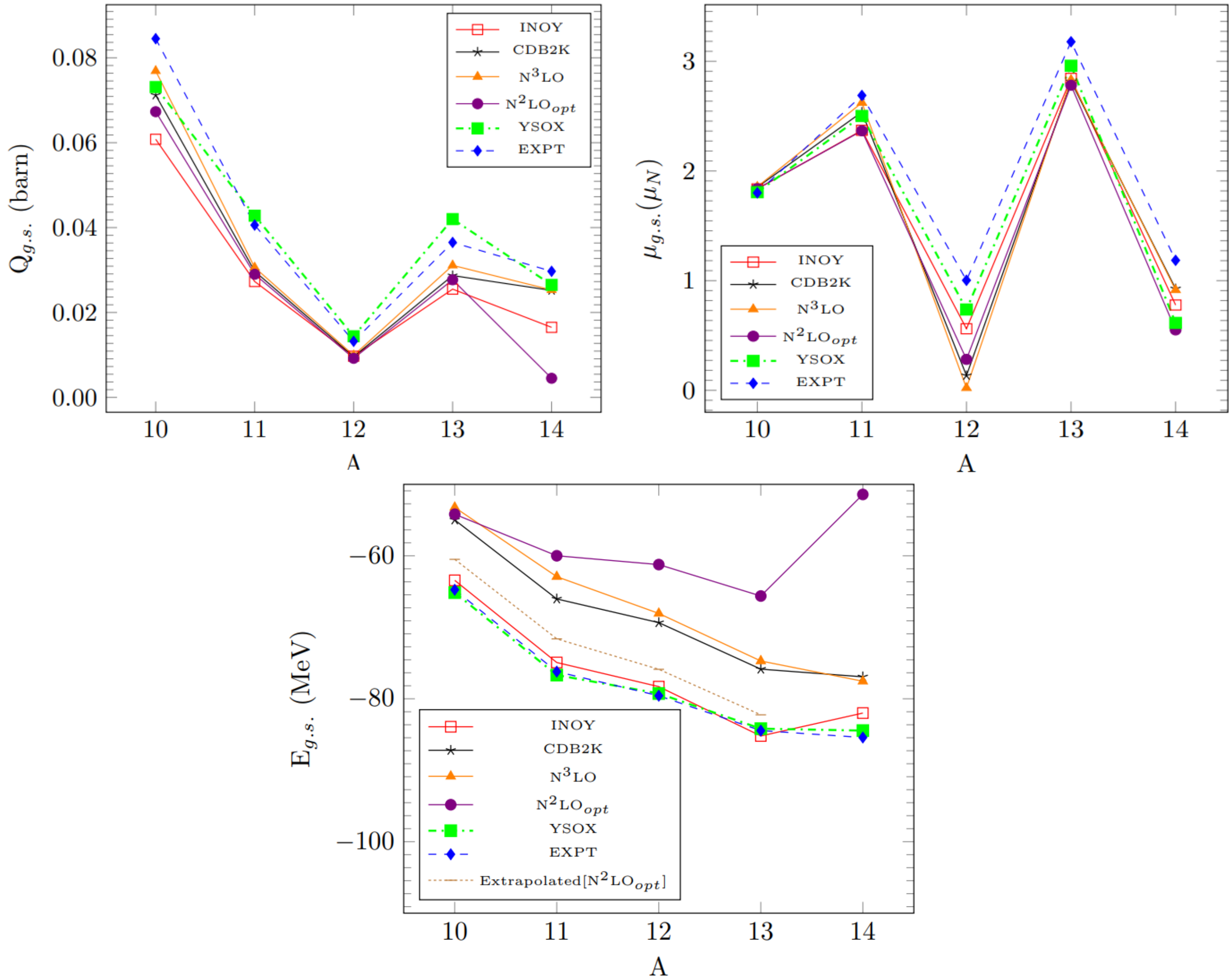


Fig: G.s. energy, quadrupole and magnetic moment dependence on the mass number of B isotopes.

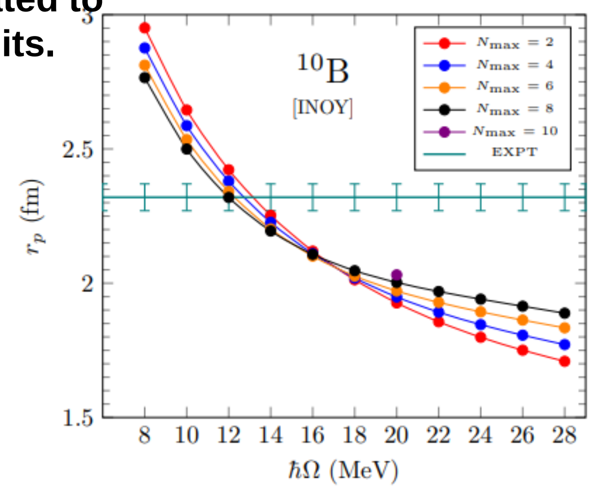
Point-proton radii of ^{10}B

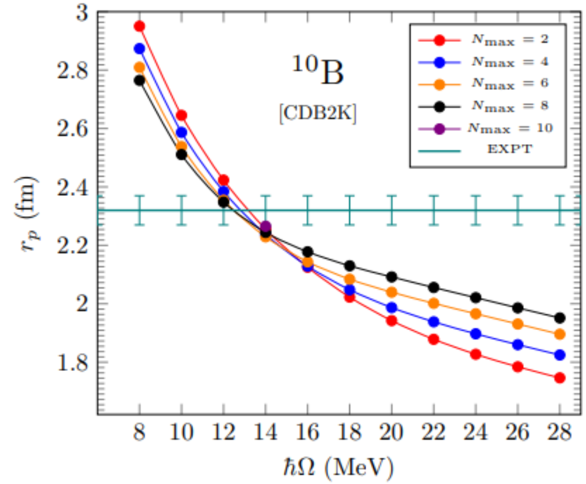
$$r_p = \sqrt{r_c^2 - R_p^2 - \frac{N}{Z}R_n^2 - \frac{3\hbar^2}{4m_p^2c^2}}$$

$$r_p^2 = \frac{1}{Z}\sum_{i=1}^{Z}|\vec{r_i} - \vec{R}_{CM}|^2$$

Last term is Darwin-Foldy term related to Relativistic correction in natural units.

$$R_p^2 = 0.8775(51)fm^2$$
$$R_n^2 = -0.1149(27)fm^2$$
$$\frac{3\hbar^2}{4m_p^2c^2} = 0.033\ fm^2$$





- ❑ r_p **from INOY, CDB2K and N3LO comes out to be 2.14fm, 2.30fm and 2.36 fm, respectively.**

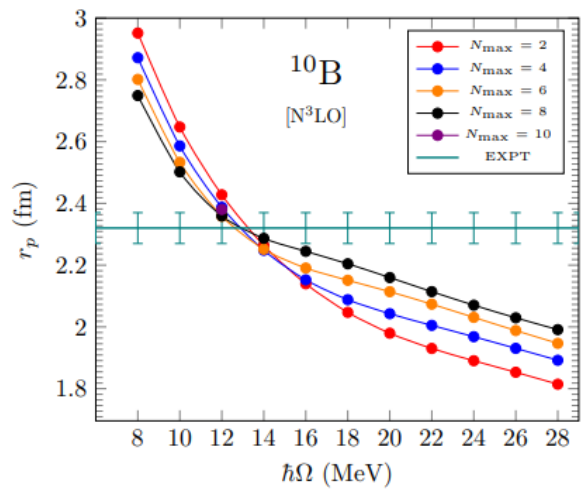


Fig: Variation of r_p for 10B with HO frequency for Nmax=2 to 10, corresponding to the INOY, N3LO and CDB2K Interactions.

PTEP
Prog. Theor. Exp. Phys. **2019**, 073D02 (8 pages)
DOI: 10.1093/ptep/ptz073

Ab initio no-core shell model study of neutron-rich nitrogen isotopes

Archana Saxena and Praveen C. Srivastava*
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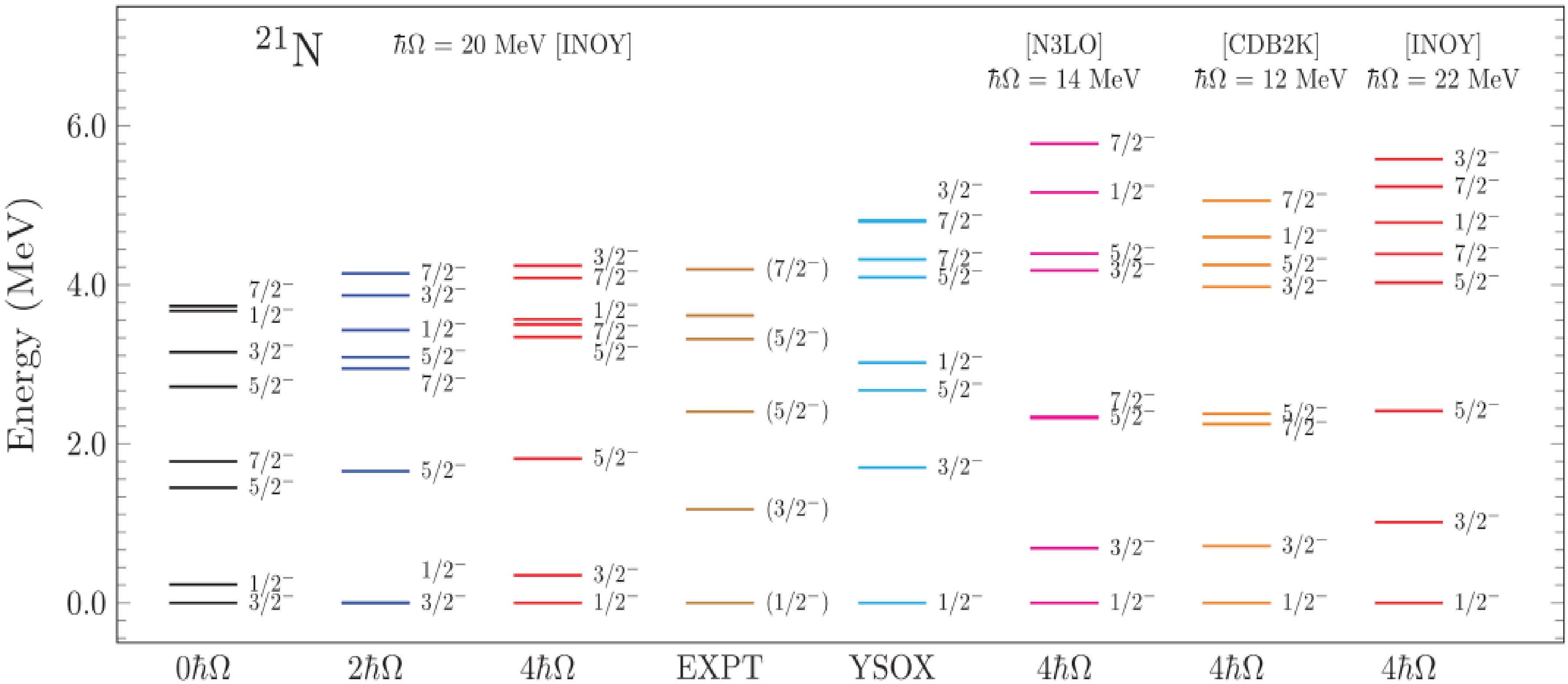
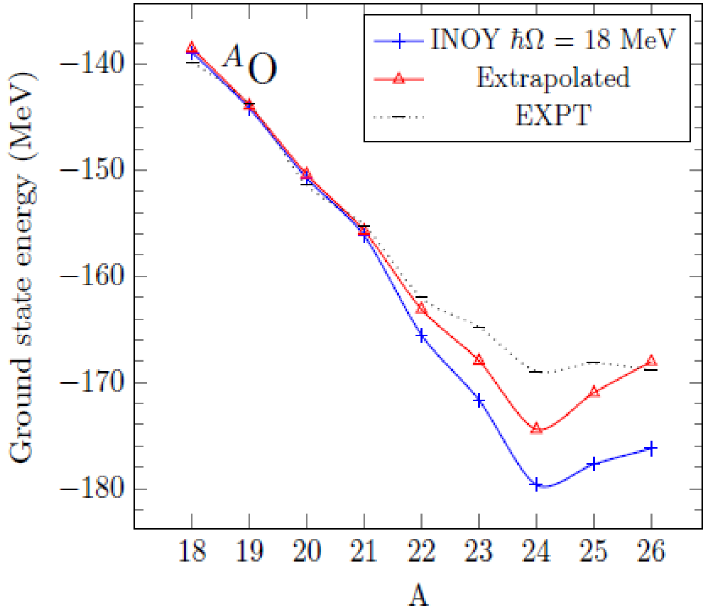
We have calculated the energy spectra for neutron-rich $^{18-22}$N isotopes using the no-core shell model.



Conclusions and Future Work :

- NCSM results for O and F isotopes. First such heavy calculations are done.



- NCSM study for B, C, N, O, F and Ne isotopes including radii.
- We need higher Nmax calculation for quadrupole moment.
- Further our aim is to locate drip line beyond O with NCSM.
- It is possible to support different experimental group with NCSM for lighter nuclei.
- Future: Quantum computing maybe one option to diagonalize the matrices for NCSM study of medium mass nuclei.
- To study beta decay using NCSM.

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Thank you for your attention !!