Neutrino-Nucleus scattering with ab initio No-Core Shell Model

尹鹏 河南科技大学





山国科学院近代物理研

Institute of Modern Physics, Chinese Academy of Sciences



合作者:

李贺, 房栋梁, 赵行波 (近物所)

Pieter Maris, James P. Vary (ISU)

Mark A. Caprio (ND)

Patrick J. Fasano (ANL)

李玉峰 (高能所)







Neutrino-nucleus interactions



Nuclear response at different energy transfer regions is crucial to make the predictions.

(Quasi-)elastic v-nucleus CC/NC interactions





Experiment	Nuclear Target	Reaction	σ_{o} [10 ⁻⁴⁶ cm ²]	ΔE _{nucl} [MeV] (no det. Thres.)
GALLEX/GNO SAGE	⁷¹ Ga ₃₃	$v_e + {}^{71}Ga \rightarrow e^- + {}^{71}Ge$	8.611 ± 0.4% (GT)	0.2327
HOMESTAKE	³⁷ Cl ₁₇	$v_e + {}^{37}Cl \rightarrow e^- + {}^{37}Ar$	1.725 (F)	0.814
SNO	² H ₁	$v_e + H \rightarrow e^- + p + p$	(GT)	1.442
DUNE, ICARUS, etc.	⁴⁰ Ar ₁₈	$v_e + {}^{40}Ar \rightarrow e^- + {}^{40}K^*$	148.58 (F) 44.367 (GT ₂)	1.505 +
		10	41.567 (GT ₆)	

From Kevin McFarland

Important for solar & supernova neutrino detection

	Channels	Threshold Signal			Event numbers		
		[MeV]		$[200~{\rm kt}{\times}{\rm yrs}]$	after cuts		
CC	$\nu_e + {}^{13}\text{C} \to e^- + {}^{13}\text{N}(\frac{1}{2}^-; \text{gnd})$	$2.2 {\rm ~MeV}$	$e^-\!+^{13}\mathrm{N}$ decay	3929	647		
NC	$\nu_x + {}^{13}\text{C} \to \nu_x + {}^{13}\text{C}(\frac{3}{2}; 3.685 \text{ MeV})$	$3.685~{\rm MeV}$	γ	3032	738		
\mathbf{ES}	$\nu_x + e \rightarrow \nu_x + e$	0	e^-	$3.0{ imes}10^5$	$6.0{ imes}10^4$		

JUNO, Astrophys.J. 965 (2024) 2, 122

Phenomenological models calculations

✤ Neutrinos-¹²C & ¹³C cross-sections calculations with phenomenological models

	$(\nu_{\mu},\mu^{-})DIF$	$(\nu_e, e^-)DAR$
	$<\sigma>_{f}(10^{-40}\ cm^{2})$	$<\sigma>_{f}(10^{-42}\ cm^{2})$
$SM(HO wf) (0+1+2)\hbar\omega$	0.70	8.42
$SM(HF wf) (0 + 1 + 2)\hbar\omega$	0.65	8.11
$SM(WS wf) (0 + 1 + 2)\hbar\omega$	0.58	8.4
RPA	2.09	49.47
QRPA	1.97	42.92
CRPA	1.06(1.03)	13.88(12.55)
EXP	$0.66 \pm 1.0 \pm 1.0$ [a]	$10.5 \pm 1.0 \pm 1.0$ [b]
		$9.1 \pm 0.4 \pm 0.9 \ [c]$
		$9.1 \pm 0.5 \pm 0.8$ [d]

Neutrinos-¹²C cross-sections from different models

Shell Model (SM) Random Phase Approximation (RPA) Quasi-particle RPA (QRPA) Continuum RPA (CRPA) a: C.Athanassopoulos and the LSND collaboration, Phys. Rev. C (1997),

- b: R.C.Allen et al., Phys. Rev. Lett (1990),
- c: C.Athanassopoulos and the LSND collaboration, Phys. Rev. C (1997),
- d: B.E.Bodmann and the KARMEN collaboration, Phys. Lett. B (1994)

The results from RPA calculations are far away from experimental data, while the SM calculations are much closer to experimental data

Phenomenological models calculations

Neutrinos-¹²C & ¹³C cross-sections calculations with shell model



Neutrino-¹²C charge current cross-sections from shell model with SFO interaction had a good agreement with experimental data

$B(GT: {}^{13}C \rightarrow {}^{13}N)$	SFO	CK	EXP.
13 N J^{π} E_x (MeV)			
$1/2^{-}$ 0.0	0.284	0.420	$0.411 {\pm} 0.004$
			$0.398 {\pm} 0.008$
$1/2^{-}$ 8.92	0.569	0.524	
$3/2^{-}$ 3.50	2.103	2.14	$1.64{\pm}0.10$
$3/2^{-}$ 9.46	0.500	0.260	
$B(M1) \ (\mu_N^2)$			
$^{13}C (3/2^{-}: 3.68 \text{ MeV}) \rightarrow ^{13}C (1/2^{-}_{g.s.})$	0.878	1.17	$0.698 {\pm} 0.072$

B(M1) and B(GT) strengths of ¹³C from shell model with SFO & CK interaction were still a little far away from experimental data

> T. Suzuki et al., Phys. Rev. C (2012) T. Suzuki et al., Phys. Rev. C (2019)

What is Ab Initio in nuclear physics?

Few-Body Syst (2023) 64:77 https://doi.org/10.1007/s00601-023-01857-2

R. Machleidt

What is *ab initio*?

Nuclear structure theory at its basic level is not about fitting data to get "good" results. Fundamental nuclear structure theory is about answering the question:

Do the same nuclear forces that explain free-space scattering experiments also explain the properties of finite nuclei and nuclear matter when applied in nuclear many-body theory?

Check for updates

OPEN ACCESS

EDITED BY Paul Stevenson, University of Surrey, United Kingdom

REVIEWED BY

Andreas Nogga, Helmholtz Association of German Research Centres (HZ), Germany Tobias Frederico, Instituto de Tecnologia da Aeronáutica (ITA), Brazil Richard Furnstahl, The Ohio State University, United States

*CORRESPONDENCE A. Ekström,

What is *ab initio* in nuc

A. Ekström¹*, C. Forssén¹, G. Hagen^{2,3}, G. F and T. Papenbrock^{2,3}

¹Department of Physics, Chalmers University of Technology, Götebo Ridge National Laboratory, Oak Ridge, TN, United States, ³Departme University of Tennessee, Knoxville, TN, United States, ⁴National Center Ridge National Laboratory, Oak Ridge, TN, United States

Ab initio has been used as a label in nuclear theory for over two decades. Its meaning has evolved and broadened over the years. We present our interpretation, briefly review its historical use, and discuss its present-day relation to theoretical uncertainty quantification.



Check for

updates



Challenges

- Self bound quantum many-body problem, with 3A degrees of freedom in coordinate (or momentum) space, as well as spin degree of freedom
- Strong interactions, with both short-range and long-range pieces
- Not only 2-body interactions, but also intrinsic 3-body interactions and possibly 4- and higher N-body interactions
- Uncertainty quantification for calculations needed
 - for comparison with experiments
 - for comparison between different methods

Computational Methods for Nuclear Structure

- Few-body methods
 - Faddeev Equation for A=3 system
 - ➤ typically in momentum space
 - Faddeev-Yakuboski Equations for A=4 system
 - \triangleright can nowadays be pushed to A=5 and 6 (Lazauskas)
 - Hyperspherical Harmonics
 - ≻ Up to A=6

Many-body methods

- Variational Monte-Carlo (A<=12)</p>
- Green's Function Monte-Carlo (A<=12)</p>

➤ Configuration Interaction (CI) methods (NCSM (A<=20), Coupled Cluster (A<=100))</p>

Nuclear Lattice Simulations (A<=32)</p>

All few- and many-body methods need some levels of High-Performance Computing

Nuclear Interactions

$$\hat{\mathbf{H}}_{\mathsf{rel}} = \hat{\mathbf{T}}_{\mathsf{rel}} + \sum_{i < j} V_{ij} + \sum_{i < j < k} V_{ijk} + \dots$$

> Nuclear interactions not well-determined

- In principle calculable from QCD
- In practice constrained by (fitting to) experimental (*NN* scattering) data

>Alphabet of realistic interactions

- Argonne potentials
- Bonn potenitals
- Chiral EFT interactions
- Daejeon16 (based on Idaho-N3LO)



➢ Most *NN* potentials need 3*N* forces for agreement with experiments

LENPIC chiral EFT NN potential up to N⁴LO



Introduction of NCSM

No-Core Configuration Interaction / No-Core Shell Model calculations

Given a Hamiltonian operator

$$\widehat{H} = \sum_{i < j} \frac{(\overrightarrow{p}_i - \overrightarrow{p}_j)}{2mA} + \sum_{i < j}^A V_{ij} + \sum_{i < j < k} V_{ijk} + \cdots$$

Solve the eigenvalue problem for wavefunction of A nucleons

$$\widehat{H}\Psi_{\alpha_1\cdots\alpha_A}=\mathbf{E}\Psi_{\alpha_1\cdots\alpha_A}$$

- > Expand wavefunction in basis states $|\psi\rangle = \sum \hat{a}_j |\phi_i\rangle$
- > Express Hamiltonian in basis $\langle \phi_j | \hat{H} | \phi_i \rangle = H_{ij}$
- > Diagonalize Hamiltonian matrix H_{ij}
- No-Core: All A nucleons are treated equally
- Complete basis ---- exact result
- In practice
 - 1. truncate basis
 - 2. study behavior of observables as function of truncation
- Computational challenge
 - 1. construct large (10¹⁰ × 10¹⁰) sparse symmetric matrix H_{ij}
 - 2. obtain lowest eigenvalues & eigenvectors corresponding to low-

lying spectrum and eigenstates

P. Maris, NCSM_NICC_YTT(2021) Barrett et al., Progress in Particle and Nuclear Physics (2013)

Main Chanllenges



> Increase of basis space dimension with A and N_{max}

- > Need calculations up to at least N_{max} =8, preferably N_{max} =10 for meaningful extrapolation and numerical error estimates
- More relevant measure for computational needs
 - Number of nonzero matrix elements
 - Current limit 10¹⁴ (Perlmutter)





National Energy Research Scientific Computing Center

MFDn in the SciDAC era

https://nuclei.mps.ohio-state.edu/nuclei_home.php

(not in NUCLEI)



- Collaborative DOE grants for domain scientists (i.e. nuclear physicists), computer scientists, and applied mathematicians to enable scientific progress through high-performance computing
- Support for students and postdocs to do the hard & tedious work
- UNEDF (2007-2012), NUCLEI(2012-2017, 2017-2022)
 - MFDn: collaboration between ISU (James Vary), Ames Lab (Masha Sosonkina), and Berkeley Lab (Esmond Ng, Chao Yang)
 - Ab Initio: Coupled Cluster, VMC & GFMC, lattice EFT, ...
 - Density Functional Theory for heavy nuclei
 - BIGSTICK: complementary/competing NCCI code (Calvin Johnson)
 - Valence Shell Model (NuShellX, BIGSTICK)



Previous calculations from ab initio NCSM

Neutrino-¹²C cross-sections calculations with NCSM



AV8': NN potential CD-Bonn: NN potential AV8' + TM'(99): NN potential + 3N NN potential

The B(M1) calculated values from AV8', CD-Bonn, AV8' + TM'(99) were still a little far away from experimental data

Experimental and calculated B(M1;0+0 \rightarrow 1+1) values for ¹²C

		CD-Bonn		AV8' + TM'(99)	
Interaction	$2\hbar\Omega$	$4\hbar\Omega$	$6\hbar\Omega$	$4\hbar\Omega$	Experiment
(ν_{e}, e^{-})	2.27	3.2	3.69	6.8	$8.9 \pm 0.3 \pm 0.9$ [a]
(ν_{μ}, μ^{-})	0.168	0.275	0.312	0.537	$0.56 \pm 0.08 \pm 0.1$ [b]
μ -capture	1.46	2.07	2.38	4.43	6.0 ± 0.4 [c]

Predicted weak interaction rates of ¹²C. The units are 10⁻⁴² cm² for the (ν_e, e^-) DAR cross section, 10⁻⁴² cm² for the (ν_{μ}, μ^-) DIF cross section, and 10³ sec⁻¹ for muon capture

a:LSND Collaboration, L. B. Auerbach et al., Phys. Rev. C 64, 065501 (2001).

- b:LSND Collaboration, L. B. Auerbach et al., Phys. Rev. C 66, 015501 (2002).
- c: G. H. Miller et al., Phys. Lett. B 41, 50 (1972);

A. C. Hayes, P. Navrátil, and J. P. Vary, Phys. Rev. Lett. 91, 012502 (2003)

Barrett et al., , Progress in Particle and Nuclear Physics (2013)

Improvements of our calculations

From the previous NCSM calculations of neutrino-¹²C scattering, we can infer that the precision of neutrino-¹²C cross-sections with Ab initio NCSM/NCCI, could be improved by applying new interaction(with the contributions from 3N force), increasing the basis space, including more reaction channels and excited states.

Highlights in our calculations

1. New interaction – Daejeon16

Dimensions of many body matrix in Nmax6: 3.26x10⁷; Nmax10: 7.83x10⁹

- 2. Larger basis space for calculations(up to Nmax=10)
- 3. Higher excitation energy (at least 20 MeV~ 30 states)
- 4. More channels(neutral current, charged current, nucleon knock-out)
- 5. Theoretical uncertainty
- 6. Extrapolation tools (Traditional and machine learning ANN)
- 7. Calculations of cross sections at reactor neutrino energies

Current progress

Ground state energy from Daejeon16



NCSM+Daejeon16 has good performance on the calculations of binding energies

We use a simple 3-point exponential extrapolation from the reference paper

$$E^{\hbar\omega}(N_{\max}) = E^{\hbar\omega}_{\infty} + a \,\mathrm{e}^{(-b\,N_{\max})}$$

P. Maris et al., Phys. Rev. C (2021)

Energy spectra from Daejeon16



The low lying spectra of ¹²C & ¹³C from Daejeon16 have good agreement with experimental data

Point Proton Radii of ground state from Daejeon16



We get the estimations and uncertainties of point proton radii from the "crossing points" The point proton radii values from Deajeon16 quite close to experimental data

Comparisons on ground state energies and point proton radii between Daejeon16 and other Chiral EFT interactions

$^{11}\mathrm{C}$	Exp.	Daej16-Extrap.	$NN+NNN_{2007}$	$N^{2}LO(450)_{2021}$	$N^{2}LO(500)_{2021}$
$E_{g.s.} MeV$	-73.441	-73.39(51)			
$r_p fm$	2.13(6)	2.36(2)			
$^{12}\mathrm{C}$	Exp.	Daej16-Extrap.	NN+NNN ₂₀₀₇	$N^{2}LO(450)_{2021}$	$N^{2}LO(500)_{2021}$
E _{g.s.} MeV	-92.162	-92.93(64)	-95.57	-98.7(4)	-101.8(4)
$r_p fm$	2.35(2)	2.30(1)	2.172		
$^{13}\mathrm{C}$	Exp.	Daej16-Extrap.	NN+NNN ₂₀₀₇	$N^{2}LO(450)_{2021}$	$N^{2}LO(500)_{2021}$
E _{g.s.} MeV	-97.108	-97.53(72)	-74.716	-108.3(4)	112.2(4)
$r_p fm$	2.29(3)	2.25(1)	2.135		

Ground state energies and point proton radii of Carbon-11, 12, 13 from Deajeon16 in good agreement with experiment, even better than NN + NNN interaction.

P. Maris et al., Phys. Rev. C (2021) P. Navrátil et al., Phys. Rev. Lett (2007)

Comparisons on ground state energies and point proton radii between Daejeon16 and other Chiral EFT interactions

-	12	² N	Exp.	Exp. Daejeon16-Extrap		N ³ LO	$N^2 LO_{opt}$	
-	$E_{g.s.}(1)$	$^+)$ MeV	-74.041	-73.99(56)				
	r _p fm		2.49(7)	2.49	(2)			
-	¹³ N		Exp.	Daejeon16	-Extrap.	LO	LO^*	
-	$E_{g.s.}(1/$	'2-) MeV	-94.105	-94.62	2(46)			
	$r_{\rm p} (1/2)$	$2_1^+) {\rm fm}$	NA	2.47	(4)	2.52	5.85	
				· · · · · · · · · · · · · · · · · · ·				
11]	3	Exp.	Daejeon	16-Extrap.	$N^2LO(4$	$(50)_{2021}$	$N^{2}LO(500)_{2}$	2021
$E_{g.s.}(3/2)$	⁻) MeV	-76.205	-75.9	99(51)	-79.8	(4)	-82.3(4)	
r _p f	m	2.21(2)	2.2	27(1)				
$^{12}]$	3	Exp.	Daejeon	16-Extrap.	$N^{2}LO(4$	$(50)_{2021}$	$N^{2}LO(500)_{2}$	2021
$E_{g.s.}(1^+$) MeV	-79.575	-79.	30(59)	-84.8	(4)	-87.5(4)	
r _p f	m	2.31(7)	2.2	27(1)				
$^{13}]$	3	Exp.	Daejeon16-Extra		$N^{2}LO(4$	$(50)_{2021}$	$N^{2}LO(500)_{2}$	2021
$E_{g.s.}(3/2)$	⁻) MeV	-84.454	-83.9	97(69)	-92.8	(5)	-95.4(5)	
r _p f	m	2.48(3)	2.2	28(1)				

Ground state energies and point proton radii of Boron 11, 12, 13 & Nitrogen 12, 13 from Deajeon16 in good agreement with experiment, even better than chiral N3LO interaction.

Comparisons on M1 and E2 transitions between

NCCI-Daejeon16 and other calculations

The CK-POT, CK, SFO interactions were performed in shell model calculations

Model space	^{12}C (1900)	Daejeon16 Extrapolatio	Chiral N on $6\hbar\Omega$	N+3N 2	+3N Chiral NN $8\hbar\Omega$		N+3N CK-F 2 2ħ		${ m SFO}\ 2\hbar\Omega$
$\begin{array}{c} B(M1;1^+0\to 0^+0) \\ B(M1;1^+1\to 0^+0) \end{array}$	$\begin{array}{c} 0.0145(21) \\ 0.951(20) \end{array}$	$0.074(1) \\ 0.712(5)$	$0.00 \\ 0.91$	0.006 0.00 [*] 0.913 1.10		0.0078 0. 1.109 0		048 71	0.0044 0.838
		$^{13}\mathrm{C}$	Daejeon16	Chiral	NN+3N	Chira	l NN	$\mathbf{C}\mathbf{K}$	SFO
Model S	pace		$6\hbar\Omega$	$6\hbar\Omega$		$6\hbar$	Ω	$2\hbar\Omega$	$2\hbar\Omega$
B(M1;3/2-:3.68 M) B(E2;3/2-:3.68 M)	$eV \rightarrow 1/2^{-}g.s.)$ $eV \rightarrow 1/2^{-}g.s.)$	$0.698(72) \\ 6.4(8)$	$0.969 \\ 5.388$	$0 \\ 2$.402 .659	1.14 2.68	48 59	1.17	0.878

Hw = 15 MeV in Daejeon16 and chiral interactions

Electromagnetic transitions of Carbon12 & 13 from Deajeon16 are not so close to experiment, but reasonable.

T. Suzuki et al., Phys. Rev. C (2012) P. Navrátil et al., Phys. Rev. Lett (2007) H. Sagawa et al., EPJ Web of Conferences (2018)

Next plan

1. Cross section

$$\begin{split} \left(\frac{d\sigma}{d\Omega}\right)_{\stackrel{\text{Ve}}{\bar{\nu}_e}} &= \frac{2}{\pi} G_F^2 \cos^2 \theta_c F(Z,\epsilon) \frac{\epsilon^2}{2J_i+1} \cos^2 \frac{\theta}{2} \Biggl\{ \sum_{J=0}^{\infty} \left| \langle J_f || \hat{\mathcal{M}}_J + \frac{\omega}{q} \hat{\mathcal{L}}_J || J_i \rangle \right|^2 \\ &+ \left[-\frac{q_\mu^2}{2q^2} + \tan^2 \frac{\theta}{2} \right] \sum_{J=1}^{\infty} \left[\left| \langle J_f || \hat{\mathcal{T}}_J^{\text{el}} || J_i \rangle \right|^2 + \left| \langle J_f || \hat{\mathcal{T}}_J^{\text{mag}} || J_i \rangle \right|^2 \right] \\ &\mp 2 \tan \frac{\theta}{2} \Biggl[-\frac{q_\mu^2}{q^2} + \tan^2 \frac{\theta}{2} \Biggr]^{1/2} \sum_{J=1}^{\infty} \operatorname{Re} \left(\langle J_f || \hat{\mathcal{T}}_J^{\text{mag}} || J_i \rangle \langle J_f || \hat{\mathcal{T}}_J^{\text{el}} || J_i \rangle^* \right) \Biggr\}, \end{split}$$

3. The multipole operators in the equation of charged-current cross section can be expressed in terms of the 7 basic operators

$$\begin{split} M_{JM_{J}}^{\pm}(q\mathbf{x}) &= F_{1}^{(1)}(q_{\mu}^{2})M_{J}^{M_{J}}(q\mathbf{x})\tau_{\pm}, \\ T_{JM_{J}}^{\text{el}\,\pm}(q\mathbf{x}) &= \frac{q}{M_{N}} \bigg(F_{1}^{(1)}(q_{\mu}^{2})\Delta_{J}^{'M_{J}}(q\mathbf{x}) + \frac{1}{2}\mu^{(1)}(q_{\mu}^{2})\Sigma_{J}^{M_{J}}(q\mathbf{x}) \bigg)\tau_{\pm}, \\ T_{JM_{J}}^{\text{mag}\,\pm}(q\mathbf{x}) &= -\frac{iq}{M_{N}} \bigg(F_{1}^{(1)}(q_{\mu}^{2})\Delta_{J}^{M_{J}}(q\mathbf{x}) - \frac{1}{2}\mu^{(1)}(q_{\mu}^{2})\Sigma_{J}^{'M_{J}}(q\mathbf{x}) \bigg)\tau_{\pm}, \\ M_{JM_{J}}^{5\,\pm}(q\mathbf{x}) &= \frac{iq}{M_{N}} \bigg(F_{A}^{(1)}(q_{\mu}^{2})\Omega_{J}^{'M_{J}}(q\mathbf{x}) + \frac{1}{2}\omega F_{P}^{(1)}(q_{\mu}^{2})\Sigma_{J}^{''M_{J}}(q\mathbf{x}) \bigg)\tau_{\pm}, \\ L_{JM_{J}}^{5\,\pm}(q\mathbf{x}) &= i \bigg(F_{A}^{(1)}(q_{\mu}^{2}) - \frac{q^{2}}{2M_{N}}F_{P}^{(1)}(q_{\mu}^{2})\bigg)\Sigma_{J}^{''M_{J}}(q\mathbf{x})\tau_{\pm}, \\ T_{JM_{J}}^{\text{el5}\,\pm}(q\mathbf{x}) &= i F_{A}^{(1)}(q_{\mu}^{2})\Sigma_{J}^{'M_{J}}(q\mathbf{x})\tau_{\pm}, \\ \end{split}$$

2. The multipole operators in the equation of charged-current cross section are defined by

$$\hat{\mathcal{M}}_{JM_J;TM_T} \equiv \int d\mathbf{x} \mathbf{M}_J^{M_J}(q\mathbf{x}) \hat{\mathcal{J}}_0(\mathbf{x})_{TM_T} = \hat{M}_{JM_J;TM_T} + \hat{M}_{JM_J;TM_T}^5,$$
$$\hat{\mathcal{L}}_{JM_J;TM_T} \equiv \frac{i}{q} \int d\mathbf{x} \left[\vec{\nabla} M_J^{M_J}(q\mathbf{x}) \right] \cdot \hat{\mathcal{J}}(\mathbf{x})_{TM_T} = \hat{\mathcal{L}}_{JM_J;TM_T} + \hat{\mathcal{L}}_{JM_J;TM_T}^5,$$
$$\hat{T}_{JM_J;TM_T}^{\text{el}} \equiv \frac{1}{q} \int d\mathbf{x} \left[\vec{\nabla} \times \mathbf{M}_{JJ}^{M_J}(q\mathbf{x}) \right] \cdot \hat{\mathcal{J}}(\mathbf{x})_{TM_T} = \hat{T}_{JM_J;TM_T}^{\text{el}} + \hat{T}_{JM_J;TM_T}^{\text{el5}},$$
$$\hat{T}_{JM_J;TM_T}^{\text{mag}} \equiv \int d\mathbf{x} \mathbf{M}_{JJ}^{M_J}(q\mathbf{x}) \cdot \hat{\mathcal{J}}(\mathbf{x})_{TM_T} = \hat{T}_{JM_J;TM_T}^{\text{mag5}} + \hat{T}_{JM_J;TM_T}^{\text{mag5}},$$

4. 7 basic operators)

$$\begin{split} M_{J}^{M_{J}}(q\mathbf{x}), \\ \Delta_{J}^{M_{J}}(q\mathbf{x}) &\equiv \mathbf{M}_{JJ}^{M_{J}}(q\mathbf{x}) \cdot \frac{1}{q} \vec{\nabla}, \\ \Delta_{J}^{'M_{J}}(q\mathbf{x}) &\equiv -i \bigg[\frac{1}{q} \vec{\nabla} \times \mathbf{M}_{JJ}^{M_{J}}(q\mathbf{x}) \bigg] \cdot \frac{1}{q} \vec{\nabla} = [J]^{-1} \big[-J^{1/2} \mathbf{M}_{JJ+1}^{M_{J}}(q\mathbf{x}) + (J+1)^{1/2} \mathbf{M}_{JJ-1}^{M_{J}}(q\mathbf{x}) \big] \cdot \frac{1}{q} \vec{\nabla} \\ \Sigma_{J}^{M_{J}}(q\mathbf{x}) &\equiv \mathbf{M}_{JJ}^{M_{J}}(q\mathbf{x}) \cdot \vec{\sigma}, \\ \Sigma_{J}^{'M_{J}}(q\mathbf{x}) &\equiv -i \bigg[\frac{1}{q} \vec{\nabla} \times \mathbf{M}_{JJ}^{M_{J}}(q\mathbf{x}) \bigg] \cdot \vec{\sigma} = [J]^{-1} \big[-J^{1/2} \mathbf{M}_{JJ+1}^{M_{J}}(q\mathbf{x}) + (J+1)^{1/2} \mathbf{M}_{JJ-1}^{M_{J}}(q\mathbf{x}) \big] \cdot \vec{\sigma}, \\ \Sigma_{J}^{''M_{J}}(q\mathbf{x}) &\equiv \bigg[\frac{1}{q} \vec{\nabla} M_{J}^{M_{J}}(q\mathbf{x}) \bigg] \cdot \vec{\sigma} = [J]^{-1} \big[(J+1)^{1/2} \mathbf{M}_{JJ+1}^{M_{J}}(q\mathbf{x}) + J^{1/2} \mathbf{M}_{JJ-1}^{M_{J}}(q\mathbf{x}) \big] \cdot \vec{\sigma}, \\ \Omega_{J}^{M_{J}}(q\mathbf{x}) &\equiv M_{J}^{M_{J}}(q\mathbf{x}) \vec{\sigma} \cdot \frac{1}{q} \vec{\nabla}, \end{split}$$

Haxton et al., Comput. Phys. Commun(2008)

Computer Resources

- •1. Perlmutter (3072 CPU nodes, 1536 GPU nodes)
- •2. Nova (ISU, ~250 CPU nodes)
- •3. ¥ 7.5 million (HAUST, 70-80 CPU nodes)

				Number of Nodes	Processors per Node	Cores per Node	Memory per Node	Interconnect	Local \$TMPDIR Disk	Accelerator Card	Job Constrain Flags
• Fu	ture ?	,		72	Two 18-Core Intel Skylake 6140	36	192 GB	100G IB	1.5 TB	N/A	nova18, intel, skylake, avx512
				40	Two 18-Core Intel Skylake 6140	36	384 GB	100G IB	1.5 TB	N/A	nova18, intel, skylake, avx512
				28	Two 24-Core Intel Skylake 8260	48	384 GB	100G IB	1.5 TB	N/A	nova18, intel, skylake, avx512
Partition	# of nodes	CPU	GPU	2	Two 18-Core Intel Skylake 6140	36	192 GB	100G IB	1.5 TB	2x NVIDIA Tesla V100-32GB	nova18, intel, skylake, avx512
GPU	GPU 1536 1x <u>AMD EPYC 77</u>	1x AMD EPYC 7763	4x <u>NVIDIA A100</u> (40GB)	1	Two 18-Core Intel Skylake 6140	36	192 GB	100G IB	1.5 TB	one NVIDIA Tesla V100-32GB	nova18, intel, skylake, avx512
	256	1× AMD EDVO 7762	4x <u>NVIDIA A100</u> (80GB)	2	Two 18-Core Intel Skylake 6140	36	384 GB	100G IB	1.5 TB	2x NVIDIA Tesla V100-32GB	nova18, intel, skylake, avx512
	230	TX AMD EFTC 7705		1	Four 16-Core Intel 6130	64	3 TB	100G IB	11 TB	N/A	nova18, intel, skylake, avx512
CPU	3072	2x <u>AMD EPYC 7763</u>	-	2	Four 24-Core Intel 8260	96	3 TB	100G IB	1.5 TB	N/A	nova18, intel, skylake, avx512
_ogin	40	1x AMD EPYC 7713	1x <u>NVIDIA A100</u> (40GB)	40	Two 32-Core AMD EPYC 7502	64	512 GB	100G IB	1.5 TB	N/A	nova21, amd, epyc-7502
				15	Two 32-Core AMD EPYC 7502	64	512 GB	100G IB	1.5 TB	four NVidia A100 80GB	nova21, amd, epyc-7502
				56	Two 32-Core Intel Icelake 8358	64	512GB	100G IB	1.6TB	N/A	nova22, intel, icelake, avx512
				5	Two 24-Core AMD EPYC 7413	48	512GB	100G IB	960GB	eight NVidia A100 80GB	nova22, amd
				16	Two 32-Core Intel Icelake8358	64	512GB	100G IB	1.5TB	N/A	nova23, intel, icelake, avx512
				14	Two 96-Core AMD EPYC 9654	192	768GB	100G IB	1.7TB	N/A	nova24, amd, epyc-9654, avx512
				3	Two 96-Core AMD EPYC 9684x	192	768GB	100G IB	1.7TB	N/A	nova24, amd, epyc-9684x, avx512

Conclusions

- Ground state energies and spectra of stable p-shell nuclei from Daejeon16 in good agreement with experiment; electromagnetic transitions are reasonable
- > Improve the accuracy of calculations: increasing the basis space
- Demanding computer resources
- > Theoretical uncertainty
- > Comparison with future experimental data