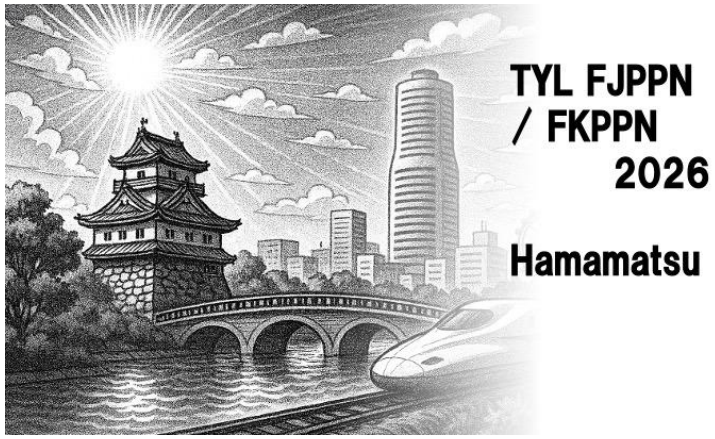
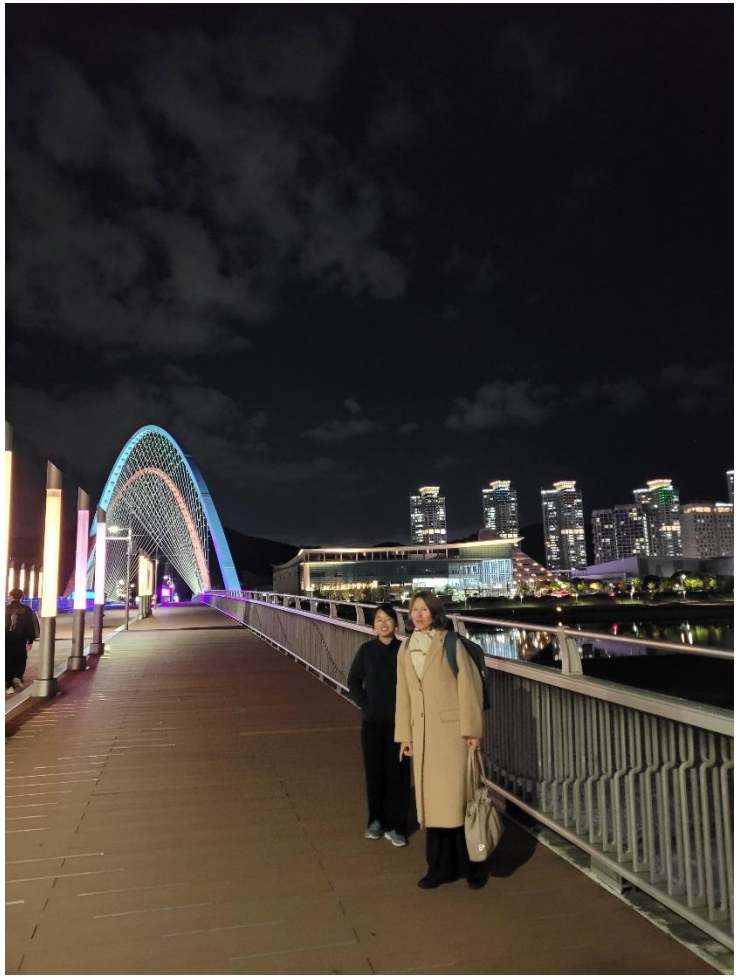


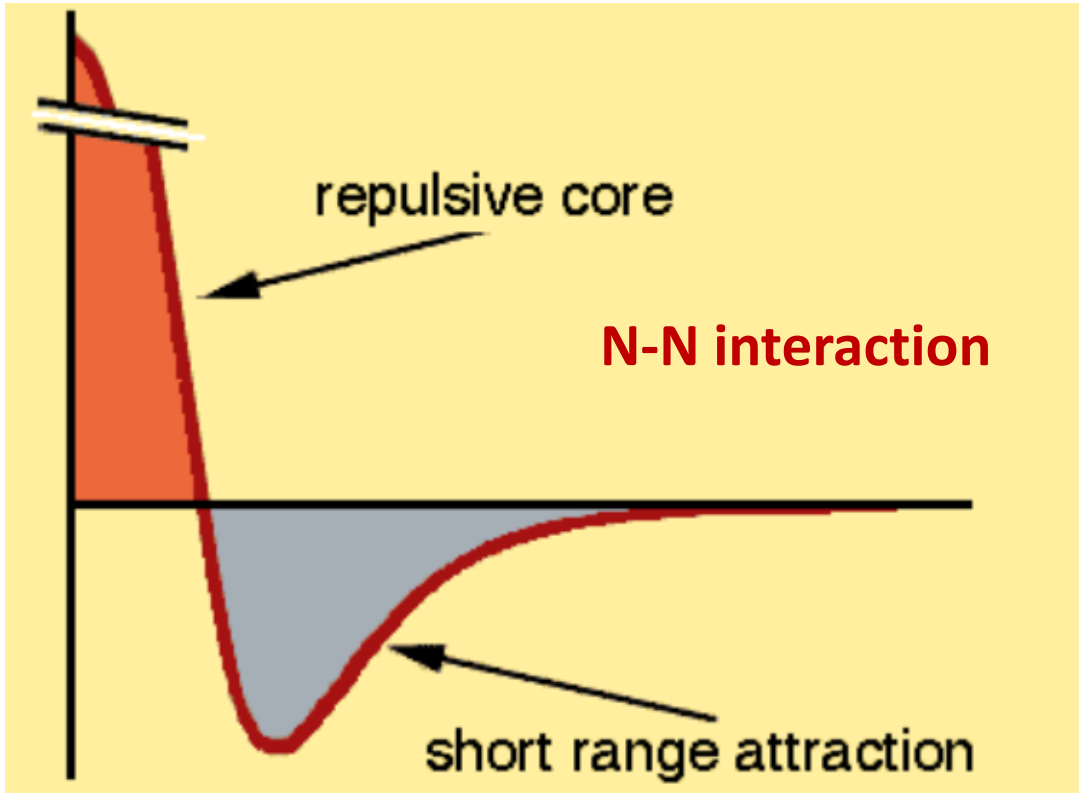
Ab-initio Shell Model for Nuclear Structure (FKPPN: ABI-SMNS)

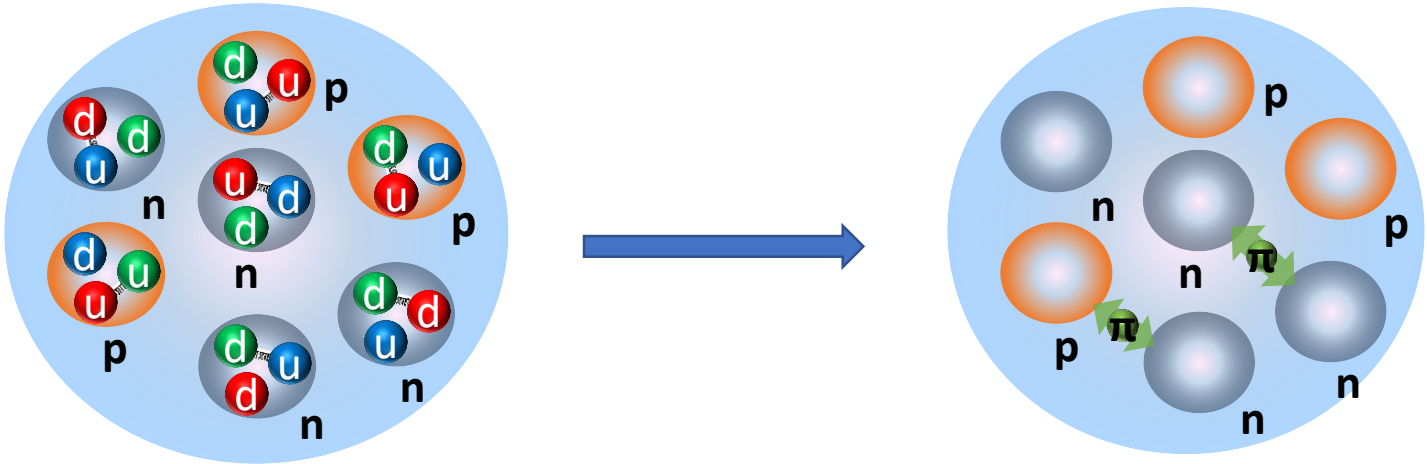
Nadezda A. Smirnova, Arturo Rivero, *LP2IB, CNRS/IN2P3 – University of Bordeaux, France*
Youngman Kim, Ik Jae Shin, Menglan Liu, *Institute for Basic Science, Daejeon, Republic of Korea*

In collaboration with
Andrey M. Shirokov*, SINP, Moscow State University, Russia*
James P. Vary, Pieter Maris, *Iowa State University, USA*



October 2025


repulsive core
N-N interaction
short range attraction


d
u
p
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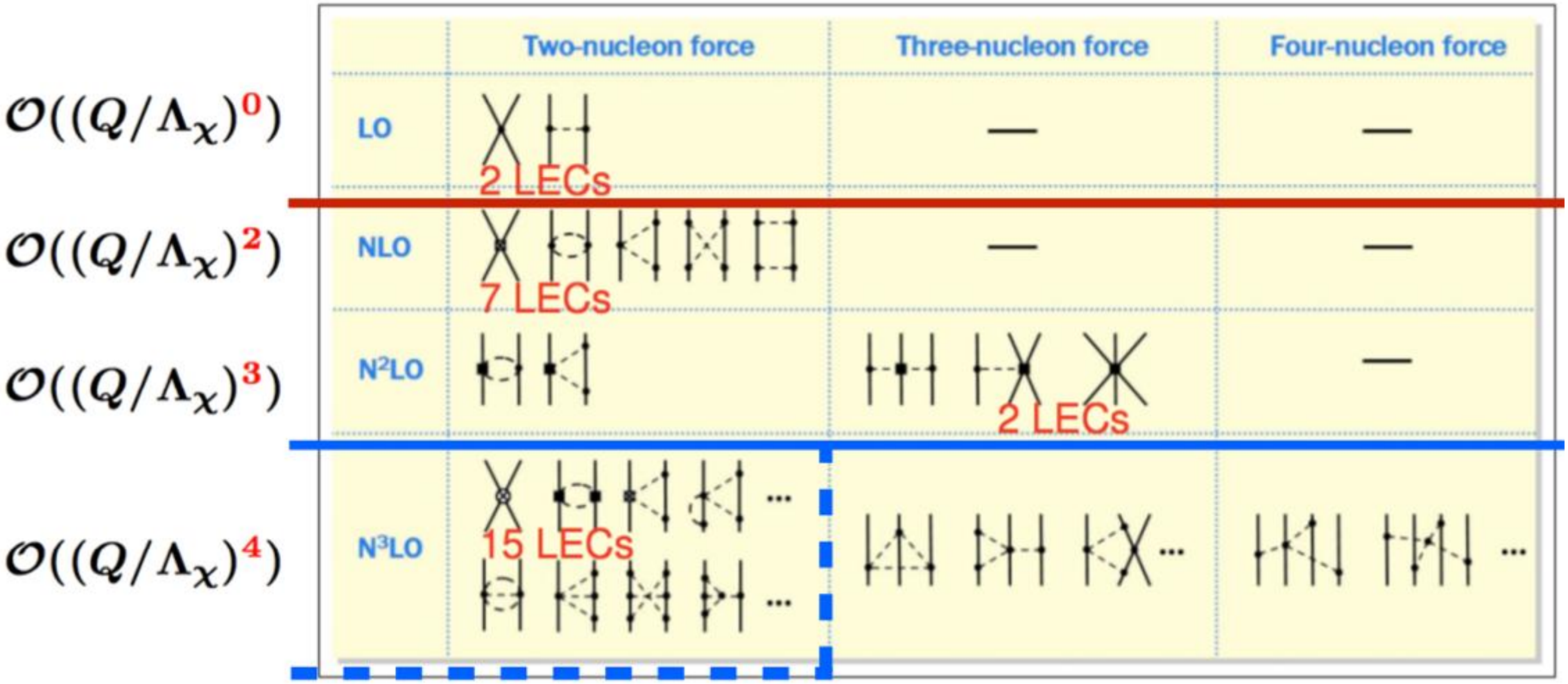
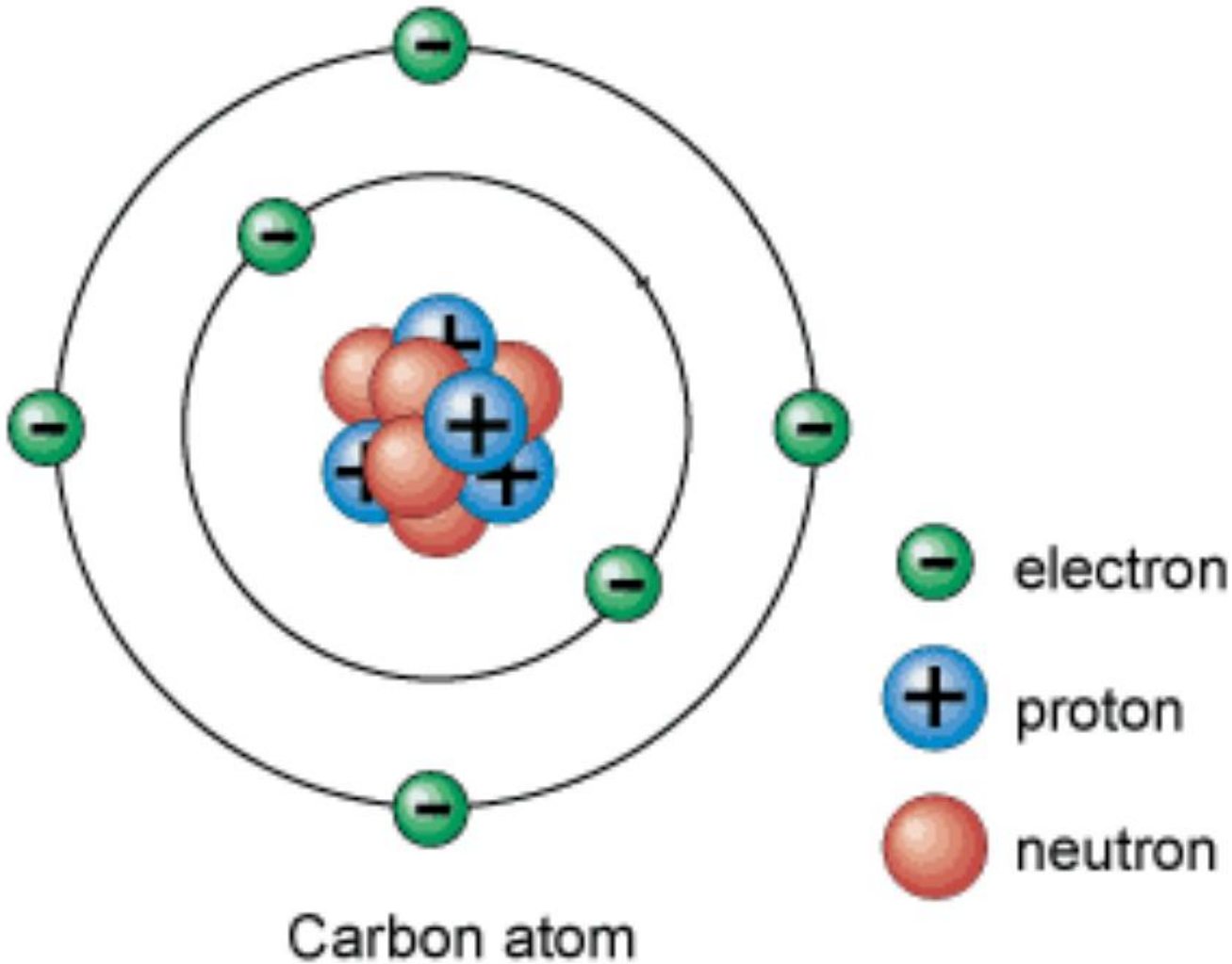
π

Modern N-N interaction



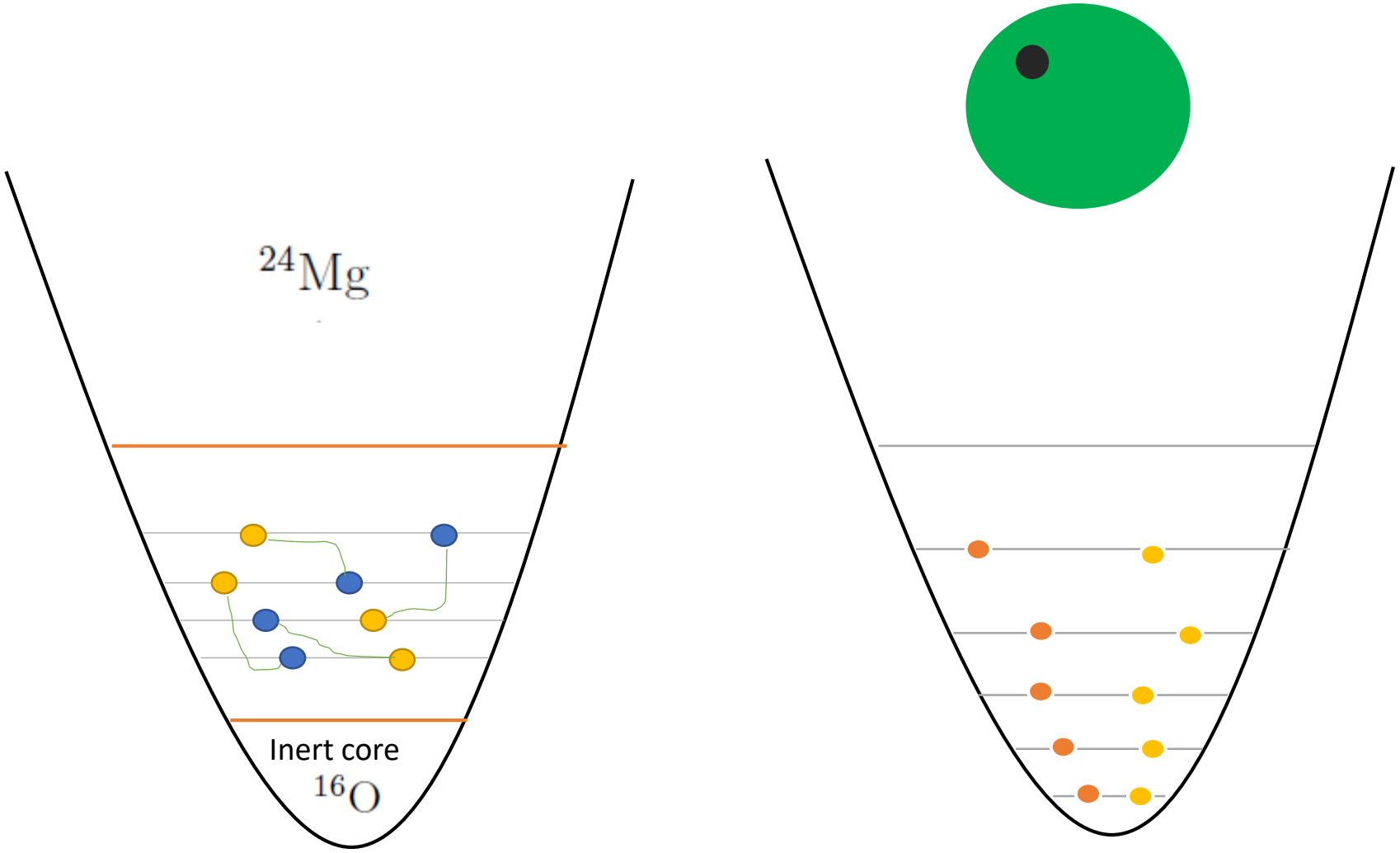
from ChPT: connected to QCD through chiral symmetry

Atoms



Carbon atom

Clusters of levels → shell structure



Interacting SM

HF

Nuclear shell model

Ingredients:

Mean-field potential. (conventional)

Residual interaction between (some of) the nucleons.

Difficulties:

Nucleonic interactions from QCD (EFT). (ab initio)

Large-matrix diagonalization.

Issues of current interest:

Changing shell structure and three-body forces in exotic nuclei.

Continuum effects (nucleus = open quantum system).

Nuclear shell model (conventional)

Many-body quantum mechanical problem:

$$\hat{H} = \sum_{k=1}^{A} \frac{p_k^2}{2m_k} + \sum_{k<l}^{A} \hat{V}_2(\boldsymbol{r}_k, \boldsymbol{r}_l)$$

$$= \underbrace{\sum_{k=1}^{A} \left[\frac{p_k^2}{2m_k} + \hat{V}(\boldsymbol{r}_k) \right]}_{\text{mean field}} + \underbrace{\left[\sum_{k<l}^{A} \hat{V}_2(\boldsymbol{r}_k, \boldsymbol{r}_l) - \sum_{k=1}^{A} \hat{V}(\boldsymbol{r}_k) \right]}_{\text{residual interaction}}$$

Independent-particle assumption. Choose *V* and neglect residual interaction:

$$\hat{H} \approx \hat{H}_{\text{IP}} = \sum_{k=1}^{A} \left[\frac{p_k^2}{2m_k} + \hat{V}(\boldsymbol{r}_k) \right]$$

- A-nucleon Schrödinger equation

$$\hat{H}\,\Psi(r_1,\cdots,r_A) = E\,\Psi(r_1,\cdots,r_A)$$

  - Hamiltonian with $NN(+NNN)$ interactions (ab initio)

$$\hat{H} = \frac{1}{A}\sum_{i<j}\frac{(\vec{p_i}-\vec{p_j})^2}{2m} + \sum_{i<j}V_{ij} + \sum_{i<j<k}V_{ijk} + \cdots$$

  - Wave functions are expanded in basis states

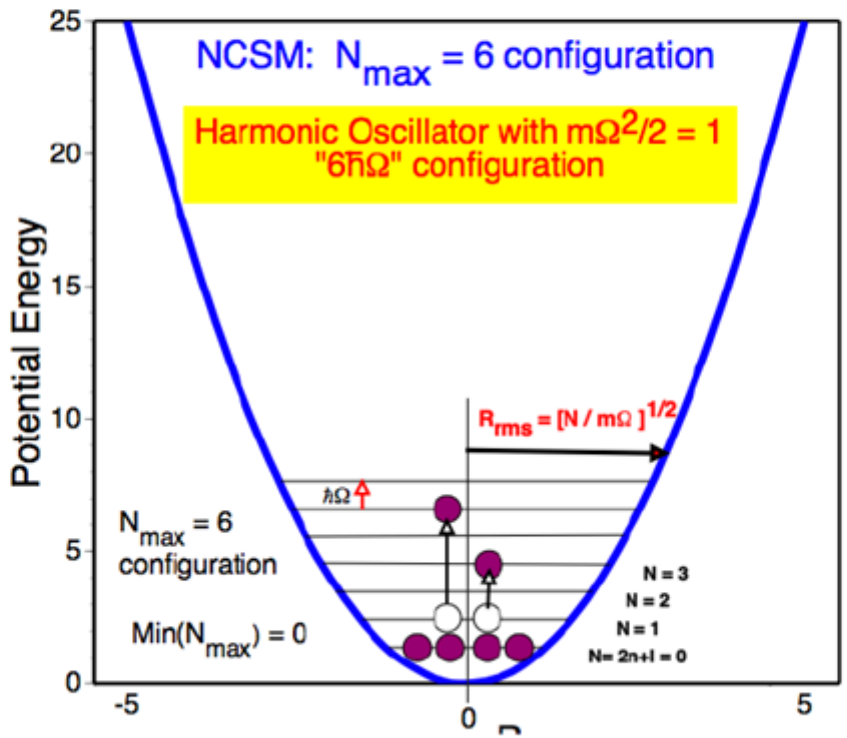
$$\Psi(r_1,\cdots,r_A) = \sum a_i \Phi_i(r_1,\cdots,r_A)$$

    basis states Φ_i : Slater determinants of single particle states

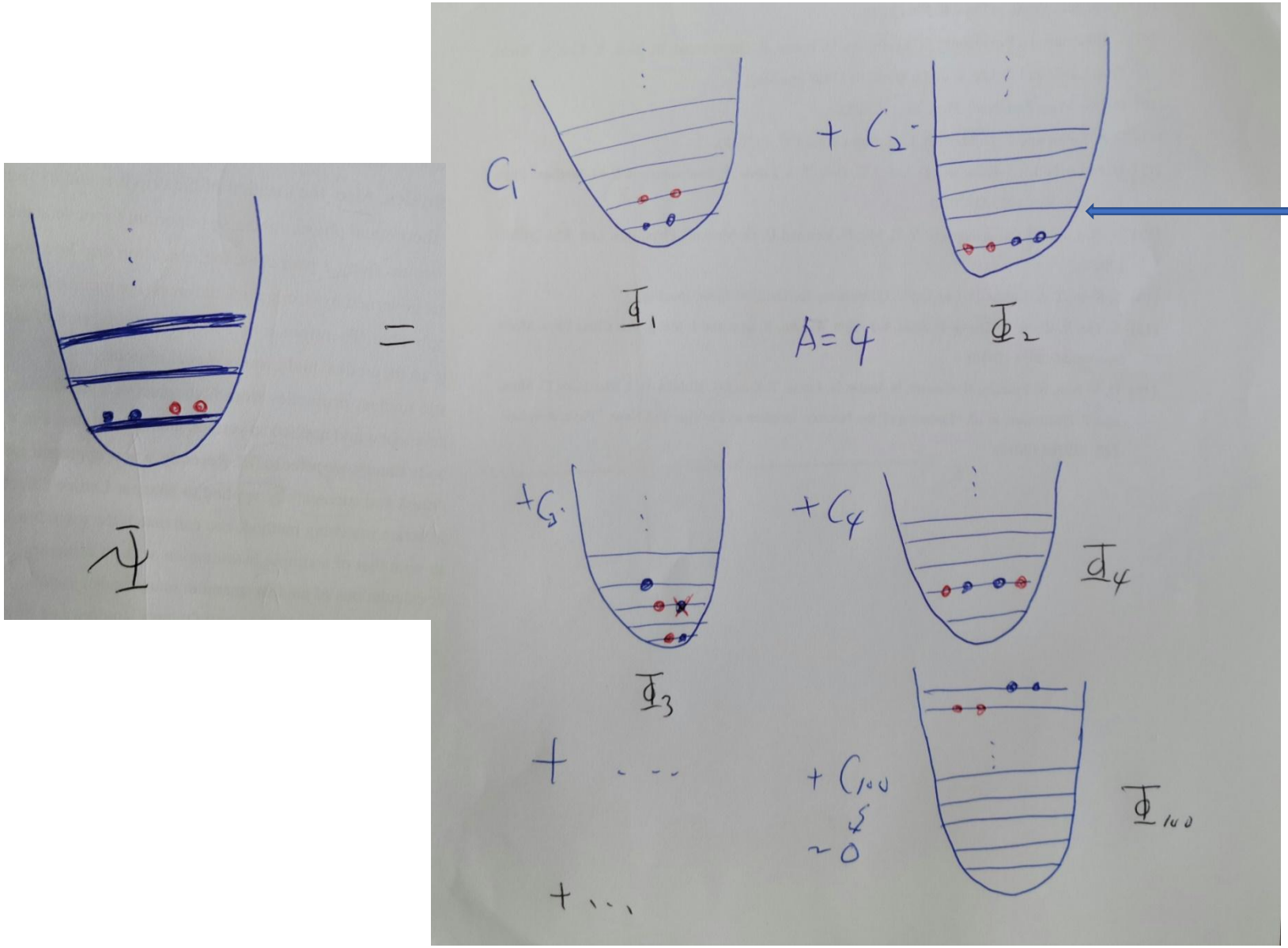
- single particle states ϕ

  for radial wave functions, harmonic oscillators are used

$$\Rightarrow \Phi_i \sim \phi_1^{(i)} \times \phi_2^{(i)} \times \cdots \times \phi_A^{(i)}$$



from the talk by J. Vary @ RISP, Mar. 2013



HF: single determinant, pre-calculated single particle basis vectors through the variational principle

- Expand wave function in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Express Hamiltonian in basis $\langle \Phi_j | \hat{\mathbf{H}} | \Phi_i \rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- Complete basis $\longrightarrow$ exact result
  - caveat: complete basis is infinite dimensional
- No-Core Configuration Interaction
  - all A nucleons are treated the same
- In practice
  - truncate basis
  - study behavior of observables as function of truncation
- Computational challenge
  - construct large $(10^{10} \times 10^{10})$ sparse symmetric real matrix H_{ij}
  - use Lanczos algorithm
    to obtain lowest eigenvalues & eigenvectors

Pieter Maris

Ab initio structure and NN interaction

- Unfortunately, the NN interaction at low energies needed for nuclear physics applications cannot be directly derived from QCD at the moment
- Ab initio theory requires, of course, a realistic NN interaction accurately describing NN scattering data and deuteron properties
- Nice to avoid NNN forces? Yes

≈30 times more Hamiltonian matrix elements when *NNN* forces are involved; hence much more computer resources are required for calculations

Daejeon 16 NN interaction

Used in many ab initio structure studies and more are planned

N3LO interaction

SRG
(similarity renormalization group)

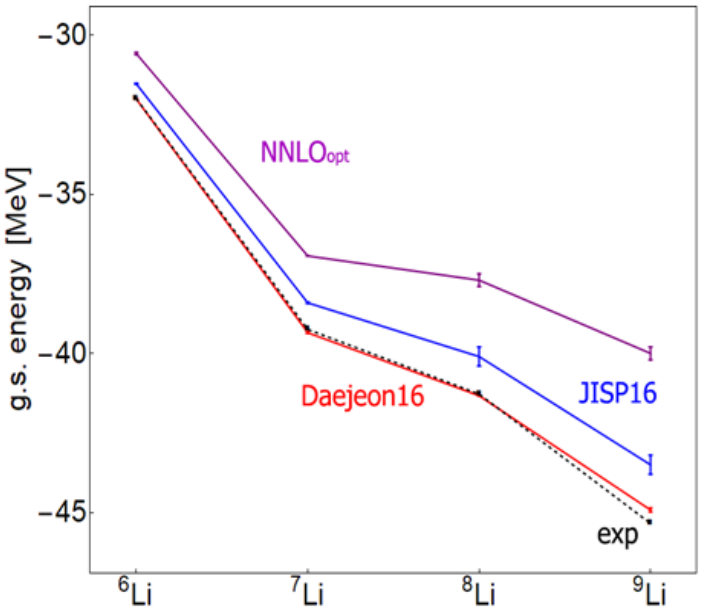
SRG-evolved N3LO

PET (phase equivalent transformation)

Daejeon16

Ground state energies of Li isotopes

calculated w/ JISP16, $NNLO_{opt}$ and Daejeon16
compared to experimental data.



- Daejeon16 shows more excellent description for the binding energies of Lithium isotopes than $NNLO_{opt}$ (from the first principle) and JISP16 (phenomenological.)
- For each result, extrapolation is adopted.
- ^{6}Li : $\sim N_{max}=18$
  $^{7}Li \sim {}^{9}Li$: $\sim N_{max}=10$

A.M. Shirokov, I.J. Shin, Y. Kim, M. Sosonkina, P. Maris, J.P. Vary, PLB761 (2016) 87

PET preserves two nucleon observables such as N N phase shifts and deuteron properties

❖ PET (phase-equivalent transformation)

Hamiltonian can be expressed as an infinite dimensional matrix $[H]$ in the oscillator basis $\{|n\rangle\}$.

$$\text{matrix elements of } [H] \ : H_{nm} = \langle \mathrm{n}|H|m\rangle$$

PET is based on the unitary transformation as

$$\left[\widetilde{H}\right] = \left[U^{\dagger}\right][H][U]$$

with the help of the unitary matrix $[U]$ which is supposed to be of the form

$$[U] = [U_0] \oplus [I] = \begin{pmatrix} [U_0] & 0 \\ 0 & [I] \end{pmatrix}$$

where $[I]$ is the infinite dimensional unit matrix.

Clearly the spectra of Hamiltonians H and $\widetilde{H}$ are identical. Corresponding eigenfunction can be written as

$$[\widetilde{\Psi}] = [U^{\dagger}]\,[\Psi]$$

in the oscillator basis $\{|n\rangle\}$. Then the difference is

$$\Delta[\Psi] = [\widetilde{\Psi}] - [\Psi] = \left([U^{\dagger}] - [I]\right)[\Psi] = \begin{pmatrix} [U_0] & 0 \\ 0 & 0 \end{pmatrix}[\Psi]\,.$$

That is, the only difference is shown as a superposition of a finite number of functions. If we consider a simple 2×2 matrix $[U_0]$ as

$$[U_0] = \begin{pmatrix} \cos\beta & \sin\beta \\ -\sin\beta & \cos\beta \end{pmatrix},$$

then only two oscillator basis $|0\rangle$ and $|1\rangle$ are related.

The superposition of a finite number of $\mathcal{L}^2$ functions cannot affect the asymptotics of scattering wave functions.

$$\tilde{\Psi} = \Psi + \sum_i^N c_i |i\rangle \quad \Rightarrow \quad \lim_{r\to\infty} \tilde{\Psi}(r) = \lim_{r\to\infty} \Psi(r) \qquad \text{when} \quad |i\rangle \in \mathcal{L}^2$$

Since the scattering phase shifts and the *S* - matrix are defined through the asymptotic behavior of the wave functions, the phase shifts δ associated with the Ψ and $\tilde{\Psi}$ are identical.

So the Hamiltonians H and $\tilde{H}$ are phase-equivalent.

Practically,

$$
\begin{aligned}
[\tilde{V}] &= [V] + [\Delta V] \\
&= [V] + \left(\left[\tilde{H}\right] - [H] \right) \\
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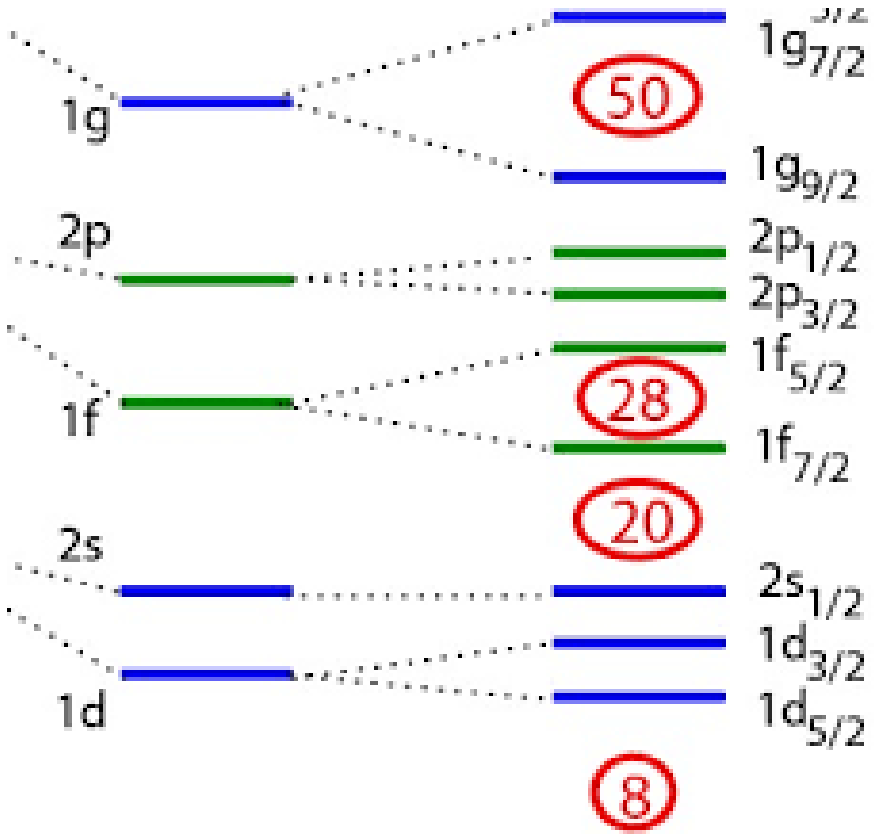

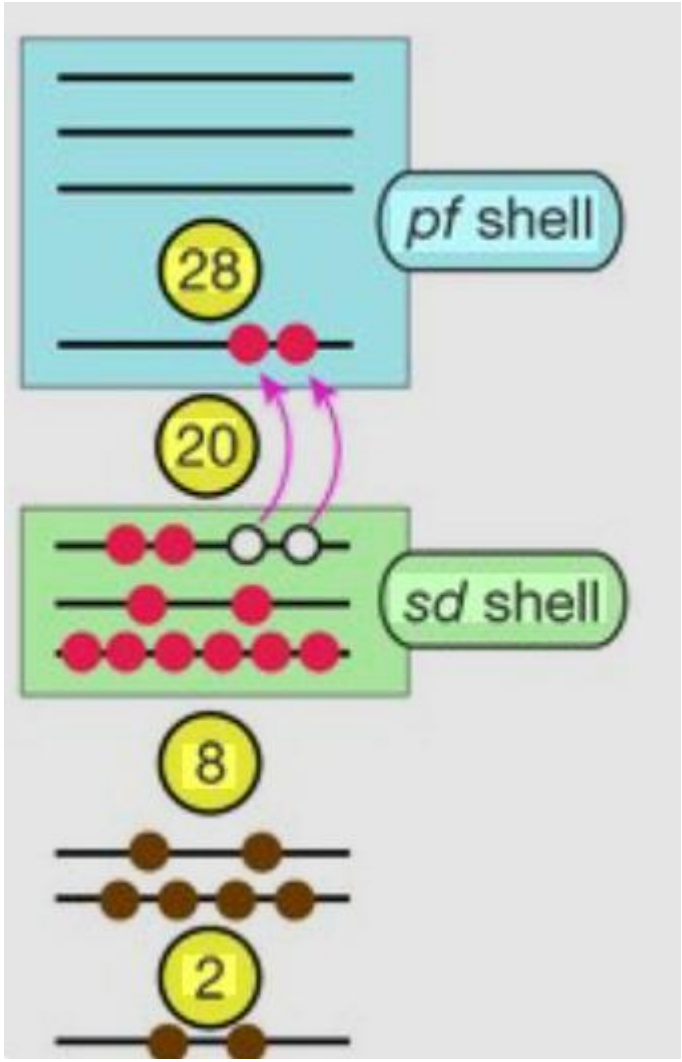

Valence nucleons in sd shell.

$0d_{5/2}$, $1s_{1/2}$, $0d_{3/2}$

Oxygen-18
Neon-20
Magnesium-24
Silicon-28
Sulfur-32
Calcium-40 (sd shell closure)

Clusters of levels with similar energies → shells

Ab initio NCSM

- Ab initio: nuclei from first principles using fundamental interactions without uncontrolled approximations.
- No core: all nucleons are active, no inert core.
- Shell model: harmonic oscillator basis
- Point nucleons

Ab initio structure and NN interaction

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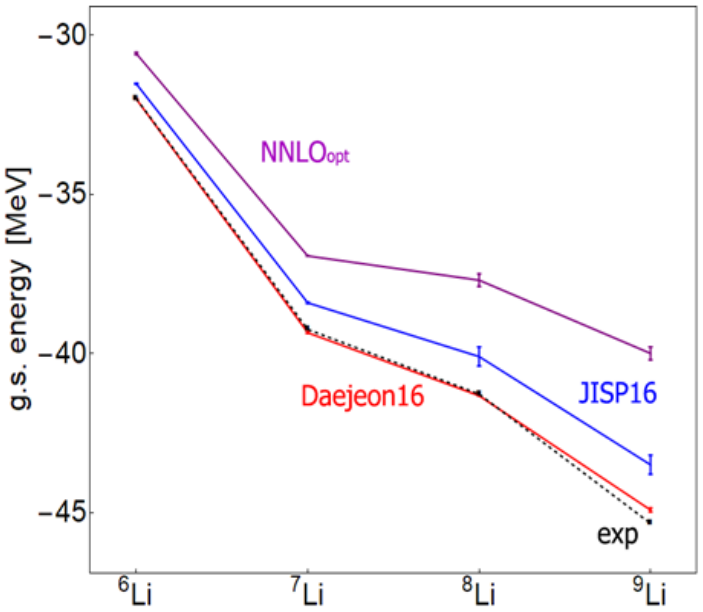

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\end{aligned}
$$

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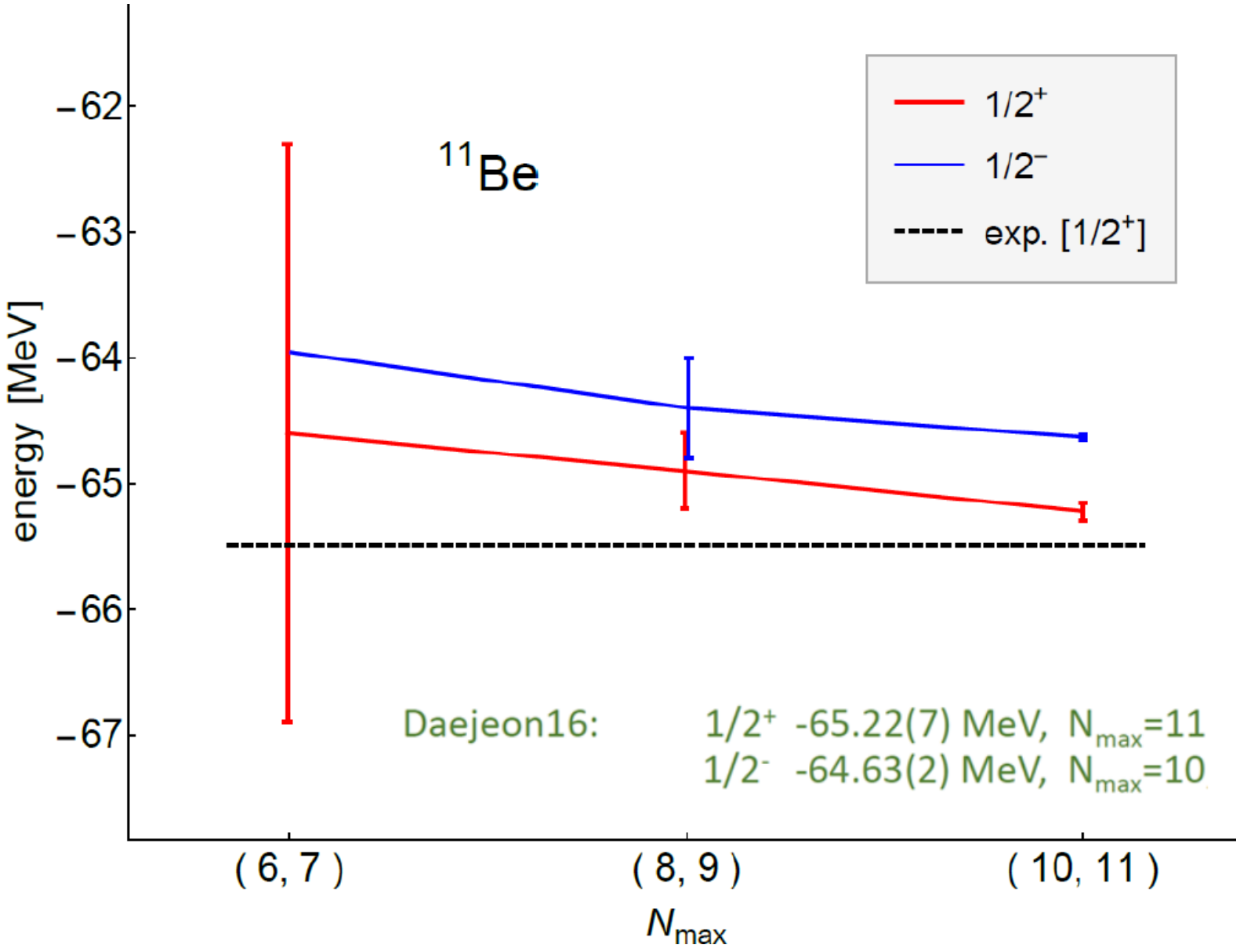
Parity Inversion in ^{11}Be

- Experimentally: $1/2^+$ -65.483(6) MeV
  $1/2^-$ -65.165(7) MeV, Exc. energy 0.318(7) MeV
- JISP16: $1/2^+$ -63.3(8) MeV, N_{max}=11
  $1/2^-$ -64.0(6) MeV, N_{max}=10



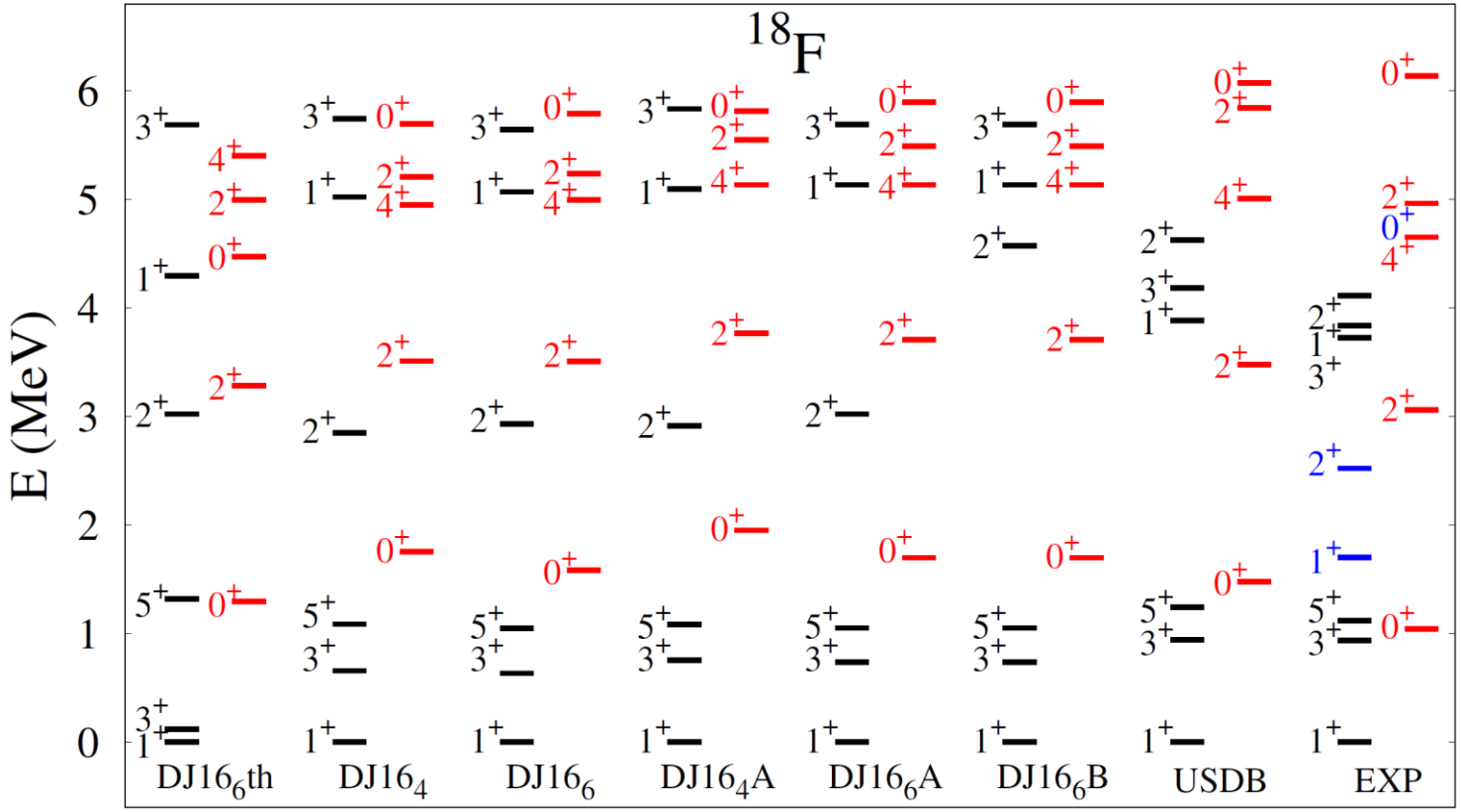
YK, Ik Jae Shin, J. Vary et al, Proceedings of NTSE 2018@IBS

Achievement

Effective shell-model interactions from Daejeon 16

A new (not fully though) microscopic effective shell-model interactions in the valence sd shell, obtained from the modern Daejeon16 nucleon-nucleon potential

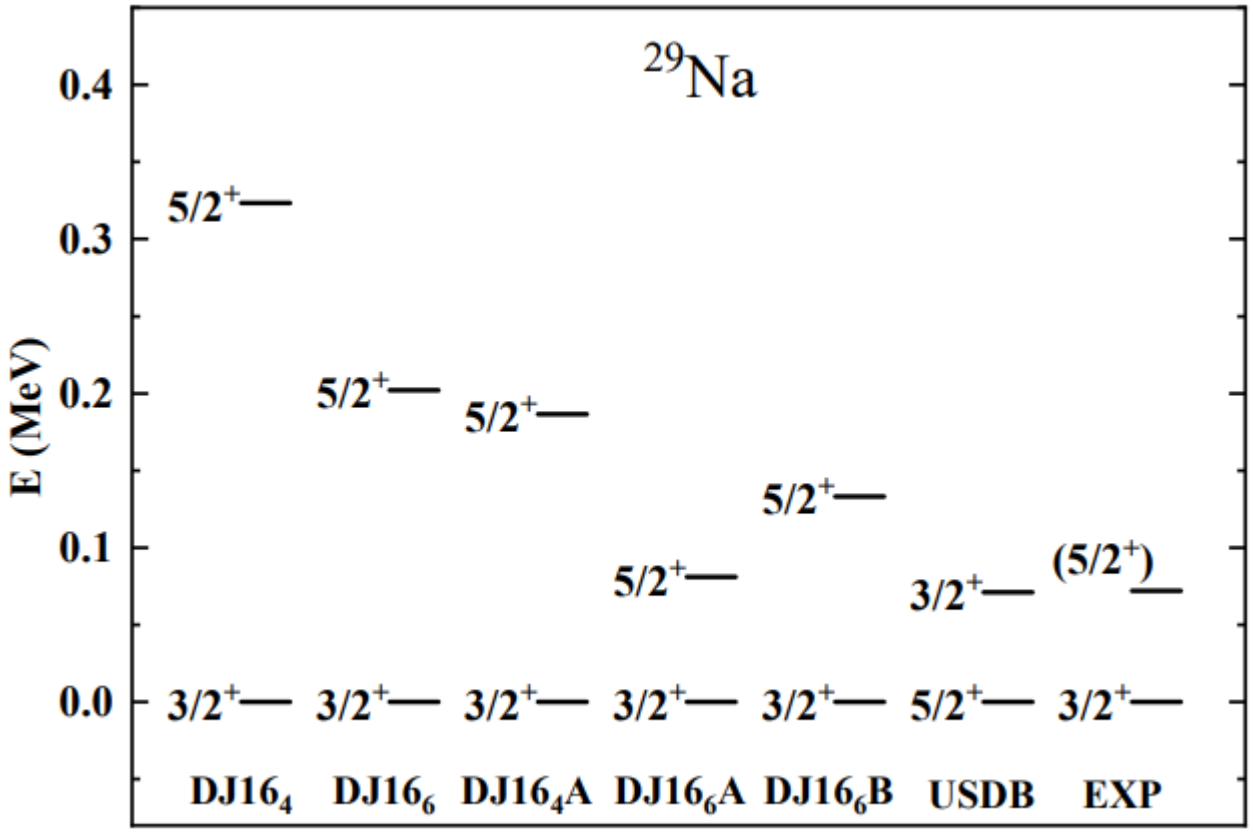
N_{max} =6



I. J. Shin, N. A. Smirnova, YK, et al, Phys.Rev.C 110 (2024) 034306

Effective shell-model interactions from Daejeon16

A new microscopic effective shell-model interactions in the valence sd shell, obtained from the Daejeon16 nucleon-nucleon potential using no-core shell-model (NCSM) wave functions of at $N_{max} = 6$



A hope!

AB INITIO NO CORE SHELL MODEL CALCULATIONS OF *sd*-SHELL NUCLEI

I. A. Mazur[1], I. J. Shin[2], N. A. Smirnova[3], A. M. Shirokov[4], Y. Kim[5]

[1]Institute for Nuclear Research of the Russian Academy of Sciences, Russia
[2]Institute for Rare Isotope Science, Institute for Basic Science, Republic of Korea
[3]Laboratory of Physics of the Two Infinities Bordeaux, CNRS – University of Bordeaux, France
[4]Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Russia
[5]Center for Exotic Nuclear Studies, Institute for Basic Science, Republic of Korea
E-mail: mazur@inr.ru

We present the first *ab initio* no-core shell-model (NCSM) [1] calculations for the entire *sd*-shell using the Daejeon16 [2] nucleon-nucleon (*NN*) interaction, obtained in a model space truncated with respect to $N_{max} = 4$ excitation quanta. Energy levels, as well as M1 and E2 transitions, are computed. We demonstrate the relative convergence of the excitation spectrum—dominated by $0\hbar\Omega$ (valence-space) configurations—throughout the *sd*-shell.

In recent years, significant progress has been achieved in the development of non-perturbative methods for constructing valence-space effective Hamiltonians based on realistic *NN* interactions. One such method employs the unitary Okubo–Lee–Suzuki transformations applied to NCSM solutions. Using this method, an effective interaction for the *sd*-shell, denoted DJ16$_4$th [3], has been derived from NCSM calculations of nuclei with $A = 16 \div 18$ nucleons using the Daejeon16 interaction in the same $N_{max} = 4$ model space. The corresponding effective electromagnetic transition operators are presented in Ref. [4]. In the present work, we discuss the agreement between the NCSM results and calculations performed with the effective DJ16$_4$th interaction.

Literature

1. B. R. Barrett, P. Navrátil, and J. P. Vary, Prog. Part. Nucl. Phys. **69**, 131 (2013).
2. A. M. Shirokov, I. J. Shin, Y. Kim, M. Sosonkina, P. Maris, and J. P. Vary, Phys. Lett. B **761**, 87 (2016).
3. I. J. Shin, N. A. Smirnova, A. M. Shirokov, Z. Yang, B. R. Barrett, Zh. Li, Y. Kim, P. Maris, and J. P. Vary, Phys. Rev. C **110**, 034306 (2024).
4. Zh. Li, N. A. Smirnova, A. M. Shirokov, I. J. Shin, B. R. Barrett, P. Maris, and J. P. Vary, arXiv: 2205.15939 (2022).

Plan

- Improvement of Daejeon16 for sd shell nuclei with preliminary results being under way
- Construction of charge-dependent versions of the Daejeon16 potential in order to get ab-initio isospin non-conserving interactions
- Construction of effective interactions in the 1hw-space shell-model space would allow the description of unnatural parity states in psdpf shell-model space, crucial for astrophysics applications

p-sd-pf shell model space

❖ Goal

- To construct valence-space effective interaction to describe **positive/negative parity** states

in ***sd*-shell nuclei**

❖ 0*p*-1*s*0*d*-1*p*0*f* shell model space

: Effective interaction consists of 5 blocks as

- 0*p* [easily done], 1*s*0*d* [published: PRC100, 054329] and 1*p*0*f* [straightforward] TBMEs
- cross-shell 0*p*-1*s*0*d* and 1*s*0*d*-1*p*0*f* TBMEs

- **^{16}O unnatural parity** states are investigated..
- For analysis, TBMEs from ^{16}N has been considered

2ja	2jb	2jc	2jd	J	T	V_2
1	1	1	1	0	1	-2.79850
1	1	3	3	0	1	2.38047
3	3	3	3	0	1	-2.38875
1	1	1	1	1	1	-1.48150
1	1	1	3	1	1	0.81100
1	1	3	1	1	1	0.47000
1	1	3	3	1	1	-0.47355
1	1	5	3	1	1	-1.98297
1	3	1	3	1	1	-1.02425

p-sd-pf shell model space

❖ Rough description of Strategy to obtain TBMEs in *sd*-shell (e.g. ^{18}F)

1. To do NCSM calculation at N_{max}=0

   ➡ Eigenstates E_i and corresponding eigenvectors $|\Psi_i\rangle$: $H\ |\Psi_i\rangle = E_i|\Psi_i\rangle$

2. Eigenvectors could be expanded as $|\Psi_i\rangle = \sum_l u_{il}|\ l\ \rangle$ where $|\ l\ \rangle = |\ n\ p\ \rangle \otimes |\ \text{core}\ \rangle \sim |\ n\ p\ \rangle$

   ➡ u_{il} could be also extracted from code

3. Then

   $\langle ab;J|H|cd;J\rangle = \langle ab;J|\ \{\sum_i |\Psi_i\rangle\langle\Psi_i|\}\ H\ \{\sum_j |\Psi_j\rangle\langle\Psi_j|\}\ |cd;J\rangle = \sum_{ilm}\langle ab;J|l\rangle\ u_{li}E_i u_{im}\langle m|cd;J\rangle$

   here, $\langle l|ab;J\rangle = \langle\alpha\beta|ab;J\rangle$ is replaced by the combination of Clebsch-Gordan coefficients

4. The core energy and SPEs, which are obtained from ^{16}O, ^{17}O and ^{17}F,

   would be subtracted appropriately to obtain TBMEs $\langle ab;J|V|cd;J\rangle$

Budget Requests

- A Short-term visit of French team members to Daejeon and
- A Short-term visit of the Korean team members to Bordeaux.