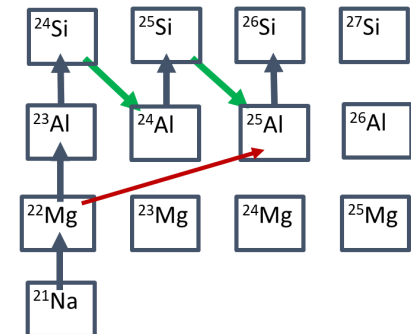
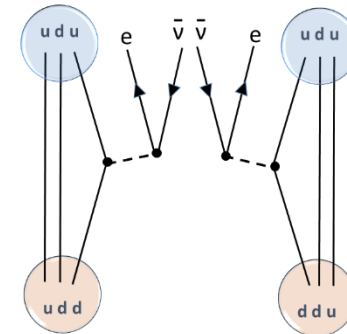
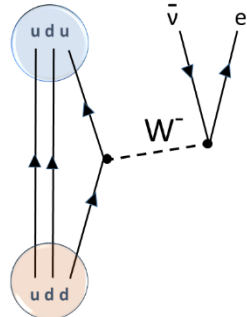
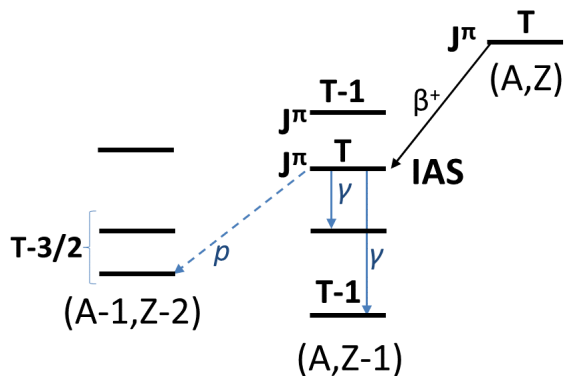


The Nuclear Shell Model: Exotic nuclei, Weak Processes and Nuclear Astrophysics

Nadezda A. Smirnova

Centre d'Etudes Nucléaires de Bordeaux-Gradignan (CENBG)
CNRS/IN2P3 – Université de Bordeaux

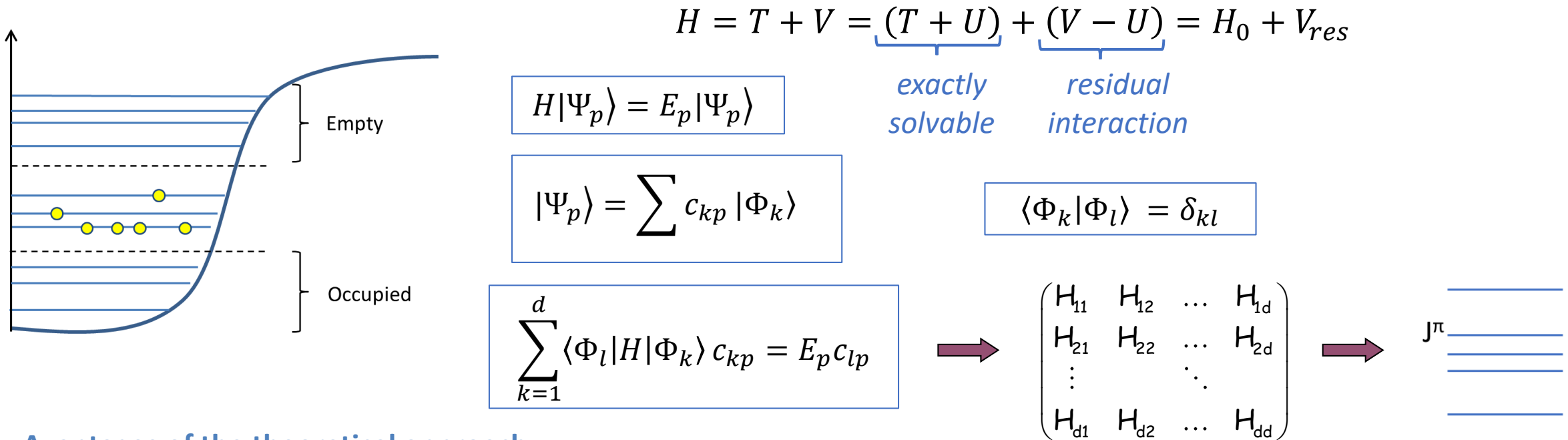


The Nuclear Shell Model: Exotic nuclei, Weak Processes and Nuclear Astrophysics

- Formalism: solution of the many-body problem by matrix diagonalization (NCSM versus Shell Model)
- Effective Hamiltonians and effective operators
- Highlights from structure of neutron-rich and neutron-deficient nuclei
- Fundamental interaction studies in nuclear decays: matrix elements
- Astrophysics applications

Shell model (full configuration-interaction approach)

Resolution of the nuclear many-body problem by Hamiltonian matrix diagonalization



Advantages of the theoretical approach:

- Conservation of symmetries of the full Hamiltonian (rotational, translation invariance, parity, particle number, etc)
- Precise information on low-energy states and transitions
- Excellent description with appropriate interactions and in suitable model space

Challenges :

- Basis dimensions !

Large-scale diagonalization

Basis construction (for example, in M-scheme)

$$\Phi(1,2,\dots,A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_{\alpha_1}(\vec{r}_1) & \phi_{\alpha_1}(\vec{r}_2) & \dots & \phi_{\alpha_1}(\vec{r}_A) \\ \phi_{\alpha_2}(\vec{r}_1) & \phi_{\alpha_2}(\vec{r}_2) & \dots & \phi_{\alpha_2}(\vec{r}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{\alpha_A}(\vec{r}_1) & \phi_{\alpha_A}(\vec{r}_2) & \dots & \phi_{\alpha_A}(\vec{r}_A) \end{vmatrix} \quad \alpha = (nljm)$$
$$\text{Dim} = \binom{D_N}{N} \cdot \binom{D_Z}{Z}$$

Computational challenges :

- (Lowest) eigenvalues of geant, but sparse matrices -> Lanczos algorithm
- Storage of the Hamiltonian matrix elements (if stored, otherwise in-fly computation)

High-performance codes (up to $10^{12} \times 10^{12}$)

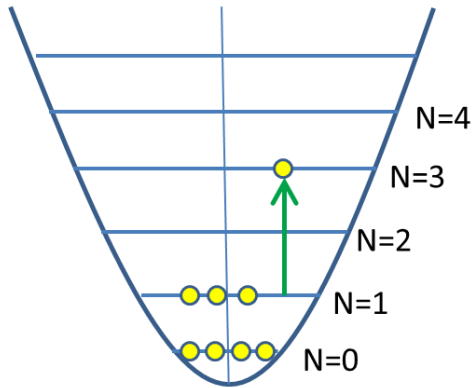
- ANTOINE, NATHAN (Strasbourg)
- NushellX (Oxford-MSU)
- Mshell , Kshell (Tokyo)
- Bigstick (St-Diego SU – LLNL-...)
- ...

Basis truncation techniques :

- Importance truncated (NC)SM (Darmstadt)
- Symmetry adapted basis (LSU)
- Monte-Carlo SM (Tokyo)
- Generalized seniority approximation, interacting boson approximation ...

No-core shell model (for light nuclei)

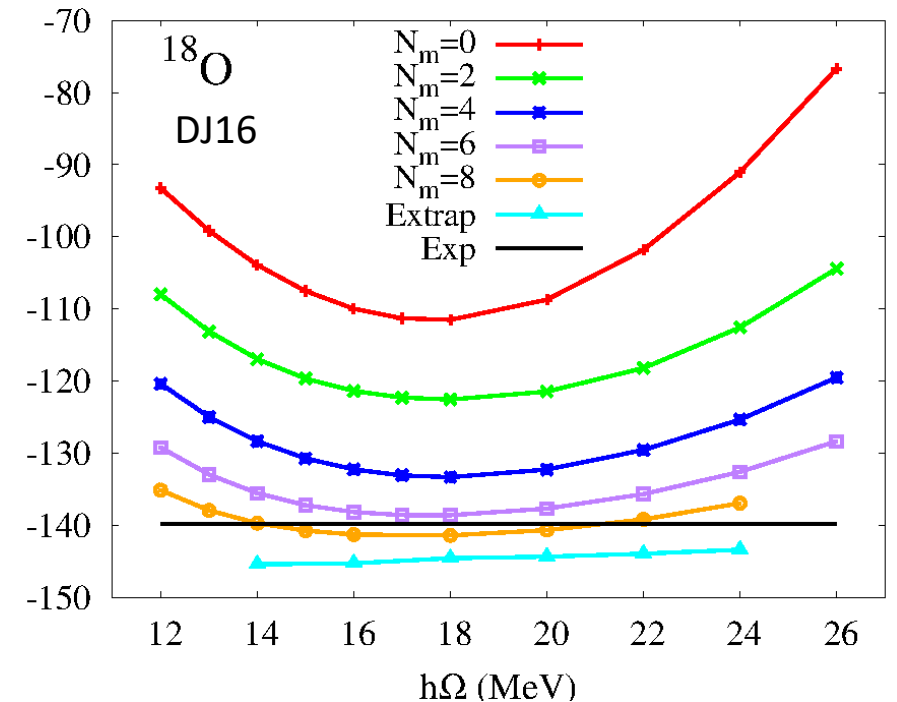
A nucleons in a (harmonic-oscillator) potential well in a large model space defined by $\hbar\Omega$ and N_{\max} .



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

Current status :

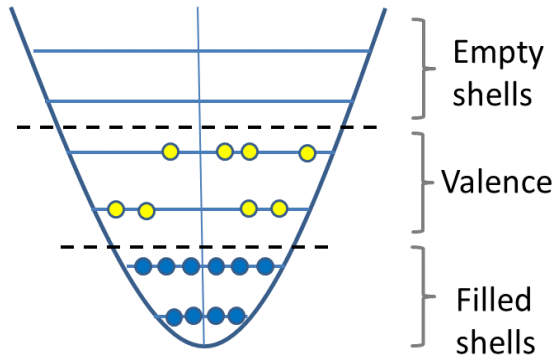
- Calculations with (bare) nucleon-nucleon forces (NN + 3NF)
- Ground state, excitation spectra, transition probabilities
=> benchmark for nuclear theory
- Reach *sd* shell nuclei (up to $A \sim 18$)
- Bridging with reaction theory



MFDn code, P. Maris, J. P. Vary et al,
Iowa State University

Valence-space shell model (heavier nuclei)

Restricted model space



Effective operators

$$H|\Psi_p\rangle = E_p|\Psi_p\rangle \quad \longrightarrow \quad H_{eff}|\Psi_p^M\rangle = E_p|\Psi_p^M\rangle$$

$$H = T + V = \underbrace{(T + U)}_{\text{exactly solvable}} + \underbrace{(V - U)}_{\text{residual interaction}} = H_0 + V_{res}$$

$$H = \sum_{\alpha} \epsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V_{res} | \delta\gamma \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta}$$

Empirical

Microscopic

Empirical

*Semi-microscopic
(microscopic,
constrained by the data)*

• **Current status :**

- Excellent description with phenomenological interactions
- Microscopic interactions -> recent progress and challenges

To prevent COMMON MISCONCEPTS about the Shell Model !

Effective Interactions : monopole-multipole decomposition

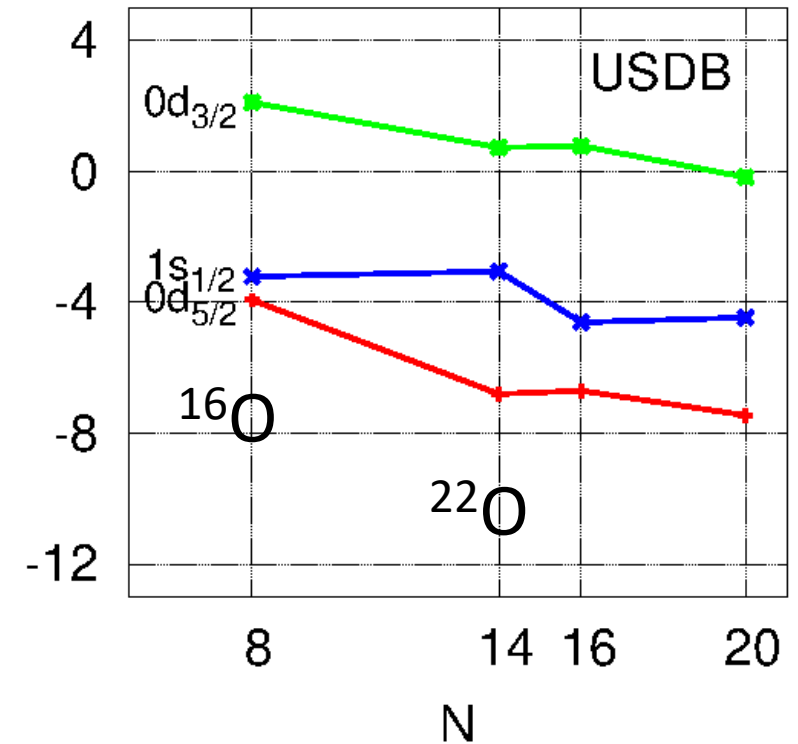
Multipole decomposition :

$$H = \sum_{\alpha} \varepsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} + \frac{1}{4} \sum_{ijkl, \lambda} w_{ijkl, \lambda} \left[a_i^{\dagger} \tilde{a}_j \right]^{(\lambda)} \left[a_k^{\dagger} \tilde{a}_l \right]^{(\lambda)} + \dots$$

$$H = \underbrace{\sum_i \varepsilon_i n_i + \sum_{i < j} \bar{V}_{ij} \frac{n_i (n_j - \delta_{ij})}{1 + \delta_{ij}}}_{\text{Monopole part (spherical mean-field)}} + \underbrace{V_{pair} + V_{quad} + \dots}_{\text{Multipole part (correlations)}}$$

- Only a physically meaningful combination of these ingredients will result in a successful description !
- Important to understand the nature of nuclear excitations (competition between sphericity and deformation)

Neutron ESPEs in O-isotopes
(from monopole part)



USDB – universal sd interaction:
W.A. Richter, B.A. Brown,
PRC74 (2006)

Effective Interactions : origin of deformation

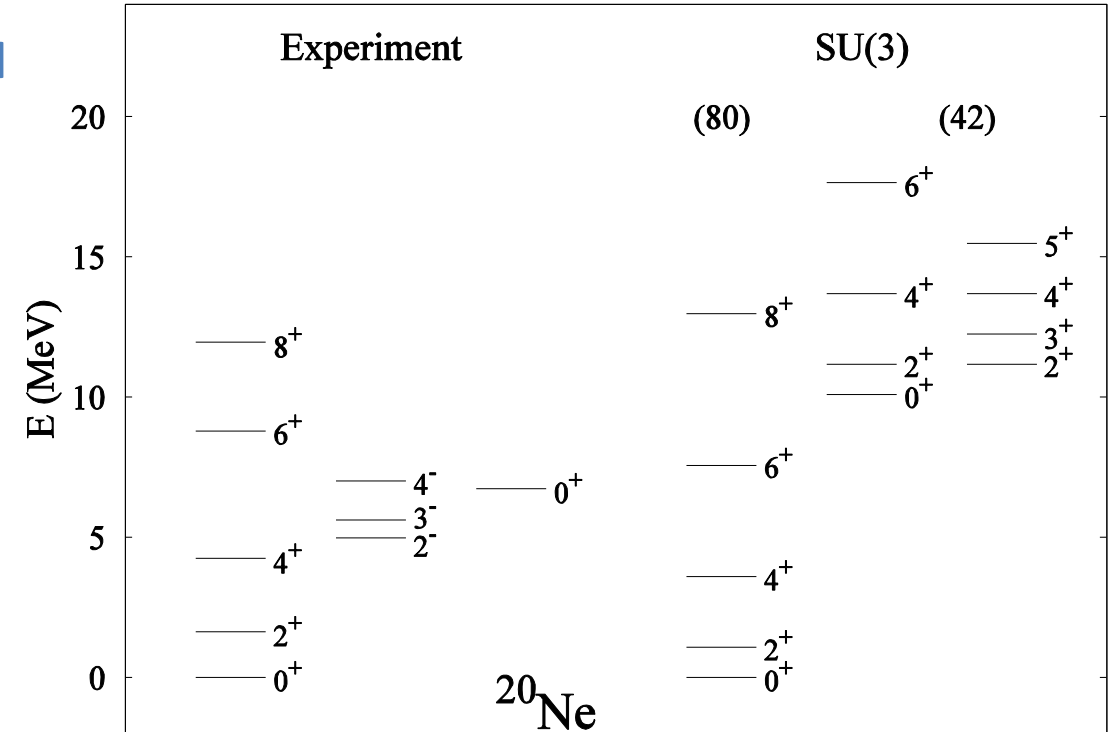
Spherical Interacting shell model and deformation : example of the algebraic SU(3) Q operator in the sd shell

J.P. Elliott, Proc. Roy. Soc. Lond. (1956, 1958)

$$H = H_0 + \chi(Q^{(2)} \cdot Q^{(2)})$$

$$U(3) \supset SU(3) \supset O(3) \supset O(2)$$

$$\begin{array}{cccc} \downarrow & \downarrow & \downarrow & \downarrow \\ n & (\lambda\mu) K & L & M \end{array}$$



- Eigenstates represent a mixing of many harmonic-oscillator configurations
- Generalization of this idea to other approximate symmetries for higher-j shells -> pseudo-SU(3), quasi-SU(3), etc => microscopic origin of deformation

Effective Interactions : link to the NN interaction

Spin-tensor decomposition

J.P. Elliott, NPA 121 (1968)

$$S_1^{(0)} = 1, S_2^{(0)} = [\vec{\sigma}_1 \times \vec{\sigma}_2]^{(0)}$$

$$S_3^{(1)} = [\vec{\sigma}_1 \times \vec{\sigma}_2]^{(1)}, S_4^{(1)} = (\vec{\sigma}_1 + \vec{\sigma}_2)^{(1)}, S_5^{(1)} = (\vec{\sigma}_1 - \vec{\sigma}_2)^{(1)}$$

$$S_6^{(2)} = [\vec{\sigma}_1 \times \vec{\sigma}_2]^{(2)}$$

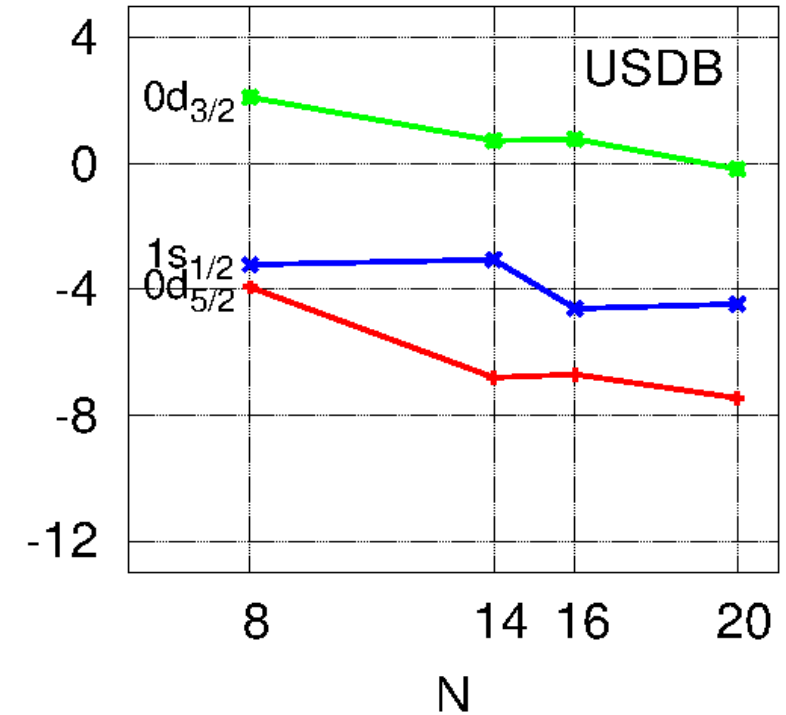
$$V_{res} = \sum_{k=0,1,2} T^{(k)} \cdot S^{(k)}$$

k=0 : central (Triplet-even, triplet-odd, ..)

k=1 : vector

k=2 : tensor

➤ Useful to understand the mechanism of a spherical mean field evolution



Microscopic approaches to valence space interactions

$$H|\Psi_p\rangle = E_p|\Psi_p\rangle$$

$$\langle\Psi_f|O|\Psi_i\rangle = O_{fi}$$

Effective operators

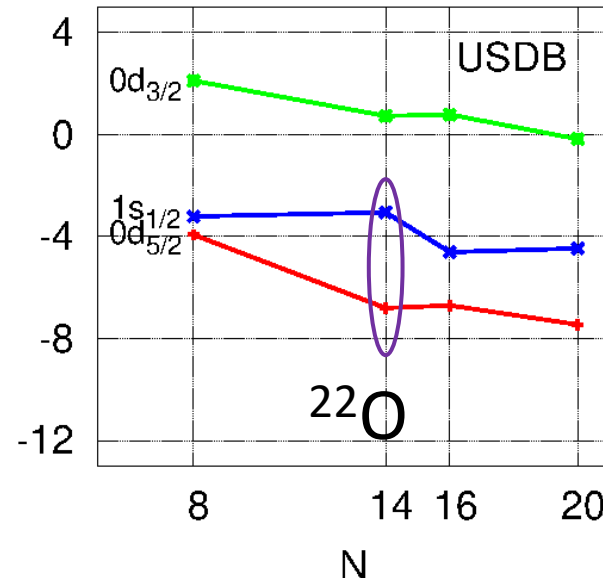
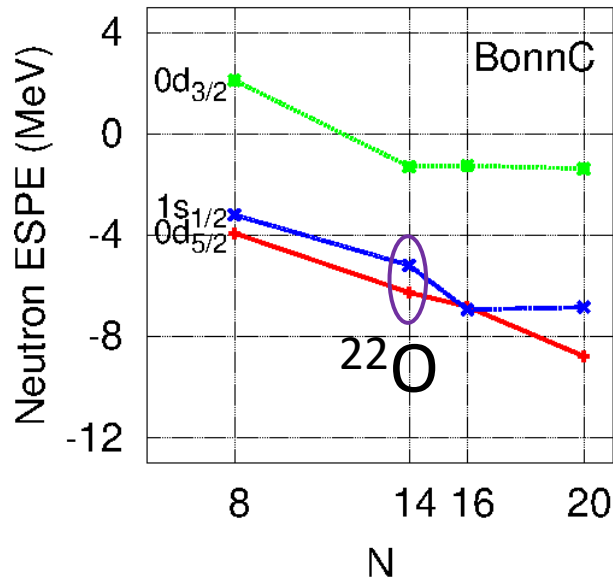
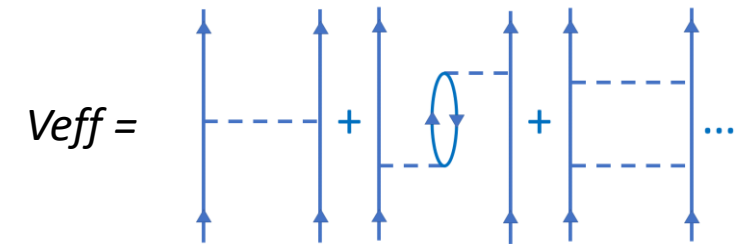


$$H_{eff}|\Psi_p^M\rangle = E_p|\Psi_p^M\rangle$$

$$\langle\Psi_f^M|O_{eff}|\Psi_i^M\rangle = O_{fi}$$

Theoretical approach: Many-body perturbation theory based on the G-matrix (NN)

G.F. Bertsch, T.T.S. Kuo, G.F. Brown, B.R.Barrett, M.Kirson, et al. (from 60's)
M. Hjorth-Jensen, T.T.S. Kuo, E. Osnes, PR261, 126 (1995)



Poor description of the
monopole term
(spherical mean-field)



Missing 3N forces

A.Poves, A.P. Zuker, PR70, 71 (1981)
A.P. Zuker, PRL90, 042502 (2003)

Microscopic approaches to valence space interactions

χ EFT

$$(\rho/\Lambda)^{\nu}, \quad Q \sim m_{\pi}, \quad \Lambda \sim M_N$$

$$|V_{2N}| \gg |V_{3N}| \gg |V_{4N}|$$

Modern theoretical approaches to effective interactions (with 3N forces)

Review : S. R. Stroberg, H. Heigert, S.K. Bogner, J.D. Holt, *ARNPS* **69**, 307 (2019).

□ Many-body perturbation theory with V_{low-k} or V_{SRG} (NN + 3N)

T. Otsuka et al, PRL105, 032501 (2010)

J.D. Holt et al, PRC90, 024312 (2014)

Y.Z. Ma, L. Coraggio et al, PRC100, 034324 (2019); L. Coraggio et al, PRC102, 054326 (2020)

□ Valence-space In-Medium Similarity Renormalization Group – IMSRG (NN + 3N)

S.R. Stroberg et al, PRC93, 051301 (2016); PRL118, 032502 (2017)

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

$$dH(s)/ds = [\eta(s), H(s)]$$

□ OLS transformation applied to NCSM results

E.Dikmen et al, PRC94 (2015); N. Smirnova, B.R. Barrett et al, PRC100 (2019)

$$H_{eff} = e^{-\omega} H e^{\omega},$$

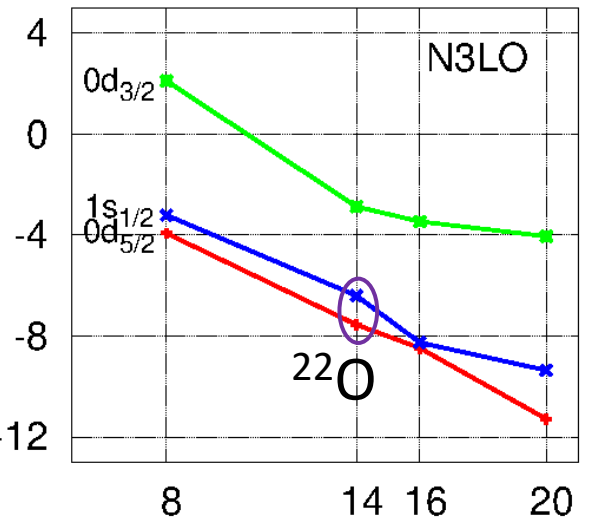
$$P H_{eff} Q = Q H_{eff} P = 0$$

□ Coupled-cluster theory (NN + 3N)

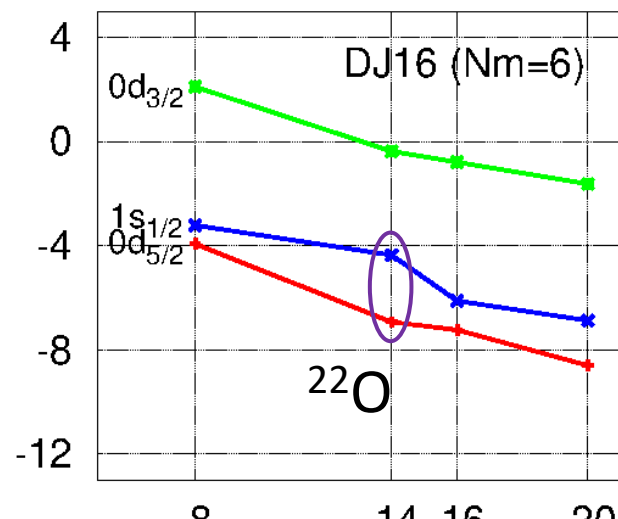
G.R. Jansen et al, PRC94, 011301 (2016); Z.H. Sun, T.D. Morris, G. Hagen et al, PRC98 (2018)

Microscopic approaches to valence space interactions

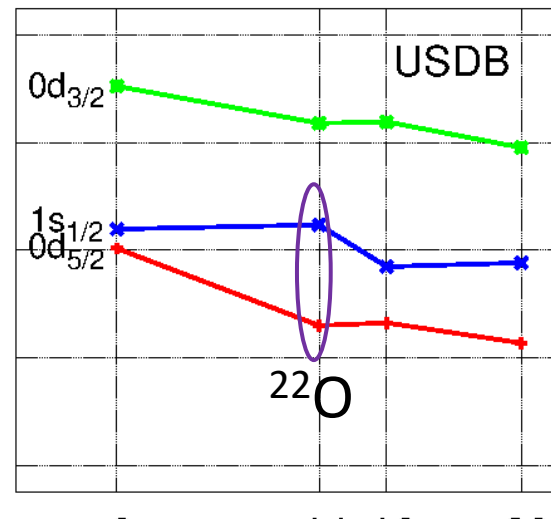
Neutron ESPEs in O-isotopes



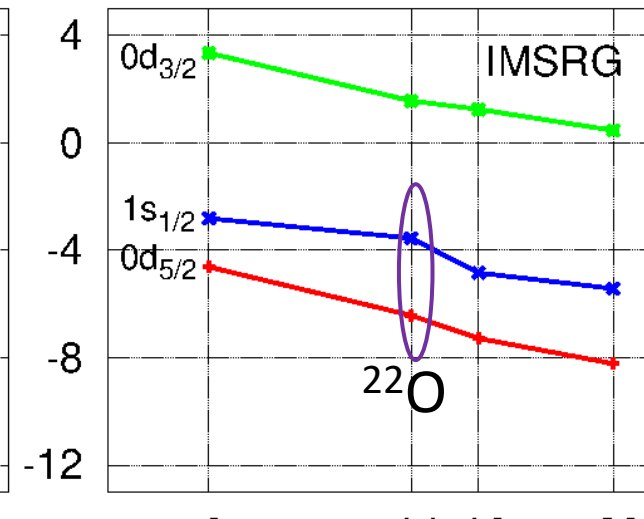
From NN interaction



From Daejeon16
NN interaction



Empirical = experiment

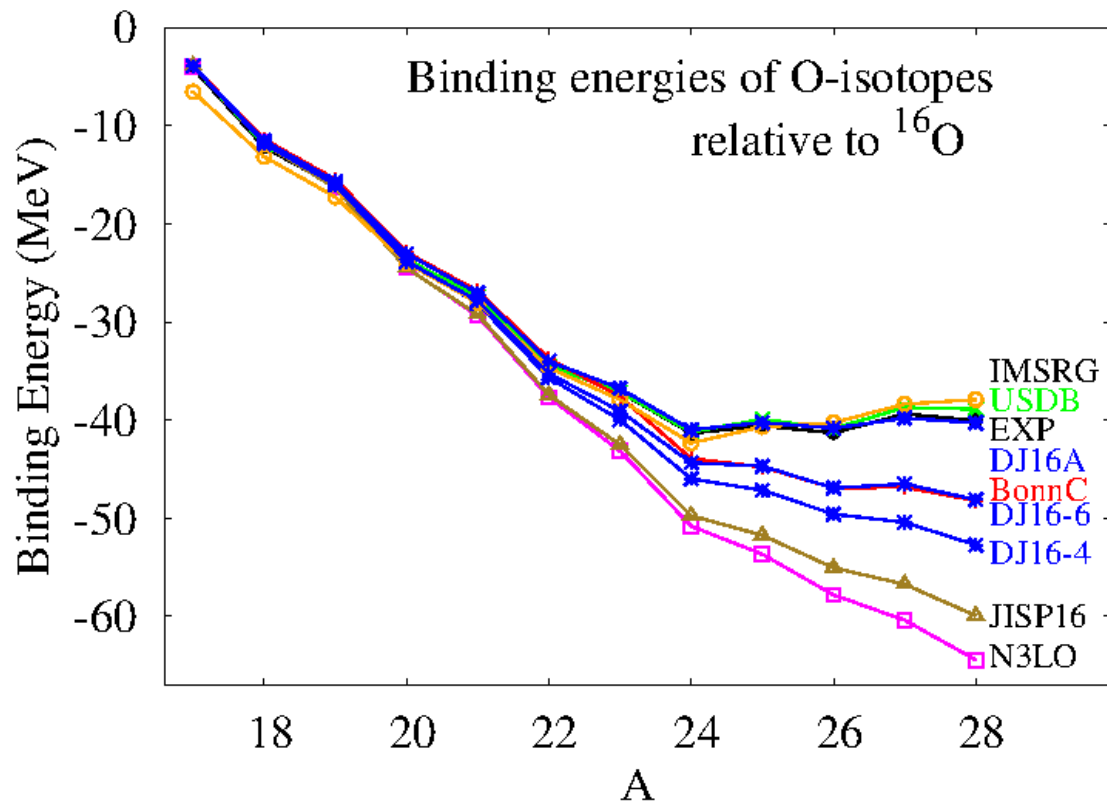


From NN+3N interaction

OLS transformation: N. Smirnova, B.R. Barrett, Y. Kim, I.J. Shin,
A.M. Shirokov, E. Dikmen, P. Maris, J.P. Vary, *PRC100*, 054329 (2019).

Daejeon16 : A.M. Shirokov et al, *PLB761*, 87 (2016) – based on N3LO + SRG evolved + phase-equivalently transformed

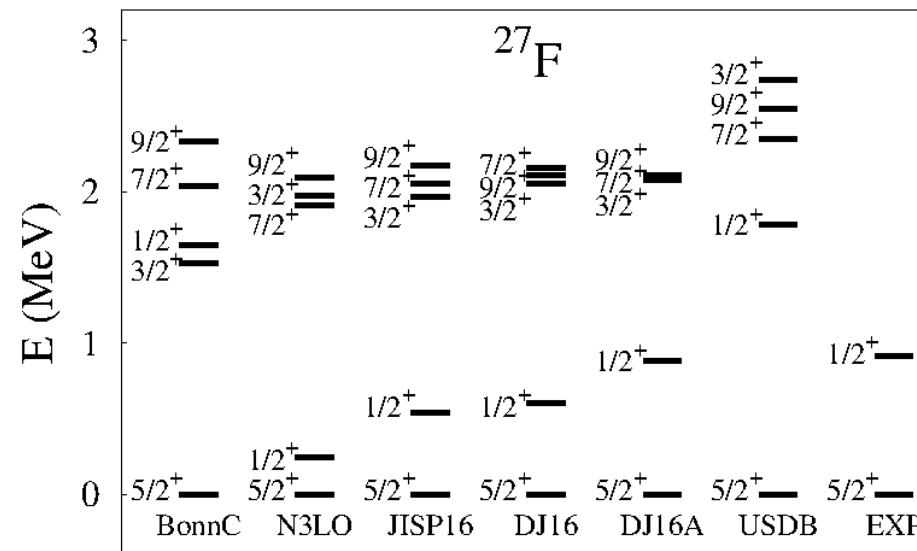
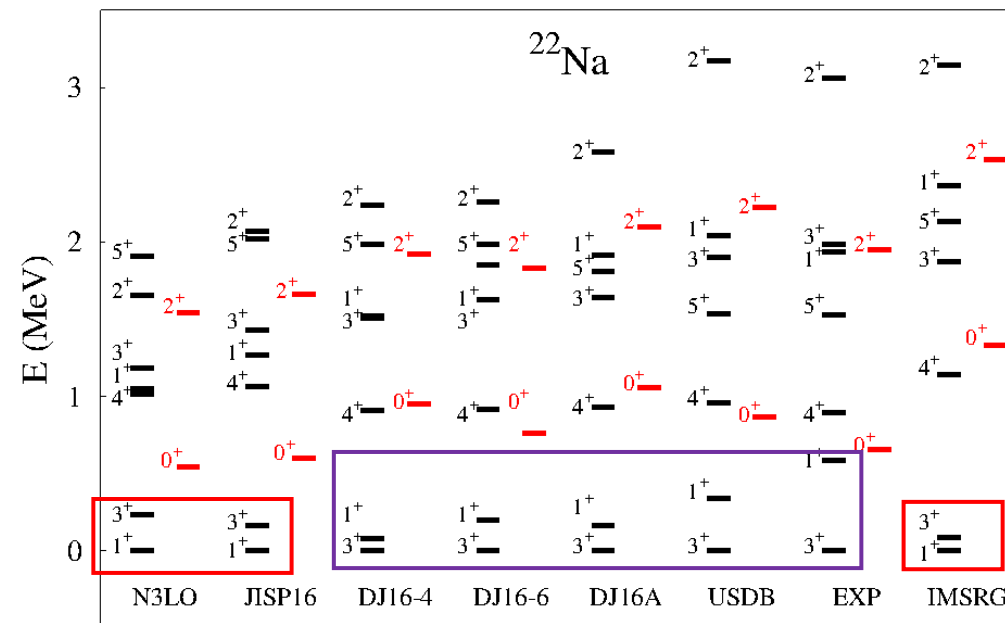
Microscopic effective interactions



RMS (microscopic) > RMS (phenomenological)

For detailed nuclear spectroscopy and applications - Experimentally constrained Interactions !

Applications beyond the Shell Model -> Talk by Duy Duc Dao later in this Session !



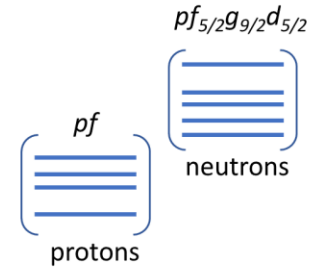
Neutron-rich nuclei

T. Otsuka, A. Gade, O. Sorlin, T. Suzuki, Y. Utsuno, RMP92, 015002 (2020)

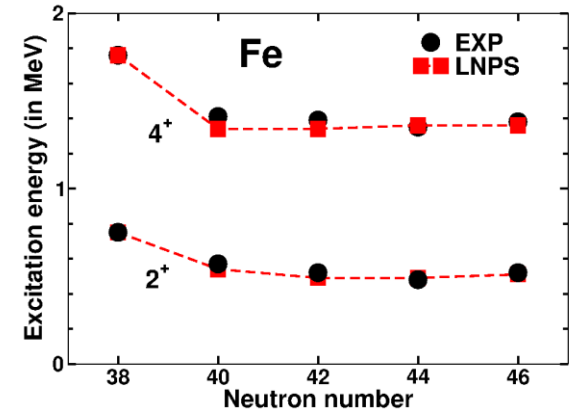
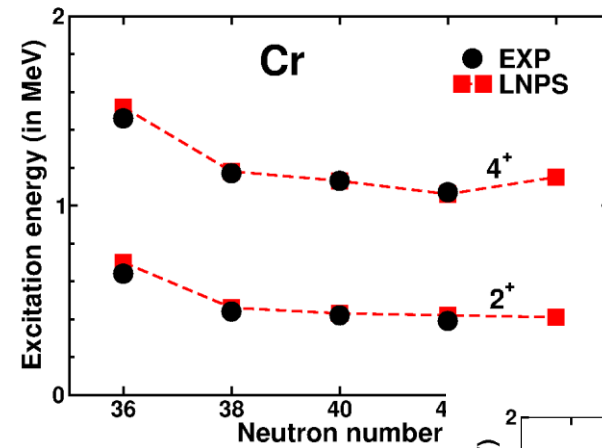
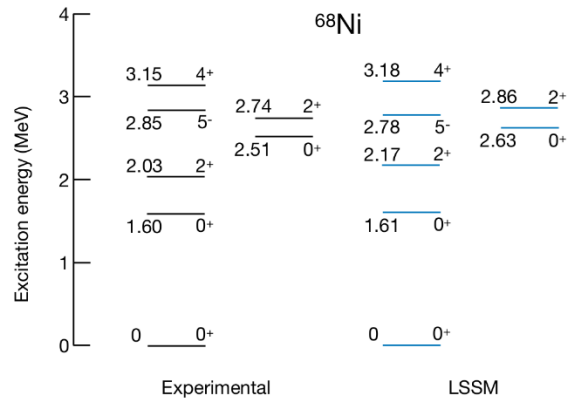
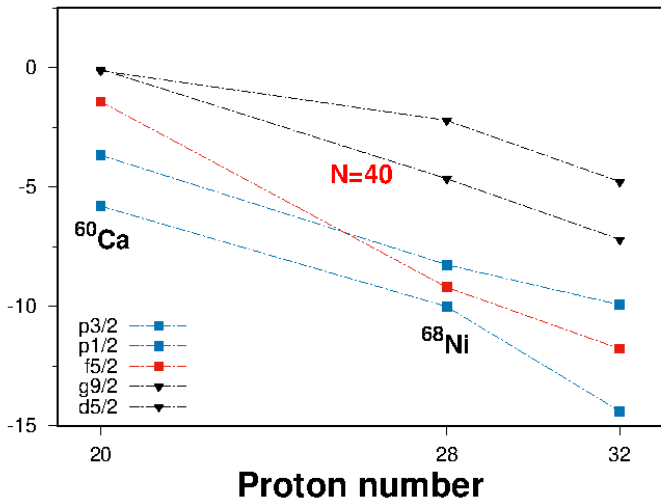
F. Nowacki, A. Obertelli, A. Poves, PPNP120, 103866 (2021)

Achievements

- Accurate and predictive interactions within **two oscillator shells**
- Explains mean-field evolution, **Islands of Inversion**, shape coexistence (competition between spherical mean-field and mainly quadrupole correlation energy)
- Provides detailed spectroscopic information



Neutron ESPEs in N=40 isotones

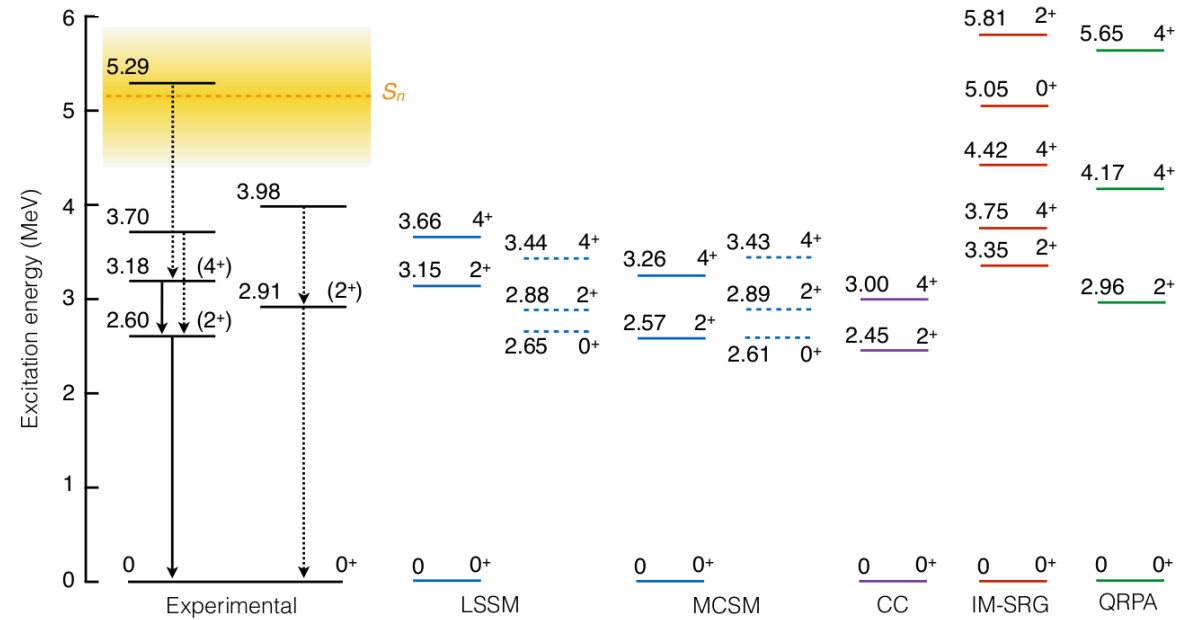
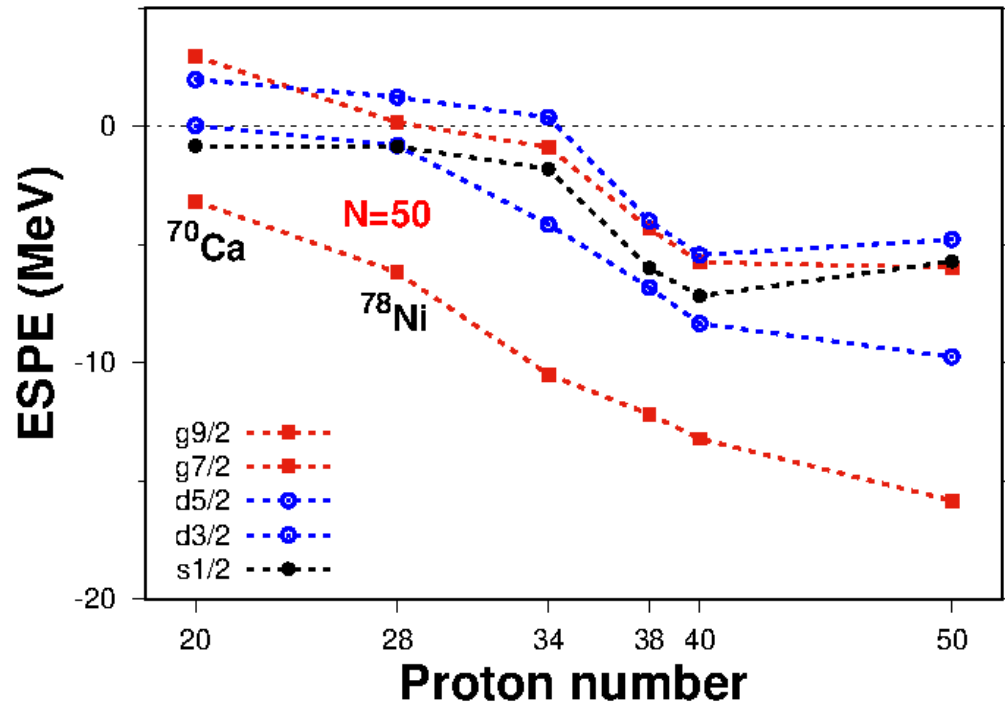
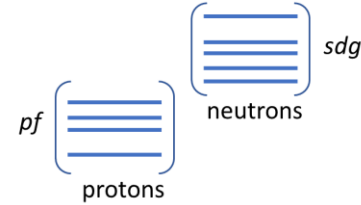


From F. Nowacki, A. Obertelli, A. Poves, PPNP120, 103866 (2021);

LPNS interaction – S.M. Lenzi, F. Nowacki, A. Poves, K. Sieja, PRC82, 054301 (2010).

Neutron-rich nuclei

Large-scale calculations in proton (pf) – neutron (sdg) model space : ^{78}Ni and neighbours



From F. Nowacki, A. Obertelli, A. Poves, PPNP120, 103866 (2021)

From R. Taniuchi et al, Nature 589, 53 (2019)

Proton-rich nuclei: isospin-symmetry breaking

Isospin non-conserving Hamiltonian
(Coulomb + effective charge-dependent components)

$$H_{INC} = H_0 + V_{res} + V_{CD}$$

$$j^\pi \frac{T=3/2}{T_z=3/2} \dots j^\pi \frac{T=3/2}{T_z=1/2} \dots j^\pi \frac{T=3/2}{T_z=-1/2} \dots j^\pi \frac{T=3/2}{T_z=-3/2}$$

$$j^\pi \frac{T=3/2}{T_z=3/2} \quad j^\pi \frac{T=3/2}{T_z=1/2} \quad j^\pi \frac{T=3/2}{T_z=-1/2}$$

Realistic situation

Isospin-symmetry limit

$$M(\eta, T, T_z) = a(\eta, T) + b(\eta, T)T_z + c(\eta, T)T_z^2$$

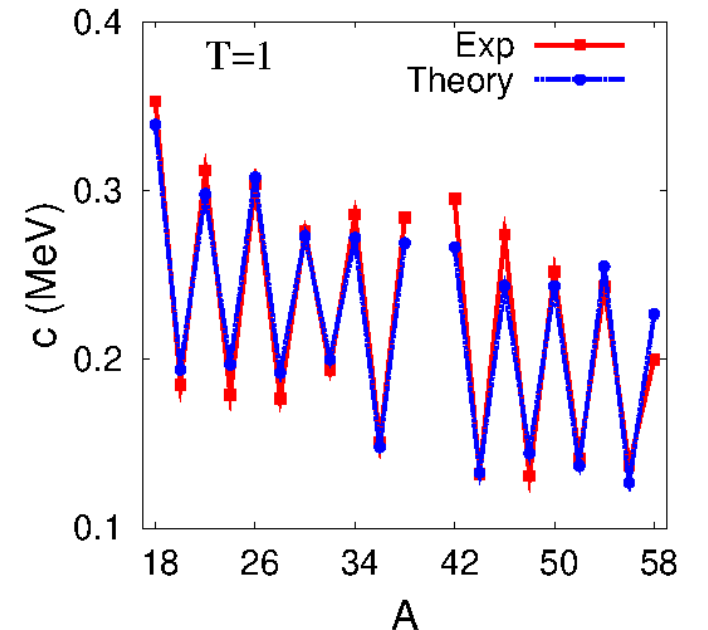
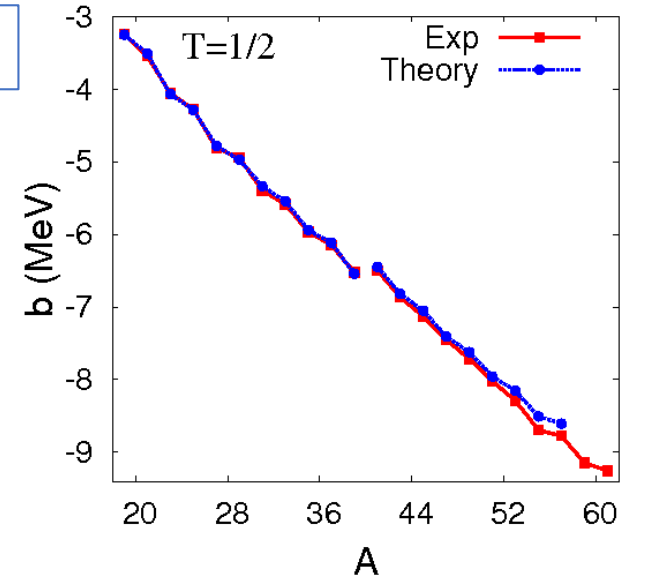
Current status :

- Phenomenological Hamiltonians (still more accurate)
 - mirror-energy differences (MED), triplet-energy differences (TED)
- => see *Lecture by Silvia Lenzi (Monday)*
 - fit of isovector s.p. e's and V_{CD} to experimental **b** and **c** coefficients

Y.H. Lam et al, PRC87 (2013); N. Smirnova et al, PRC96 (2017),...

- Microscopic charge-dependent Hamiltonians

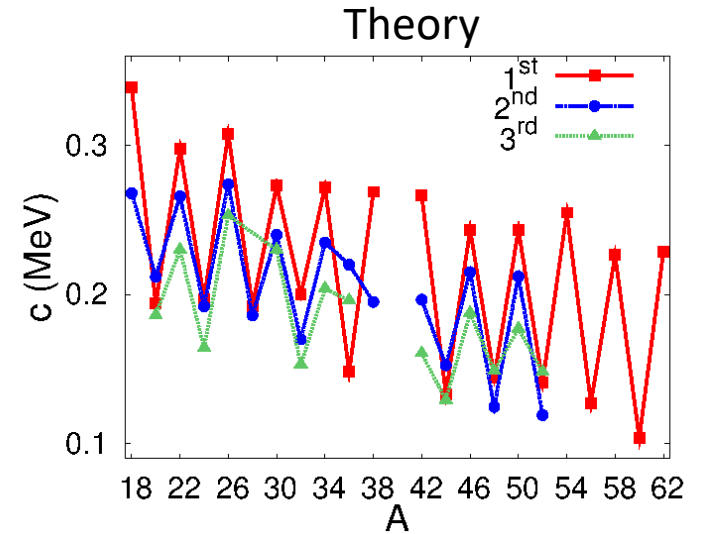
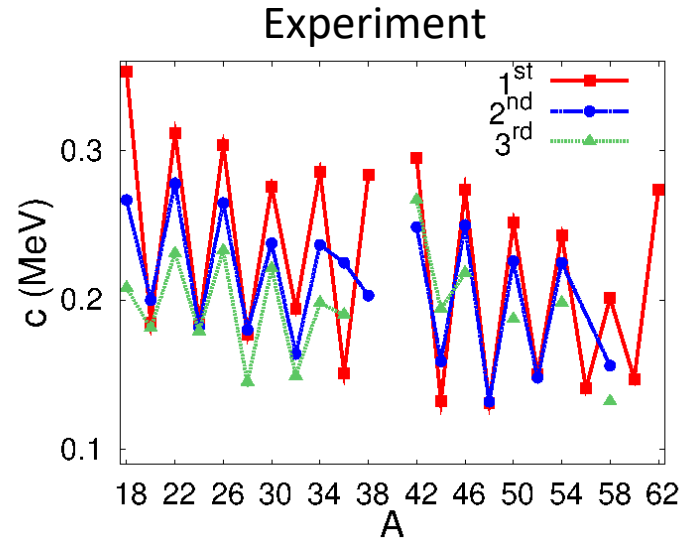
J.D. Holt et al, PRL (2013); W.E.Ormand, B.A. Brown, M.Hjorth-Jensen, PRC96 (2017),...



IMME b and c coefficients of lowest and excited multiplets

Fine structure (staggering) of b and c coefficients

$$M_{T_z} = a + bT_z + cT_z^2$$



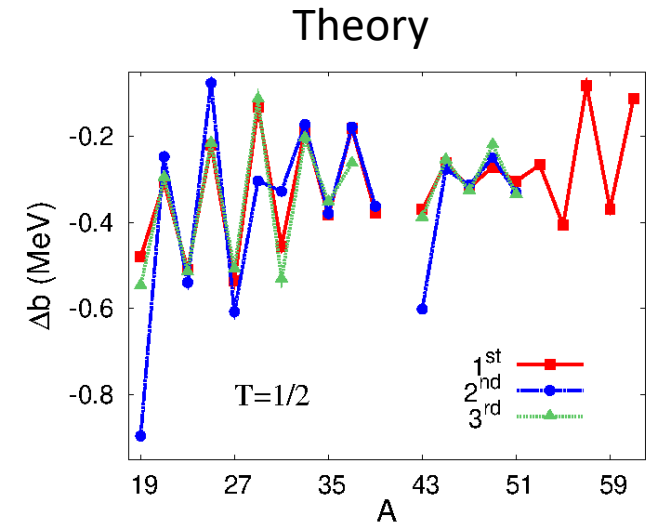
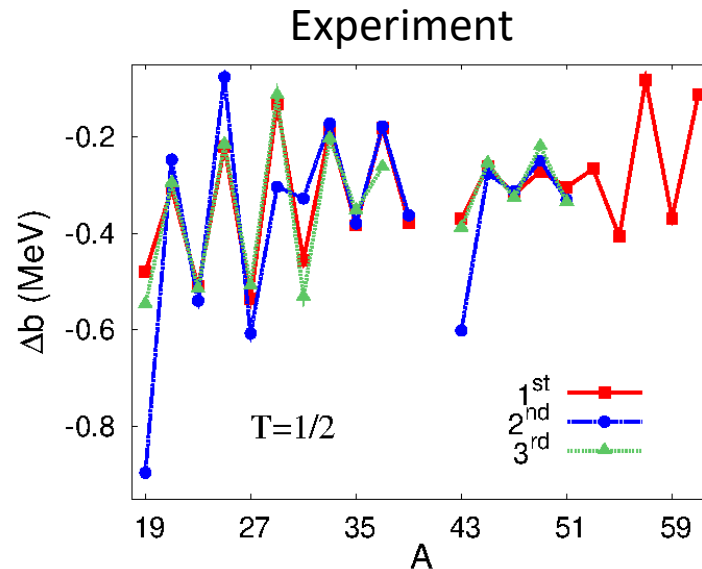
Importance :

- Prediction of masses and excited levels in proton-rich nuclei, e.g. if $T_z > 0$:

$$M_{-T_z} = M_{T_z}^{exp} + 2b^{th}T_z$$

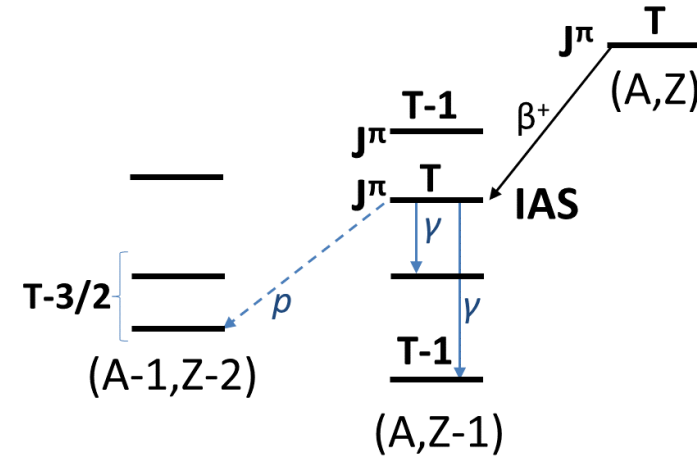
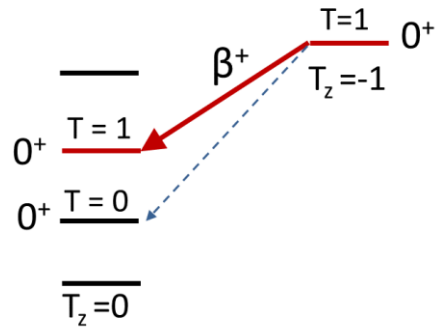
- Particular case of triplets :

$$M_{-1} = 2M_0^{exp} - M_1^{exp} + 2c^{th}$$



Important for nuclear astrophysics applications!

Isospin-forbidden decays and isospin mixing



$$H_{INC} = H_0 + V + V_{CD}$$

$$\alpha^2 \sim \frac{\langle V_{CD} \rangle^2}{\Delta E^2}$$

Combination of Theory and Experiment:

Current status :

- Prediction of isospin-forbidden decay rates and of isospin mixing: challenging, because of poor ΔE
- Safe predictions of Coulomb mixing matrix elements

$$\Gamma_p = \frac{I_p}{I_\gamma} \Gamma_\gamma^{th}$$

$$S_p = \frac{I_p}{\Gamma_{sp}^{th} I_\gamma} \Gamma_\gamma^{th}$$

$$\alpha^2 = \frac{I_p}{S_{ad} \Gamma_{sp}^{th} I_\gamma} \Gamma_\gamma^{th}$$

Fundamental interactions studies

Nuclear Matrix elements are needed to probe fundamental interactions and to search for or to constrain physics beyond the Standard Model

- Neutrinoless double-beta decay process (nature of neutrino and effective mass)
e.g. J. Engel, J. Menendez, RPP 80, 046301 (2017)
- Dark matter particle interactions (^{136}Xe , ...)

*beyond the scope
of the workshop*

- **Fermi type beta decay** => tests of the **Conserved Vector Current Hypothesis** and $|V_{ud}|$ matrix element of the Cabibbo-Kobayasi-Maskawa (CKM) quark-mixing matrix for unitarity tests

Current status:

J.C. Hardy, I. S. Towner, PRC102. 045501 (2020) ;

M. Gonzalez-Alonzo, O. Navillat-Cuncic, N. Severijns, PPNP104, 165 (2019)

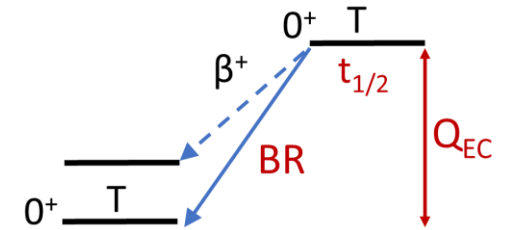
$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}$$

Superaligned $0^+ \rightarrow 0^+$ beta decay

^{10}C , ^{14}O , ^{18}Ne , ^{22}Mg , ^{26}mAl , ^{26}Si , ^{34}Cl , ^{34}Ar , ^{38}mK , ^{38}Ca , ^{42}Sc , ^{46}V , ^{50}Mn , ^{54}Co , ^{62}Ga , ^{66}Br , ^{74}Rb

(Précision de ft : $\sim 0.4\%$)

$$\mathcal{F}t = (1 + \delta_R)(1 + \delta_{NS} - \delta_C)ft = \frac{K}{M_0^2 G_F^2 |V_{ud}|^2 (1 + \Delta_R)}$$



- $\Delta_R, \delta_R, \delta_{NS}$ Radiative corrections
- δ_C Isospin-symmetry breaking correction to the Fermi matrix element

$$M_F^2 = M_0^2 (1 - \delta_C)$$

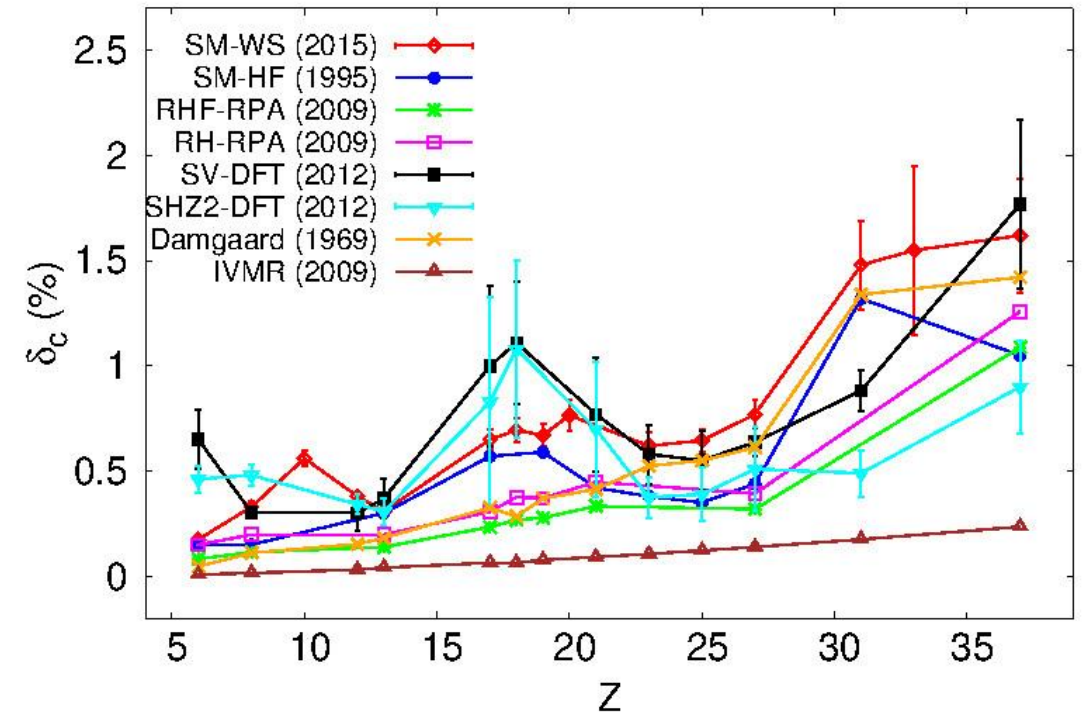
Current status: J.C. Hardy, I. S. Towner, PRC102, 045501 (2020) :

$$\mathcal{F}t = 3072.24 \pm 0.57 \text{ sec}$$

$$\chi^2/\nu = 0.47$$

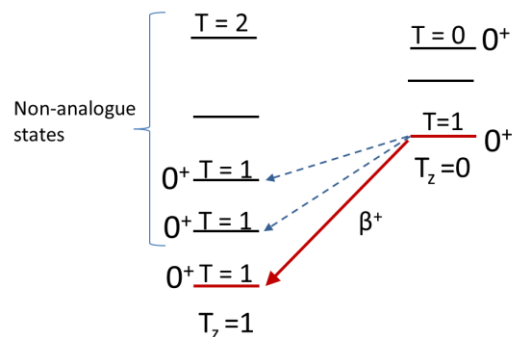
$$|V_{ud}| = 0.97373(31)$$

$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.9985(5)$$

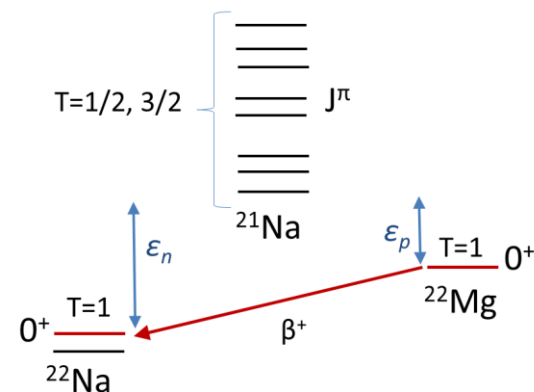


Nuclear-structure correction to Fermi β decay

Large-scale shell model + WS or HF radial wave functions



$$\delta_C = \delta_{IM} + \delta_{RO}$$



Results and perspectives :

- Large-scale calculations with global parametrization lead to the results similar to those of Towner and Hardy (2015)

$$ft = 3073.8 \pm 0.7 \text{ sec}$$

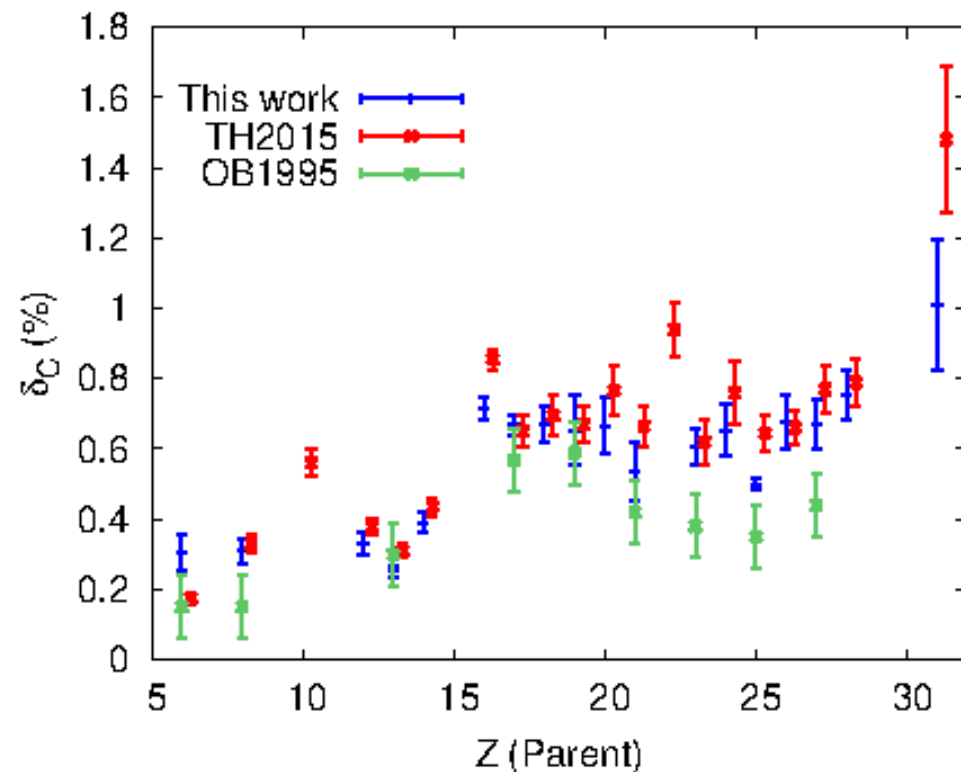
$$\chi^2/\nu = 1.4$$

- New techniques to calculate single-particle strength distribution
- Calculations with the Skyrme HF wave functions are in progress
- Mirror decays ($T=1/2$), exact Fermi operator ...

L. Xayavong, N. Smirnova, *Phys. Rev. C* 97, 024324 (2018)

L. Xayavong et al, *Proc. NTSE2018* (2019) and in preparation

L. Xayavong, N. Smirnova, M. Bender, K. Bennaceur, *Acta Phys. Pol. B Supp* 10, 285 (2017) and in preparation)



Nuclear astrophysics applications



From <https://www.ligo.caltech.edu>

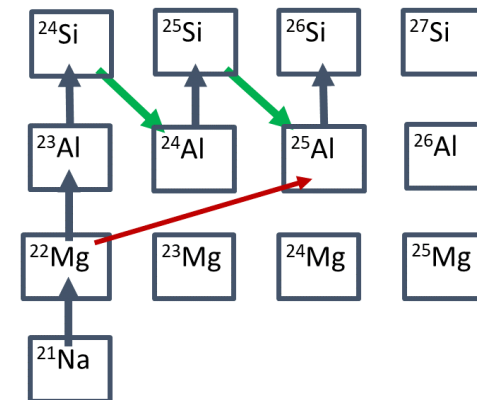


From <https://www.ztf.caltech.edu/image/binary-white-dwarf-stars-and-accretion-disk>

Necessary nuclear physics input for stellar models:

- *Masses of very exotic nuclei*
- *Reaction rates in stellar environment :*
 - *weak interaction rates (e- capture, ..)*
 - *nucleon capture rates (r- or rp-process)*
 - *transfer reactions,*

Theoretical estimations are needed when cross sections are too small



Neutron or proton capture rates

Neutron capture rates (r-process)

- Direct reaction rates with nuclear structure input from the shell model -> *r-process* simulations
- Gamma strength function evaluation
- Beta decay half-lives

K. Sieja, PRC98 (2018); S. Goriely, S. Hilaire, S. Peru, K. Sieja, PRC98 (2018); K. Sieja, S. Goriely, EPJA57, 110 (2021)

Proton capture rates (explosive hydrogen burning – X-ray bursts and novae)

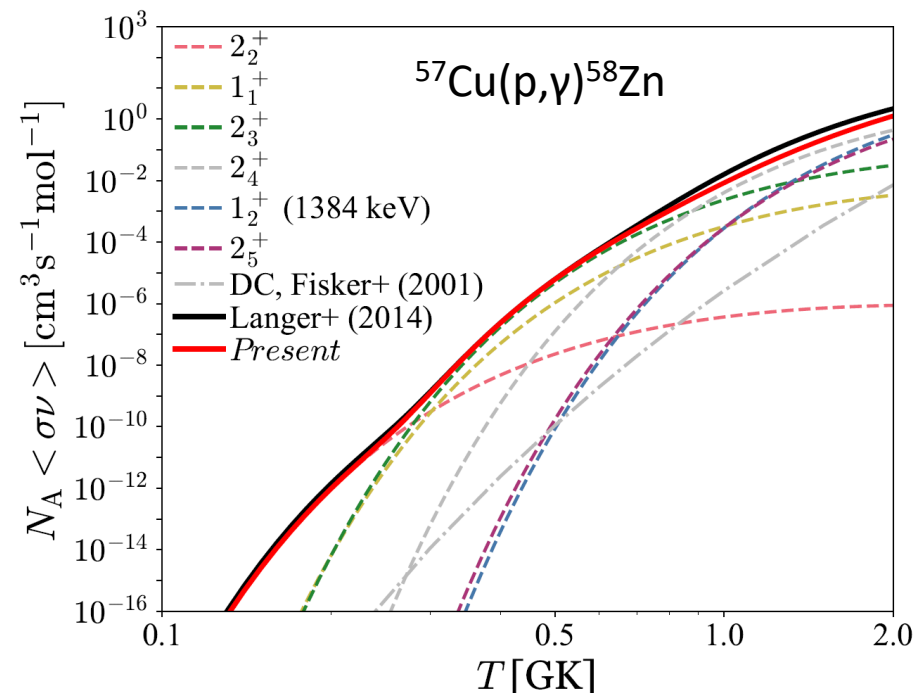
- Reactions on pf-shell nuclei are achievable
- Impact of the Thomas-Ehrman shift (specific role of s1/2)
- Theoretical database of (p,γ) reaction rates

H. Herndl et al (1995); W.A. Richter, B.A. Brown et al, PRC83 (2011)

Reactions of high impact (Cybert et al, AAJ, 2016) :

$^{56}\text{Ni}(\alpha, p)^{59}\text{Cu}$, $^{59}\text{Cu}(p, \gamma)^{60}\text{Zn}$, $^{61}\text{Ga}(p, \gamma)^{62}\text{Ge}$, etc.

$$N_A \langle \sigma v \rangle = 1.54 \cdot 10^{15} (\mu T_9)^{-3/2} \omega \gamma \exp\left(\frac{-11.605 E_r}{T_9}\right) \text{cm}^3 \text{s}^{-1} \text{mol}^{-1}$$



From Y.H. Lam et al, submitted to ApJ (2021)

Conclusions and Perspectives

- The nuclear shell model still keeps its particular (honoured) place among modern many-body approaches capable to provide a deep physics insight into properties of atomic nuclei
=> support to experimental projects
- Technical developments -> towards larger model spaces
- Effective interaction theory -> towards microscopic foundations of the model and link to the ab-initio nuclei theory
- Precision nuclear theory for spectroscopy, fundamental interaction studies and astrophysics applications
- Important, but skipped topics :
Gamow shell model or Continuum coupling (*N. Michel et al, JPG36, 013101 (2009)*)
Alpha clustering within configuration interaction approach (*K. Kravvaris, A. Volya, PRC100, 034321 (2019)*)
.....

Acknowledgements

B. Blank, Z. Li, M. Sanchez (CENBG)

E. Caurier, F. Nowacki (IPHC, Strasbourg)

Y. H. Lam, Z. Yang (IMP, Lanzhou, China)

L. Xayavong (National University of Laos, Vientiane, Laos)

B.A. Brown (NSCL, MSU, East Lansing, USA)

B.R. Barrett (University of Arizona, USA)

J.P. Vary, P. Maris (Iowa State University, Ames, USA)

A.M. Shirokov (Moscow State University, Moscow, Russia)

I.J. Shin, Y. Kim (ISB, Daejeon, South Korea)

+ support from IN2P3/CNRS via « Isospin » and « ENFIA » master projects