Shell model calculations for exotic nuclei with realistic potentials: reliability and predictiveness

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From Rare Isotopes to Neutron Stars
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Part I

The theoretical framework
Introductory remark

What is a realistic effective shell-model hamiltonian?
An example: $^{19}\text{F}$

- 9 protons & 10 neutrons interacting
- spherically symmetric mean field (e.g. harmonic oscillator)
- 1 valence proton & 2 valence neutrons interacting in a truncated model space

The degrees of freedom of the core nucleons and the excitations of the valence ones above the model space are not considered explicitly.
An example: $^{19}$F

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Effective shell-model hamiltonian

The shell-model hamiltonian has to take into account in an effective way all the degrees of freedom not explicitly considered.

Two alternative approaches
- phenomenological
- microscopic

\[ V_{NN} ( + V_{NNN} ) \Rightarrow \text{many-body theory} \Rightarrow H_{\text{eff}} \]

Definition
The eigenvalues of \( H_{\text{eff}} \) belong to the set of eigenvalues of the full nuclear hamiltonian.
Choose a realistic $NN$ potential ($NNN$)

2. Pin down the model space better tailored to study the system under investigation

3. Derive the effective shell-model hamiltonian by way of the many-body theory

4. Calculate the physical observables (energies, e.m. transition probabilities, ...)

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Several realistic potentials $\chi^2/datum \simeq 1$: CD-Bonn, Argonne V18, Nijmegen, ...

How to handle the short-range repulsion?
- Brueckner $G$ matrix
- EFT inspired approaches
- $V_{\text{low}}-k$, SRG, chiral potentials
Realistic nucleon-nucleon potential: $V_{NN}$

Several realistic potentials $\chi^2/\text{datum} \simeq 1$: CD-Bonn, Argonne V18, Nijmegen, ...

How to handle the short-range repulsion?

- Brueckner $G$ matrix
- EFT inspired approaches
  - $V_{\text{low}-k}$, SRG chiral potentials

Strong short-range repulsion

![Graph showing the inter-nucleon potential vs. separation, with regions marked for $2\pi$, $p$, $\omega$, and $\sigma$.]
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**Strong short-range repulsion**
Realistic nucleon-nucleon potential: $V_{NN}$

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How to handle the short-range repulsion?

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Strong short-range repulsion
The shell-model effective hamiltonian

A-nucleon system Schrödinger equation

\[ H |\psi_\nu\rangle = E_\nu |\psi_\nu\rangle \]

with

\[ H = H_0 + H_1 = \sum_{i=1}^A (T_i + U_i) + \sum_{i<j} (V_{i}\!\!_{j}^{NN} - U_i) \]

Model space

\[ |\Phi_i\rangle = [a_1^\dagger a_2^\dagger \ldots a_n^\dagger]_i |c\rangle \Rightarrow P = \sum_{i=1}^d |\Phi_i\rangle \langle \Phi_i| \]

Model-space eigenvalue problem

\[ H_{\text{eff}} P |\psi_\alpha\rangle = E_\alpha P |\psi_\alpha\rangle \]
The shell-model effective hamiltonian

\[
\begin{pmatrix}
    PHP & PHQ \\
    QHP & QHQ
\end{pmatrix}
\begin{matrix}
    \mathcal{H} = X^{-1} H X \\
    \Rightarrow
\end{matrix}
\begin{pmatrix}
    PHP & PHQ \\
    QHP & QHQ
\end{pmatrix}

Q\mathcal{H} P = 0

\[
H_{\text{eff}} = PHP
\]

Suzuki & Lee \Rightarrow X = e^{\omega} \text{ with } \omega = \begin{pmatrix}
    0 & 0 \\
    Q\omega P & 0
\end{pmatrix}

\[
H_{\text{eff}}^1(\omega) = PH_1 P + PH_1 Q \frac{1}{\epsilon - QHQ} QH_1 P - PH_1 Q \frac{1}{\epsilon - QHQ} \omega H_{\text{eff}}^1(\omega)
\]
The shell-model effective hamiltonian

Folded-diagram expansion

$\hat{Q}$-box vertex function

$$\hat{Q}(\epsilon) = PH_1 P + PH_1 Q \frac{1}{\epsilon - QHQ} QH_1 P$$

⇒ Recursive equation for $H_{\text{eff}}$ ⇒ iterative techniques (Krenciglwa-Kuo, Lee-Suzuki, ...)

$$H_{\text{eff}} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} \ldots ,$$
The perturbative approach to the shell-model $H^{\text{eff}}$

\[ \hat{Q}(\epsilon) = PH_1 P + PH_1 Q \frac{1}{\epsilon - QHQ} QH_1 P \]

The $\hat{Q}$-box can be calculated perturbatively

\[ \frac{1}{\epsilon - QHQ} = \sum_{n=0}^{\infty} \frac{(QH_1 Q)^n}{(\epsilon - QH_0 Q)^{n+1}} \]

The diagrammatic expansion of the $\hat{Q}$-box
The perturbative approach to the shell-model $H^{\text{eff}}$

- $H^{\text{eff}}$ for systems with one and two valence nucleons
- $\hat{Q}$-box $\Rightarrow$ Goldstone diagrams up to third order in $V_{NN}$ (up to 2p-2h core excitations)
- Padè approximant $[2|1]$ of the $\hat{Q}$-box

\[
[2|1] = V_{Qbox}^0 + V_{Qbox}^1 + V_{Qbox}^2 (1 - (V_{Qbox}^2)^{-1} V_{Qbox}^3)^{-1},
\]
Test case: $p$-shell nuclei

- $V_{NN} \Rightarrow$ chiral N$^3$LO potential by Entem & Machleidt (smooth cutoff $\simeq 2.5$ fm$^{-1}$)
- $H_{\text{eff}}$ for two valence nucleons outside $^4$He
- Single-particle energies and residual two-body interaction are derived from the theory. **No empirical input**

First, some convergence checks!

Convergence checks

The intermediate-state space $Q$

$Q$-space is truncated: intermediate states whose unperturbed excitation energy is greater than a fixed value $E_{max}$ are disregarded

$$|\epsilon_0 - QH_0 Q| \leq E_{max} = N_{max} \hbar \omega$$

$^6$Li yrast states

Results stable for $N_{max} \geq 20$
Convergence checks

Order-by-order convergence

Compare results from $H_{1\text{st}}^{\text{eff}}$, $H_{2\text{nd}}^{\text{eff}}$, $H_{3\text{rd}}^{\text{eff}}$ and $H_{\text{Padé}}^{\text{eff}}$.
Convergence checks

Dependence on $\hbar \omega$

Auxiliary potential $U \Rightarrow$ harmonic oscillator potential

HF-insertions

- zero in a self-consistent basis
- neglected in most applications
- disregard of HF-insertions introduces relevant dependence on $\hbar \omega$
Approximations are under control ... and what about the accuracy of the results?

Compare the results with the “exact” ones

*ab initio* no-core shell model (NCSM)


To compare our results with NCSM we need to start from a translationally invariant Hamiltonian

\[ H_{int} = (1 - \frac{1}{A}) \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} \left( V_{ij}^{NN} - \frac{p_i \cdot p_j}{mA} \right) = \]

\[ = \left[ \sum_{i=1}^{A} \left( \frac{p_i^2}{2m} + U_i \right) \right] + \left[ \sum_{i<j=1}^{A} \left( V_{ij}^{NN} - U_i - \frac{p_i^2}{2mA} - \frac{p_i \cdot p_j}{mA} \right) \right] \]

(a) not translationally invariant Hamiltonian  
(b) purely intrinsic hamiltonian
Remark

$H^{\text{eff}}$ derived for 2 valence nucleon systems $\Rightarrow$ 3-, 4-, .. $n$-body components are neglected

- ground-state energies for $N = Z$ nuclei
- discrepancy grows with the number of valence nucleons
Benchmark calculation

$^10\text{B}$ relative spectrum

- discrepancy $\leq 1$ MeV
- minor role of many-body correlations
Part II

Reliability
Large-scale realistic shell-model calculations

Neutron-rich isotopic chains

Approaching neutron drip line:
Shell-model study of the onset of collectivity at $N = 40$


Proton-rich isotopic chains

Approaching proton drip line:
Enhanced quadrupole collectivity of neutron-deficient tin isotopes

Collectivity at $N = 40$

$\Rightarrow$ shell-model study of neutron-rich isotopic chains outside $^{48}$Ca

$\Rightarrow$ Collective behavior framed within the quasi-SU(3) approximate symmetry

$\Rightarrow$ Two model spaces with $^{48}$Ca inert core, including or not the neutron $1d_{5/2}$ orbital
Collectivity at \( N = 40 \) in neutron-rich \(^{40}\)Cr

A. Gade, 1,2 R. V. F. Janssens, 1 T. Bangher, 1,2 D. Bazar, 1 B. A. Brown, 1,3 M. P. Carpenter, 1 C. J. Chiara, 1,3 A. N. Deacon, 4 S. J. Freeman, 1 G. F. Grinyer, 1 C. R. Hoffman, 1 B. P. Kay, 1 G. G. Kondev, 1 T. Lauritsen, 1 S. McDaniel, 1,2 K. Meierbachtol, 1,2 A. Ratkiewicz, 1,2 S. R. Stoberg, 1 K. A. Walsh, 1,2 D. Weisshaar, 1 R. Winkler, 1 and S. Zhu 1

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(Rceived 19 March 2010; published 28 May 2011)

Re-induced inelastic scattering of \(^{60}\)Fe and \(^{62}\)Cr was performed at intermediate beam energies. Excited states in \(^{40}\)Cr were measured for the first time. Energies and population patterns of excited states in these neutron-rich Fe and Cr nuclei are compared and interpreted in the framework of large-scale shell-model calculations in different model spaces. Evidence for increased collectivity and for distinct structural changes between the neighboring Fe and Cr isotopic chains near \( N = 40 \) is presented.

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The collectivity at \( N = 40 \)

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Collectivity at $N = 40$

(a) Expt.
- Model space (I)
- Model space (II)

(b) ENSDF
- Rother 2011
- Crawford 2013

(c) Expt.
- Model space (I)
- Model space (II)

(d) ENSDF
- Marchi 2013
shell-model study of neutron-deficient tin isotopes using $^{88}$Sr as a core

Quadrupole collectivity enhanced by the $Z = 50$ cross-shell excitations

Model space spanned by proton $1p_{1/2}, 0g_{9/2}, 0g_{7/2}, 1d_{5/2}$ and $0g_{7/2}, 1d_{5/2}$ orbitals

Theoretical single-particle energies, two-body matrix elements, and effective charges have been employed
Calculation of the effective charges

\[ \langle a | e_p | b \rangle \]

| \( n_a | l_a a \) | \( n_b | l_b b \) | \( \langle a | e_p | b \rangle \) |
|------------------|------------------|------------------|
| \( 0g_{9/2} \)   | \( 0g_{9/2} \)   | 1.62             |
| \( 0g_{9/2} \)   | \( 0g_{7/2} \)   | 1.67             |
| \( 0g_{9/2} \)   | \( 1d_{5/2} \)   | 1.60             |
| \( 0g_{7/2} \)   | \( 0g_{7/2} \)   | 1.73             |
| \( 0g_{7/2} \)   | \( 1d_{5/2} \)   | 1.74             |
| \( 0g_{7/2} \)   | \( 1d_{3/2} \)   | 1.76             |
| \( 1d_{5/2} \)   | \( 1d_{5/2} \)   | 1.73             |
| \( 1d_{5/2} \)   | \( 1d_{3/2} \)   | 1.72             |
| \( 1d_{5/2} \)   | \( 2s_{1/2} \)   | 1.76             |
| \( 1d_{3/2} \)   | \( 1d_{3/2} \)   | 1.74             |
| \( 1d_{3/2} \)   | \( 2s_{1/2} \)   | 1.76             |
| \( 0h_{11/2} \)  | \( 0h_{11/2} \)  | 1.72             |

| \( n_a | l_a a \) | \( n_b | l_b b \) | \( \langle a | e_n | b \rangle \) |
|------------------|------------------|------------------|
| \( 0g_{7/2} \)   | \( 0g_{7/2} \)   | 0.94             |
| \( 0g_{7/2} \)   | \( 1d_{5/2} \)   | 0.96             |
| \( 0g_{7/2} \)   | \( 1d_{3/2} \)   | 0.95             |
| \( 1d_{5/2} \)   | \( 1d_{5/2} \)   | 0.94             |
| \( 1d_{5/2} \)   | \( 1d_{3/2} \)   | 0.97             |
| \( 1d_{5/2} \)   | \( 2s_{1/2} \)   | 0.79             |
| \( 1d_{3/2} \)   | \( 1d_{3/2} \)   | 0.96             |
| \( 1d_{3/2} \)   | \( 2s_{1/2} \)   | 0.79             |
| \( 0h_{11/2} \)  | \( 0h_{11/2} \)  | 0.87             |
Enhanced quadrupole collectivity in light tin isotopes

Enhanced quadrupole collectivity is observed in light tin isotopes, as depicted in the figure. The plots show the comparison between experimental data (Expt.) and theoretical predictions from the Shell model with an $^{88}$Sr core.

(a) 
- **Expt.**
- **Shell model – $^{88}$Sr core**

(b) 
- **NSCL**
- **Riken**
- **REX–ISOLDE**
- **GSI**

The plots illustrate the $2^+_1$ excitation energy [MeV] and $B(E2; 0^+ \rightarrow 2^+)$ [e$^2$ fm$^4$] as a function of the neutron number (N) for tin isotopes ranging from $N = 50$ to $N = 58$.
Part III

Predictiveness
Nuclear models and predictive power

RIBs & advances in detection techniques ⇒ unknown structure of nuclei towards the drip lines
Realistic shell-model calculations in different mass regions

\[ \Rightarrow \]

results in good agreement with experimental data

Can realistic shell-model calculations be predictive?

few selected examples
Few selected physics cases

- Sn isotopes beyond $N = 82$
- heavy calcium isotopes
- neutron-rich titanium and nickel isotopes

Single-particle energies from the experiment $\Rightarrow$ reduced role of $3N$ force
Sn isotopes beyond $N = 82$

Shell-model study of exotic Sn isotopes with a realistic effective interaction

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⇒ shell-model study of Sn isotopes beyond $N = 82$
⇒ $V_{\text{low-k}}$ from CD-Bonn $NN$ potential
⇒ $h_{9/2}fpi_{13/2}$ model space with $^{132}\text{Sn}$ inert core
⇒ SP energies from $^{133}\text{Sn}$
Shell-model study of exotic Sn isotopes with a realistic effective interaction

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⇒ shell-model study of Sn isotopes beyond N = 82

... It is the aim of our study to compare the results of our calculations with the available experimental data and to make predictions for the neighboring heavier isotopes ...
Sn isotopes beyond $N = 82$

Excitation energies of the $2^+_1$, $4^+_1$, and $6^+_1$ states in Sn isotopes

![Graph showing excitation energies of different states in Sn isotopes](image-url)
Sn isotopes beyond $N = 82$

Excitation energies of the $2^+_1$, $4^+_1$, and $6^+_1$ states in Sn isotopes

[Graph showing excitation energies for $A = 134, 136, 138, 140$.]

Yrast $6^+$ Seniority Isomers of $^{136, 138}\text{Sn}$

Heavy calcium isotopes

LETTER

Masses of exotic calcium isotopes pin down nuclear forces

F. Wienholtz¹, D. Beck², K. Blaum³, Ch. Borgmann⁴, M. Breitenfeldt⁵, R. B. Cakirli⁶,⁷, S. George⁸, F. Herfurth², J. D. Holt⁵,⁷, M. Kowalska⁸, S. Kreim³,⁸, D. Lunney⁹, V. Manea⁴, J. Menéndez⁶,⁷, D. Niedherr³, M. Rosenbusch¹, L. Schweikhard⁶, A. Schwenk⁴, J. Simonis⁶,⁷, J. Starja¹⁰, R. N. Wolf¹ & K. Zuber¹⁰

general:
⇒ first mass measurements of $^{53}$Ca and $^{54}$Ca
⇒ new method of precision mass spectroscopy with ISOLTRAP
“... pronounced decrease in $S_{2n}$ revealed by the new $^{53}\text{Ca}$ and $^{54}\text{Ca}$ ISOLTRAP masses ...”
Heavy calcium isotopes

**LETTER**

Evidence for a new nuclear ‘magic number’ from the level structure of $^{54}$Ca

D. Steppenbeck$^1$, S. Takeuchi$^3$, N. Aoi$^3$, P. Doornenbal$^3$, M. Matsushita$^1$, H. Wang$^2$, H. Baba$^2$, N. Fukuda$^2$, S. Go$^1$, M. Honma$^2$, J. Lee$^2$, K. Matsui$^3$, S. Michimasa$^3$, T. Motobayashi$^3$, D. Nishimura$^6$, T. Otsuka$^{1,5}$, H. Sakurai$^{2,5}$, Y. Shiga$^7$, P.-Å. Söderström$^2$, T. Sumikama$^8$, H. Suzuki$^2$, R. Taniuchi$^9$, Y. Utsuno$^{10}$, J. J. Valiente-Dobón$^{10}$ & K. Yoneda$^7$

⇒ spectroscopic study of $^{54}$Ca
⇒ proton knockout reactions involving $^{55}$Sc and $^{56}$Ti projectiles

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Heavy calcium isotopes

⇒ shell-model study of neutron-rich calcium isotopes
⇒ $fp$ model space with $^{40}$Ca inert core
⇒ predictions for the (at that time) unknown spectra of $^{53-56}$Ca
Heavy calcium isotopes: shell-model results

Different monopole properties

\begin{align*}
S_{\alpha/2} & \quad \text{[MeV]} \\
22 & 24 & 26 & 28 & 30 & 32 & 34 \\
\text{Expt.} & \quad \text{V}_{\text{low}-k} \ (2009) & \quad \text{GXPF1A} \ (2005)
\end{align*}

\begin{align*}
\text{excitation energy} & \quad \text{[MeV]} \\
2_+ & 1_+ \\
\text{Present calculations} & \quad \text{GXPF1A}
\end{align*}

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Heavy calcium isotopes: shell-model results

different monopole properties
Realistic shell-model calculations for isotopic chains “north-east” of $^{48}$Ca in the $(N,Z)$ plane

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We perform realistic shell-model calculations for nuclei with valence nucleons outside $^{48}$Ca, employing two different model spaces. The matrix elements of the effective two-body interaction and electromagnetic multipole operators have been calculated within the framework of many-body perturbation theory, starting from a low-momentum potential derived from the high-precision CD-Bonn free nucleon-nucleon potential. The role played by the neutron orbital $1d_{5/2}$ has been investigated by comparing experimental data on yrast quadrupole excitations of isotopic chains north-east of $^{48}$Ca with the results of calculations including or not including this single-particle state in the model space.

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⇒ shell-model study of neutron-rich isotopic chains outside $^{48}$Ca
⇒ $fpgd$ model space with $^{48}$Ca inert core
⇒ predictions for the (at that time) unknown spectra exotic Ti isotopes and of $^{78}$Ni shell closure
Isotopic chains “north-east” of $^{48}$Ca: shell-model results

![Graphs showing $B(E2; 2^+ \rightarrow 0^+)$ and excitation energy vs. N]
Isotopic chains “north-east” of $^{48}\text{Ca}$: shell-model results

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Conclusions and outlook

- The agreement of our results with the experimental data testifies the reliability of a microscopic shell-model calculation with realistic potentials.
- We have now evidence of the predictive power of realistic shell model.
- Role of real three-body forces and three-body correlations should be investigated.
- Perspectives: benchmark calculations with other many-body approaches.
These terms introduce density dependence into the effective shell-model hamiltonian
Conclusions and outlook

- The agreement of our results with the experimental data testifies the reliability of a **microscopic shell-model calculation** with **realistic potentials**.
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- Perspectives: **benchmark calculations** with other many-body approaches.