THE REALISTIC SHELL MODEL AND THE KSHELL IMPLEMENTATION





OUTLINE

The Shell Model

- > The basic framework
- ➤ The shell-model effective Hamiltonian
- Dimensionality of the SM basis and SM codes
- > Calculations of physical observables
- Some examples of calculations within SM

SHELL MODEL (non interacting)

Each nucleon is assumed to be moving in an external field created by the remaining nucleons, with the mean field consisting in an isotropic harmonic oscillator plus a strongly attractive spin-orbit potential and an orbit-orbit term

 $U = U(r) + U_{ls}l \cdot s + U_{b}l^{2}$

J. Hans D. Jensen Maria Goeppert Mayer



Noble Prize in 1963





 $n \equiv radial$ quantum number $I \equiv orbital$ angular momentum $j \equiv total$ angular momentum

TWO OR MORE VALENCE NUCLEONS



Non interacting shell model
$(f_{5/2}p_{3/2}) J^{\pi} = I^+, 2^+, 3^+, 4^+$
$(f_{5/2})^2 J^{\pi} = 0^+, 2^+, 4^+$



TOWARDS THE INTERACTING SHELL MODEL



SHELL MODEL (interacting)

Mean-field ansatz \rightarrow we obtain a set of single-particle states, where all nucleons are distributed starting from the lowest energy level



SHELL MODEL HAMILTONIAN

$$H_{\text{eff}} = \sum_{i} U_i + \sum_{i < j} V_{ij}$$

defined in the model space for only valence nucleons

$H_{\rm eff}$ should take into account <u>in an effective way</u> all the degrees of freedom not considered explicitly



EXAMPLE



$$= \sum_{\alpha\beta\in \text{ valence space}} C^{i}_{\alpha\beta}[a^{\dagger}_{\alpha}a^{\dagger}_{\beta}]_{i}|c\rangle, \quad i = 1, ..., d,$$

$$|c\rangle = \prod_{\alpha\in filled \ shells} a^{\dagger}_{\alpha}|0\rangle$$

$$0f1p \xrightarrow{|2p\ 0h>} |3p\ 1h> |4p\ 2h>$$

$$0f1p \xrightarrow{0} |p \xrightarrow{0} |p$$

<

<

<

H

EXAMPLE

SHELL-MODEL HAMILTONIAN

$$H = H_0 + V = \sum_{i=1}^{N} h_i + \sum_{i,j=1}^{N} V_{ij}$$

$$H_0 = \sum_a \varepsilon_a N_a \qquad \qquad N_j = \sum_a a_{jm}^+ a_{jm}$$

$$V = -\frac{1}{4} \sum_{J} \sum_{abcd} [\mathcal{N}_{ab}(J)\mathcal{N}_{cd}(J)]^{-1} \widehat{J} \langle ab; J|V|cd; J \rangle \left[[a_a^+ a_b^+]_J [\tilde{a}_c \tilde{a}_d]_J \right]_{00}$$

$$V = -\frac{1}{4} \sum_{\substack{J \\ T=0,1}} \sum_{abcd} [\mathcal{N}_{ab}(JT)\mathcal{N}_{cd}(JT)]^{-1} \widehat{J}\widehat{T}\langle ab; JT|V|cd; JT \rangle$$
$$\times [[a_a^+ a_b^+]_J^T [\tilde{a}_c \tilde{a}_d]_J^T]_{00}^{00}$$

$$\begin{aligned} A_{JM}^{+}(ab) &= [a_{a}^{+}a_{b}^{+}]_{JM} \\ A_{JM}(ab) &= [a_{b}a_{a}]_{JM} \\ \tilde{A}_{JM}(ab) &= (-1)^{J-M}A_{J-M}(ab) \end{aligned}$$

SHELL-MODEL HAMILTONIAN

Two alternative approaches:

Phenomenological Microscopic

PHENOMENOLOGICAL SHELL-MODEL HAMILTONIAN

SPE and interaction TBMEs are considered as adjustable parameters and they - or their linear combinations - are fitted to experimental data in order reproduce experimental low-energy spectra by a least-square fit procedure

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A very simple case:
two valence nucleons in the 0f_{7/2} orbit: (0f_{7/2})^2
8 TBME
J=0, 2, 4, 6 T=1 & J=1, 3, 5, 7 T=0
1 SPE
```

0р	l s0d	l s0d	lp0f
I 5 TBME + 2 SPE	63 TBME + 3 SPE	63 TBME + 3 SPE	195 TBME + 4 SPE
A=5-16	A=17-40 (389 data)	A=17-40 (608 nuclei)	A=47-66 (699 data)
Cohen-Kurath (1965)	USD-Brown et al (1980)	USDA-Brown et al (2006)	GXPFI-Honma et al (2002)

the number of ME to be fitted becomes too large for increasing spaces

MONOPOLE MODIFIED SHELL-MODEL HAMILTONIAN

Start from interactions derived from the free nuclear potentials and use a readjusting procedure in which only the monopole component is modified

$$H = H_{mon} + H_{multi}$$

Monopole: spherical mean field as extracted from the interacting shell model Multipole: correlations like pairing, gradrupole, octupole,...

The case of ⁴⁹Ca

KB: Kuo-Brown interaction for the *fp* valence space KB3: monopole modified interactions from KB





E. Caurier, G. Martínez-Pinedo, F. Nowacki, A. Poves, A. P. Zuker, Rev. Mod. Phys. 77 (2005) 427

SOME SEMI-PHENOMENOLOGICAL SHELL-MODEL HAMILTONIANS

Label	Model space	Ref
KB3	I p0f	A. Poves, A.P. Zuker. Phys. Rep, 70, 235 (1981)
SDPF-U	ls0d-lp0f	F. Nowacki,A. Poves. PRC 79, 014310 (2009)
LNPS	$0f_{5/2}I_{p}0g_{9/2}Id_{5/2}$	S. M. Lenzi et al, PRC 82, 054301 (2010)
SVD GCN5082	0g _{7/2} 1d2s0h _{11/2}	C. Qi, Z.X.Xu, PRC,86, 044323 (2012) J. Menéndez et al, NPA 818, 139 (2009)
	above 78Ni	K. Sieja et al, PRC 79, 064310 (2009)
•••	•••	•••

MICROSCOPIC SHELL-MODEL HAMILTONIAN

$$V_{NN}(+V_{NNN}) \Longrightarrow many \ body \ theory \Longrightarrow H_{eff}$$

Hilbert space $H = T + V_{NN} = (T + U) + (V_{NN} - U) = H_0 + H_1 \Longrightarrow |\psi_{\alpha}\rangle; E_{\alpha}$

Model space

 $H_{\text{eff}} = H_0 + H_1^{\text{eff}} \Longrightarrow |\psi_\beta\rangle = P|\psi_\beta\rangle; \ E_\beta \in \{E_\alpha\}$

A well-established approach "folded-diagrams expansion" is based on the many-body perturbation theory and has started with the seminal paper by Tom Kuo and Gerry Brown on sd-shell nuclei [Nucl. Phys. 85, 40 (1966)]



+ 1 and 2-body third order diagrams (~200) + ...

MODEL SPACE & DIMENSIONALITY OF SHELL-MODEL CALCULATIONS

Table 1. *M*-scheme and *J*-scheme dimensions of several nuclei. The dimension of the $M^{\pi} = 0^+$ $(J^{\pi} = 0^+)$ subspace is shown. See text for details.

Nuclide	Model Space	M-Scheme Dim	J-Scheme Dim
¹² C	$2 \leq N, Z \leq 8$ (<i>p</i> shell)	51	9
²⁸ Si	$8 \le N, Z \le 20$ (sd shell)	93,710	3372
⁵⁶ Ni	$20 \le N, Z \le 40 \ (pf \text{ shell})$	$1.08 imes 10^9$	$1.54 imes10^7$
⁷⁸ Y	$28 \le N, Z \le 50 \ (f_5 pg_9, jj44)$	$1.31 imes 10^{10}$	$1.11 imes 10^8$
¹³⁰ Sm	$50 \le Z, N \le 82 \ (jj55)$	$2.06 imes10^{15}$	$9.58 imes10^{12}$
¹⁷² Dy	$50 \le Z \le 82, 82 \le N \le 126$	$1.71 imes 10^{19}$	$5.54 imes10^{16}$
	(<i>jj</i> 56)		

N. Shimizu,, Physics 2022, 4, 1081–1093

PERFORMANCE OF SHELL MODEL CODES

Manageable Hamiltonian size as a function of the year



Current limit of the Hamiltonian size ~ 10¹¹

N. Shimizu, T. Mizusaki, Y. Utsuno et al. Computer Physics Communications 244 (2019) 372–384

SHELL MODEL CODES



PHYSICAL OBSERVABLES



We need

- \checkmark the value of the operator between SP states
- \checkmark the one body transition density matrix elements

ELECTROMAGNETIC OBSERVABLES

$$\langle \phi_f \| \hat{O}^{\lambda} \| \phi_i \rangle = \sum_{k_{\alpha} k_{\beta}} \text{OBTD}(fik_{\alpha} k_{\beta} \lambda) \langle k_{\alpha} \| \hat{O}^{\lambda} \| k_{\beta} \rangle$$

• <u>electric</u>

 $O(E\lambda) = r^{\lambda} Y^{\lambda}_{\mu}(\hat{r}) e_{t_z} e,$

Free charges $e_n = 0$, $e_p = 1$

• <u>magnetic</u>

$$O(M\lambda) = \sqrt{\lambda(2\lambda+1)} \left[[Y^{\lambda-1} \otimes \vec{\ell}]^{\lambda}_{\mu} \frac{2g^{\ell}_{t_z}}{(\lambda+1)} + [Y^{\lambda-1} \otimes \vec{s}]^{\lambda}_{\mu} g^s_{t_z} \right] r^{\lambda-1} \mu_N$$

Free g factors $g_p^{\ell} = 1$, $g_n^{\ell} = 0$, $g_p^s = 5.586$ and $g_n^s = -3.826$.

EFFECTIVE OPERATORS

$$\langle \phi_f | \hat{O}_{\text{eff}}^{\lambda} | \phi_i \rangle = \langle \psi_f | \hat{O}^{\lambda} | \psi_i \rangle$$

• $\phi_{\nu} \equiv$ eigenstate of the H_{eff} corresponding to the eigenvalue E_{ν} : $H_{\rm eff} |\phi_{\nu}\rangle = E_{\nu} |\phi_{\nu}\rangle$

• $\psi_{\nu} \equiv$ eigenstate of the full Hamiltonian corresponding to the eigenvalue E_{ν} : $H |\psi_{\nu}\rangle = E_{\nu} |\psi_{\nu}\rangle$

$$\langle k_{\alpha} || \hat{O}^{\lambda} || k_{\beta} \rangle \Longrightarrow \langle k_{\alpha} || \hat{O}_{\text{eff}}^{\lambda} || k_{\beta} \rangle$$

• empirical effective charges and empirical gyromagnetic factors

 microscopic effective operators derived consistently with SM Hamiltonian

One-body operator



GLOSSARY

- **STATE:** a solution of the Schrödinger equation for the effective SM Hamiltonian
- **ORBITAL:** the ensemble of SP states with the same quantum numbers nlj, e.g. 0d5/2. with degeneracy is (2j+1)
- SHELL: an ensemble of orbitals quasi-degenerated in energy, e.g. the sd shell
- MAGIC NUMBERS: the numbers of protons or neutrons that fill sequentially a certain number of shells
- **SHELL GAP:** the energy difference between two shells
- **MODEL SPACE:** the ensemble of orbitals included in the SM calculation
- SPE: SP energies, namely the eigenvalues of the one-body component of the Hamiltonian
- **TBME:** two-body matrix elements of the effective interaction

FLOWCHART OF SHELL-MODEL CALCULATIONS

Identify the best model space for the nucleus under investigation: the set of orbitals that are accessible by the valence nucleons

Fix the Hamiltonian: the one-body term U_i and the V_{ii}

Construct the basis, and the ME of the Hamiltonian

Diagonalize the shell-model Hamiltonian \rightarrow energies, wave functions

Calculate physical observables by using the SM wave functions and effective operators

SOMETHING TO CONSIDER

The shell structure known so far is based on stable nuclei

New data on light nuclei with N >> Z show significant modifications \rightarrow in neutron-rich exotic nuclei, traditional magic numbers (N=8, 20, etc.) can disappear, while new ones (N=6, 16, etc.) may emerge



How do magic numbers evolve as a function of the neutron-to-proton ratio and what are the underlying mechanisms?

- Large-scale shell-model calculations (LSSM) including more than one major shell
- 3 body forces

. . .

SOME STUDY CASES

¹³²Sn REGION



The only region around a heavy, neutron rich doubly-closed shell nucleus far-off stability experimentally accessible today

➤ shell evolution & underlying driving forces to search for effects similar to those observed in lighter nuclei

- provide predictions for nuclei
 still inaccessible for present
 - experiments
- ✓ involved in 0vββ decay (¹³⁰Te, ¹³⁶Xe)
 ✓ of great relevance for the rapid neutron-capture process,

THE MAGICITY OF ¹³²Sn



RSM CALCULATIONS FOR NUCLEI IN ¹³²Sn REGION



¹³⁴Sn - ¹³⁴Te - ¹³⁴Sb



SHELL EVOLUTION IN Sn ISOTOPES FOR N>82



No significant upshift of the 2+ state in ¹⁴⁰Sn \rightarrow No significant changes of the $If_{7/2}-2p_{3/2}$ gap \rightarrow No shell gap @N=90

NEUTRON ESPE IN Sn ISOTOPES FOR N>82



$$ESPE(a\tau) = \epsilon_{a\tau} + \sum_{b\tau'} \bar{V}_{ab}^{\tau\tau'} n_b^{\tau}$$
$$\bar{V}_{ab}^{\tau\tau'} = \frac{\sum_J \hat{J} \langle a\tau b\tau'; J \mid V_{\text{eff}} \mid a\tau b\tau'; J \rangle}{\sum_J \hat{J}}$$

 $n_b^{\tau} \equiv$ number of neutrons in the *b* orbital

Neutron ESPE as a function of the valence neutron number

E2 PROPERTIES IN Sn ISOTOPES FOR N>82



Theory deviates from expt at A=136.

B(E2)	calc	expt
$2^+ \rightarrow 0^+$	117	
4⁺ → 2⁺	34	
$6^+ \rightarrow 4_1^+$	5	24(4)
$4^+_2 \rightarrow 2^+$	74	
$6^+ \rightarrow 4_2^+$	66	

¹³⁶ Sn

	E	calc	expt
	0+	0	0
	2+	737	688
	4+	1020	1079
	6+	1133	1295
~	4+	1180	

E2 PROPERTIES IN Sn ISOTOPES FOR N>82

Small changes (~50/100 keV) in the (f7/2)² J=2,4,6 diagonal MEs to favor the mixing between the two 4⁺ states

	E	calc	expt	E	calc	expt
0	+	0	0	0+	0	0
2	+	737	688	2+	658	688
4	+	1020	1079	4+	1054	1079
6	+	1133	1295	4+	1176	
4	+	1180		6+	1280	1295

B(E2)	calc	expt	B(E2)	calc
2 ⁺ → 0 ⁺	117		$2^+ ightarrow 0^+$	119
4 ⁺ → 2 ⁺	34		4+> 2+	90
6 ⁺ → 4 ⁺	5	24(4)	6+>4+	32
$6^+ \rightarrow 4^+_2$	66		6 ⁺ → 4 ⁺ ₂	41

THE MAGICITY OF ¹³²Sn VIA ELECTROMAGNETIC MOMENTS

 μ moments in 7/2⁻ ground state of even Z \geq 50, N = 83 nuclei



 $|7/2^{-}\rangle = \approx 85\% |\pi 0^{+}_{1} \otimes \nu f_{7/2}\rangle + (5-6)\% |\pi 2^{+}_{1} \otimes \nu f_{7/2}\rangle + \cdots$ for Z>50

L.V. Rodríguez et al., PRC 102, 051301(R) (2020)

THE MAGICITY OF ¹³²Sn VIA ELECTROMAGNETIC MOMENTS

 μ moments in 7/2⁺ ground state of odd Z>50, N = 82 nuclei



 $g_{eff}^{l}(\mathbf{p})=1.18 g_{eff}^{l}(\mathbf{n})=0$ $g_{eff}^{s}(\mathbf{p},\mathbf{n})=0.7 g_{s}(\mathbf{p},\mathbf{n})$ emprical g factors

→ Relevance of first-order core polarization renormalization induced by spin-flip $\pi 0g_{9/2} \rightarrow \pi 0g_{7/2}$ transitions. Need to explicitly include proton cross shell excitations (see calculations with ⁸⁸Sr core



S. Lechner et al, Phys. Rev. C 104, 014302 (2021)

EMERGE OF COLLECTIVITY NEAR ¹³²Sn: ¹²⁹Sb



$$\sum B(E2;\uparrow) = B(E2; 0_{gs}^+ \to 2^+)_{core}$$

When does this scheme break down and collectivity develop owing to the np interaction?

EMERGE OF COLLECTIVITY NEAR ¹³²Sn: ¹²⁹Sb



T. J. Gray et al, Phys. Rev. Lett. 124, 032502 (2020)

ONE-PHONON 2⁺ VIBRATIONAL STATES:¹³²TE



Two one-phonon 2⁺ states may appear as a symmetric or antisymmetric combinations of the π & ν configurations:

 $|2_{FSS}^{+}\rangle = \alpha |0^{+}(\pi)\rangle |2^{+}(\nu)\rangle + \beta |0^{+}(\nu)\rangle |2^{+}(\pi)\rangle \qquad |2_{MS}^{+}\rangle = \alpha |0^{+}(\pi)\rangle |2^{+}(\nu)\rangle - \beta |0^{+}(\nu)\rangle |2^{+}(\pi)\rangle$

|2⁺_{MS}⟩ characterized by
 > strong MI to 2⁺_{FSS} due its isovector nature
 > weak E2 to 0⁺ due to the partial cancellation of the neutron and proton contributions

ONE-PHONON 2⁺ VIBRATIONAL STATES: ¹³²TE



$B(E2; 2_1^+ \to 0^+)$	10(1) Wu
$B(E2; 2_2^+ \to 0^+)$	0.5(1) ₩u
$B(M1; 2_2^+ \rightarrow 2_1^+)$	5.4(35) - >0.23 μ _N ²

M. Danchev, Phys. Rev. C 84, 061306(R) (2011)

			~	0		
			Expt	Calc		
			Expt	Calc		
	$B(E2; 2_1^+)$	$\rightarrow 0^+)$	10(1) Wu	7.8 Wu		
	$B(E2; 2_2^+)$	$\rightarrow 0^+)$	0.5(1) Wu	0.21 Wu		
	B(M1; 2 ⁺ ₂	$\rightarrow 2^+_1)$	5.4(35) - > 0.23 μ_N^2	0.20 μ_N^2		
($ 0_{1}^{+}\rangle = 0.94 0_{1}^{+}\rangle_{\nu} 0_{1}^{+}\rangle_{\pi} + \cdots,$					
2	$ 2_1^+\rangle = 0.62 2_1^+\rangle_{\nu} 0_1^+\rangle_{\pi} + 0.66 0_1^+\rangle_{\nu} 2_1^+\rangle_{\pi} + \cdots,$					
2	$2_{2}^{+}\rangle = 0.63 2\rangle$	$_{1}^{+}\rangle_{\nu} 0_{1}^{+}\rangle_{\pi}$	$-0.58 0_{1}^{+}\rangle_{\nu} 2_{1}^{+}\rangle_{\pi}+\cdots$, .		

0.97 MeV

¹³²**Te**



THANK YOU FOR YOUR ATTENTION

&

ENJOY EXPLORING SHELL-MODEL CALCULATIONS