Shell-Model Applications in nuclear physics and astrophysics

Gabriel Martínez Pinedo





- Introduction
- Shell-Model Basics
- Effective Interaction
- Lanczos Strength Function
- Astrophysical Applications

Nucleus as a many body problem

• Nucleus is made of quarks interacting by exchange of gluons. We need to solve Quantum Chromodinamics.

Nucleus as a many body problem

- Nucleus is made of quarks interacting by exchange of gluons. We need to solve Quantum Chromodinamics.
- Nucleus is made of nucleons (neutrons and protons) that interact by meson exchange. Interaction could be described by a non-relativistic potential.

Nucleus as a many body problem

- Nucleus is made of quarks interacting by exchange of gluons. We need to solve Quantum Chromodinamics.
- Nucleus is made of nucleons (neutrons and protons) that interact by meson exchange. Interaction could be described by a non-relativistic potential.

We need to solve the Schrödinger equation:

$$H\Psi = E\Psi$$

$$\boldsymbol{H} = \sum_{i=1}^{A} \frac{\boldsymbol{p}_{i}}{2m} + \sum_{i < j=1}^{A} V_{ij} + \sum_{i < j < k=1}^{A} V_{ijk}$$

Basic symmetries

• Invariance under translations. Potential depends only on relative coordinates.

Basic symmetries

- Invariance under translations. Potential depends only on relative coordinates.
- Invariance under rotations (space, spin, isospin).
 - \succ States are eigenstates of total angular momentum (J=L+S) and isospin.
 - > Tensor operators (multipole operators).

$$[J_{\pm}, T_q^k] = \hbar \sqrt{k(k+1) - q(q \pm 1)} T_{q+1}^k$$
$$[J_0, T_q^k] = \hbar q$$

Basic symmetries

- Invariance under translations. Potential depends only on relative coordinates.
- Invariance under rotations (space, spin, isospin).
 - \succ States are eigenstates of total angular momentum (J=L+S) and isospin.
 - > Tensor operators (multipole operators).

$$[J_{\pm}, T_q^k] = \hbar \sqrt{k(k+1) - q(q \pm 1)} T_{q+1}^k$$
$$[J_0, T_q^k] = \hbar q$$

• invariance under parity and time reversal

Example of Potential

Potential consistent with two-nucleon scattering data and deuteron structure Potential AV8':

$$V(r) = V_c(r) + V_{\tau}(r)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + V_{\sigma}(r)(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) + V_{\sigma\tau}(r)(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + V_t(r)S_{12} + V_{t\tau}(r)S_{12}(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + V_b(\boldsymbol{L} \cdot \boldsymbol{S}) + V_{b\tau}(r)(\boldsymbol{L} \cdot \boldsymbol{S})(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)$$

Solution only possible for light systems

Benchmark test calculations for ⁴He

[H. Kamada, et al., Phys. Rev. C 64, 044001 (2001)]

$E_{\rm exp} = 28.296~{\rm MeV}$

TABLE I. The expectation values $\langle T \rangle$ and $\langle V \rangle$ of kinetic and potential energies, the binding energies E_b in MeV, and the radius in fm.

Method	$\langle T \rangle$	$\langle V \rangle$	E_b	$\sqrt{\langle r^2 \rangle}$
FY	102.39(5)	-128.33(10)	-25.94(5)	1.485(3)
CRCGV	102.30	-128.20	-25.90	1.482
SVM	102.35	-128.27	-25.92	1.486
HH	102.44	-128.34	-25.90(1)	1.483
GFMC	102.3(1.0)	-128.25(1.0)	-25.93(2)	1.490(5)
NCSM	103.35	-129.45	-25.80(20)	1.485
EIHH	100.8(9)	-126.7(9)	-25.944(10)	1.486

TABLE II. Expectation values of the eight potential operators in Eq. (24) in MeV.

Method	$\langle V_c \rangle$	$\langle V_{\tau} \rangle$	$\langle V_\sigma \rangle$	$\langle V_{\sigma\tau} \rangle$
FY	16.54	-5.038	-9.217	-57.55
CRCGV	16.54	-5.035	-9.215	-57.51
SVM	16.54	-5.036	-9.213	-57.51
HH	16.57	-5.034	-9.255	-57.59
GFMC	16.5(5)	-5.03(6)	-9.21(7)	-57.3(5)
NCSM	16.16	-4.92	-9.77	-57.89
Method	$\langle V_t \rangle$	$\langle V_{t\tau} \rangle$	$\langle V_b \rangle$	$\langle V_{b\tau} \rangle$
FY	0.707	-69.06	10.79	-15.50
CRCGV	0.708	-68.99	10.60	-15.30
SVM	0.707	-69.03	10.78	-15.49
HH	0.702	-69.03	10.76	-15.46
GFMC	0.71(3)	-68.8(5)	10.62(15)	-15.40(15)
NCSM	0.68	-69.13	11.23	-15.80

GFMC calculations for light nuclei



Theoretical models



Shell-Model basics

- Shell-Model assumes the existence of shells. Magic numbers are obtained when a shell is completely fill.
- Shells results from the bunching (grouping) of levels coming from a independent particle average potential.

Independent-Particle Model

• Assume the existence of some single-particle wave functions that are the solution of a Schrödinger equation

$$\boldsymbol{h}\phi(r) = \{\boldsymbol{T} + \boldsymbol{U}\}\phi_a(r)\} = \varepsilon_a\phi_a(r)$$

The independent-particle motion hamiltonian is then:

$$\boldsymbol{H}_0 = \sum_{k=1}^{A} \boldsymbol{T}(k) + U(r_k)$$

Eigenfunctions are the product of single-particle wave functions:

$$\Phi_{a_1 a_2 \dots a_A}(1, 2, \dots, A) = \prod_{k=1}^A \phi_{a_k}(r_k)$$

System identical particles

Wave function should be antisymmetric. For two particles:

$$\Phi_{ab}(1,2) = \frac{1}{\sqrt{2}} [\phi_a(1)\phi_b(2) - \phi_a(2)\phi_b(1)] = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_a(1) & \phi_b(2) \\ \phi_a(2) & \phi_b(1) \end{vmatrix}$$

A-particle Wave function:

$$\Phi_{a_1a_2...a_A}(1,2,...,A) = \sqrt{\frac{1}{A!}} \begin{vmatrix} \phi_{a_1}(r(1)) & \phi_{a_1}(r(2)) & \cdots & \phi_{a_1}(r(A)) \\ \phi_{a_2}(r(1)) & \phi_{a_2}(r(2)) & \cdots & \phi_{a_2}(r(A)) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{a_A}(r(1)) & \phi_{a_A}(r(2)) & \cdots & \phi_{a_A}(r(A)) \end{vmatrix}$$

Simple single-particle potential

Empirical construction based in an harmonic oscillator potential plus a spin-orbit term to reproduce the magic numbers (M. Goeppert-Mayer and H. Jensen)

$$\boldsymbol{U}(r) = \frac{1}{2}m\omega^2 r^2 + D\boldsymbol{l}^2 + \boldsymbol{l} \cdot \boldsymbol{s}$$

$$\varepsilon_{nlj} = \hbar\omega[2(n-1)+l+3/2)] + Dl(l+1) + C \begin{cases} l+1 & j=l-1/2\\ -l & j=l+1/2 \end{cases}$$

$$\hbar\omega = \frac{41}{A^{1/3}} \,\mathrm{MeV}$$

Spherical mean-field



Solution to the many-nucleon problem

$$\boldsymbol{H}\Psi(1,2,\ldots,A) = \left[\sum_{k=1}^{A} T(k) + \sum_{k$$

Hamiltonian rewritted:

$$\boldsymbol{H} = \sum_{k=1}^{A} [T(k) + U(k)] + \left[\sum_{k$$

Hartree-Fock theory provides method to derive single-particle potential. The criterium is to search for the "best" A-particle slater determinant such us the value of H is minimum. Next, one assumes that the resulting residual interaction is small and that:

$$\Psi(1, 2, \dots, A) = \Phi_{a_1 a_2 \dots a_A}(1, 2, \dots, A)$$

Validity shell structure



A. deWitt Huberts, Rev. mod. Phys. 69, 981 (1997)



Limits of the IPM



Limits of the IPM



Limits of the IPM

Example ¹⁶0



Two-particle wave function

Let's consider the possible isospin values for two nucleons:

$$|T = 1, T_z = 1\rangle = |n\rangle|n\rangle, \quad |1, -1\rangle = |p\rangle|p\rangle$$
$$|1, 0\rangle = \frac{1}{\sqrt{2}} [|n\rangle|p\rangle + |p\rangle|n\rangle] \qquad q$$
$$|0, 0\rangle = \frac{1}{\sqrt{2}} [|n\rangle|p\rangle - |p\rangle|n\rangle]$$

N-particle system: T = odd (symmetric), T = even (antisymmetric).

We can also couple the angular momentum:

$$|JM\rangle = \sum_{m_1m_2} \langle j_1m_1j_2m_2|JM\rangle |j_1m_1\rangle |j_2m_2\rangle$$

In N = Z nuclei protons and neutrons occupy the same orbits. Low lying states fulfill (J + T = odd number).

Example ⁶Li

posible two-particle states $(j_1 j_2)^{JT}$

$$(p_{3/2}p_{3/2})^{J=1,3,5;T=0}, \quad (p_{3/2}p_{3/2})^{J=2,4,6;T=1} (p_{3/2}p_{1/2})^{J=1,2;T=0} \quad (p_{3/2}p_{1/2})^{J=1,2;T=1} (p_{1/2}p_{1/2})^{J=1;T=0} \quad (p_{1/2}p_{1/2})^{J=0;T=1}$$



10th Euro Summer School on Exotic Beams

Correlations (residual interaction)

In order to incorporate the correlations, one has to go beyond mean-field



Possible solution

• Take the basics formed by the A-particle Slater determinants:

$$\Phi_a = \Phi_{a_1 a_2 \dots a_A}(1, 2, \dots, A)$$

Possible solution

• Take the basics formed by the A-particle Slater determinants:

$$\Phi_a = \Phi_{a_1 a_2 \dots a_A}(1, 2, \dots, A)$$

• build the (infinite) matrix:

 $\langle \Phi_b | oldsymbol{H} | \Phi_a
angle$

Possible solution

• Take the basics formed by the A-particle Slater determinants:

$$\Phi_a = \Phi_{a_1 a_2 \dots a_A}(1, 2, \dots, A)$$

• build the (infinite) matrix:

 $\langle \Phi_b | oldsymbol{H} | \Phi_a
angle$

• diagonalize

Shell-Model approximation

The space of orbits generated by the mean-field potential are grouped in three blocks

- Inner core: orbits that are always full.
- Valence space: orbits that contain the physical degrees of freedom relevant to a given property. The distribution of the valence particles among these orbitals is governed by the interaction.
- External space: all the remaining orbits that are always empty.



Shell-Model approximation

The exact solution on the infinite Hilbert space spanned by the mean field orbits is approximated in the large scale shell-model calculation by the solution of the Schrödinger equation in the valence space using an effective interaction.

$$H\Psi = E\Psi \rightarrow H_{\text{eff}}\Psi_{\text{eff}} = E\Psi_{\text{eff}}$$

In general, effective operators have to be introduced to account for the restrictions of the Hilbert space

$$\langle \Psi | oldsymbol{O} | \Psi
angle = \langle \Psi_{ ext{eff}} | oldsymbol{O}_{ ext{eff}} | \Psi_{ ext{eff}}
angle$$

Shell-Model calculation

A shell model calculation needs the following ingredients:

• A valence space

Shell-Model calculation

A shell model calculation needs the following ingredients:

- A valence space
- An effective interaction

Shell-Model calculation

A shell model calculation needs the following ingredients:

- A valence space
- An effective interaction
- A code to build and diagonalize the hamiltonian matrix.

The choice of the valence space:

• In light nuclei the <u>harmonic oscillator</u> closures determine the natural valence spaces.



• In heavier nuclei:

 $\longrightarrow jj$ closures due to the spin-orbit term show up

N=28, 50, 82, 126

- In heavier nuclei: $\longrightarrow jj$ closures due to the spin-orbit term show up N=28, 50, 82, 126
- the transition $HO \longrightarrow jj$: occurs between 40 Ca and 100 Sn where the protagonism shifts from the $1f_{7/2}$ to the $1g_{9/2}$

- In heavier nuclei: $\longrightarrow jj$ closures due to the spin-orbit term show up N=28, 50, 82, 126
- the transition $HO \longrightarrow jj$: occurs between 40 Ca and 100 Sn where the protagonism shifts from the $1f_{7/2}$ to the $1g_{9/2}$
- A valence space can be adequate to describe some properties and completely wrong for others

^{48}Cr	$(f_{\frac{7}{2}})^8$	$(f_{\frac{7}{2}}p_{\frac{3}{2}})^8$	$(fp)^8$
Q(2 $^+$) (e.fm 2)	0.0	-23.3	-23.8
E(2 ⁺) (M <i>e</i> V)	0.63	0.44	0.80
E(4 ⁺)/E(2 ⁺)	1.94	2.52	2.26
BE2(2 $^+ ightarrow$ 0 $^+$) (e 2 .fm 4)	77	150	216
B(GT)	0.90	0.95	3.88
Second quantization

• Creation and destruction operators:

$$a_k^{\dagger}|0\rangle = |k\rangle, \qquad a_k|k\rangle = |0\rangle$$

vacuum $|0\rangle$, such $a_k|0\rangle$ $\forall k.$ For fermions antisymmetry given by anti-commutation rules

$$\{a_i^{\dagger}, a_j^{\dagger}\} = \{a_i, a_j\} = 0, \qquad \{a_i^{\dagger}, a_j\} = \delta_{ij}$$

• Slater determinant:

$$\Phi_{\alpha_1\alpha_2\dots\alpha_A}(1,2,\dots,A) = a^{\dagger}_{\alpha_A}\cdots a^{\dagger}_{\alpha_2}a^{\dagger}_{\alpha_1}|0\rangle$$

Second quantization

• One body operators:

$$\mathcal{O} = \sum_{k=1}^{A} \mathbf{O}(k) \to \mathcal{O} = \sum_{\alpha\beta} \langle \alpha | \mathbf{O} | \beta \rangle a_{\alpha}^{\dagger} a_{\beta}$$

number of particles $N=\sum_{\alpha}n_{\alpha}=\sum_{\alpha}a_{\alpha}^{\dagger}a_{\alpha}$

• Two-body operators:

$$\mathcal{O} = \sum_{i < j=1}^{A} \boldsymbol{O}(i,j) \to \mathcal{O} = \sum_{\alpha \beta \gamma \delta} \langle \alpha \beta | \boldsymbol{O} | \gamma \delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}$$

The interaction in second quantization

$$\boldsymbol{H} = \sum_{\alpha} \varepsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} = \boldsymbol{H}_{0} + \boldsymbol{V}_{\text{res}}$$

The interaction in second quantization

In general it is convenient to work in a couple basis: Defining $\tilde{a}_{jm} = (-1)^{j+m} a_{j-m}$, and the coupling:

$$[a_{j_1}^{\dagger}a_{j_2}^{\dagger}]_M^J = \sum_{m_1m_2} \langle j_1m_1j_2m_2 | JM \rangle a_{j_1m_1}^{\dagger}a_{j_2m_2}^{\dagger}$$

$$\mathbf{H} = \sum_{\alpha} \varepsilon_{\alpha} n_{\alpha} - \frac{1}{4} \sum_{j_{1} j_{2} j_{3} j_{4} JT} \langle j_{1} j_{2} | V | j_{3} j_{4} \rangle^{JT} \\
 \sqrt{(2J+1)(2T+1)(1+\delta_{12})(1+\delta_{23})} \\
 \left[[a_{j_{1}}^{\dagger} a_{j_{2}}^{\dagger}]^{JT} \times [\tilde{a}_{j_{3}} \tilde{a} j_{4}]^{JT} \right]^{00}$$

The shell-model interaction

All the information needed for a shell-model calculation are the independent particle energies (ε_{α}) and the two-body matrix elements $\langle j_1 j_2; JT | V | j_3 j_4; JT \rangle$ Example USD interaction ($d_{5/2}, s_{1/2}, d_{3/2}$)

```
USD
   3 205
         1001 203
  -3.94780 -3.16354 1.64658
  0 205 205 205 205 0
                              5
  0.0000 -1.6321 0.0000 -1.5012
                                  0.0000 - 4.2256
 -2.8197
         0.0000 -1.0020 0.0000 -0.1641 0.0000
     205 1001 205 1001
                         2
                              3
  \left( \right)
 -1.4474 -3.8598
 -0.8183
         0.7626
     205 203 205 203
                         1
  0
                              4
 -6.5058 -3.8253 -0.5377 -4.5062
  1.0334 -0.3248 0.5894 -1.4497
  0 1001 1001 1001 1001 0 1
  0.0000 -3.2628
 -2.1246 0.0000
  0 1001 203 1001
                   203
                      1
                              2
 -4.2930
         -1.8194
  0.6066
         -0.4064
     203
         203 203 203
                         0
  \cap
                              3
  0.0000
         -1.4151 0.0000 -2.8842
 -2.1845
         0.0000 -0.0665 0.0000
```

10th Euro Summer School on Exotic Beams

Application

Spectrum of 0^+ states in $^{\rm 18}{\rm O}$

we build a 3×3 matrix:





Large scale Shell-Model basis and codes

pf-shell valence space: $1f_{7/2}, 2p_{3/2}, 2p_{1/2}, 1f_{5/2}$

nucleus	m-scheme	jj-scheme
	(ANTOINE)	(NATHAN)
48 Cr	1,963,461	41,355
54 Fe	345,400,174	5,220,621
56 Fe	501,113,392	7,413,488
56 Ni	1,087,455,228	15,443,684

Impossible to store Hamiltonian matrix! Still possible to compute $oldsymbol{H}\Psi$. Diagonalization using an iterative algorithm.

Shell-Model code ANTOINE

http://sbgat194.in2p3.fr/~theory/antoine/



Lanczos algorithm

Construction of a orthonormal basis: Initial vector $|\mathbf{1}\rangle.$

$$E_{12}|\mathbf{2}\rangle = (\mathbf{H} - E_{11})|\mathbf{1}\rangle$$

$$E_{23}|\mathbf{3}\rangle = (\mathbf{H} - E_{22})|\mathbf{2}\rangle - E_{12}|\mathbf{1}\rangle$$

...

$$E_{NN+1}|\mathbf{N} + \mathbf{1}\rangle = (\mathbf{H} - E_{NN})|\mathbf{N}\rangle - E_{N-1N}|\mathbf{N} - \mathbf{1}\rangle$$

where

$$E_{NN} = \langle \mathbf{N} | \boldsymbol{H} | \mathbf{N} \rangle, \qquad E_{NN+1} = E_{N+1N}$$

Lanczos algorithm

$$\begin{pmatrix} E_{11} & E_{12} & 0 & 0 & \dots & 0 \\ E_{12} & E_{22} & E_{23} & 0 & \dots & 0 \\ 0 & E_{23} & E_{33} & E_{34} & \dots & 0 \end{pmatrix}$$

- Diagonalize and obtain an approximation to the energy and wave function.
- Do a few more iterations
- Diagonalize again and check that $\Delta E = E_{N+k} E_N < \epsilon$

Lanczos convergence

RANDOM STARTING VECTOR

З					
S C	-6.345165	11.335118	29.120687		
0	-21.344259	-7.802025	4.637278	16.927858	29.308309
9	-30.092574	-19.653950	-9.343311	0.467972	10.265731
12	-32.722076	-24.462806	-17.104890	-9.353111	-1.628857
15	-32.930624	-26.709841	-22.335011	-15.957805	-9.401645
18	-32.952147	-28.028244	-24.233122	-19.625844	-14.772679
21	-32.953570	-28.413699	-25.350732	-22.676041	-18.180356
24	-32.953655	-28.537584	-26.244093	-23.883982	-20.534298
27	-32.953658	-28.559930	-26.542899	-24.362551	-22.197866
30	-32.953658	-28.563001	-26.646165	-24.887184	-23.559799
33	-32.953658	-28.564277	-26.912739	-26.199181	-24.299165
36	-32.953658	-28.564535	-27.102898	-26.382496	-24.409357
39	-32 953658	-28 564567	-27 148522	-26 416873	-24 529055
42	-32 953658	-28 564570	-27 156735	-26 /25250	-24 724078
45	22.052650	20.504570	27.150755	20.423230	24.724070
48	-32.953658	-28.564570	-27.158085	-26.42/319	-24.910915
	-32.953658	-28.564570	-27.158371	-26.428021	-25.107898

Lanczos convergence





Isospin symmetry

Nuclear spectra are almost unchanged under the exchange of neutrons and protons.



Isospin representation

Neutron and proton are considered different states of the same particle: the nucleon

$$|n\rangle = \begin{pmatrix} 1\\ 0 \end{pmatrix}, \qquad |p\rangle = \begin{pmatrix} 0\\ 1 \end{pmatrix}$$

Isospin operators:

$$oldsymbol{t} = rac{1}{2}oldsymbol{ au}, oldsymbol{t}_{\pm} = oldsymbol{t}_1 \pm oldsymbol{t}_2$$
 ,

$$\boldsymbol{\tau}_1 = \left(egin{array}{cc} 0 & 1 \ 1 & 0 \end{array}
ight), \quad \boldsymbol{\tau}_2 = \left(egin{array}{cc} 0 & -i \ i & 0 \end{array}
ight), \quad \boldsymbol{\tau}_3 = \left(egin{array}{cc} 1 & 0 \ 0 & -1 \end{array}
ight)$$

States are eigenstates of total isospin ($m{T} = \sum_{i=1}^A t^i$)

$$T^2 = T(T+1)|T, T_z\rangle, \qquad T_z|T, T_z\rangle$$

$$T \ge T_z = \frac{|N - Z|}{2}$$

	Exp.	KB	KLS	Bonn A	Bonn B	Bonn C
		${f 2}_1^+$ excita	ation ener	ſду		
44 Ca	1.16	1.45	1.43	1.31	1.25	1.26
46 Ca	1.35	1.45	1.42	1.26	1.22	1.23
48 Ca	3.83	1.80	1.60	1.23	1.30	1.41
50 Ca	1.03	1.41	1.35	1.27	1.10	1.17
$\langle (f_{7/2})^8 \Psi_{GS} \rangle$		0.468	0.381	0.214	0.345	0.437

	Exp.	KB	KLS	Bonn A	Bonn B	Bonn C	
		2 $_1^+$ excita	ation ener	ду			
44 Ca	1.16	1.45	1.43	1.31	1.25	1.26	
46 Ca	1.35	1.45	1.42	1.26	1.22	1.23	
48 Ca	3.83	1.80	1.60	1.23	1.30	1.41	
50 Ca	1.03	1.41	1.35	1.27	1.10	1.17	
$\langle (f_{7/2})^8 \Psi_{GS} \rangle$		0.468	0.381	0.214	0.345	0.437	
56 Ni model space (f $_{\frac{7}{2}}$ p $_{\frac{3}{2}}$) 16							
⁵⁶ Ni	2.70	0.39	0.31	0.43	0.42	0.42	
$\langle (f_{\frac{7}{2}})^{16} \Psi_{GS} \rangle$	$\langle \rangle$	0.04	0.015	0.018	0.011	0.019	
$\langle n_{p_{3/2}} angle$		4.5	5.2	5.7	5.2	5.0	

	Exp.	KB	KLS	Bonn A	Bonn B	Bonn C
	•	2_1^+ excita	ation ener	ЗЛ		
44 Ca	1.16	1.45	1.43	1.31	1.25	1.26
46 Ca	1.35	1.45	1.42	1.26	1.22	1.23
48 Ca	3.83	1.80	1.60	1.23	1.30	1.41
50 Ca	1.03	1.41	1.35	1.27	1.10	1.17
$\langle (f_{7/2})^8 \Psi_{GS} \rangle$		0.468	0.381	0.214	0.345	0.437
	⁵⁶ N	Ni model e	pace (f $\frac{7}{2}$	$p_{\frac{3}{2}})^{16}$		
⁵⁶ Ni	2.70	0.39	0.31	0.43	0.42	0.42
$\langle (f_{\frac{7}{2}})^{16} \Psi_{GS} \rangle$	\rangle	0.04	0.015	0.018	0.011	0.019
$\langle n_{p_{3/2}} angle$		4.5	5.2	5.7	5.2	5.0

The realistic interactions do not reproduce the shell closure $N \mbox{ or } Z{=}28$

	-			-				
	Exp.	KB	KLS	Bonn A	Bonn B	Bonn C		
		2^+_1 excita	ation ener	Зλ				
44 Ca	1.16	1.45	1.43	1.31	1.25	1.26		
46 Ca	1.35	1.45	1.42	1.26	1.22	1.23		
48 Ca	3.83	1.80	1.60	1.23	1.30	1.41		
50 Ca	1.03	1.41	1.35	1.27	1.10	1.17		
$\langle (f_{7/2})^8 \Psi_{GS} \rangle$		0.468	0.381	0.214	0.345	0.437		
	⁵⁶ Ni model space $(f_{\frac{7}{2}}p_{\frac{3}{2}})^{16}$							
⁵⁶ Ni	2.70	0.39	0.31	0.43	0.42	0.42		
$\langle (f_{\frac{7}{2}})^{16} \Psi_{GS} \rangle$	\rangle	0.04	0.015	0.018	0.011	0.019		
$\langle n_{p_{3/2}} angle$		4.5	5.2	5.7	5.2	5.0		

The realistic interactions do not reproduce the shell closure $N \mbox{ or } Z{=}28$

Why?

The structure of the Hamiltonian

From the work of M. Dufour and A. Zuker (PRC 54 1996 1641) Separation theorem:

Any effective interaction can be split in two parts:

 $H = H_m(monopole) + H_M(multipole)$

 H_m contains all the terms that are affected by a spherical Hartree-Fock variatition, hence reponsible of the global saturation properties and of the evolution of the spherical single particle field. Important property:

 $\langle CS \pm 1 | \boldsymbol{H} | CS \pm 1 \rangle = \langle CS \pm 1 | \boldsymbol{H}_m | CS \pm 1 \rangle$

The structure of the Hamiltonian

For all the realistic G-matrices,

- $oldsymbol{H}_m$ is not accurate enough.
- $oldsymbol{H}_M$ is almost the same.

The monopole part has to be empirically corrected to reproduce the structure of the "simple" nuclei $|CS\pm1\rangle$

Multipole Hamiltonian

Can be characterized as the sum of simple terms:

- L = 0 isovector and isoscalar pairing
- Elliot's quadrupole-quadrupole force.
- $(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)$
- Octupole and hexadecapole terms $r^{\lambda}Y_{\lambda}\cdot r^{\lambda}Y_{\lambda}$

All the interactions contains similar terms:

Interaction	JT = 01	JT = 10	$\lambda \tau = 20$	$\lambda \tau = 40$	$\lambda \tau = 11$
KB3	-4.75	-4.46	-2.79	-1.39	+2.46
FPD6	-5.06	-5.08	-3.11	-1.67	+3.17
GOGNY	-4.07	-5.74	-3.23	-1.77	+2.46

 H_m contains terms that depend in n and T. Assume that we have a constant potential and single particle energy:

$$E = n\varepsilon + \frac{n(n-1)}{2}V$$

If we consider also isospin:

$$E = n\varepsilon + \frac{n(n-1)}{2}V + bT(T+1)$$

In general we have different orbits each with different average interactions:

$$E = \sum_{i} n_i \varepsilon_i + \sum_{i} \frac{n_i (n_i - 1)}{2} V_{ii} + \sum_{i \neq j} n_i n_j V_{ij}$$

If we consider also the fact that we have isospin:

$$\boldsymbol{H}_{m} = \sum_{i} \varepsilon_{i} \boldsymbol{n}_{i} + \sum_{ij} \left[\frac{1}{1 + \delta_{ij}} a_{ij} \boldsymbol{n}_{i} (\boldsymbol{n}_{j} - \delta_{ij}) + \frac{1}{1 + \delta_{ij}} b_{ij} \left(\boldsymbol{T}_{i} \cdot \boldsymbol{T}_{j} - \frac{3\boldsymbol{n}_{i}}{4} \delta_{ij} \right) \right)$$

Where a and b are defined from the centroids (average interaction):

$$V_{ij}^{T} = \frac{\sum_{J} (2J+1) W_{ijij}^{JT}}{\sum_{J} (2J+1)}$$
$$a_{ij} = \frac{3V_{ij}^{1} + V_{ij}^{0}}{4}, \qquad b_{ij} = V_{ij}^{1} - V_{ij}^{0}$$

Influence of monopole hamiltonian

The evolution of effective spherical single particle energies with the number of particles in the valence space can be extracted from H_m . In the case of identical particles the expression is:

$$\varepsilon_j(n) = \varepsilon_j(n=1) + \sum_i V_{ij} n_i$$

The monopole hamiltonian $oldsymbol{H}_m$ also governs the relative position of the various T-values in the same nucleus, via the terms:

$$b_{ij} T_i \cdot T_j$$

Even small defects in the centroids can produce large changes in the relative position of the different configurations due to the appearance of quadratic terms involving the number of particles in the different orbits

Effect of monopole corrections



Evolution SPE



Figure 3. Comparison of bare single-particle energies (ε) and effective single-particle energies ($\varepsilon + H_m$) of ⁵⁶Ni. Far right column shows experimental energy levels of ⁵⁷Ni and the shell-gap evaluated by using the binding energies: $\Delta = 2BE({}^{56}\text{Ni}) - BE({}^{57}\text{Ni}) - BE({}^{55}\text{Ni})$. Data are taken from ref. [16]

Limits of IPM



Limits of IPM



Limits of IPM

Example ¹⁶0



Monopole explanation



$$E_{0ph} = 12\varepsilon_p + \frac{12 \cdot 11}{2} V_{pp}$$

$$E_{1ph} = 11\varepsilon_p + \varepsilon_r + 55V_{pp} + 11V_{pr}$$

$$E_{2ph} = 10\varepsilon_p + 2\varepsilon_r + 45V_{pp} + 20V_{pr} + V_{rr}$$

$$E_{4ph} = 8\varepsilon_p + 4\varepsilon_r + 28V_{pp} + 32V_{pr} + 6V_{rr}$$

Monopole explanation



$$\Delta_{1\text{ph}} = \varepsilon_r - \varepsilon_p + 11(V_{pr} - V_{pp})$$

$$\Delta_{2\text{ph}} = 2(\varepsilon_r - \varepsilon_p) + V_{pp} + 20(V_{pr} - V_{pp}) + (V_{rr} - V_{pp})$$

$$\Delta_{4\text{ph}} = 4(\varepsilon_r - \varepsilon_p) + 32(V_{pr} - V_{pp}) + 6(V_{rr} - V_{pp})$$

Evolution SPE far off stability

Given H_m , the effective single particle energies [from Otsuka et al, Phys. Rev. Lett. 87, 82502 (2001)],



Evolution SPE far off stability

N=20



10th Euro Summer School on Exotic Beams

Vanishing of shell closure at N=20



10th Euro Summer School on Exotic Beams
Computation of transition operators

Given a one-body transition operator \mathcal{O} , how do we compute

 $\langle \Psi_f | \mathcal{O} | \Psi_i \rangle$

here Ψ_i and Ψ_f are many-body wave functions obtained from shell-model diagonalization

• One body operators:

$$\mathcal{O} = \sum_{i=1}^{A} o(r(i)) \longrightarrow \mathcal{O} = \sum_{i,j} \langle i | \mathbf{O} | j \rangle a_i^{\dagger} a_j$$

- We need to know
 - \succ the value of our one body operator between single particle wave functions $\langle i|{\cal O}|j\rangle$
 - \succ the one body density matrix elements $\langle \Psi_f | a_i^\dagger a_j | \Psi_i
 angle$

Computation of transition operators

• for $\langle i|O|j\rangle$, one needs (eventually) to know the radial part of the wave function: usually harmonic oscillator, sometimes wood-saxon.

$$\langle i | \boldsymbol{O} | j \rangle = \int d^3 r \; \phi_i^*(\boldsymbol{r}) \boldsymbol{O}(\boldsymbol{r}) \phi_j(\boldsymbol{r})$$

for the one body density matrix elements (same procedure as for the hamiltonian):

$$a_5^{\dagger}a_2|001011\rangle = |011001\rangle$$

now we know the procedure to compute:

- EL transitions: $r^L Y_{L0}$
- β decay :
 - \succ Fermi decay : τ_{\pm}
 - \succ Gamow-Teller decay: $\sigma \tau_{\pm}$

Example calculation

 β decay half-life calculation

- Determine initial state $|\Psi_i\rangle$.
- Determine all posible final states $|\Psi_f
 angle$.
- Compute <u>matrix elements</u> $\langle \Psi_f | {oldsymbol O} | \Psi_i
 angle$

$$\lambda_f = \frac{\ln 2}{K} f(Z, W_0^f) [B_f(F) + B_f(GT)]$$

• Determine total decay rate:

$$\lambda = \frac{\ln 2}{T_{1/2}} = \sum_{f} \lambda_f$$

- $|\Psi
 angle$ ground state given nucleus.
- Sum rule state (or doorway): $|\Omega
 angle=\mathbf{\Omega}|\Psi
 angle.$
- Total sum rule (sum over all final states of the matrix element squared) is the norm of state $|\Omega\rangle$:

$$\langle \Omega | \Omega \rangle = \langle \Psi | \mathbf{\Omega}^{\dagger} \mathbf{\Omega} | \Psi \rangle = \sum_{i} | \langle i | \mathbf{\Omega} | \Psi \rangle |^{2}$$

• We can think of the state $|\Omega\rangle$ as a (probability) distribution over the eigenvalues $|i\rangle$ of H with values $|\langle i|\Omega\rangle|^2 = |\langle i|\Omega|\Psi\rangle|^2$

Any distribution can be characterized by the moments of the distribution.

$$\bar{E} = \langle \Omega | \boldsymbol{H} | \Omega \rangle = \sum_{i} E_{i} |\langle i | \boldsymbol{\Omega} | \Psi \rangle|^{2}$$
$$m_{n} = \langle \Omega | (\boldsymbol{H} - \bar{E})^{n} | \Omega \rangle = \sum_{i} (E_{i} - \bar{E})^{n} |\langle i | \boldsymbol{\Omega} | \Psi \rangle|^{2}$$

Gaussian distribution characterized by two moments ($\bar{E}, \sigma^2 = m_2$) $g(E) = \frac{1}{\sigma\sqrt{2\pi}} \exp(-\frac{(E-\bar{E})^2}{2\sigma^2})$



In general we only need a finite number of momenta. We can define a basis of $|\alpha\rangle$ states.

$$m_n = \langle \Omega | (\boldsymbol{H} - \bar{E})^n | \Omega \rangle = \sum_{\alpha}^N (E_\alpha - \bar{E})^n | \langle \alpha | \boldsymbol{\Omega} | \Psi \rangle |^2 \quad (\forall n \le M)$$

$$E_{\alpha} \approx \langle \alpha | \boldsymbol{H} | \alpha \rangle$$

With N states we can reproduce 2N moments of the distribution.

Example: Beta half-life

$$\lambda \sim \sum_{i} f(Z, W_0^i) |\langle i | \mathbf{\Omega} | \Psi \rangle|^2$$
$$f(Z, W_0^i) \approx \int_1^{W_0^i} W^2 (W_0^i - 1)^2 dW \approx \frac{(W_0^i)^5}{30}$$

Lanczos method provides a natural way of determining the basis $|\alpha\rangle.$

Initial vector $|\mathbf{1}
angle=rac{|\Omega
angle}{\sqrt{\langle\Omega|\Omega
angle}}.$

$$E_{12}|\mathbf{2}\rangle = (\mathbf{H} - E_{11})|\mathbf{1}\rangle$$

$$E_{23}|\mathbf{3}\rangle = (\mathbf{H} - E_{22})|\mathbf{2}\rangle - E_{12}|\mathbf{1}\rangle$$

...

$$E_{NN+1}|\mathbf{N} + \mathbf{1}\rangle = (\mathbf{H} - E_{NN})|\mathbf{N}\rangle$$

$$-E_{N-1N}|\mathbf{N} - \mathbf{1}\rangle$$

Each Lanczos iteration gives information about two new moments of the distribution.

$$E_{11} = \langle \mathbf{1} | \mathbf{H} | \mathbf{1} \rangle = \bar{E}$$

$$E_{12}^2 = \langle \Omega | (\mathbf{H} - E_{11})^2 | \Omega \rangle = m_2$$

$$E_{22} = \frac{m_3}{m_2} + \bar{E}$$

$$E_{23}^2 = \frac{m_4}{m_2} - \frac{m_3^2}{m_2^2} - m_2$$

where $E_{NN} = \langle \mathbf{N} | \boldsymbol{H} | \mathbf{N} \rangle, \quad E_{NN+1} = E_{N+1N}$

Diagonalizing Lanczos matrix after N iterations gives an approximation to the distribution with the same lowest 2N moments.



















GT Strength on $^{\rm 48}{\rm Sc}$



GT Strength on $^{\rm 48}{\rm Sc}$



$$B(F) = \frac{1}{2J_i + 1} \sum_{M_i, M_f} |\langle J_f M_f; T_f T_{z_f}| \sum_{k=1}^A \boldsymbol{t}_{\pm}^k |J_i M_i; T_i T_{z_i}\rangle|^2$$

 $B(F) = [T_i(T_i + 1) - T_{z_i}(T_{z_i} \pm 1)]\delta_{J_i, J_f}\delta_{T_i, T_f}\delta_{T_{z_f}, T_{z_i} \pm 1}$

$$B(F) = \frac{1}{2J_i + 1} \sum_{M_i, M_f} |\langle J_f M_f; T_f T_{z_f}| \sum_{k=1}^A \boldsymbol{t}_{\pm}^k |J_i M_i; T_i T_{z_i}\rangle|^2$$

$$B(F) = [T_i(T_i + 1) - T_{z_i}(T_{z_i} \pm 1)]\delta_{J_i, J_f}\delta_{T_i, T_f}\delta_{T_{z_f}, T_{z_i} \pm 1}$$

Energetics:

$$E_{\text{IAS}} = Q_{\beta} + \text{sign}(T_{z_i})[E_C(Z+1) - E_C(Z) - (m_n - m_H)]$$

$$B(F) = \frac{1}{2J_i + 1} \sum_{M_i, M_f} |\langle J_f M_f; T_f T_{z_f}| \sum_{k=1}^A \boldsymbol{t}_{\pm}^k |J_i M_i; T_i T_{z_i}\rangle|^2$$

$$B(F) = [T_i(T_i + 1) - T_{z_i}(T_{z_i} \pm 1)]\delta_{J_i, J_f}\delta_{T_i, T_f}\delta_{T_{z_f}, T_{z_i} \pm 1}$$

Energetics:

$$E_{\text{IAS}} = Q_{\beta} + \text{sign}(T_{z_i})[E_C(Z+1) - E_C(Z) - (m_n - m_H)]$$

Selection rule:

$$\Delta J = 0 \qquad \Delta T = 0 \qquad \pi_i = \pi_f$$

$$B(F) = \frac{1}{2J_i + 1} \sum_{M_i, M_f} |\langle J_f M_f; T_f T_{z_f}| \sum_{k=1}^A \boldsymbol{t}_{\pm}^k |J_i M_i; T_i T_{z_i}\rangle|^2$$

$$B(F) = [T_i(T_i + 1) - T_{z_i}(T_{z_i} \pm 1)]\delta_{J_i, J_f}\delta_{T_i, T_f}\delta_{T_{z_f}, T_{z_i} \pm 1}$$

Energetics:

$$E_{\text{IAS}} = Q_{\beta} + \text{sign}(T_{z_i})[E_C(Z+1) - E_C(Z) - (m_n - m_H)]$$

Selection rule:

$$\Delta J = 0 \qquad \Delta T = 0 \qquad \pi_i = \pi_f$$

Sum rule (sum over all the final states):

$$S(F) = S_{-}(F) - S_{+}(F) = 2T_{z_{i}} = (N - Z)$$

Gamow-Teller matrix elements

back

$$B(GT) = \frac{g_A^2}{2J_i + 1} |\langle J_f; T_f T_{z_f}|| \sum_{k=1}^A \sigma^k t_{\pm}^k ||J_i; T_i T_{z_i}\rangle|^2$$

$$g_A = -1.2720 \pm 0.0018$$

Selection rule:

$$\Delta J = 0, 1 \text{ (no } J_i = 0 \to J_f = 0) \qquad \Delta T = 0, 1 \qquad \pi_i = \pi_f$$

Ikeda sum rule:

$$S(GT) = S_{-}(GT) - S_{+}(GT) = 3(N - Z)$$

SN1987A

Type II supernova in LMC (\sim 55 kpc)



- $E_{\rm grav} \approx 10^{53} \, {\rm erg}$
- $E_{\rm rad} \approx 8 \times 10^{49} \, {\rm erg}$
- $E_{\rm kin} \approx 10^{51} \, {\rm erg} = 1$ foe



 $E_{\nu} \approx 2.7 \times 10^{53} \text{ erg}$

Evolution Massive Stars

Evolution 20 solar mass star



10th Euro Summer School on Exotic Beams

Late stages core evolution



10th Euro Summer School on Exotic Beams

Semileptonic Weak Processes in Stars



 $O_{\rm F} \sim e^{i \boldsymbol{q} \boldsymbol{r}} \boldsymbol{\tau} \qquad O_{\rm GT} \sim e^{i \boldsymbol{q} \boldsymbol{r}} \boldsymbol{\sigma} \boldsymbol{\tau}$

Presupernova evolution



• T = 0.1-0.8 MeV, $\rho = 10^7-10^{10}$ g cm⁻³. Composition of iron group nuclei

(A = 45–65)

- Important processes:
 - \succ electron capture:

$$e^{-} + (N, Z) \to (N + 1, Z - 1) + \nu_e$$

- > β^- decay: $(N,Z) \rightarrow (N-1,Z+1) + e^- + \bar{\nu}_e$
- Dominated by allowed transitions (Fermi and Gamow-Teller)
- Evolution decreases number of electrons (Y_e) and Chandrasekar mass ($M_{\rm Ch} \approx 1.4(2Y_e)^2 \, {\rm M}_{\odot}$)
 - Fenomenological model (Fuller, Fowler, Newman, 1985)
 - Charge exchange reactions (n, p), $(d, {}^{2}\mathrm{He})$
 - Microscopic model (Shell-Model) (Langanke & Martínez-Pinedo, 2001)



GT in charge exchange reactions

GT strength could be measured in CE reactions:

- GT_{-} proved in (p, n), $({}^{3}He, t)$.
- GT_+ proved in (n, p), $(t, {}^{3}He)$, $(d, {}^{2}He)$.

Mathematical relationship ($E_p \ge 100$ MeV/nucleon):

$$\frac{d\sigma}{d\Omega dE}(0^\circ) \approx S(E_x)B(GT)$$

$$B(GT) = \left(\frac{g_A}{g_V}\right)^2 \frac{\langle f||\sum_k \boldsymbol{\sigma}^k \boldsymbol{t}_{\pm}^k||i\rangle^2}{2J_i + 1}$$

Ikeda sum rule:

$$S_{-} - S_{+} = 3(N - Z)$$

Independent Particle Model



Gamow-Teller strength

 GT_{+} strength measured in charge-exchange (n, p) experiments (TRIUMF).



10th Euro Summer School on Exotic Beams

GT_+ strength measured in $(d,^2He)$



High resolution Gamow-Teller distributions on ⁵¹V,⁵⁸Ni (⁶⁴Ni,...) measured at KVI (Groningen) by EuroSupernova Collaboration.



Shell-model (LMP) vs FFN rates



Most important nuclei

Most important nuclei to determine the electron capture rate



Collapse phase



Important processes:

• Neutrino transport (Boltzman equation): $\nu + A \rightleftharpoons \nu + A$ (trapping) $\nu + e^- \rightleftarrows \nu + e^-$ (thermalization) cross sections $\sim E_{\nu}^2$

• electron capture on protons: $e^- + p \rightleftharpoons n + \nu_e$

What is the role of electron capture on nuclei?

$$e^- + (N, Z) \rightleftharpoons (N+1, Z-1) + \nu_e$$

What is the role of inelastic neutrino-nucleus scattering?

$$\nu + A \rightleftarrows \nu + A^*$$
Collapse abundances



(Un)blocking electron capture at N=40





Weak Rates for nuclei with A=65– 112 computed using the Shell Model Monte Carlo plus RPA approach

Electron capture: nuclei vs protons



10th Euro Summer School on Exotic Beams

Reaction rates



Electron capture on nuclei dominates over capture on protons

Consequences

With Rampp & Janka (General Relativic model) 15 M_{\odot} presupernova model from A. Heger & S. Woosley



Consequences

With Hix, Liebendörfer, Mezzacappa, Messer (Newtonian Gravity)



Shock evolution



Neutrino interactions in the collapse



- Elastic scattering: $\nu + A \rightleftharpoons \nu + A$ (trapping)
- Absorption: $\nu_e + (N, Z) \rightleftharpoons e^- + (N-1, Z+1)$
- ν -e scattering: $\nu + e^- \rightleftharpoons \nu + e^-$
- Inelastic ν -nuclei scattering: $\nu + A \rightleftharpoons \nu + A^*$

ν_e absorption cross section on ⁵⁶Fe

 56 Fe $(\nu_e, e^-)^{56}$ Co measured by KARMEN collaboration: $\sigma_{exp} = 2.56 \pm 1.08 (stat) \pm 0.43 (syst) \times 10^{-40} cm^2$ $\sigma_{th} = 2.38 \times 10^{-40} cm^2$



Neutrino nucleosynthesis

Neutrinos interact with abundant nuclear species

- Neutral current (ν, ν') : Nucleus excited to particle unbound states that decay by particle emission.
- Charged current (ν_e, e^-) and $(\bar{\nu}_e, e^+)$.

Product	Parent	Reaction
¹¹ B	¹² C	(u, u'n),(u, u'p)
¹⁵ N	¹⁶ 0	(u, u'n),(u, u'p)
¹⁹ F	²⁰ Ne	(u, u'n),(u, u'p)
¹³⁸ La	¹³⁸ Ba	(ν, e^-)
	¹³⁹ La	(u, u'n)
¹⁸⁰ Ta	¹⁸⁰ Hf	(ν, e^-)
	¹⁸¹ Ta	(u, u'n)



¹¹B/¹⁰B traces galactic evolution:

- Big ratio (100) predicted by u-process.
- Cosmic rays spallation reactions on C give a ratio of 2.
- Solar system ratio is 4.

 138 La, 180 Ta production is sensitive to neutrino oscillations.

Nucleosynthesis with and without ν

With Heger (Los Alamos)



The production of ¹³⁸La



The production of ¹⁸⁰Ta



Presupernova abundances

