# The Interacting shell model

Silvia M. Lenzi University of Padova and INFN

#### The shell model potential

Nuclei are made up of protons and neutrons held together by the strong interaction inside of a volume with a radius of a few Fermi.

One might expect that the motions of these nucleons in this closely packed system should be very complex because of the large number of frequent collisions. Due to these collisions nucleons could not maintain a single-particle orbit.

But, because of Pauli exclusion the nucleons are restricted to only a limited number of allowed orbits.

#### **Nuclear Potentials**

There are two approaches:

- 1. An empirical form of the potential is assumed, e.g. square well, harmonic oscillator, Woods-Saxon
- 2. The mean field is generated self-consistently from the nucleon-nucleon interaction

N nucleons in a nucleus



A nucleon in the Mean Field of N-1 nucleons

- Assumption ignore detailed two-body interactions
- Each particle moves in a state independent of the other particles
- The Mean Field is the average smoothed-out interaction with all the other particles
- An individual nucleon only experiences a central force

#### The one-body potential

This is an independent particle model where the nucleus is described in terms of non-interacting particles in the orbits of a spherical symmetric (central) potential U(r) which is itself produced by all the nucleons.

Then, the resulting orbit energies are mass dependent.

This model is applicable to nuclei with one single nucleon outside closed shell.

When more valence nucleons are considered, we have to include the residual interaction between these nucleons.

The simplest potentials are the square well and the harmonic oscillator.

#### Wrong magic numbers



## The magic numbers: H.O. + l.l + l.s



# The nuclear shell model with residual interactions

#### **Global and local properties**



3 orders of magnitude of difference between the two scales!

Are we able to describe both global and local properties using the same, original nucleon-nucleon interaction?



#### The nucleon-nucleon potential

The bare nucleon-nucleon (or nucleon-nucleon-nucleon) interactions are inspired by meson exchange theories or more recently by chiral perturbation theory, and must reproduce the NN phase shifts, and the properties of the deuteron and other few body systems



#### Independent Particle Motion and correlations

In the nucleus, due to the very **strong short range repulsion** and the **tensor force**, the **independent particle** motion or Hartree-Fock approximation, based upon the **bare nucleon-nucleon force,** are **impracticable**.

However, at low energy, the nucleus do manifest itself as a system of independent particles in many cases, and when it does not, it is due to the medium range correlations that produce strong configuration mixing and not to the short range repulsion.

#### The unique interaction

To have a tractable problem, the critical point is the choice of the model space and the "effective" nucleon-nucleon interaction.

The starting point should be a realistic interaction that reproduces the nucleon-nucleon scattering properties in the energy region 0-500 MeV

#### **Deriving a realistic effective interaction**

All modern NN potentials fit equally well ( $\chi^2/N_{data} \sim 1$ ) the deuteron properties and the NN scattering data up to the inelastic threshold: CD-Bonn, Argonne V18, Nijm I, Nijm II, N<sup>3</sup>LO potentials,...

However, these potentials cannot be used directly in the derivation of  $V_{eff}$  due to the strong short-range repulsion, but a renormalization procedure is needed.



#### Many-body methods:

Brueckner G-matrix

-  $V_{\text{low-K}}$  : smooth low-momentum potential that is used in a perturbative approach to derive  $V_{\text{eff}}$ 

#### The full problem

The challenge is to find  $\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_A)$  such that  $H\Psi = E\Psi$ , with

$$H = \sum_{i}^{A} T_{i} + \sum_{i,j}^{A} V_{2b}(\vec{r}_{i},\vec{r}_{j}) + \sum_{i,j,k}^{A} V_{3b}(\vec{r}_{i},\vec{r}_{j},\vec{r}_{k})$$

The knowledge of the eigenvectors  $\Psi$  and the eigenvalues E make it possible to obtain electromagnetic moments, transition rates, weak decays, cross sections, spectroscopic factors, etc.

Only very recently and only for very light nuclei A $\leq$ 10 the problem has been solved "exactly",

#### Ab initio and 3-body forces



#### **Approaches for heavy systems**

For medium-heavy systems, ab initio calculations are not possible and one is obliged to resort to an effective force

We are simply forced to simplify the force (B.R. Mottelson)

Two main approaches:

Shell Model based on the bare forces, introduces correlations in the many-body states, or in the associated matrix elements. Spherically symmetric average potential + residual interaction in a subspace of the Hilbert space.

Mean-field methods devise a complementary strategy: defines an energy-density functional to produce directly the appropriate single particle potential. Search for the 'best' mean-field potential starting from a phenomenological energy functional + correlations. Self-consistent potentials.



Inspired by the effective field theory and renormalization group for low-energy systems

Realistic  $V_{NN}$  Construct  $V_{low-k}$  integrating out potential the high-momentum part of  $V_{NN}$ B. Bogner et al. Phys Rev. C 65 (2002) 05130(R)

preserves the physics of  $V_{NN}$  up to a cutoff momentum  $\Lambda$ 

S. Bogner et al. Phys Rev. C 65 (2002) 05130(R) T.T.S. Kuo and E. Osnes, Lecture Notes in Physics, vol 364 (1990) L. Coraggio et al. Prog. Part. Nucl. Phys 62 (2009) 135

#### Features of V<sub>low-k</sub>

- eliminates sources of non-perturbative behavior
- real potential in the k-space
- gives an approximately unique representation of the NN potentials for  $\Lambda \cong 2 \text{ fm}^{-1} \Rightarrow E_{Lab} \cong 350 \text{ MeV}$

 V<sub>low-k</sub> is used to derive V<sub>eff</sub> in a perturbative approach: folded diagrams expansion, in the framework of the Q-box formalism

To what extent the nuclear structure results depend on the choice of the starting potential?

#### V<sub>low-k</sub> in the <sup>132</sup>Sn region: the 2p case



A. Covello, L. Coraggio, A. Gargano, N. Itaco PPNP 59 (2007) 401

#### **The Interacting Shell Model**

Is an approximation to the exact solution of the nuclear A-body problem using effective interactions in restricted spaces.

The effective interactions are obtained from the bare nucleon-nucleon interaction by means of a regularization procedure aimed to soften the short range repulsion.

The only way to obtain a tractable problem is to define a new reference "vacuum".

#### Some hypothesis

The microscopic description of the nucleus we adopt is that of a non-(explicitly)-relativistic quantum many body system.

Therefore we assume:

- nucleon velocities small enough to justify the use of non-relativistic kinematics
- hidden meson and quark-gluon degrees of freedom
- two body interactions

#### The many-body hamiltonian

We want to solve the Schrödinger equation

$$H|\psi\rangle = \left(\sum_{i} T_{i} + \sum_{i < j} V_{ij}\right)|\psi\rangle = E|\psi\rangle$$

To treat this perturbatively, we express the Hamiltonian as

$$H|\psi\rangle = (H_0 + H_1)|\psi\rangle = E|\psi\rangle$$

with the unperturbed Hamiltonian

$$H_0 = \sum_i h_{0i} \qquad h_0 |\varphi_i\rangle = (T_i + U_i) |\varphi_i\rangle = \varepsilon_i |\varphi_i\rangle$$

and the perturbation

$$H_1 = \sum_{i < j} V_{ij} - \sum_i U_i$$

Where the auxiliary one-body potential U is chosen to make  $H_1$  small

#### The interacting shell model

We want to solve the eigenvalue problem

$$H|\psi\rangle = (H_0 + H_1)|\psi\rangle = E|\psi\rangle$$

and E is the true energy of the system.

However we work in the model space, not in the full Hilbert space. We thus need to construct an effective Hamiltonian  $H_{eff}$  acting in the model space, such as

$$H_{eff}|\psi'\rangle = E|\psi'\rangle$$

### Reducing the model space (2)

To reduce the Schrödinger equation of the A-body system

to a secular equation acting only in the selected subspace, with the condition

$$\left\langle \psi' \left| H_{eff} \right| \psi' \right\rangle = E$$

We divide the full Hilbert space into a model space P and an excluded space Q which is achieved using projection operators

$$P = \sum_{i=1}^{d} |\psi_i 
angle \! \left\langle \psi_i 
ight| \qquad Q = \sum_{i=d+1}^{\infty} \! \left| \psi_i 
angle \! \left\langle \psi_i 
ight|$$

$$P^2 = P, \quad Q^2 = Q, \quad PQ = QP = 0$$



#### The model space

The success of the independent particle model strongly suggests that the very singular free NN interaction can be regularized in the nuclear medium.

For a given number of protons and neutrons the mean field orbitals can be grouped in three blocks

- Inert core: orbits that are always fully occupied
- 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 approach

β decays

ββ decays



#### **Ingredients for the Shell Model calculations**



#### The effective interaction



*microscopic* effective interaction (*realistic* interaction)

$$V_{NN} \implies \mathbf{G} \implies V^{e\!f\!f}$$

M. Hjorth-Jensen et al, Phys.Rep.261 (1995)

*empirical* interaction (fitted to the data)

B.A.Brown, B.H.Wildenthal, Ann. Rev. Nucl.Part.Sci. 38 (1988)

schematic interaction (delta-force, etc)

#### A simple case: <sup>18</sup>O

5.08 $1d_{3/2}$ We will calculate some states of  ${}^{18}O$ <br/>as an example of ISM calculation<br/>Two neutrons above a core of  ${}^{16}O$ 0.87 $2s_{1/2}$ The lowest states have nucleons in the<br/> $1d_{5/2}$  orbit:0.0 $1d_{5/2}$ The lowest states have nucleons in the<br/> $1d_{5/2}$  orbit:17O $1d_{5/2}$ with  $(1d_{5/2})^2$  : we can construct only 3 states<br/> $(J^{\pi} = 0+, 2+ \text{ or } 4+)$ 

To construct other states, we have to consider a wider valence space: we thus include the  $2s_{1/2}$  level.

The strength of the effective interaction V(1,2) depends on the valence space

#### The states in the model space

We can then construct the following states:

$$J^{\pi} = 0^{+} \rightarrow (1d_{5/2})_{0^{+}}^{2}; \quad (2s_{1/2})_{0^{+}}^{2}$$
$$J^{\pi} = 2^{+} \rightarrow (1d_{5/2})_{2^{+}}^{2}; \quad (1d_{5/2}2s_{1/2})_{2^{+}}$$
$$J^{\pi} = 3^{+} \rightarrow (1d_{5/2}2s_{1/2})_{3^{+}}$$
$$J^{\pi} = 4^{+} \rightarrow (1d_{5/2})_{4^{+}}^{2}$$

The energy values for these states will be the corresponding of the eigenstates of the hamiltonian:

$$H = H_0 + H_{res} = \sum_{i=1}^{2} h_0(i) + V_{12}$$

where the core energy corresponding to the closed shell system (16O)  $E_0$  is taken as a reference value

#### eigenfunctions

The wave functions will be linear combinations of the possible basis functions. For J=0+ we obtain two eigenfunctions

$$\Psi_{0^{+};1} \rangle = \sum_{k=1}^{n} a_{k,1} | \psi_{k}^{0}; 0^{+} \rangle$$
$$\Psi_{0^{+};2} \rangle = \sum_{k=1}^{n} a_{k,2} | \psi_{k}^{0}; 0^{+} \rangle$$

For the particular case of <sup>18</sup>O we define

$$|\psi_1^0;0^+\rangle = |(1d_{5/2})^2;0^+\rangle$$
  
 $|\psi_2^0;0^+\rangle = |(2s_{1/2})^2;0^+\rangle$ 

#### The general case

If the basis set is defined as  $|\psi_k^0\rangle (k=1,...,n)$ 

$$\psi_{k}^{0}(\vec{r}_{1},\vec{r}_{2},...,\vec{r}_{A}) = \frac{1}{\sqrt{A!}} \det \begin{pmatrix} \varphi_{1}(\vec{r}_{1}) & \varphi_{1}(\vec{r}_{1}) & \cdots & \varphi_{1}(\vec{r}_{A}) \\ \vdots & \ddots & \vdots \\ \varphi_{A}(\vec{r}_{1}) & \varphi_{A}(\vec{r}_{1}) & \cdots & \varphi_{A}(\vec{r}_{A}) \end{pmatrix}$$

The total wave function can be expanded as:  $|\Psi|$ 

$$|\Psi_p\rangle = \sum_{k=1}^n a_{kp} |\Psi_k^0\rangle$$

The coefficients  $a_{kp}$  have to be determined by solving the Schrödinger equation

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

$$(H_{0} + H_{res})\sum_{k=1}^{n} a_{kp} |\psi_{k}^{0}\rangle = E_{p}\sum_{k=1}^{n} a_{kp} |\psi_{k}^{0}\rangle$$
  
or  
$$\sum_{k=1}^{n} \langle\psi_{l}^{0} | H_{0} + H_{res} |\psi_{k}^{0}\rangle a_{kp} = E_{p}a_{lp}$$

#### the matrix to be diagonalized

Since  $|\Psi_k^0\rangle$  corresponds to eigenfunctions of H<sub>0</sub> with eigenvalues (unperturbed energies)  $E_{0}$ , calling

$$\left\langle \psi_{\ell}^{0} \left| H_{0} + H_{res} \left| \psi_{k}^{0} \right\rangle = H_{\ell k} \right.$$

we obtain:

$$\sum_{k=1}^{n} H_{lk} a_{kp} = E_p a_{lp}$$

$$\boldsymbol{H}_{lk} = \boldsymbol{E}_{k}^{0} \boldsymbol{\delta}_{lk} + \left\langle \boldsymbol{\psi}_{l}^{0} \left| \boldsymbol{H}_{res} \right| \boldsymbol{\psi}_{k}^{0} \right\rangle$$

The eigenvalue equation becomes a matrix equation:

$$[H][A] = [E][A]$$

#### The matrix equation

The eigenvalue equation becomes a matrix equation:

$$[H][A] = [E][A]$$

This forms a secular equation for the eigenvalues  $E_p$ :

$$\begin{vmatrix} H_{11} - E_p & H_{12} & \dots H_{1n} \\ H_{21} & H_{22} - E_p & \dots H_{2n} \\ \vdots & \vdots & \vdots \\ H_{n1} & \dots & H_{22} - E_p \end{vmatrix} = 0$$

This is a nth degree equation for the n-roots  $E_p$  (p=1,2,...n)

#### The solutions

Once we have the energies  $E_p$ , we can use

$$\left|\sum_{k=1}^{n} E_{k}^{0} \delta_{lk} a_{kp} + \sum_{k=1}^{n} \langle \psi_{l}^{0} | H_{res} | \psi_{k}^{0} \rangle a_{kp} = E_{p} a_{lp}\right|$$

to obtain the coefficients  $a_{kp}$ . Using the orthonormalization:

$$\sum_{k=1}^{n} a_{kp} a_{kp'} = \delta_{pp'}$$

We can then write

$$\sum_{l,k=1}^{n} a_{lp'} E_{k}^{0} \delta_{lk} a_{kp} + \sum_{l,k=1}^{n} a_{lp'} \left\langle \psi_{l}^{0} \left| H_{res} \right| \psi_{k}^{0} \right\rangle a_{kp} = E_{p} \delta_{pp'}$$

Which is a matrix equation of the form

$$[A]^{-1}[H][A] = [E]$$

This equation indicates a similarity transformation to a new basis that makes [H] diagonal

If n is large this process needs a high-speed computer

### **Configuration mixing**

If the non-diagonal matrix elements are of the order of the unperturbed energy differences

$$|H_{ij}|\approx |E_i^0-E_j^0|$$

large configuration mixing will result and the final energy eigenvalues  $E_p$  will be very different from the unperturbed ones.

On the contrary, if the non-diagonal matrix elements are small, these energy shifts will be small and we can use perturbation theory to solve the problem

$$|H_{ij}| << |E_i^0 - E_j^0|$$

#### Back to the <sup>18</sup>O problem

We now consider the case of the J=0<sup>+</sup> states in <sup>18</sup>O in the  $1d_{5/2}$ ,  $2s_{1/2}$  model space.

$$|\psi_1^0;0^+\rangle = |(1d_{5/2})^2;0^+\rangle$$
  
 $|\psi_2^0;0^+\rangle = |(2s_{1/2})^2;0^+\rangle$ 

The Hamiltonian matrix is now

$$H = \begin{bmatrix} 2\varepsilon_{d_{5/2}} + \langle (d_{5/2})^2; 0^+ | V_{12} | (d_{5/2})^2; 0^+ \rangle & \langle (d_{5/2})^2; 0^+ | V_{12} | (s_{1/2})^2; 0^+ \rangle \\ \langle (s_{1/2})^2; 0^+ | V_{12} | (d_{5/2})^2; 0^+ \rangle & 2\varepsilon_{s_{1/2}} + \langle (s_{1/2})^2; 0^+ | V_{12} | (s_{1/2})^2; 0^+ \rangle \end{bmatrix}$$

These diagonal matrix elements yield the first correction to the unperturbed single-particle energies  $2\varepsilon_{s_{1/2}}$  e  $2\varepsilon_{d_{5/2}}$ 

#### The diagonalization

The secular equation can thus be written:

$$\begin{vmatrix} H_{11} - \lambda & H_{12} \\ H_{12} & H_{22} - \lambda \end{vmatrix} = 0$$

We then get the quadratic equation:

$$\lambda^2 - \lambda (H_{11} + H_{22}) - H_{12}^2 + H_{11}H_{22} = 0$$

With the roots:

$$\lambda_{\pm} = \frac{H_{11} + H_{22}}{2} \pm \frac{1}{2} [(H_{11} - H_{22})^2 + 4H_{12}^2]^{1/2}$$

$$\Delta \lambda = \lambda_{+} - \lambda_{-} = [(H_{11} - H_{22})^{2} + 4H_{12}^{2}]^{1/2}$$

Even if the **unperturbed states are degenerate** there is a repulsion between them that separates the two solutions.

#### in perturbation theory...

$$\lambda_{\pm} = \frac{H_{11} + H_{22}}{2} \pm \frac{1}{2} [(H_{11} - H_{22})^2 + 4H_{12}^2]^{1/2}$$

If: 
$$|H_{12}| << |H_{11} - H_{22}| \implies \Delta \lambda \rightarrow |H_{11} - H_{22}|$$

We can write the series,

$$\begin{split} \lambda_{+} &= \lambda_{1} = H_{11} + \frac{H_{12}^{2}}{H_{11} - H_{22}} + \dots \\ \lambda_{-} &= \lambda_{2} = H_{22} + \frac{H_{12}^{2}}{H_{11} - H_{22}} + \dots \end{split}$$

#### Final spectrum for the O<sup>+</sup> in <sup>18</sup>O



#### **Eigenvalues and eigenvectors**

The problem consists on diagonalizing a matrix in the model space. The basis is formed by the eigenfunctions of the mean field

For "normal"  $0^+$  states, one needs to diagonalize the  $4 \times 4$  matrix:



shell model

n<sup>+</sup>\_\_\_\_5292

2+ \_\_\_\_\_4071

exp.

#### **Basic Shell Model**



#### **Shell model basis**

#### **Shell-model basis states**

The basis states have good angular momentum (coupling all j values to J), good parity and good isospin.

The slater determinants can also be constructed with good M and Tz e.g., 4 particles in the sd shell with M=0:

$$\left|1d_{5/2}, -\frac{1}{2}; 1d_{5/2}, -\frac{3}{2}; 1d_{5/2}, +\frac{3}{2}; 1d_{5/2}, +\frac{1}{2}\right\rangle$$

The number of basis states can be estimated approximately as ( $\Omega$ : shell degeneracy, n: valence particles)

For example for <sup>60</sup>Zn with 10 valence protons and 10 valence neutrons in the *fp* shell

$$N_{basis} = \begin{pmatrix} \Omega_p \\ n_p \end{pmatrix} \begin{pmatrix} \Omega_n \\ n_n \end{pmatrix}$$



#### **Configuration mixing**

$$\phi = \frac{1}{\sqrt{A!}} \det \begin{pmatrix} \psi_1(r_1) & \cdots & \psi_1(r_A) \\ \vdots & \ddots & \vdots \\ \psi_A(r_1) & \cdots & \psi_A(r_A) \end{pmatrix}$$





due to the residual interaction



#### An example

sd MODEL SPACE



#### What can be achieved



#### **Accessible regions**



#### **Algorithms and codes**

Algorithms include Direct Diagonalisation, Lanczos, Monte Carlo Shell Model, Quantum Monte Carlo Diagonalization, DMRG etc. There are also a number of different extrapolation ansatzs

The Strasbourg-Madrid codes (Antoine, Nathan), can deal with problems involving basis of 10<sup>10</sup> Slater determinants, using relatively modest computational resources. Other competitive ones in the market are OXBACH, NUSHELL and MSHELL

Can shell model describe collective states?

# Example: the $f_{7/2}$ shell

The  $1f_{7/2}$  shell is isolated in energy from the rest of fp orbitals

Wave functions are dominated by  $(1f_{7/2})^n$  configurations

High-spin states experimentally reachable





N=Z

#### Shell model and collective phenomena



![](_page_49_Figure_0.jpeg)

How well shell model describes the nuclear structure far from stability?

# Bibliography

- P. J. Brussaard, P. W. M. Glaudemans, Shell-Model Applications in Nuclear Spectroscopy (North-Holland, Amsterdam, 1977).
- K. Heyde, The Nuclear Shell Model (Springer-Verlag, Heidelberg, 2004)
- A. DeShalit, I. Talmi, Nuclear Shell Theory (Academic Press, New York and
- London, 1963)
- I. Talmi, Simple Models of Complex Nuclei, The Shell Model and the Interacting Boson Model (Harwood Academic Publishers, New York, 1993)
- R. D. Lawson, Theory of the Nuclear Shell Model (Clarendon Press, 1980).
- Review article: E. Caurier et al, The shell model as a unified view of nuclear structure, Rev. Mod. Phys. 77 (2005) 427.