# Nuclear structure theory II: Pairing, deformation, and collective nuclear structure 

Mark A. Caprio<br>Department of Physics and Astronomy<br>University of Notre Dame

Exotic Beam Summer School
Notre Dame, IN
June 10, 2022

## From simple shell structure to collective dynamics



## From simple shell structure to collective dynamics



## From simple shell structure to collective dynamics



## Shell model and collective correlations

$$
\begin{aligned}
H= & \sum_{i=1}^{A}-\frac{\hbar^{2}}{2 m_{i}} \nabla_{i}^{2}+\sum_{i, j=1}^{A} V\left(\mathrm{r}_{i}-\mathrm{r}_{j}\right)
\end{aligned}
$$

Independent particle model $\left(H \approx H_{0}\right)$ : Eigenstate approximated as single configuration Classic shell model ("configuration interaction" calculation):

Many-body problem restricted to valence shell
Neglected ("inert") core leads to effective interaction of valence nucleons
Open shell $\left[\Delta \varepsilon \lesssim\left\langle V_{\text {res }}\right\rangle\right]$ permits collective phenomena:
Large number of single-particle configurations energetically accessible
Little energy required for excitation

Flow chart for ab initio nuclear theory


Quarks


Flow chart for phenomenological nuclear theory (extreme case)


Quarks

...then a miracle occurs...



Obtain detailed information on physical structure and excitation phenomena from spectroscopic properties

- Level energies and quantum numbers
- Electromagnetic transition probabilities and multipolarities

$$
\begin{array}{|lc|}
\left.\hline \text { Fermi's golden rule } \quad T_{i \rightarrow f} \propto\left|\left\langle\Psi_{f}\right| \hat{T}\right| \Psi_{i}\right\rangle\left.\right|^{2} \\
\hline
\end{array}
$$

Electromagnetic probes ( $e$-scattering), $\alpha$ decay, $\beta$ decay, nucleon transfer reactions, ...

## Multipolarity of nuclear radiation

Homogeneous charged fluid


Electric quadrupole ( $E 2$ )
Relative motion of proton and neutron density


Electric dipole (E1)


Magnetic dipole (M1)

## Multipole operator definitions

Electric quadrupole ( $E 2$ ) operator

$$
\mathbf{Q}_{2}=\sum_{i=1}^{A} e_{i} r_{i}^{2} Y_{2 u}\left(\hat{\mathbf{r}}_{i}\right) \quad=\mathbf{Q}_{p}+\mathbf{Q}_{n} \quad e_{p}=e \quad e_{n}=0
$$

Magnetic dipole (M1) operator

$$
\begin{aligned}
\mathbf{M}_{1} & =\sqrt{\frac{3}{4 \pi}} \mu_{N} \sum_{i=1}^{A}\left(g_{\ell}^{(i)} \boldsymbol{\ell}_{i}+g_{s}^{(i)} s_{i}\right) \quad \begin{array}{lll}
g_{\ell, p}=1 & g_{\ell, n}=0 \\
g_{s, p} \approx 5.585 & g_{s, n} \approx-3.826
\end{array} \\
& =g_{\ell, p} \mathbf{L}_{p}+g_{\ell, n} \mathbf{L}_{n}+g_{s, p} \mathbf{S}_{p}+g_{s, n} \mathbf{S}_{n} \\
\mathbf{L}_{p} & =\sum_{i=1}^{Z} \boldsymbol{\ell}_{p, i} \quad \mathbf{L}_{n}=\sum_{i=1}^{N} \boldsymbol{\ell}_{n, i} \quad \mathbf{S}_{p}=\sum_{i=1}^{Z} \mathbf{s}_{p, i} \quad \mathbf{S}_{n}=\sum_{i=1}^{N} \mathbf{s}_{n, i}
\end{aligned}
$$

## Nuclear structure with transfer reactions

- transfer reactions probe nuclear response to the addition of nucleon
- information about nuclear structure from:
- angular differential cross section
- absolute value
- position
- width (in the continuum)


## A standard approach to reactions:

$$
\sigma=S_{i}^{2} \tilde{\sigma}
$$

spectroscopic factor cross section from from structure model few-body/reaction models

can suffer from inconsistency between the two schemes!

## Outline

- Isospin
- Pairing
- Deformation: Rotation


## Observed energy levels for $A=6$ nuclei



Figure from D.R. Tilley et al., Nucl. Phys. A 708, 3 (2002).

## Observed energy levels for $A=7$ nuclei



## Observed energy levels for $A=12$ nuclei



Figure from F. Ajzenberg-Selove, Nucl. Phys. A 506, 1 (1990).

## What is a Lie algebra?

A vector space...

$$
\begin{array}{ll}
X, Y \in \mathscr{V} \Rightarrow X+Y \in \mathscr{V}, a X \in \mathscr{V} & \text { Closure } \\
a(X+Y)=a X+a Y & \text { Linearity }
\end{array}
$$

...with a vector product ("Lie product")

$$
\begin{array}{ll}
{[X, Y] \in \mathscr{V}} & \text { Closure } \\
{[a X+b Y, Z]=a[X, Z]+b[Y, Z]} & \text { Linearity } \\
{[X, Y]=-[Y, X]} & \text { Antisymmetry } \\
{[A,[B, C]]+[C,[A, B]]+[B,[C, A]]=0} & \text { Jacobi identity }
\end{array}
$$

Note: A vector space is spanned by $d$ basis vectors $X_{1}, X_{2}, \ldots, X_{d}$.

$$
\mathscr{V}=\left\{\sum_{i=1}^{d} a_{i} X_{i} \mid a_{i} \in \mathbb{R} \text { or } \mathbb{C}\right\} \quad d=" \text { dimension" of } \mathscr{V}
$$

## Why should we care?

There are Lie algebras hidden inside our QM problems! Two vector spaces...

1) Space of states - "Hilbert space"
2) Space of operators (!)

$$
\begin{aligned}
& a(\hat{X}+\hat{Y})=a \hat{X}+a \hat{Y} \\
& {[\hat{X}, \hat{Y}] \equiv \hat{X} \hat{Y}-\hat{Y} \hat{X} \quad \text { is a "Lie product" }}
\end{aligned}
$$

Example Angular momentum algebra [SU(2)] basis $J_{x}, J_{y}, J_{z}$ closure? $\quad\left[J_{x}, J_{y}\right]=i J_{z} \quad\left[J_{y}, J_{z}\right]=i J_{x} \quad\left[J_{z}, J_{x}\right]=i J_{y}$

Lie algebra operators as "generators" for continuous transformations
Lie algebra $g \stackrel{R=e^{i X}}{\Longleftrightarrow}$ Lie group $G \quad$ e.g., $R(\theta)=e^{i\left(\theta_{x} J_{x}+\theta_{y} J_{y}+\theta_{z} J_{z}\right)}$
Symmetry - invariance of Hamiltonian under tranformation

$$
R(\theta) H R(\theta)^{\dagger}=H \quad \Leftrightarrow \quad\left[J_{i}, H\right]=0 \quad(i=1,2,3)
$$

Eigenvalues form degenerate multiplets $\quad(M=-J, \ldots, J-1, J)$
Eigenstates rotate into each other $\quad R(\theta)|J M\rangle=\sum_{M^{\prime}=-J}^{J} \mathscr{D}_{M^{\prime} M}^{(J)}(\theta)\left|J M^{\prime}\right\rangle$

## $\mathrm{SU}(2)$ in a nutshell

$\mathrm{SU}(2) \sim \mathrm{SO}(3) \quad(2 \times 2$ spin rotation or $3 \times 3$ Euler rotation matrices $)$
Ladder operators $\quad J_{ \pm}=J_{x} \pm i J_{y} \quad$ Raises or lowers $M$ value
Weight operator $J_{0}=J_{z} \quad$ "Weighs" a state for its $M$ value
Everything follows from the commutators*...

$$
\left[J_{0}, J_{+}\right]=+J_{+} \quad\left[J_{0}, J_{-}\right]=-J_{-} \quad\left[J_{+}, J_{-}\right]=2 J_{0}
$$

Action of generators

$$
J_{ \pm}|J M\rangle=\sqrt{(J \mp M)(J \pm M+1)}|J(M \pm 1)\rangle \quad J_{0}|J M\rangle=M|J M\rangle
$$

States form "irreducible representation" connected by ladder operators


Set may be labeled by its "highest weight" $M_{\max }(\equiv J)$
${ }^{*}$ Actually, these plus the relations $J_{+}^{\dagger}=J_{-}$and $J_{0}^{\dagger}=J_{0} \ldots$

## Symmetries in nuclei

Fundamental symmetries

- Rotation [SU(2)] \& parity $\quad \Rightarrow \quad J, P$

Approximate symmetries of the many-body problem

- Isospin [SU(2)] \& Wigner spin-isospin [SU(4)]
- Pairing quasispin symmetries: $\mathrm{SU}(2), \mathrm{SO}(5), \ldots$
- Phase space (or oscillator) symmetries: Elliott $\operatorname{SU}(3) \& \operatorname{Sp}(3, \mathbb{R})$

Symmetries of collective degrees of freedom

- Bosonic models: U(6), ...
- Symplectic collective model [ $\mathrm{Sp}(3, \mathbb{R})$ again!] Collective flow
D. J. Rowe, A. E. McCoy, and M. A. Caprio, Physica Scripta 91, 033003 (2016).

But symmetries are broken, so... Why symmetries?

- Identifying and characterizing emergent correlations
E.g., isospin multiplets, Elliott rotation
- Symmetry as computational tool $H=H_{s y m m}^{(0)}+H^{\prime}$
"Right" basis for decomposing and truncating many-body space


## Outline

- Isospin
- Pairing
- Deformation: Rotation

Figure 1.8: One-neutron separation energies, $S_{n}$, for the calcium isotopes. Note the odd-even staggering between neighbouring nuclei and the strong discontinuities that occur between $A=40$ and 41 and between $A=48$ and 49 (cf. Figure 1.9). (The data are from Audi G., Wapstra A.H. and Thibault C. (2003), Nucl. Phys. A729, 337.)


Figure 1.9: Two-neutron separation energies, $S_{2 n}$, for the calcium isotopes. The odd-even staggering is smoothed away, leaving a clear indication of discontinuities at $A=41$ and 49. (The data are from Audi G., Wapstra A.H. and Thibault C. (2003), Nucl. Phys. A729, 337.)

## Single-particle energies in the $p f$ shell



Figure courtesy United States Postal Service

Figure 1.28: Low-energy states in the $A=42$ isobars ${ }^{42} \mathrm{Ca},{ }^{42} \mathrm{Sc}$, and ${ }^{42} \mathrm{Ti}$. Excitations are in MeV . Levels are labelled by their spinparity, $J^{\pi}$. The vertical arrows indicate the energies above which there are excited states known but which are omitted from the figure. The states shown for ${ }^{42} \mathrm{Sc}$ result from the various spin couplings of the configuration $\pi 1 f_{7 / 2} \nu 1 f_{7 / 2}$. The $J=0,2,4,6 \mathrm{mem}-$ bers of this multiplet are connected with the corresponding $\left(\pi 1 f_{7 / 2}\right)^{2}$ and $\left(\nu 1 f_{7 / 2}\right)^{2}$ states in ${ }^{42} \mathrm{Ti}$ and ${ }^{42} \mathrm{Ca}$, respectively. (The data are taken from Endt P.M. (1990), Nucl. Phys. A521, 1.)


## Pairing as approximation to short-range interaction

$$
\begin{aligned}
& V_{\mathrm{RES}}=-\frac{1}{2} \sum_{J} \widehat{J}\langle j j ; J| V|j j ; J\rangle\left[\left[c_{j}^{\dagger} c_{j}^{\dagger}\right]_{J}\left[\tilde{c}_{j} \tilde{c}_{j}\right]_{J}\right]_{00} \\
& \stackrel{\text { pairing }}{\approx}-\frac{1}{2}\langle j j ; 0| V|j j ; 0\rangle\left[c_{j}^{\dagger} c_{j}^{\dagger}\right]_{0}\left[\tilde{c}_{j} \tilde{c}_{j}\right]_{0} \\
& =-\frac{1}{2}\langle j j ; 0| V|j j ; 0\rangle \widehat{j}^{-2} \sum_{m m^{\prime}}(-1)^{j-m+j-m^{\prime}} c_{j m}^{\dagger} c_{j,-m}^{\dagger} \tilde{c}_{j m^{\prime}} \tilde{c}_{j,-m^{\prime}} \\
& =\frac{1}{2}\langle j j ; 0| V|j j ; 0\rangle \widehat{j}^{-2} \sum_{m m^{\prime}} c_{j m}^{\dagger} \tilde{c}_{j m}^{\dagger} \tilde{c}_{j m^{\prime}} c_{j m^{\prime}}
\end{aligned}
$$

## Seniority relates states obtained by adding pairs

$$
\begin{aligned}
{\left[A, A^{\dagger}\right] } & =1-\hat{n} / \Omega \\
{\left[A^{\dagger}, \hat{n}\right] } & =-2 A^{\dagger}, \\
{\left[V_{\mathrm{PAIR}}, A^{\dagger}\right] } & =-G A^{\dagger}(\Omega-\hat{n})=-G(\Omega-\hat{n}+2) A^{\dagger}
\end{aligned}
$$



$$
\begin{aligned}
& \text { (42) } \underline{V=4} \\
& (J=2,4,5,8) \\
& \text { (27) } \underline{v=2} \\
& \text { (27) } \underline{\mathrm{V}=2} \\
& \text { (27) } \xrightarrow{\mathrm{V}=2} \quad(\mathrm{~J}=2,4,6) \\
& \text { (48) } \mathrm{v}=3 \\
& \text { (48) } \mathrm{V}=3 \\
& \text { ( } \mathrm{J}=3 / 2,5 / 2,9 / 2,11 / 2,15 / 2 \text { ) } \\
& \text { (1) } \frac{\mathrm{v}=0}{\mathrm{~N}=2} \\
& \text { (8) } \frac{v=1}{\mathrm{~N}=3} \\
& \text { (1) } \frac{\mathrm{v}=0}{\mathrm{~N}=4} \\
& \text { (8) } \frac{\mathrm{v}=1}{\mathrm{~N}=5} \\
& \text { (1) } \frac{\mathrm{v}=0}{\mathrm{~N}=6} \\
& \text { (8) } \frac{\mathrm{v}=1}{\mathrm{~N}=7} \\
& \text { (1) } \frac{\mathrm{v}=0}{\mathrm{~N}=8}
\end{aligned}
$$

(8) $\frac{\mathrm{v}=1}{\mathrm{~N}=1}$

Fig. 12.3. Excitation spectra in the seniority scheme for different numbers $N$ of particles occupying the $0 f_{7 / 2}$ shell. The seniority $v$ is indicated for each level. The numbers in parentheses to the left of the levels give the degeneracies. The angular momentum content of the levels is given on the far right


Figure 1.29: Low-energy states in the even-mass $\operatorname{tin}(Z=50)$ isotopes. The $0^{+}$ground states and $2^{+}$first excited states are discussed in the text. (The data are taken from Nuclear Data Sheets and Juutinen S. et al. (1997), Nucl. Phys. A617, $74-{ }^{106}$ Sn; Górska M. et al. (1998), Phys. Rev. C58, $108-{ }^{104}$ Sn.)


Figure 1.30: Low-energy states in the odd-mass tin isotopes. Levels are labelled by their spin-parity. The vertical arrows indicate the energies above which there are excited states known but which are omitted from the figure. The lowest three states are a selection from the spin-parities $5 / 2^{+}, 7 / 2^{+}, 1 / 2^{+}, 3 / 2^{+}$, $11 / 2^{-}$, corresponding to the single-particle configurations $2 d_{5 / 2}, 1 g_{7 / 2}, 3 s_{1 / 2}, 2 d_{3 / 2}, 1 h_{11 / 2}$, respectively. Information on states in ${ }^{103,105,107,109} \mathrm{Sn}$ is very limited. The identification of $2 \mathrm{~d}_{5 / 2}$ in ${ }^{117} \mathrm{Sn}$ and $1 g_{9 / 2}$ in ${ }^{123,129} \mathrm{Sn}$ is ambiguous. (The data are taken from Nuclear Data Sheets and Fahlander C. et al. (2001), Phys. Rev. C63, 021307(R) - ${ }^{103} \mathrm{Sn}$.)

## The Fermi surface and quasiparticle excitation


D. J. Rowe, Nuclear Collective Motion: Models and Theory (World Scientific, Singapore, 2018).


Figure 1.31: Fractional occupation probabilities, $v_{j}^{2}$, of single-particle orbitals in ${ }^{112-124} \mathrm{Sn}$. The uncertainties in $v_{j}^{2}$ shown are typical for each subshell (other uncertainties are omitted to avoid cluttering the figure). (The data are taken from Fleming D.G. (1982), Can. J. Phys. 60, 428.)

## Outline

- Isospin
- Pairing
- Deformation: Rotation


## Separation of rotational degree of freedom

Factorization of wave function $\left|\psi_{J K M}\right\rangle \quad J=K, K+1, \ldots$

$$
\begin{aligned}
& \left|\phi_{K}\right\rangle \quad \text { Intrinsic structure } \quad(K \equiv \text { a.m. projection on symmetry axis }) \\
& \mathcal{D}_{M K}^{J}(\vartheta) \quad \text { Rotational motion in Euler angles } \vartheta
\end{aligned}
$$

Rotational energy

$$
\text { Coriolis } \underbrace{K=1 / 2)}
$$

$$
E(J)=E_{0}+A\left[J(J+1)+a(-)^{J+1 / 2}\left(J+\frac{1}{2}\right)\right] \quad A \equiv \frac{\hbar^{2}}{2 \mathcal{J}}
$$

Rotational relations (Alaga rules) on electromagnetic transitions

$$
B\left(E 2 ; J_{i} \rightarrow J_{f}\right) \propto\left(J_{i} K 20 \mid J_{f} K\right)^{2}\left(e Q_{0}\right)^{2} \quad e Q_{0} \propto\left\langle\phi_{K}\right| Q_{2,0}\left|\phi_{K}\right\rangle
$$





Figure 1.58: The low-lying states of ${ }^{168} \mathrm{Er}$ arranged into rotational bands. The positive-parity bands are shown also in Figure 1.59. (The data are taken from Nuclear Data Sheets.)

Figure from D. J. Rowe and J. L. Wood, Fundamentals of Nuclear Models: Foundational Models (World Scientific, Singapore, 2010).


Figure 1.59: Plots of the excitation energies of the low-lying positive-parity states of ${ }^{168} \mathrm{Er}$ (cf. Figure 1.58) versus $I(I+1)$, cf. Equation (1.53) to reveal rotational behaviour. Note the left and right energy scales, with the lefthand scale applying to all but the groundstate band.

Figure from D. J. Rowe and J. L. Wood, Fundamentals of Nuclear Models: Foundational Models (World Scientific, Singapore, 2010).


Figure from D. J. Rowe and J. L. Wood, Fundamentals of Nuclear Models: Foundational Models (World Scientific, Singapore, 2010).

## Separation of rotational degree of freedom

Factorization of wave function $\left|\psi_{J K M}\right\rangle \quad J=K, K+1, \ldots$

$$
\begin{aligned}
& \left|\phi_{K}\right\rangle \quad \text { Intrinsic structure } \quad(K \equiv \text { a.m. projection on symmetry axis }) \\
& \mathcal{D}_{M K}^{J}(\vartheta) \quad \text { Rotational motion in Euler angles } \vartheta
\end{aligned}
$$

Rotational energy

$$
\text { Coriolis ( } \underbrace{K=1 / 2)}
$$

$$
E(J)=E_{0}+A[J(J+1)+\overbrace{a(-)^{J+1 / 2}\left(J+\frac{1}{2}\right)}] \quad A \equiv \frac{\hbar^{2}}{2 \mathcal{J}}
$$

Rotational relations (Alaga rules) on electromagnetic transitions

$$
B\left(E 2 ; J_{i} \rightarrow J_{f}\right) \propto\left(J_{i} K 20 \mid J_{f} K\right)^{2}\left(e Q_{0}\right)^{2} \quad e Q_{0} \propto\left\langle\phi_{K}\right| Q_{2,0}\left|\phi_{K}\right\rangle
$$





Figure 1.71: A Nilsson diagram for protons in nuclei with $50 \leq Z \leq 82$. Energies, in units of $\hbar \omega_{0}$, are plotted against the deformation parameter, $\epsilon$. Energy levels are labelled by their spherical shell model quantum numbers, $l$ and $j$, at $\epsilon=0$, and by the asymptotic quantum numbers $\Omega\left[N n_{z} \Lambda\right]$ for $\epsilon \neq 0$. (The figure is adapted from Lamm I.-L. (1969), Nucl. Phys. A125, 504.)

## Observed energy levels for $A=7$ nuclei



## Rotational features emerge in $a b$ initio calculations

P. Maris, M. A. Caprio, and J. P. Vary, Phys. Rev. C 91, 014310 (2015 C. W. Johnson, Phys. Rev. C 91, 034313 (2015).
M. A. Caprio, P. J. Fasano, P. Maris, A. E. McCoy, J. P. Vary, Eur. Phys. J. A 56, 120 (2020).
Valence shell structure? $\quad \mathrm{SU}(3)$
T. Dytrych et al., Phys. Rev. Lett. 111, 252501 (2013).

Multishell dynamics? $\quad \operatorname{Sp}(3, \mathbb{R})$
A. E. McCoy et al., Phys. Rev. Lett. 125, 102505 (2020).

Cluster rotation?




## Elliott SU(3) symmetry

Generators of $\mathrm{SU}(3) \supset \mathrm{SO}(3)$

$$
L_{M}^{(1)} \sim\left(b^{\dagger} \times \tilde{b}\right)_{M}^{(1)} \quad Q_{M}^{(2)} \sim\left(b^{\dagger} \times \tilde{b}\right)_{M}^{(2)}
$$

States classified into $\operatorname{SU}(3)$ irreps $\quad(\lambda, \mu)$

- States are correlated linear combinations of configurations over $\ell$-orbitals
- Branching of $\mathrm{SU}(3) \rightarrow \mathrm{SO}(3)$ gives rotational bands (in $L$ )



## $S p(3, \mathbb{R}) \supset U(3)$ dynamical symmetry for ${ }^{7} B e$



$$
H=\alpha C_{\mathrm{Sp}(3, \mathbb{R})}+\varepsilon H_{0}+\beta C_{\mathrm{SU}(3)}+a_{L} \mathbf{L}^{2}+a_{S} \mathbf{S}^{2}+\xi \mathbf{L} \cdot \mathbf{S}
$$

A. E. McCoy, M. A. Caprio, T. Dytrych, and P. J. Fasano, Phys. Rev. Lett. 125, 102505 (2020).

## Decomposition by U(3) content

Yrast band up to maximal "valence" angular momentum has $\mathrm{U}(3)$
$N_{\text {ex }}(\lambda, \mu)=0(3,0) S=1 / 2$



JISP16 (no Coulomb), SpNCCI, $N_{\sigma, \text { max }}=N_{\text {max }}=6, \hbar \omega=20 \mathrm{MeV}$

## FUNDAMENTALS of NUCLEAR MODELS

Foundational Models
David J Rowe John L Wood
$1 / 3$ world Scientific

## Chapter 1

Elements of nuclear structure


David Rowe, Playa del Carmen, 2003.

## Further reading

D. J. Rowe and J. L. Wood, Fundamentals of Nuclear Models: Foundational Models (World Scientific, Singapore, 2010).

```
http://www.worldscibooks.com/physics/6209.html
```

D. J. Rowe, Nuclear Collective Motion: Models and Theory (World Scientific, Singapore, 2018).
J. Suhonen, From Nucleons to Nucleus (Springer-Verlag, Berlin, 2007).
http://dx.doi.org/10.1007/978-3-540-48861-3
Richard F. Casten, Nuclear Structure from a Simple Perspective, 2ed (Oxford Univ. Press, 2000).
P. Ring and P. Schuck, The Nuclear Many-Body Problem (Springer-Verlag, New York, 1980).

