

An algebraic mean-field theory of nuclear shape-coexistence in nuclei

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Introduction

This contribution shows, without approximation, that the Hilbert space \mathbb{H}^A of an A -nucleon nucleus is a sum of subspaces

$$\mathbb{H}^A = \mathbb{H}_{\text{CM}} \otimes \sum_{\alpha\sigma} \mathbb{H}_{\alpha\sigma ST},$$

where \mathbb{H}_{CM} is a centre-of-mass Hilbert space and $\mathbb{H}_{\alpha\sigma ST}$ is the Hilbert space for a microscopic version of the unified model with an intrinsic state defined by an eigenstate with the quantum numbers $\{\sigma_1, \sigma_2, \sigma_3\}$ of a triaxial harmonic oscillator: S and T are spin and isospin quantum numbers, and α is a multiplicity index.

The subspaces $\mathbb{H}_{\alpha\sigma ST}$ are defined such that there are no isoscalar E2 transitions and no non-zero matrix elements of the many-nucleon kinetic energy of a nucleus between the states of different subspaces. Thus, they are ideal collective model subspaces and it is possible, by a simple algebraic extension of mean-field theory to explore their dynamics and energy-level spectra.

A first result to emerge is that the low-energy rotational states of heavy strongly deformed nuclei lie predominantly in spherical harmonic-oscillator shells of energy $\sim 20\hbar\omega$ above those of a standard valence shell. A second result is the large number of coexisting states of widely different deformation that fall into the low-energy region of a nucleus, very few of which could be coupled by a two-body interaction.

Particularly significant is the observation that the many developments in the beyond-mean-field and Monte-Carlo methods, reviewed at this workshop by Bender, Rodriguez and Otsuka, already provide the essential computational methods needed for applications of the algebraic mean-field developments.

Shape co-existence and algebraic mean-field theory

Nuclear shapes were among the first properties of nuclei to be measured.

T. Schmidt. *Naturwiss*, 28:565, 1940

(see K. Lieb: *Hyperfine Interactions*,
136/137:783–802, 2001)

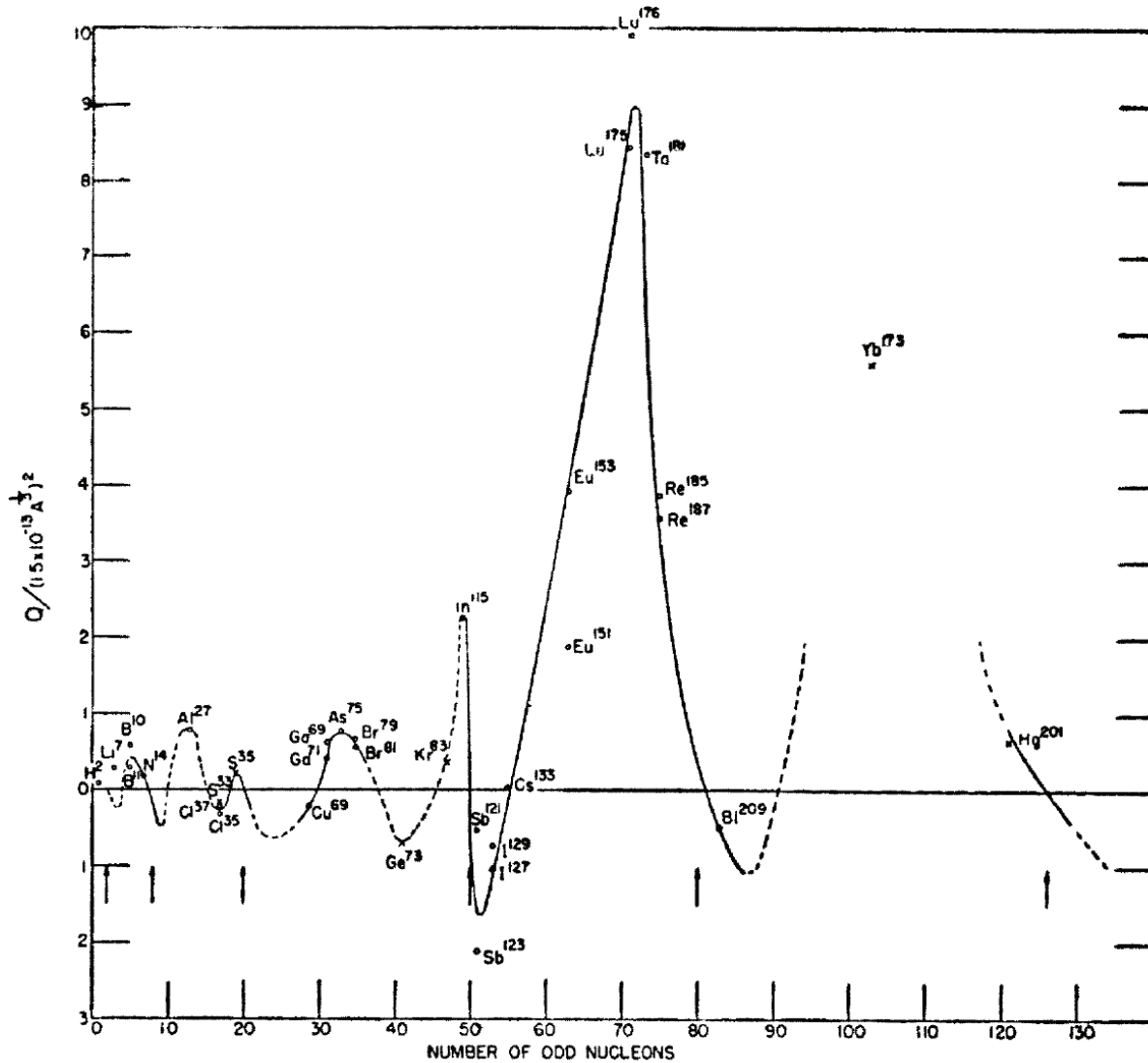
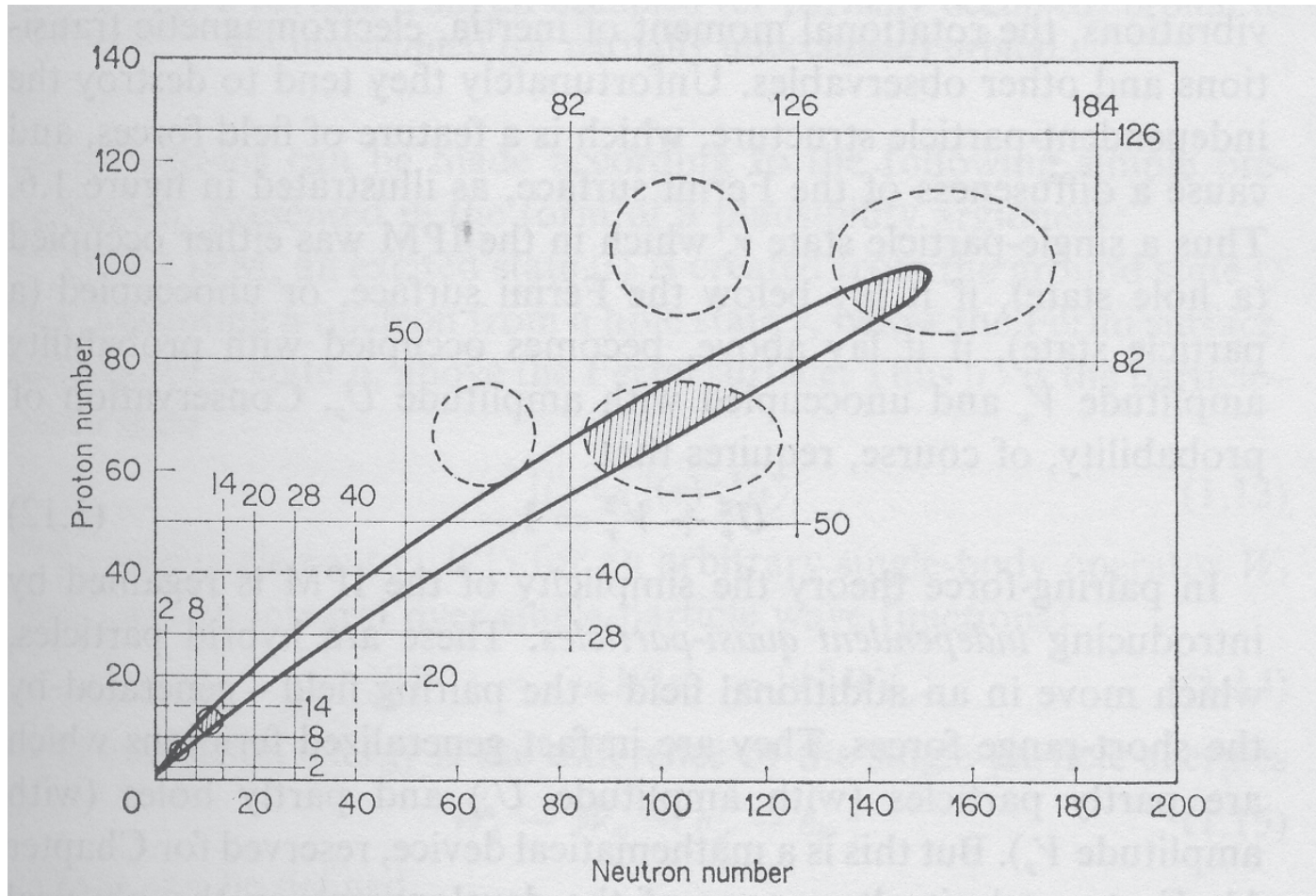


Figure from
C. H. Townes, H. M. Foley, and W. Low. Nuclear
quadrupole moments and nuclear shell
structure. *Phys. Rev.*, 76:1415–1416, 1949.

The early days of the spherical shell model

The general perception

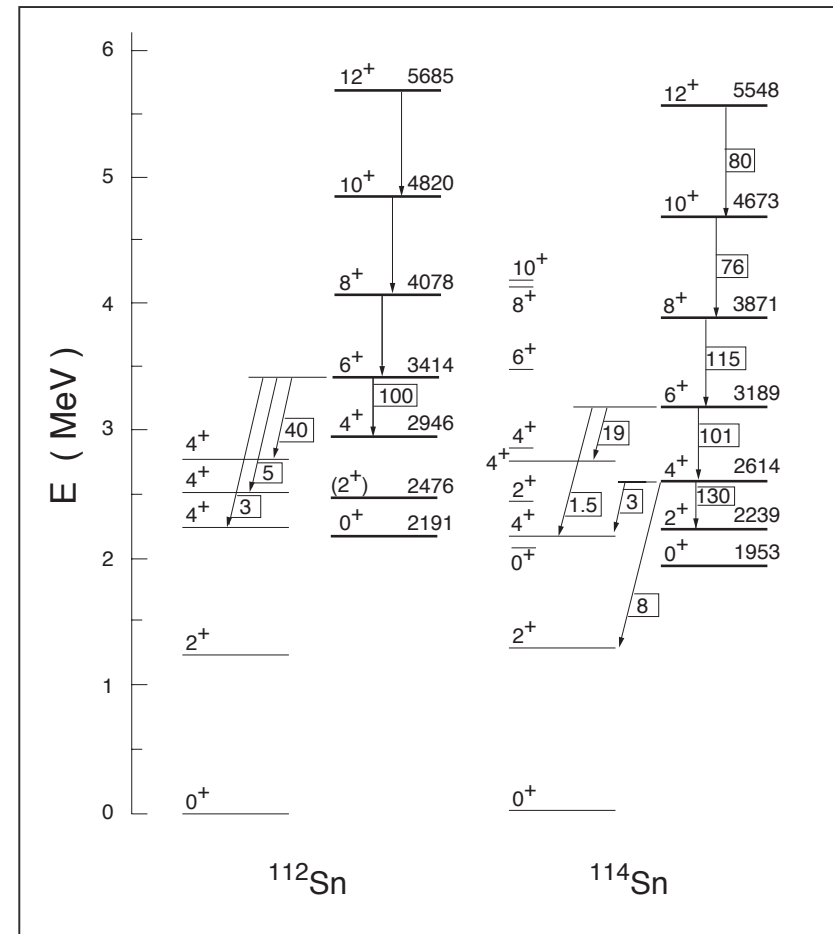
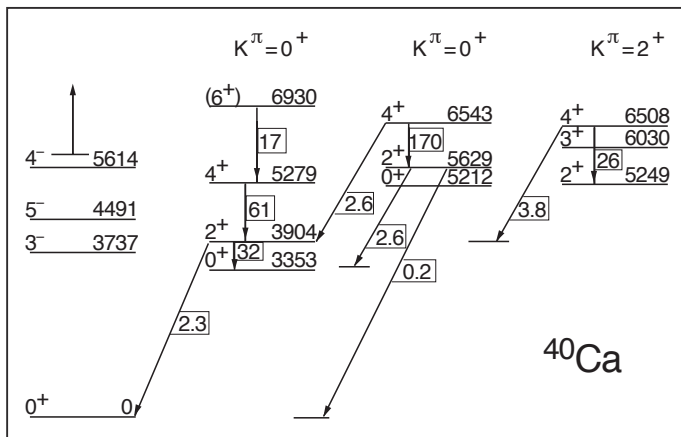
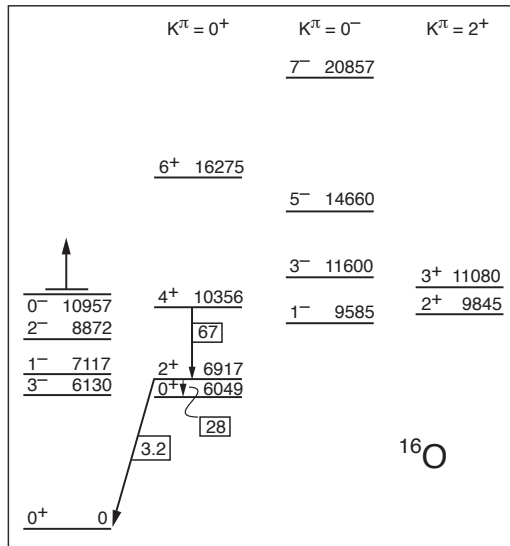
**CLOSED AND SINGLY-CLOSED SHELL NUCLEI ARE ESSENTIALLY SPHERICAL
NUCLEI IN THE MIDDLE OF DOUBLY OPEN SHELL ARE DEFORMED**



(Figure from:Marshalek et al. 1963)

Shape coexistence

- Strongly deformed nuclei are not restricted to the middles of doubly open-shell nuclei.
e.g., the first excited state of ^{16}O is the ground state of a rotational band (Morinaga 1956).
- They are now observed in essentially all nuclei (shape coexistence: Heyde and Wood 1983, 1992).**



EXCITED STATES OF CLOSED-SHELL NUCLEI ARE OPEN-SHELL STATES

THE ALGEBRAIC STRUCTURE OF NUCLEAR PHYSICS

- Many-nucleon quantum mechanics as an algebraic model.
It is really simple compared with it might have been.
- The spherical shell model perspective.
Three classes of nuclear states.
- Pair coupling of nucleons --- spherical nuclei.
Singly closed-shell states are spherical.
- Deformation aligned coupling of nucleons --- deformed rotational nuclei.
Doubly open-shell states are deformed.
- The standard Hartree-Fock and Hartree-Fock-Bogolyubov mean-field theories.
- **ALGEBRAIC MEAN-FIELD THEORY:**
It is a unification and generalization of Lie algebra and mean-field theory. It also provides a microscopic version of the unified model and an understanding of shape coexistence.

Many-nucleon quantum mechanics is an algebraic model

It starts with the quantization of nucleon position and momentum coordinates

$$\{x_{ni}\}, \quad \{p_{ni}\}, \quad n = 1, \dots, A, \quad i = 1, 2, 3.$$

$$x_{ni} \rightarrow \hat{x}_{ni}, \quad p_{ni} \rightarrow \hat{p}_{ni},$$
$$\hat{x}_{ni}\psi(x) = x_{ni}\psi(x), \quad \hat{p}_{ni}\psi(x) = -i\hbar \frac{\partial}{\partial x_{ni}}\psi(x).$$

This gives the Heisenberg-Weyl (HW) Lie algebra of quantum mechanics

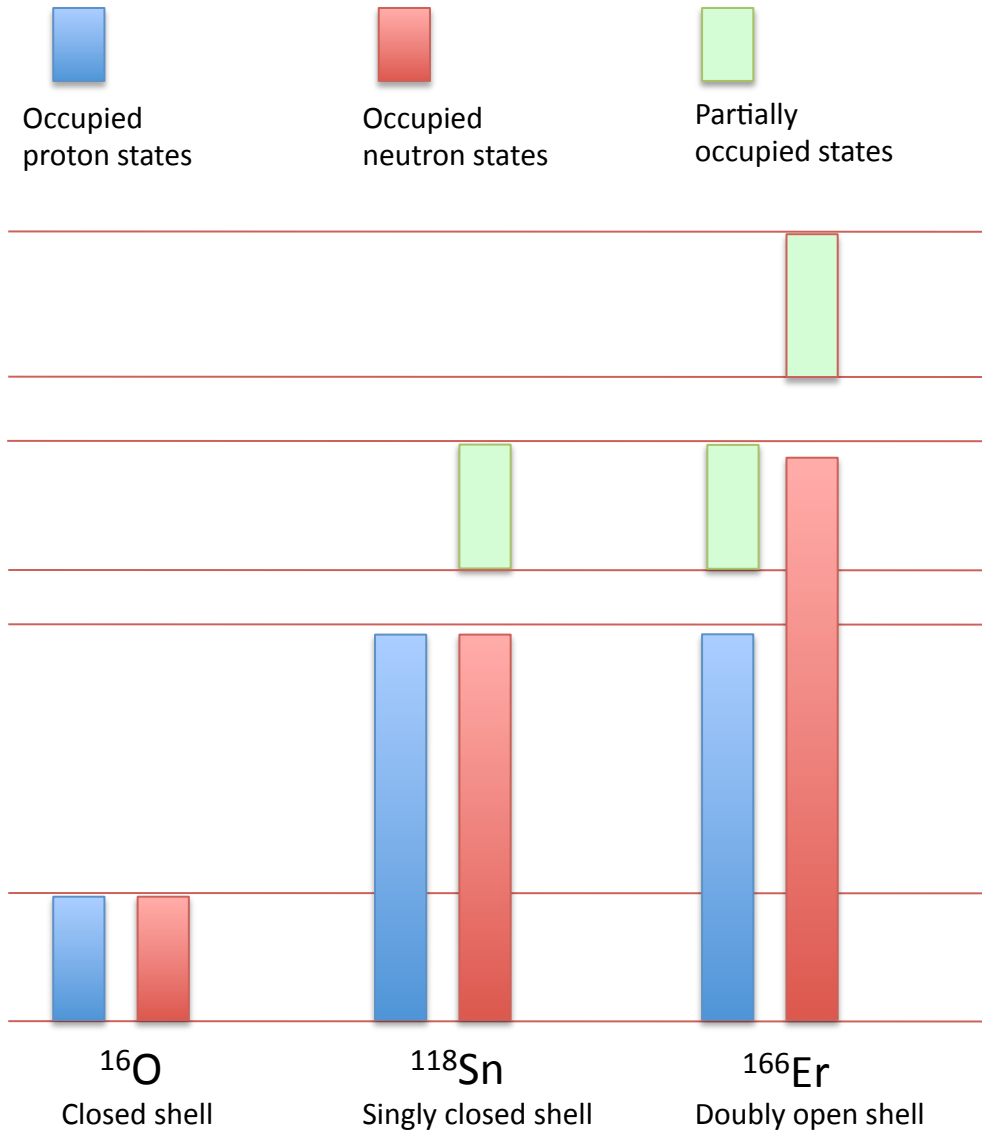
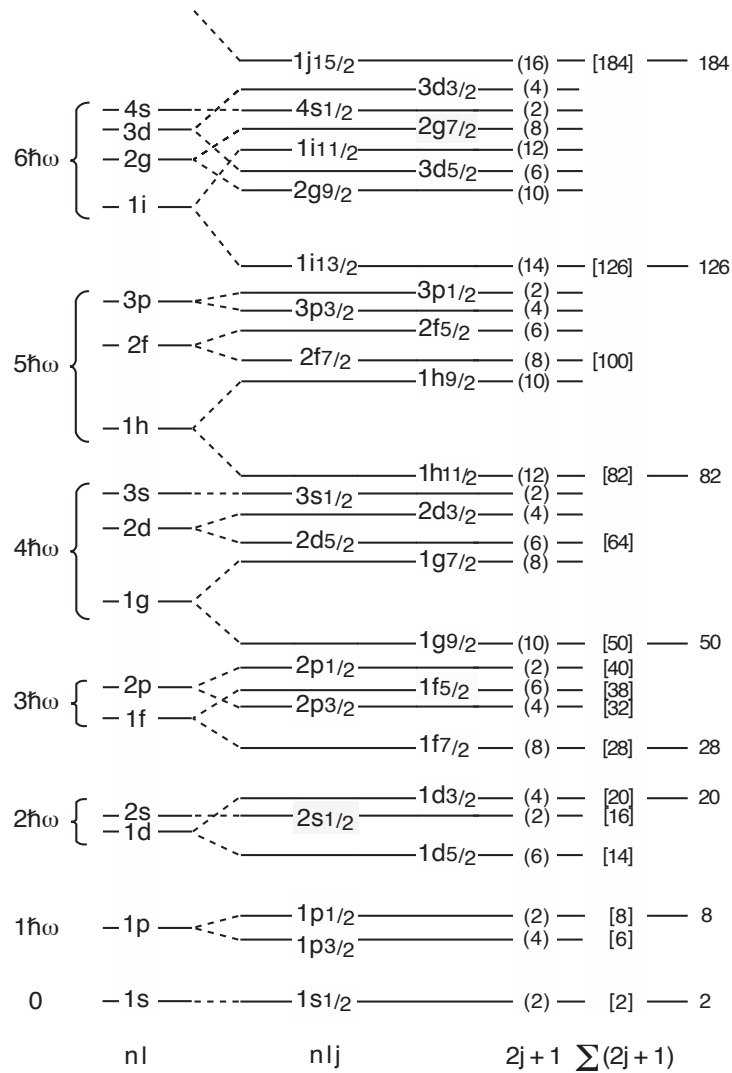
$$[\hat{x}_{ni}, \hat{p}_{mj}] = i\hbar \delta_{n,m} \delta_{i,j}$$

The quantum mechanics of an A-nucleon nucleus is a fully anti-symmetric tensor product of A copies of the single-particle representations of the group

$$\text{HW} \times \text{SU}(2)_S \times \text{SU}(2)_T.$$

⇒ The many-nucleon Hilbert space is spanned by independent-particle states (Slater determinants). Note, however, that an independent-particle basis does not imply an independent-particle approximation.

Three classes of nuclear states in the spherical harmonic-oscillator shell model



The shell model is a very poor approximation for doubly open-shell states

Pair-coupling of nucleons in singly closed-shell states

There are two basic coupling schemes in nuclear physics (Mottelson 1962)

PAIR COUPLING AND DEFORMATION-ALIGNED COUPLING

Pair coupling is the standard jj coupling-scheme of the spherical shell model. It favours the coupling of nucleon in pairs to states of zero angular momentum.

Basis states for this coupling scheme are generated by the raising operators of Kerman's so-called quasi-spin algebra acting on quasi-spin lowest-weight states.

$$\begin{aligned}\hat{S}_+^j &= \sum_m a_{jm}^\dagger a_{j\bar{m}}^\dagger = \sum_m (-1)^{j+m} a_{jm}^\dagger a_{j,-m}^\dagger, \\ \hat{S}_-^j &= (\hat{S}_+^j)^\dagger = \sum_m (-1)^{j+m} a^{j,-m} a^{j,m}, \\ \hat{S}_0^j &= \frac{1}{2} \sum_m (a_{jm}^\dagger a^{jm} - 1).\end{aligned}$$

Pair coupling is favoured for nucleons of the same type, as in singly closed-shell states.

Deformation-aligned coupling of nucleons in doubly open-shell states

It is apparent, from numerous experimental observations, that states, in which there are both neutrons and protons in open shells, are deformed and rotational. This is attributed to the lowering in energy of states in which the densities of many nucleons have maximal overlaps with one another.

Thus, for neutrons with wave functions $\{\psi_{jm}^{(n)}\}$ and protons with wave functions $\{\psi_{j'm}^{(p)}\}$, the strongly interacting aligned combinations are of the form

$$\Psi = \psi_{j,1/2}^{(n)} \psi_{j,-1/2}^{(n)} \psi_{j,3/2}^{(n)} \psi_{j,-3/2}^{(n)} \cdots \psi_{j',1/2}^{(p)} \psi_{j',-1/2}^{(p)} \psi_{j',3/2}^{(p)} \psi_{j',-3/2}^{(p)} \cdots \quad (\text{prolate})$$

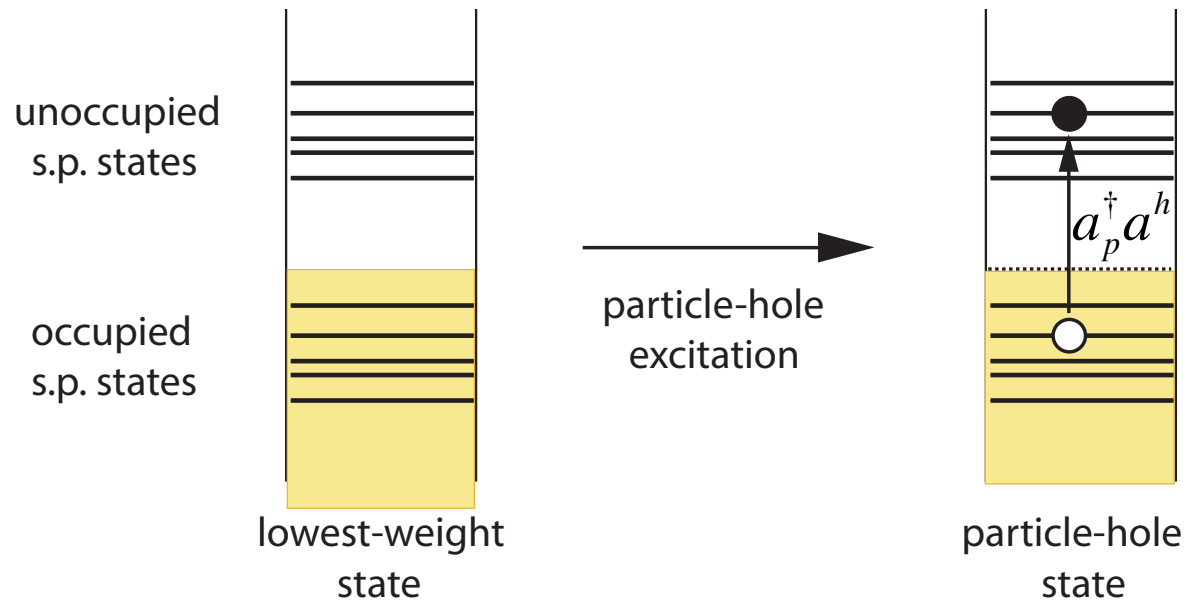
or

$$\Psi = \psi_{j,j}^{(n)} \psi_{j,-j}^{(n)} \psi_{j,j-1}^{(n)} \psi_{j,-j+1}^{(n)} \cdots \psi_{j',j'}^{(p)} \psi_{j',-j'}^{(p)} \psi_{j',j'-1}^{(p)} \psi_{j',-j'+1}^{(p)} \cdots \quad (\text{oblate})$$

More generally one can have deformation-aligned states of many j values. Such states are Slater determinants of the type that emerge in Hartree-Fock theory: they define the intrinsic state of a fully quantal unified model.

The Pauli principle allows two unlike nucleons (a neutron and a proton) to be in the same state. Thus, aligned coupling is more effective than pair coupling for doubly open-shell states.

Mean-field theory from a Lie algebra perspective



Any Slater determinant of occupied single-particle states is a lowest-weight state for a unitary irrep of the Lie algebra of one-body operators with raising and lowering operators given, respectively, by particle-hole creation and particle-hole annihilation operators

The set of all lowest-weight states is a very special manifold:

it is an orbit of the group of one-body unitary transformation,

it is a classical phase space. and

it spans the Hilbert space for the quantum mechanics of the Lie algebra.

The minimum-energy lowest-weight is even more special:

it is a minimum-uncertainty coherent state.

Properties of a minimum-energy particle-hole state

- Starting from any lowest-weight state for an irrep of a Lie algebra and a set of raising operators, one can construct a basis for the Hilbert space of the irrep.

- A minimal energy lowest-weight state is special because it is not coupled by the Hamiltonian to any state excited from the lowest-weight state by an elementary (e.g., particle-hole) raising operator, e.g.,

$$\langle \phi | \hat{H} a_p^\dagger a^h | \phi \rangle = 0$$

- The smooth manifold of A-particle Slater determinants is a classical phase space and the infinite set of A-particle Slater determinants spans the Hilbert space of the A-nucleon nucleus.
- A Hartree-Fock minimum-energy Slater determinant, if spherically symmetric, is in one-to-one correspondence with a classical equilibrium state and is a variational approximation to the quantum-mechanical ground state of the nucleus.
- The small-amplitude time-dependent Hartree-Fock ‘normal-mode’ equations correspond, in quantum mechanics, to the one-phonon vibrational excitations of the RPA (Random Phase Approximation), as shown in 1966.
- If the minimum-energy Slater determinant is not spherically symmetric, its rotated states are all stationary states of zero angular momentum consistent with the Nambu-Goldstone interpretation of a broken symmetry. The rotated stationary states are then all classical equilibrium states and rotational states in quantum mechanics.
- The RPA/normal-mode equations then give the intrinsic vibrational states of a microscopic version of the unified model.

Parallel properties apply to the minimum-energy lowest-weight state of any algebraic model.

Mean-field theory for an algebraic model

Mean-field methods can be applied to any irreducible representation of a Lie algebra that has a lowest- (and/or highest-) weight state.

(It can also be applied to irreps without lowest or highest weight states but it then has fewer and less useful properties.)

If G is the dynamical group of an algebraic model, a set of all possible lowest-weight states is an orbit of the group G ; i.e., it is the set of states generated by the transformations of a given lowest-weight state by the elements of the G .

This set of lowest-weight states is the classical phase space of all possible mean-field states and it spans a Hilbert space for its quantisation

A minimum-energy lowest-weight state invariably has additional and invaluable properties.

Algebraic mean-field theory

Algebraic mean-field theory is simply the extension of Hartree-Fock theory to any algebraic model whose dynamical group has a lowest-weight state. The lowest-weight state then corresponds to a particle-hole vacuum state, and the raising and lowering operators, correspond to particle-hole creation and annihilation operators.

Such an extension is useful when the Hilbert space of a nucleus can be expressed as a sum of the Hilbert space for irreps of a suitable algebraic collective model.

It is particularly useful when the irreps are those of a collective model that has a dynamical group and a Lie algebra that contains the nuclear quadrupole moments, the angular-momentum operators, and the nuclear kinetic energy. The smallest Lie group that satisfies these condition in the so-called symplectic group $Sp(3,R)$.

The decomposition of the Hilbert space of a nucleus into irreducible $Sp(3,R)$ subspaces is optimal because these Hilbert subspaces are ideal collective model spaces in the sense that they have no non-zero E2 transitions nor matrix elements of the nuclear kinetic energy between their states.

The plan is to calculate the properties of the pure unmixed collective model states for a reasonable many-nucleon Hamiltonian, and subsequently explore the mixing of these states both theoretically and experimentally.

The $\text{Sp}(3, \mathbb{R})$ Lie algebra

The $\text{Sp}(3, \mathbb{R})$ Lie algebra consists of all bilinear combinations of the nucleon position and momentum operators. It includes the following:

$$\hat{Q}_{ij} = \sum_n \hat{x}_{ni} \hat{x}_{nj} = \frac{1}{2a^2} (2\hat{Q}_{ij} + \hat{A}_{ij} + \hat{B}_{ij}), \quad (\text{monopole, quadrupole moments})$$

$$\hat{K}_{ij} = \sum_n \hat{p}_{ni} \hat{p}_{nj} = \frac{1}{2} a^2 \hbar^2 (2\hat{Q}_{ij} \hat{A}_{ij} - \hat{B}_{ij}), \quad (\text{kinetic energy tensor})$$

$$\hat{P}_{ij} = \sum_n (\hat{x}_{ni} \hat{p}_{nj} + \hat{p}_{ni} \hat{x}_{nj}) = i\hbar (\hat{A}_{ij} - \hat{B}_{ij}), \quad (\text{infinitesimal generators of deformation})$$

$$\hbar L_{ij} = \sum_n (\hat{x}_{ni} \hat{p}_{nj} - \hat{p}_{ni} \hat{x}_{nj}) = -i(\hat{C}_{ij} - \hat{C}_{ji}), \quad (\text{angular momentum operators})$$

with n summed over the effective number of $A-1$ nucleons (with exclusion of the linear combinations that involve the nuclear centre-of-mass degrees of freedom).

These elements of the $\text{Sp}(3, \mathbb{R})$ Lie algebra are all required elements of a many-nucleon theory of collective states.

The $\text{Sp}(3, \mathbb{R})$ Lie algebra is a spectrum generating algebra for any three-dimensional harmonic oscillator

If the nucleon position and momentum coordinate are expressed in terms of harmonic oscillator raising and lower operators

$$\hat{x}_{ni} = \frac{1}{\sqrt{2} a_i} (c_{ni}^\dagger + c_{ni}), \quad \hat{p}_{ni} = i\hbar \frac{a_i}{\sqrt{2}} (c_{ni}^\dagger - c_{ni})$$

where $a_i = \sqrt{M\omega_i / \hbar}$ are arbitrary units of inverse length for a generally tri-axial harmonic oscillator with a triple of frequencies $\{\omega_1, \omega_2, \omega_3\}$. The $\text{Sp}(3, \mathbb{R})$ Lie algebra is expressed in terms of the operators

$$\begin{aligned} \hat{A}_{ij} = \hat{A}_{ji} &= \sum_n c_{ni}^\dagger c_{nj}^\dagger, & \hat{B}_{ij} = \hat{B}_{ji} &= \sum_n c_{ni} c_{nj}, \\ \hat{C}_{ij} &= \sum_n (c_{ni}^\dagger c_{nj} + \frac{1}{2} \delta_{i,j}), & \hat{Q}_{ij} &= \frac{1}{2} (\hat{C}_{ij} + \hat{C}_{ji}) \end{aligned}$$

with n summed over the effective number of A-1 nucleons (with exclusion of the linear combinations that involve the nuclear centre-of-mass degrees of freedom).

Note that the above basis for the $\text{Sp}(3, \mathbb{R})$ Lie algebra is defined for any choice of the harmonic-oscillator frequencies.

Sp(3,ℝ) irreps from a mean-field perspective

An Sp(3,ℝ) irrep is defined by the quantum numbers $(\sigma_1, \sigma_2, \sigma_3)$ of a lowest-weight state $|\phi\rangle$, for which

$$\begin{aligned}\hat{B}_{ij} |\phi\rangle &= 0, \quad i, j = 1, 2, 3, \\ \hat{C}_{ij} |\phi\rangle &= 0, \quad i < j = 1, 2, 3, \\ \hat{C}_{ii} |\phi\rangle &= \sigma_i |\phi\rangle, \quad i = 1, 2, 3,\end{aligned}$$

However, there are many lowest-weight states, which satisfy these equations: they are given by the eigenstates

$$\hat{H}_0(\omega) = \frac{1}{2} \sum_i \hbar \omega_i \hat{C}_{ii}$$

for arbitrary values of $\omega = \{\omega_1, \omega_2, \omega_3\}$.

Thus, for a given nuclear Hamiltonian, one can select the lowest-weight state for which the energy $\langle \phi(\omega) | \hat{H} | \phi(\omega) \rangle$ is a minimum. This minimum-energy lowest-weight state will be given when the mean-field that it generates has the same shape as its density distribution; **i.e., when the shape-consistency condition is satisfied:**

$$\sigma_1 \omega_1 = \sigma_2 \omega_2 = \sigma_3 \omega_3$$

Together with a knowledge of the desired nuclear volume, the shape-consistent mean-field state is simple to determine, whether or not it is a Slater determinant: it is an eigenstate of a harmonic oscillator.

Some predictions of $Sp(3, \mathbb{R})$ mean-field theory?

The Hilbert space of a nucleus is a sum of ideal collective model spaces: i.e., irreducible $Sp(3, \mathbb{R})$ subspaces for which there are no E2 transition matrix elements between different subspaces.

Each irrep has a lowest-weight state that is an eigenstate of a spherical harmonic-oscillator Hamiltonian of energy $N_0 \hbar \omega_0$ and a shape-consistent lowest-weight state of triaxial harmonic-oscillator energy $E_\sigma \hbar \omega_0 = (\sigma_1 \omega_1 + \sigma_2 \omega_2 + \sigma_3 \omega_3) \hbar \omega_0$.

The magnitude of the difference $(N_0 - E_\sigma) \hbar \omega_0$ is remarkably large for irreps of large deformation as characterised by the values of $2\lambda + \mu$. Also remarkable is the number and the wide range of strongly deformed irreps that are predicted to fall into and below the expectations of the spherical shell model.

^{12}C				
N_0	λ	μ	$2\lambda + \mu$	E_σ
24.5	0	4	4	23.75
28.5	12	0	24	24.27
26.5	6	2	14	24.68
30.5	10	2	22	26.91
32.5	12	2	26	27.90

^{16}O				
N_0	λ	μ	$2\lambda + \mu$	E_σ
34.5	0	0	0	34.50
38.5	8	4	20	35.68
36.5	4	2	10	35.78
46.5	24	0	48	36.30
42.5	16	2	34	36.61
40.5	10	4	28	36.86

^{168}Er				
N_0	λ	μ	$2\lambda + \mu$	E_σ
812.5	30	8	68	811.11
824.5	96	20	212	811.38
822.5	82	26	190	811.47
826.5	104	20	228	811.49
814.5	40	16	96	811.51
820.5	70	28	168	811.53
816.5	52	20	124	811.58
818.5	60	26	146	811.59
828.5	114	16	244	811.66

$$N_0 = \sigma_1 + \sigma_2 + \sigma_3, \quad \lambda = \sigma_1 - \sigma_2, \quad \mu = \sigma_2 - \sigma_3,$$

$$E_\sigma = \hbar(\omega_1 \sigma_1 + \omega_2 \sigma_2 + \omega_3 \sigma_3)$$

The inclusion of spin and isospin

Irreducible $Sp(3, \mathbb{R})$ subspaces can be further labelled by their spins and isospins and classified by the quantum numbers of the groups

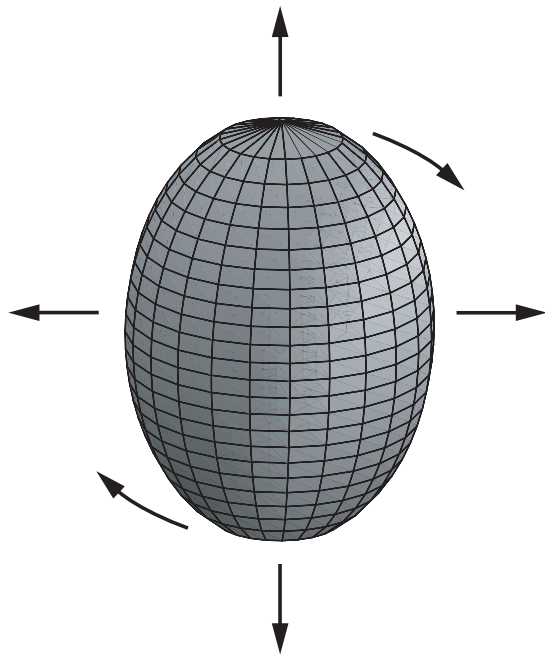
$$Sp(3, \mathbb{R}) \times U(4) \supset Sp(3, \mathbb{R}) \times SU(2)_S \times SU(2)_T$$

where $U(4)$ is Wigner's supermultiplet group.

The inclusion of these extra degrees of freedom is essential for a complete algebraic mean-field theory of doubly open-shell nuclei. However, for present purposes, it will suffice to note that the lowest-energy states of nuclei are predominantly those of maximum space symmetry.

The unified model

A unified model of nuclear rotational states is characterised by an intrinsic state $|\phi\rangle$ that is an eigenstate of each of its commuting quadrupole moments. The orientation of the intrinsic state is then uniquely defined, to within the rotations of an intrinsic symmetry group that leaves its quadrupole moments invariant.



Thus, for a small rotation $|\phi\rangle \rightarrow |\phi(\Omega)\rangle$ of a triaxial intrinsic state, it is understood in the unified model that

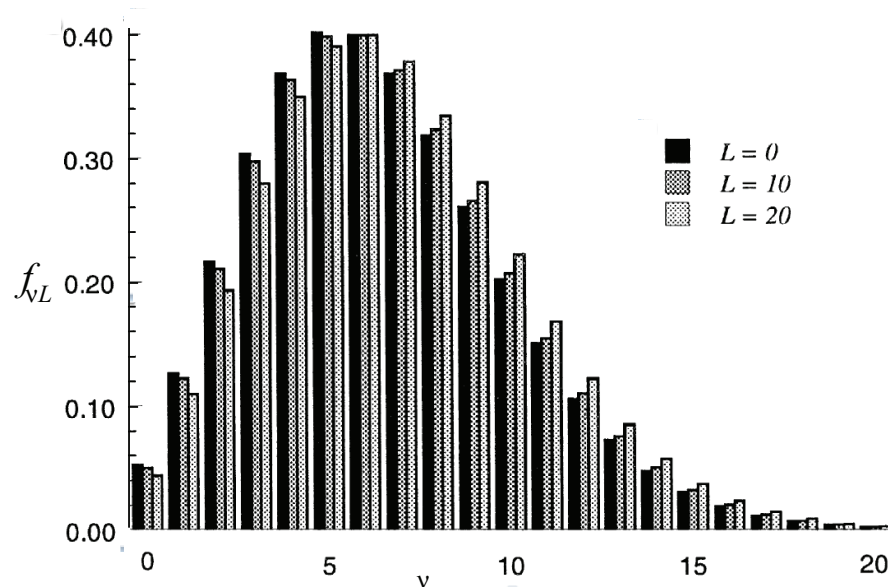
$$\langle\phi|\phi(\Omega)\rangle = \delta(\Omega)$$

This is only possible in quantum mechanics in a delta-function limit.

The remarkable fact is that this limit is achieved in the symplectic model in the large-deformation limit. Thus, the algebraic mean-field treatment of the symplectic model is a many-nucleon version of the unified model

Some preliminary results

We can now construct the intrinsic states for all collective model irreps of a nucleus and have the potential to calculate the properties of the states of these irreps and their mixing with the states of other irreps.



Amplitudes of the angular-momentum states projected from a shape-consistent state for an ^{166}Er irrep with

$$N_0 = 826.5 \quad \lambda = 78, \mu = 0,$$

$$\text{and} \quad N_0 \neq \sigma_1 + \sigma_2 + \sigma_3$$

The figure shows the angular-momentum components of states spread over ~ 15 spherical harmonic-oscillator shells of which the lowest is at an energy of $\sim 10\hbar\omega$ in spherical harmonic oscillator units above that of a conventional shell model calculation for this nucleus.

Kinetic-energy moments of inertia

It is now possible (and straightforward for axially symmetric irreps) to calculate the intrinsic expectation values of any element of the $\text{Sp}(3, \mathbb{R})$ Lie algebra.

For example, the following table gives the expectation values of the nuclear kinetic energy in the above determined rotational states for ^{166}Er .

L	$K.E.$	$\frac{1}{2}L(L+1)/K.E.$
2	30	99.5
4	101	99.3
6	212	99.1
8	364	98.9
10	568	98.5
12	795	98.1
14	1,076	97.6
16	1,401	97.1

The kinetic-energy contribution to the moments of inertia for the 2+ rotational state (left).

Below are comparisons with observed moment-of-inertia values for rigid and irrotational-flow rotations

$$\mathcal{I}_{KE}/\hbar^2 = 99.5 \text{ MeV}^{-1}, \quad \mathcal{I}_{\text{expt}}/\hbar^2 = 37.6 \text{ MeV}^{-1}.$$

$$\mathcal{I}_{\text{rig}}/\hbar^2 = 84.4 \text{ MeV}^{-1}, \quad \mathcal{I}_{\text{irr}}/\hbar^2 = 5.8 \text{ MeV}^{-1}.$$

Note that the kinetic energies, for this calculation (which are accurately calculated subject to mistakes), are less than half the excitation energies of the observed rotational states and close to those of rigid-body flow.

The difference from experimental observations must be due to potential energy contributions and/or mixing of irreps.

Conclusions

- The standard spherical-shell model in a pair-coupling scheme is expected to describe the structure of the spherical states of closed and singly-closed-shell states of nuclei reasonably well but requires an impossibly large space to begin to describe the doubly open-shell rotational states of almost any nucleus.
- In contrast, the deformation-aligned symplectic coupling scheme is tailor made for the doubly open-shell states of all nuclei.
- The relevance of the symplectic coupling-scheme is exposed, as a result of three major developments: **the experimental observation of shape coexistence** associated with doubly open-shell states of almost all nuclei (Wood and Heyde 2016); **the emergence of $Sp(3,R)$ as an extraordinarily good dynamical symmetry** in the doubly open-shell states of light nuclei (Dytrych et al., LSU), and **its application in terms algebraic mean-field theory.**
- **Algebraic mean-field theory now provides a simple and rigorous framework for understanding the collective structure of the doubly open-shell states of essentially all nuclei.**

Remaining challenges

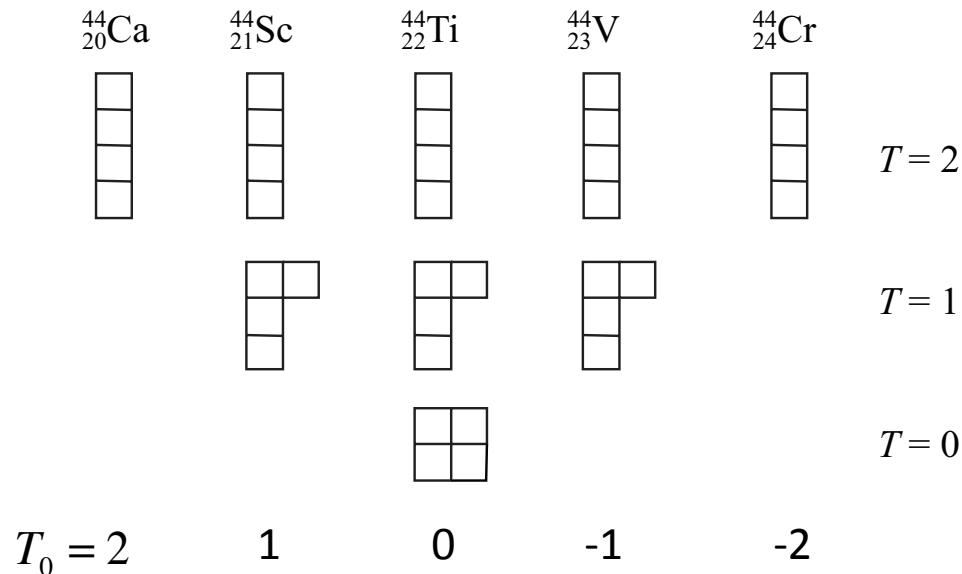
- **Develop the necessary technology for applications of the algebraic mean theory: e.g., efficient angular-momentum projection methods that exploit the harmonic oscillator and $SU(3)$ substructure of the intrinsic states as already done for axially symmetric irreps.**
- **Develop the theory for irreps with non-zero intrinsic spin states and for all nuclei: even, odd and odd-odd.**
- **Develop the techniques for mixing different collective states within the framework of quasi-dynamical symmetry. Find out why nuclear rotations are (or appear to be) axially symmetric.**

An addendum pertinent to the final discussions on a relationship between isospin and nuclear deformation

A relationship between isospin and nuclear deformation pertinent to the final discussion

Closed- and singly closed-shell states of nuclei, e.g. ^{44}Ca , are states of isospin $T = \frac{1}{2}(N - Z)$. Moreover, by a sequence of charge exchange reactions one can identify a sharply defined isobaric analog of the ^{44}Ca ground state in each of the other isobaric nuclei listed below.

However, whereas the four extra closed-shell core neutrons in ^{44}Ca are all in $T = 2$ anti-symmetric combinations, the neutrons and protons in ^{44}Sc , ^{44}Ti and ^{44}Cr can also be in states of $T = 1$ and ^{44}Ti can also be in a $T = 0$ state.



The Young diagrams shows that, in a state of maximal isospin, the nucleons are maximally antisymmetric, hence pair-coupled and and the nucleus is spherical. Similarly in a states of minimum isospin the nucleons are maximally symmetric and the nucleus is most likely to be deformed. This is illustrated dramatically by the energy level spectrum of ^{44}Ti .

The energy levels and isospins of ^{44}Ti ;
 note that, whereas the double isobaric analog T=2 state is spherical the lower-energy T=0 states exhibit rotational bands.

