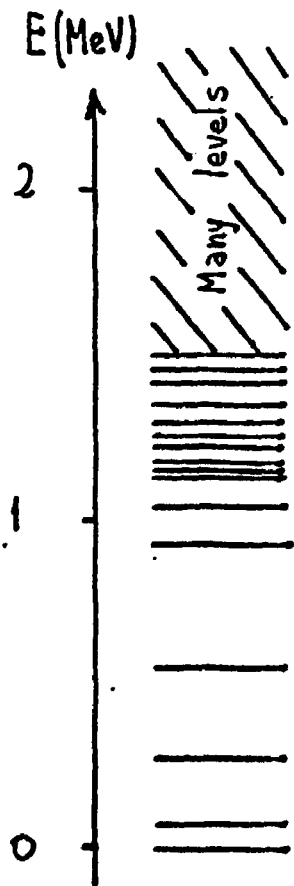


SYMMETRIES IN MOLECULAR AND NUCLEAR PHYSICS

F. Iachello - Dept. of Physics, Yale University

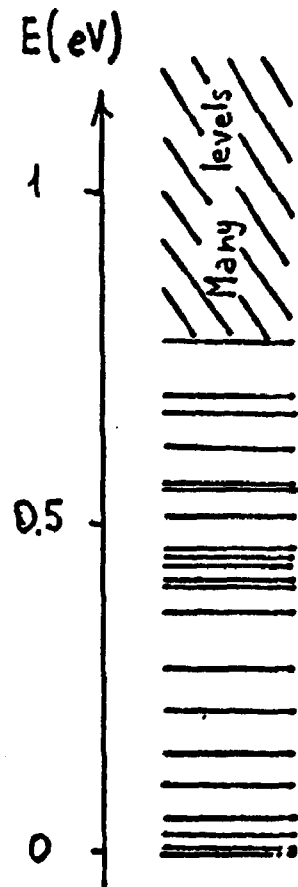
NUCLEI

$^{156}_{64}\text{Gd}_{92}$

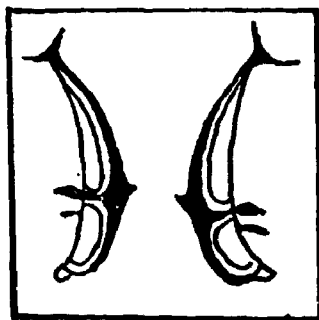


MOLECULES

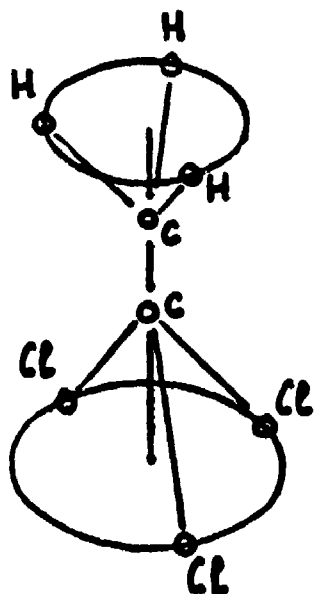
H_2



⇒ Symmetries



FLOOR PATTERN FOUND AT THE MEGARON
IN TYRINS, GREECE (ABOUT 1200 B.C.)



GEOMETRIC SYMMETRIES : THE TWISTED
 H_3C-CCl_3 MOLECULE (C_3 SYMMETRY)

Symmetries in physics

(i) Exact symmetries

(a) Poincaré invariance

$$\mathcal{L}(x) = \bar{\psi}(x) \left[i \gamma^\mu \frac{\partial}{\partial x^\mu} - m \right] \psi(x)$$

(b) Rotational invariance

$$H = \frac{\mathbf{p}^2}{2m} + V(r)$$

(ii) Dynamic symmetries

(a) The Hamiltonian has group structure

G

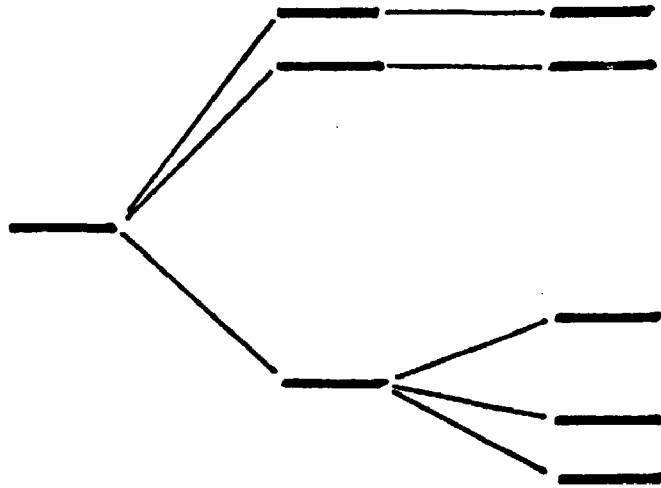
(b) The Hamiltonian can be written in terms only of Casimir invariants of a chain of groups $G \supset G' \supset \dots$

\Rightarrow Properties of the system given in closed form in terms of quantum numbers

\Rightarrow Classification scheme

\Rightarrow Splitting of the representations of G by successive addition of invariant

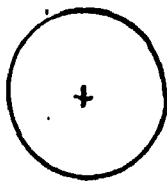
operators



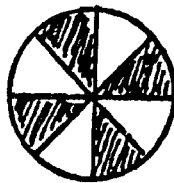
$G \supset G' \supset G'' \supset \dots$

$$H = \alpha C(G) + \alpha' C(G') + \alpha'' C(G'') + \dots$$

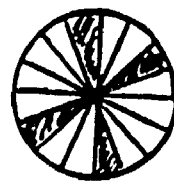
ILLUSTRATION OF DYNAMIC SYMMETRIES BY
REGULAR BREAKING OF ROTATIONAL INVARIANCE



$O(2)$



C_4

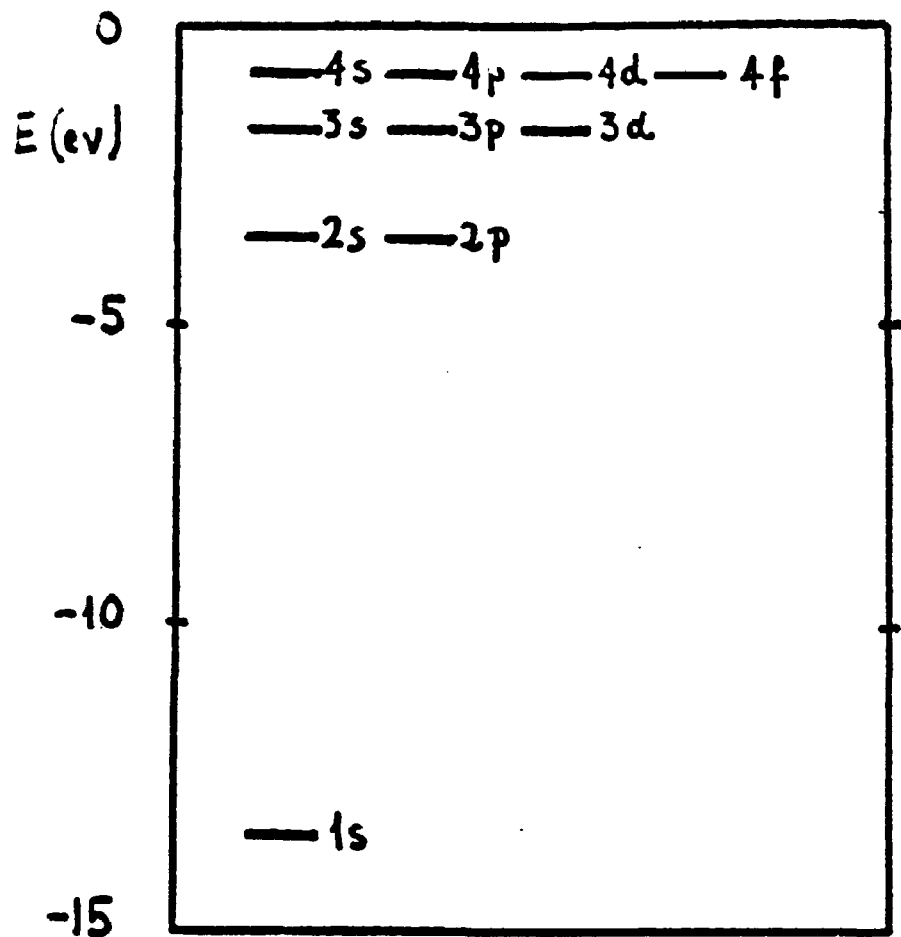


C_2

Examples

(a) The hydrogen atom

$$E(n, l, m_l) = -A/n^2$$



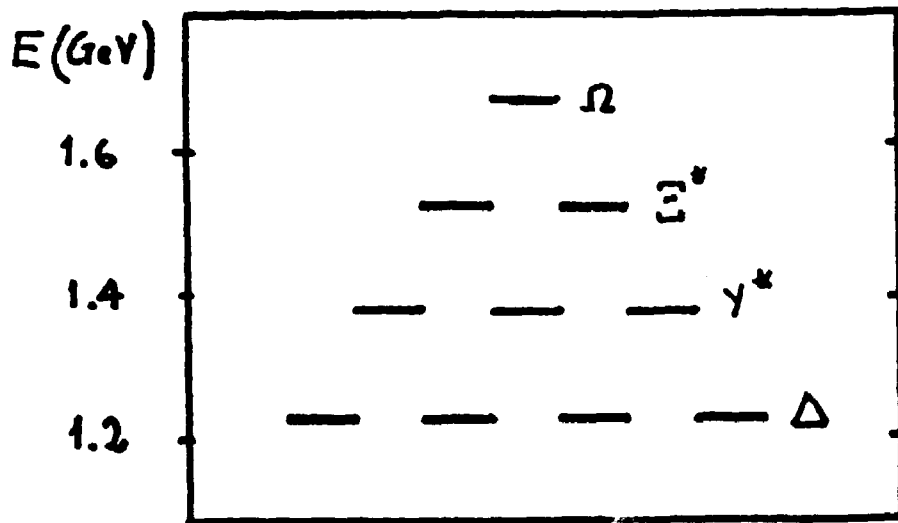
(b) Gell-Mann - Ne'eman $SU(3)$

$$\begin{pmatrix} u \\ d \\ s \end{pmatrix} \leftarrow \text{quarks}$$

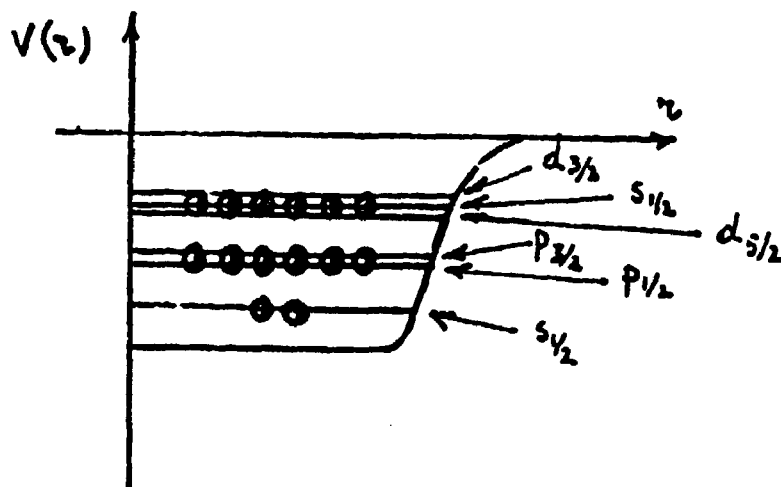
$$\begin{array}{ccccc} G & & G' & & G'' \\ \downarrow & & \downarrow & & \downarrow \\ SU(3) & \supset & SU(2) \otimes U(1) & \supset & SO(2) \otimes U(1) \\ \uparrow & & \uparrow & & \uparrow \\ I & & Y & & I_3 \end{array}$$

\Rightarrow Energy formula (Gell-Mann - Okubo)

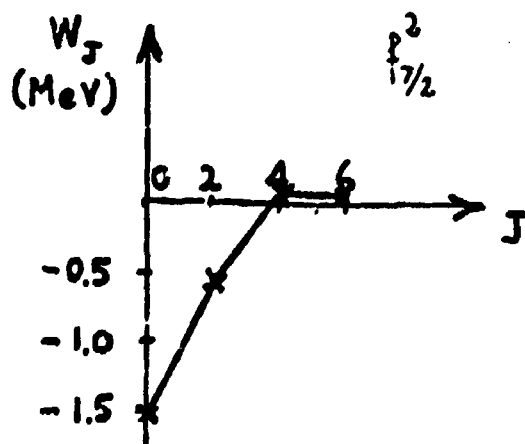
$$E(I, I_3, Y) = a + bY + c \left[\frac{1}{4} Y^2 - I(I+1) \right]$$



NUCLEAR STRUCTURE
CENTRAL FIELD



CORRELATIONS



COOPER PAIRS



S-BOSON



D-BOSON

INTERACTING BOSON MODEL

A. Arima and F. Iachello, *Ann. Phys. (N.Y.)* 99, 253 (1976);
111, 201 (1978); 123, 468 (1979).

(a) Building blocks

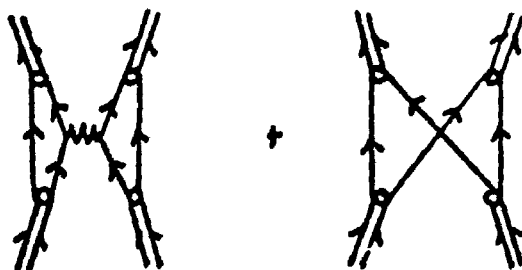
Boson operators

$$b_{\alpha}^{\dagger} (\alpha=1, \dots, 6) \equiv s^{\dagger}, d_{\mu}^{\dagger} (\mu=\pm 2, \pm 1, 0)$$

(b) Hamiltonian

$$H = E_0 + \sum_{\alpha\beta} \epsilon_{\alpha\beta} b_{\alpha}^{\dagger} b_{\beta} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} u_{\alpha\beta\gamma\delta} b_{\alpha}^{\dagger} b_{\beta}^{\dagger} b_{\gamma} b_{\delta}$$

Boson-boson interaction



(c) The interacting boson model $U(6)$

$$\begin{array}{l}
 \nearrow U(5) \supset SO(5) \supset SO(3) \supset SO(2) \quad (I) \\
 \rightarrow SU(3) \supset SO(3) \supset SO(2) \quad (II) \\
 \searrow SO(6) \supset SO(5) \supset SO(3) \supset SO(2) \quad (III)
 \end{array}$$

\Rightarrow Energy formulas

$$\begin{array}{l}
 \nearrow E(N, n_d, v, n_\Delta, L, M_L) = \epsilon n_d + \alpha n_d (n_d + 4) + \beta v (v + 3) + \gamma L(L + 1) \quad (I) \\
 \rightarrow E(N, \lambda, \mu, \kappa, L, M_L) = \kappa (\lambda^2 + \mu^2 + 2\mu + 3\lambda + 3\mu) + \kappa' L(L + 1) \quad (II) \\
 \searrow E(N, \sigma, \tau, \nu_\Delta, L, M_L) = A \sigma(\sigma + 4) + B \tau(\tau + 3) + C L(L + 1) \quad (III)
 \end{array}$$

\Rightarrow Classification scheme for even-even nuclei

(d) Dual interpretation of the bosons

(i) Quantal (or particle)

Correlated pairs of nucleons with $J=0$
and $J=2$ (Cooper-like pairs)

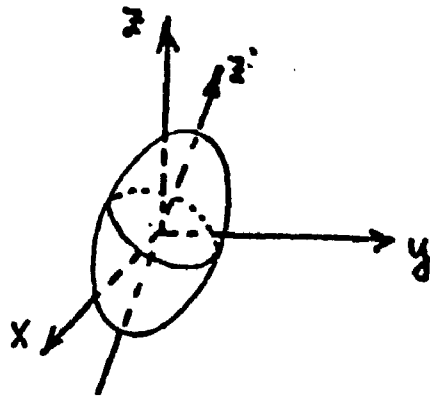


(ii) Classical (or geometric)

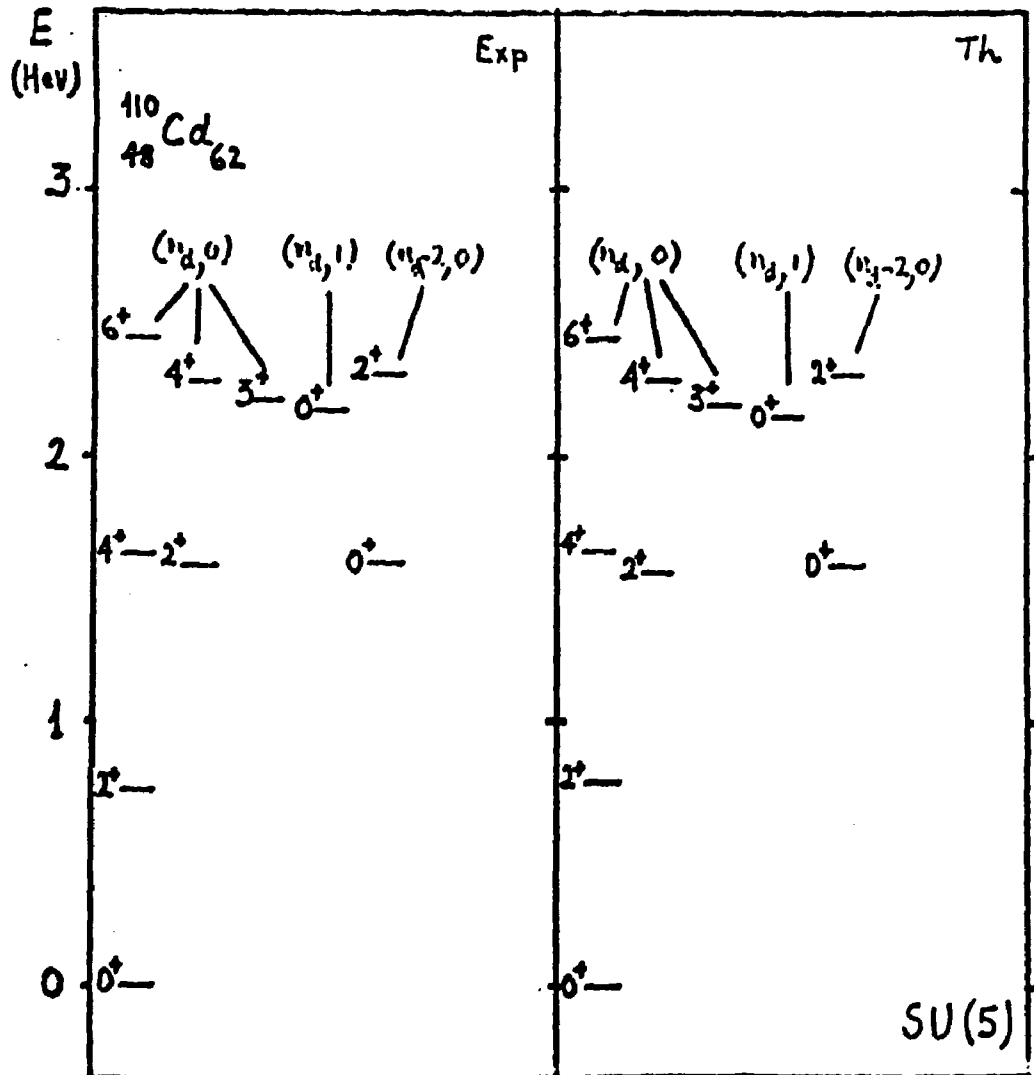
Coherent state

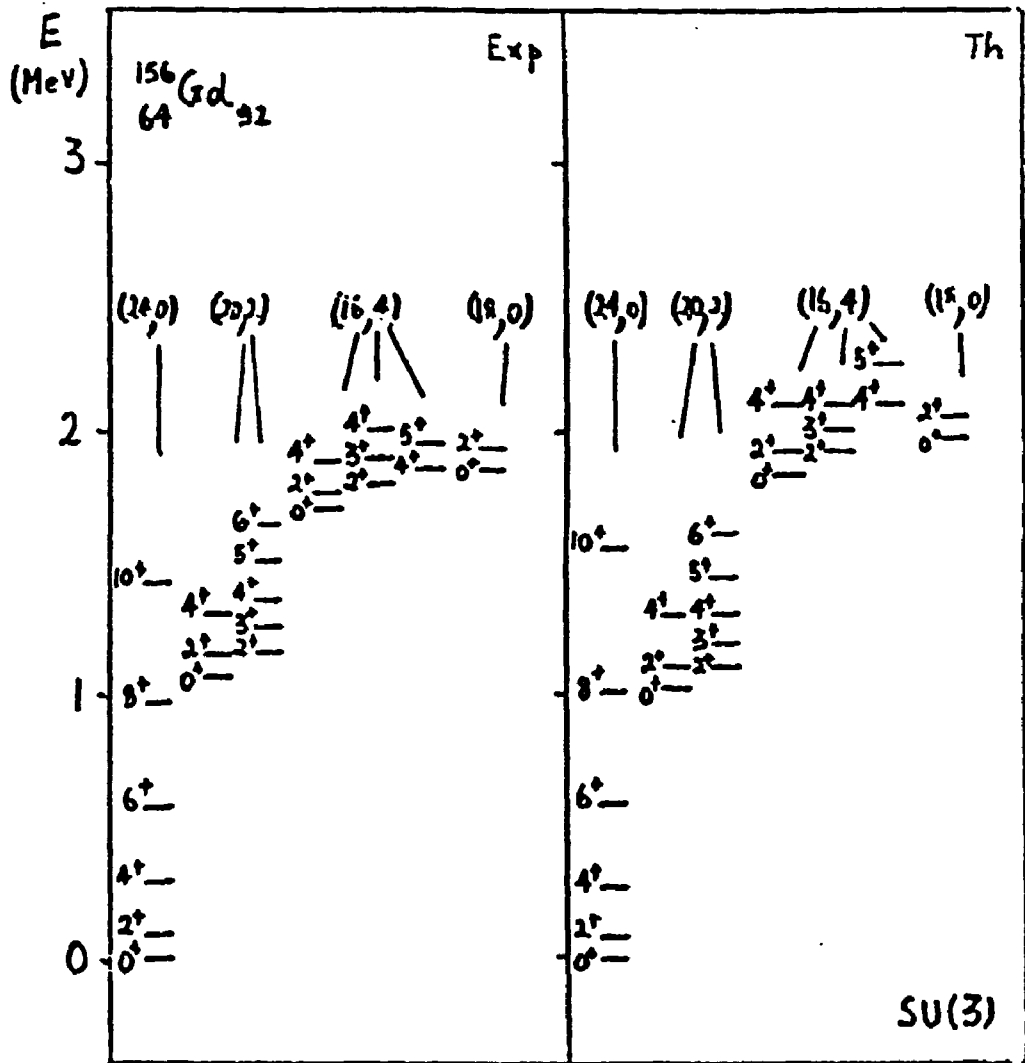
$$|N, \alpha_\mu\rangle = (s^\dagger + \sum_\mu \alpha_\mu d_\mu^\dagger)^N |0\rangle$$

↑
Classical variables



$$R = R_0 \left(1 + \sum_\mu \alpha_\mu y_{2\mu}(\theta, \varphi) \right)$$



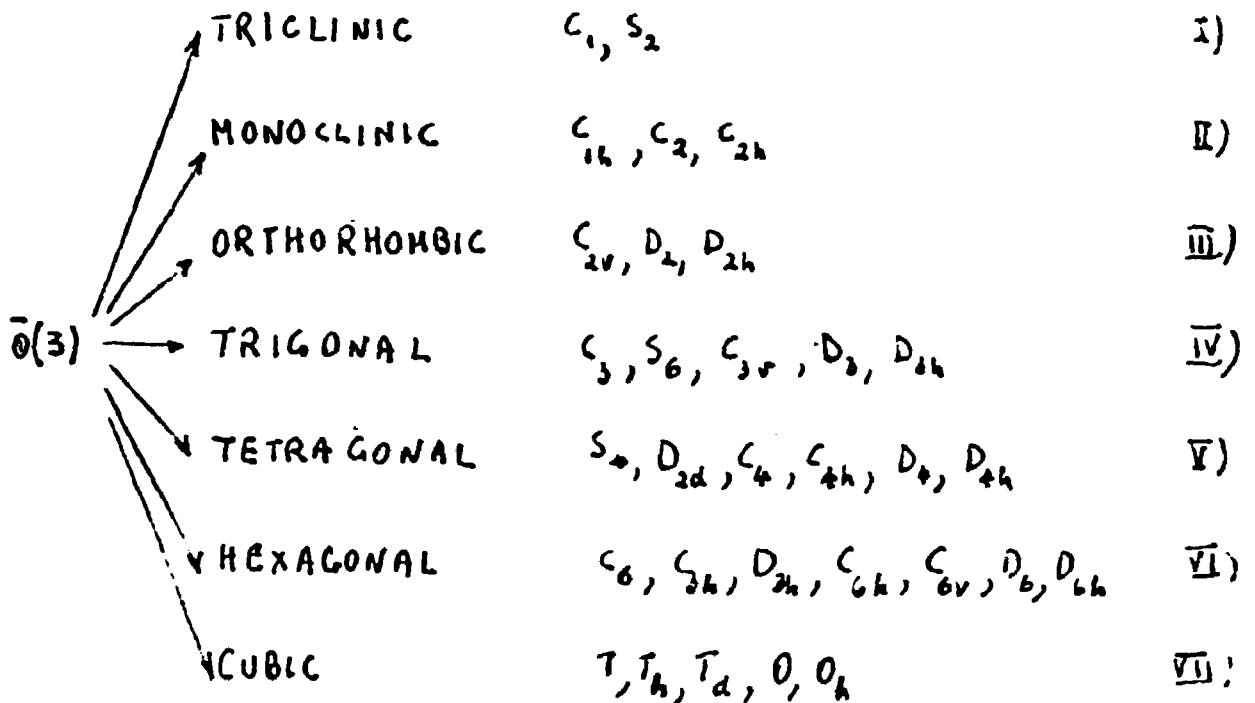


⇒ Classification of shapes of nuclei in terms of symmetry groups

- (I) Spherical shape
- (II) Axially symmetric deformed shape
- (III) Non-axially symmetric deformed shape

CLASSIFICATION OF THE SHAPES OF CRYSTALS

BY MEANS OF POINT GROUPS

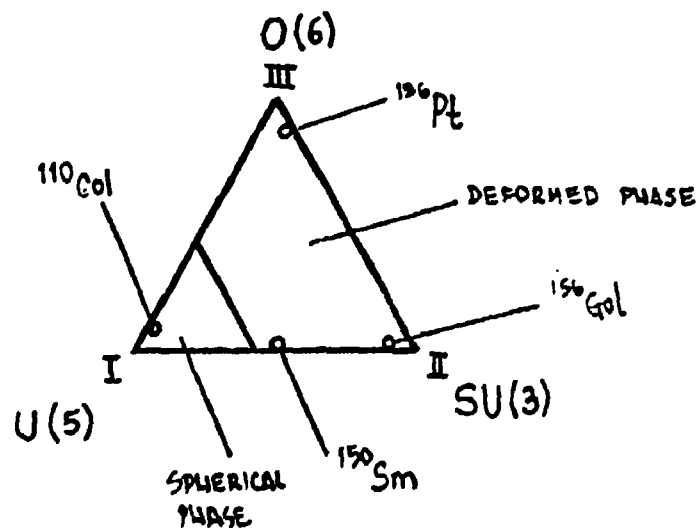


(I) SPHERICAL SHAPE

(II) AXIALLY DEFORMED SHAPE

(III) γ -UNSTABLE DEFORMED SHAPE

SHAPE PHASE DIAGRAM



NORMAL SYMMETRIES

BOSONS \longleftrightarrow BOSONS

OR

FERMIONS \longleftrightarrow FERMIONS

SUPERSYMMETRIES

BOSONS \longleftrightarrow FERMIONS

DYNAMIC SUPERSYMMETRIES

- (i) THE HAMILTONIAN HAS SUPERGROUP STRUCTURE G^* .
- (ii) THE HAMILTONIAN CAN BE WRITTEN IN TERMS ONLY OF INVARIANT OPERATORS OF A COMPLETE CHAIN OF GROUPS (OR SUPERGROUPS).

SUPERSYMMETRIES IN PHYSICS

(i) EXACT SUPERSYMMETRIES

(a) WESS-ZUMINO SUPERSYMMETRIES

$$\mathcal{L}(x) = -\frac{1}{2} (\partial_\mu A(x))^2 - \frac{1}{2} (\partial_\mu B(x))^2 - \frac{1}{2} i \bar{\psi}(x) \gamma^\mu \partial_\mu \psi(x)$$

$$-\frac{1}{2} m^2 A^2(x) - \frac{1}{2} m^2 B^2(x) - \frac{1}{2} i m \bar{\psi}(x) \psi(x)$$

$$-g m A(x) [A^2(x) + B^2(x)] - \frac{1}{2} g^2 [A^2(x) + B^2(x)]$$

$$-i g \bar{\psi}(x) [A(x) - \gamma_5 B(x)] \psi(x)$$

(ii) DYNAMIC SUPERSYMMETRIES

(a) THE HAMILTONIAN HAS SUPERGROUP STRUCTURE G^*

(b) THE HAMILTONIAN CAN BE WRITTEN IN TERMS ONLY OF CASIMIR OPERATORS OF A COMPLETE CHAIN OF GROUPS (OR SUPERGROUPS)

$$G^* \supset G' \supset G'' \supset \dots$$

MATHEMATICAL FRAMEWORK

Graded Lie groups

(a) Generators

$$\begin{array}{cc} G_\alpha & , & F_i \\ \uparrow & & \uparrow \\ \text{Bosonic} & & \text{Fermionic} \end{array}$$

(b) Commutation relations

$$[G_\alpha, G_\beta] = c_{\alpha\beta}^\gamma G_\gamma$$

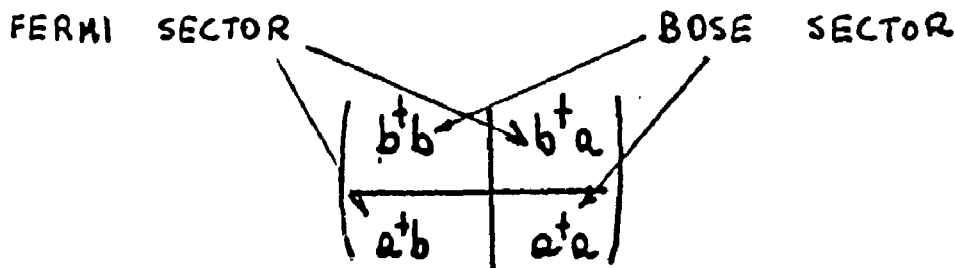
$$[G_\alpha, F_i] = f_{\alpha i}^j F_j$$

$$\{F_i, F_j\} = g_{ij}^\alpha G_\alpha$$

SUPERALGEBRAS $U(m|m)$

GENERATORS

$$\begin{array}{ll}
 G_{\alpha_i}^{(b)} = b_{\alpha}^{\dagger} b_{\alpha} & m^2 \\
 G_{i\bar{i}}^{(f)} = a_i^{\dagger} a_{\bar{i}} & m^2 \\
 F_{\alpha_i}^{\dagger} = b_{\alpha}^{\dagger} a_i & mn \\
 F_{i\bar{\alpha}} = a_i^{\dagger} b_{\alpha} & mn \\
 \hline
 & (m+n)^2
 \end{array}$$



REPRESENTATIONS

YOUNG SUPERTABLEAUX

$$[N] \equiv \overbrace{\square \square \dots \square}^N$$

INTERACTING BOSON-FERMION MODEL

F. Iachello and O. Scholten, Phys. Rev. Lett. 43, 679 (1979)

F. Iachello and S. Kiryucok, Ann. Phys. (N.Y.) 136, 19 (1981)

(a) Building blocks



S-BOSON



D-BOSON

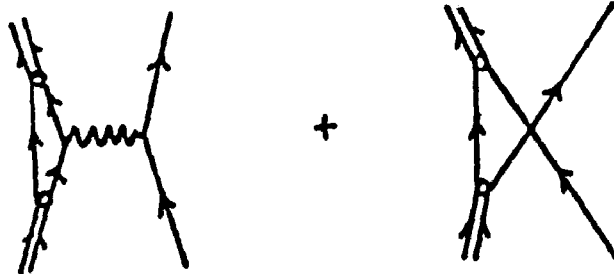


J-FERMION

(b) Hamiltonian

$$H = H_B + H_F + V_{BF}$$

Boson - fermion interaction

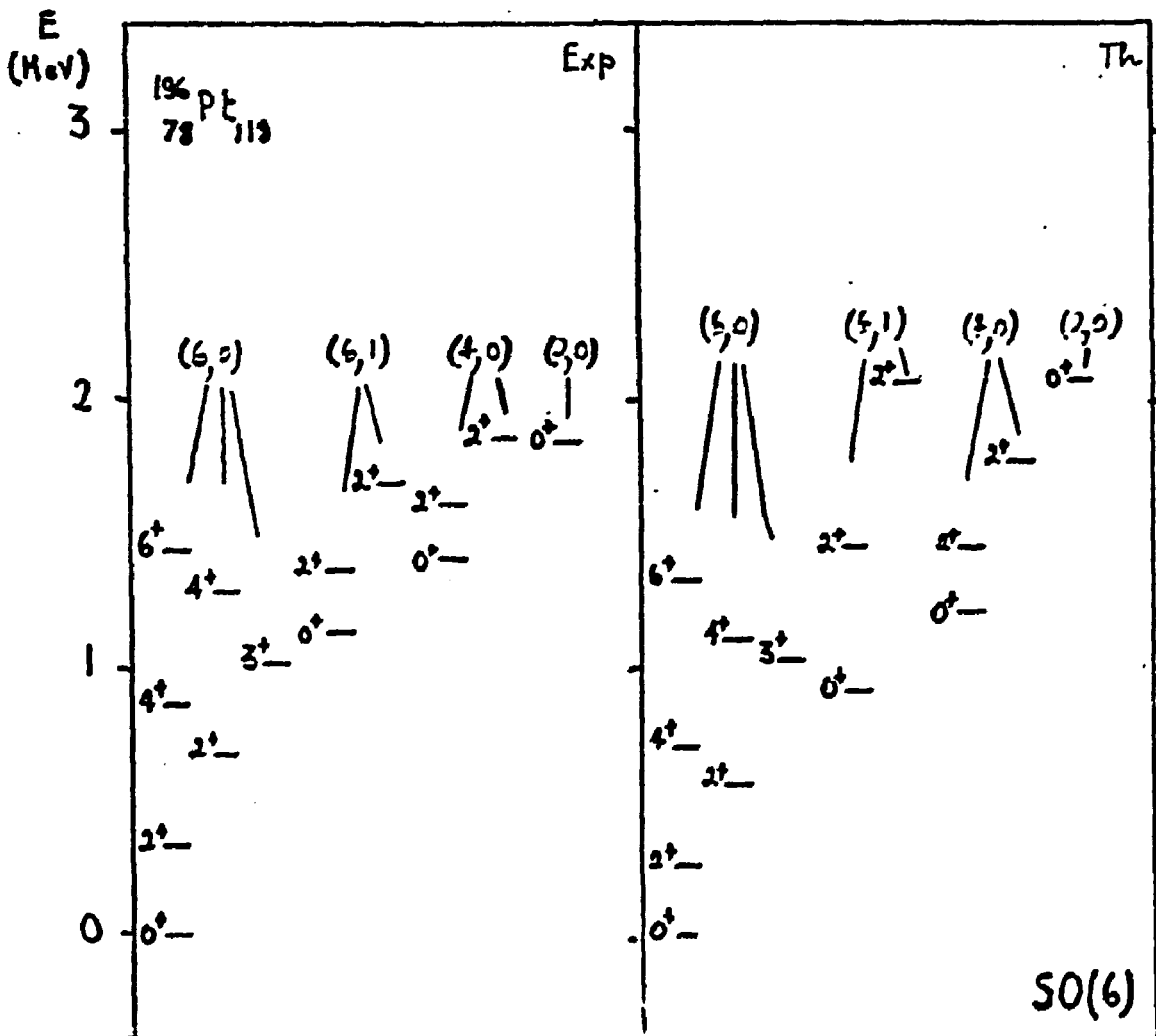
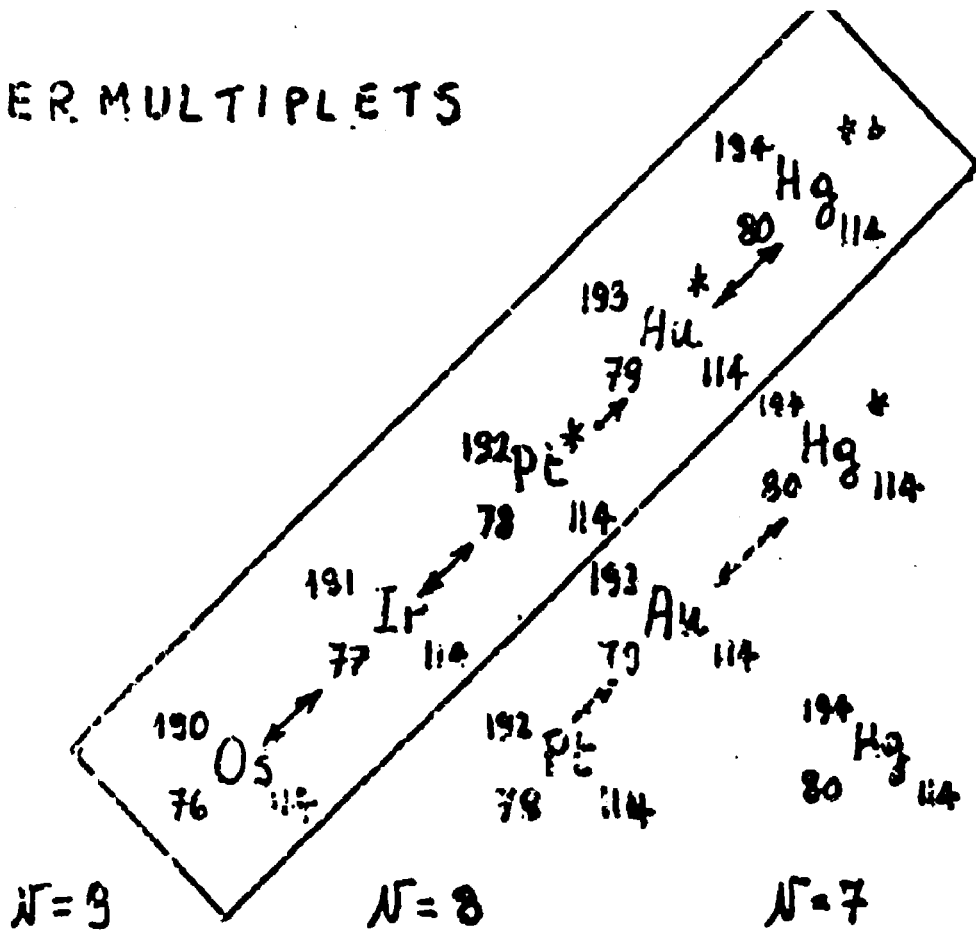


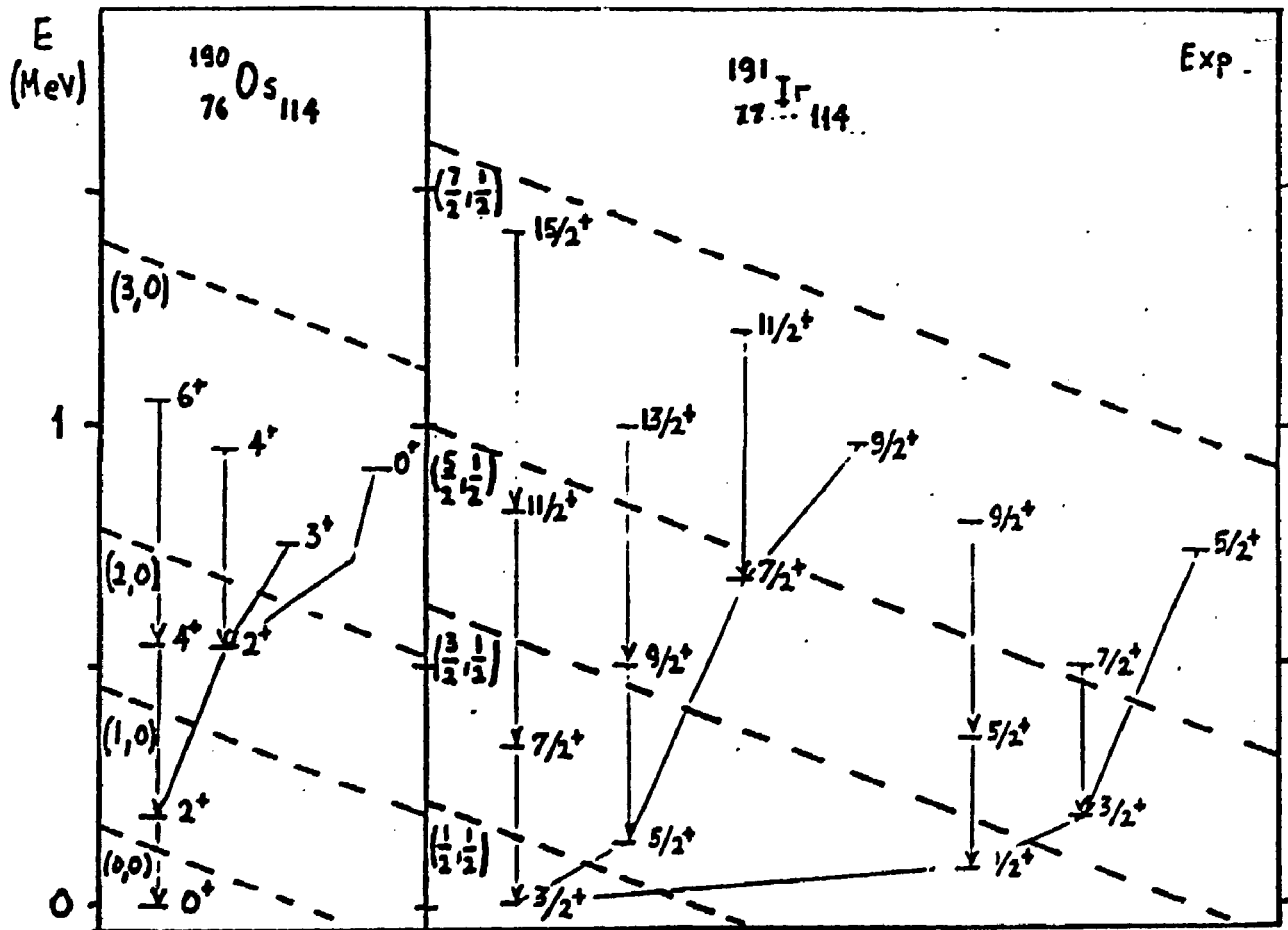
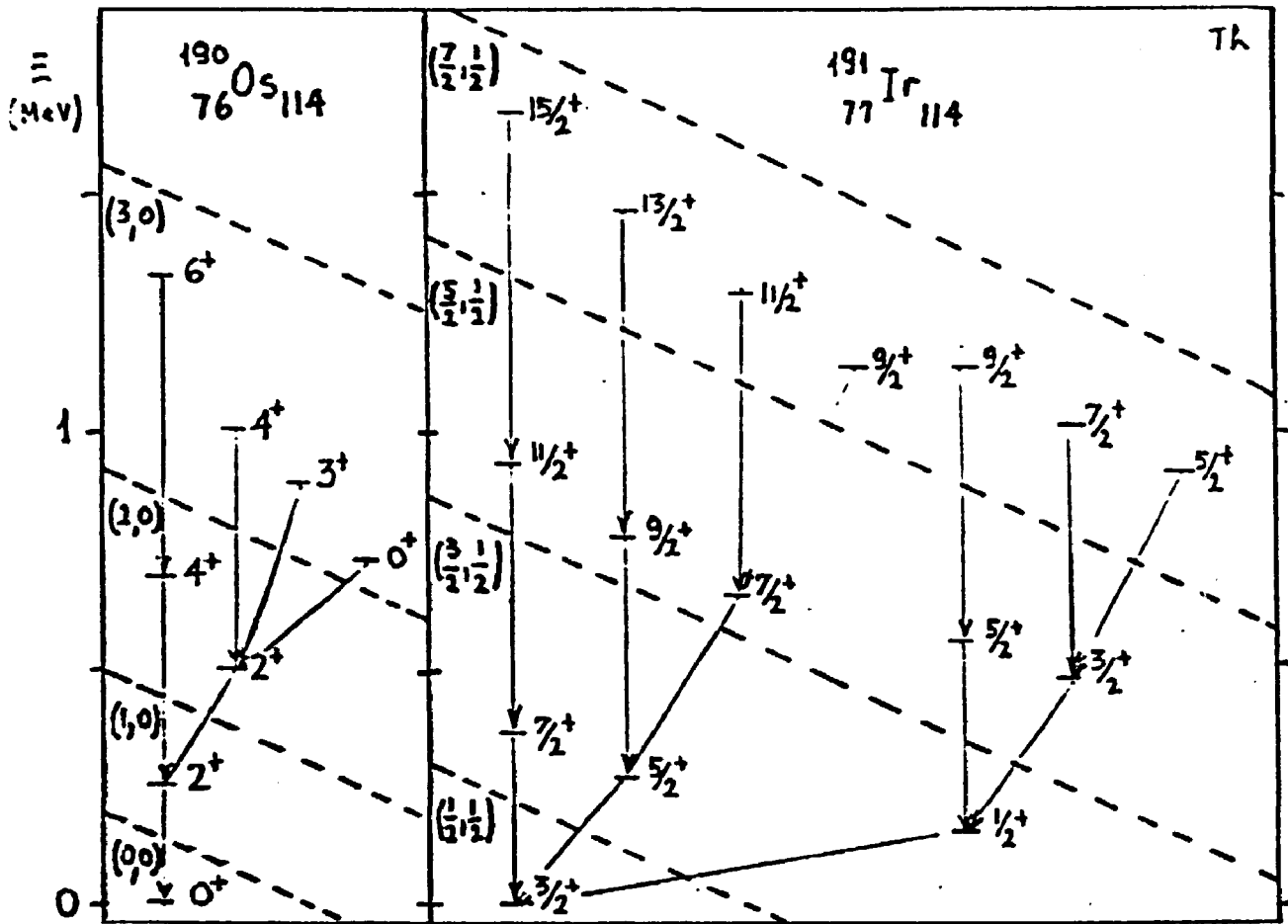
(c) Supersymmetries

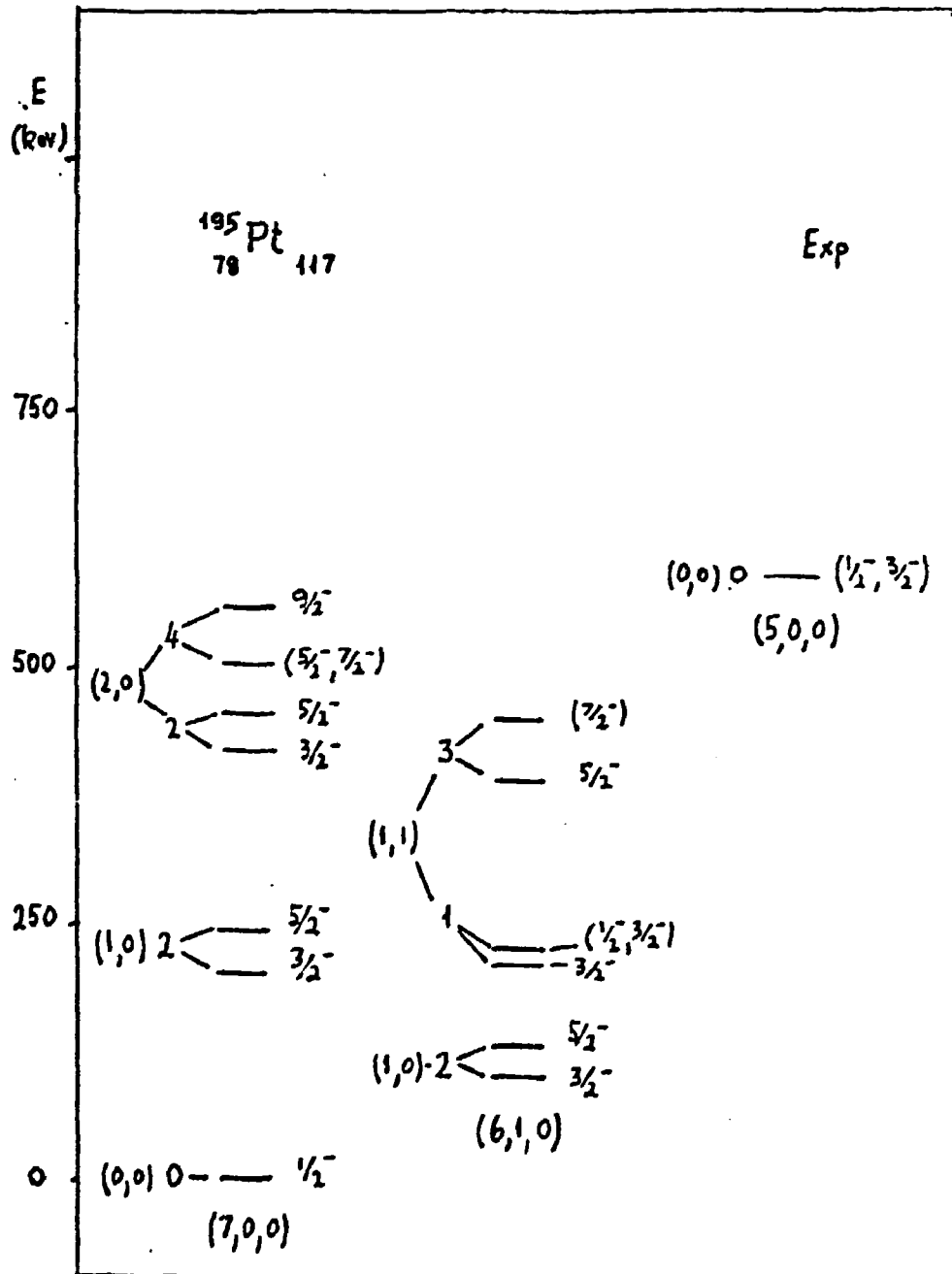
⇒ Many classes

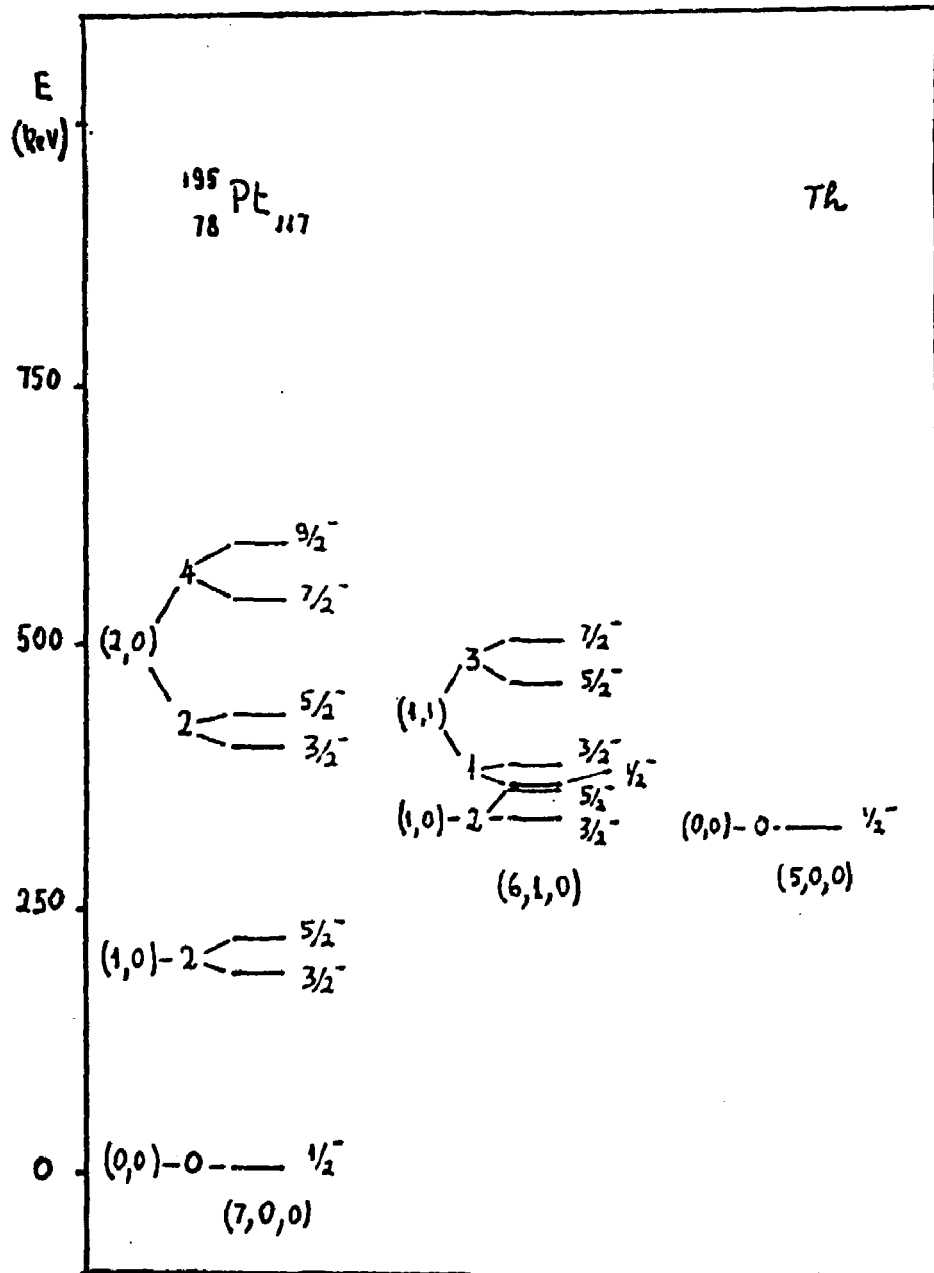
⇒ Provide a classification scheme for odd-even nuclei

SUPER MULTIPLETS









EXPERIMENTAL RESULTS

		$U(6 4)$	(P, P')	Coupling
^{194}Pt ($\sigma=7$)	2_1^+	1.00	1.00	1.00
	2_2^+	0.00	<0.01	0.005
^{193}Ir ($\sigma=15/2$)	$1/2_1^+$	0.11	≈ 0.08	0.068
	$5/2_1^+$	0.33	0.48	0.44
	$3/2_2^+$	0.00	0.07	0.052
	$7/2_1^+$	0.44	0.40	0.30
	$3/2_2^+$	0.00	0.019	0.017
	$7/2_2^+$	0.00	0.01	0.056
^{191}Ir ($\sigma=17/2$)	$1/2_1^+$	0.14	0.04	0.051
	$5/2_1^+$	0.41	0.64	0.55
	$3/2_2^+$	0.00	0.08	0.068
	$7/2_1^+$	0.54	0.46	0.31
	$7/2_2^+$	0.00	0.07	<0.01

$$1542 \text{ } 0^+$$

$$192 \text{ Pt }^*$$

$$78 \text{ } 114$$

$$N=7, M=2$$

$$\tau = \frac{3}{2} \left\{ \begin{array}{l} 343 \text{ } 7\frac{1}{2}^+ \\ 129 \text{ } 5\frac{1}{2}^+ \\ 87 \text{ } 3\frac{1}{2}^+ \\ \tau = \frac{1}{2} \text{ } 0 \text{ } 3\frac{1}{2}^+ \end{array} \right.$$

$$191 \text{ Ir }^*$$

$$77 \text{ } 114$$

$$N=8, M=1$$

$$\tau = 2 \left\{ \begin{array}{l} 784 \text{ } 4^+ \\ 612 \text{ } 2^+ \end{array} \right.$$

$$\tau = \frac{3}{2} \left\{ \begin{array}{l} 539 \text{ } 7\frac{1}{2}^+ \\ 258 \text{ } 5\frac{1}{2}^+ \\ 38 \text{ } 1\frac{1}{2}^+ \\ \tau = \frac{1}{2} \text{ } 0 \text{ } 3\frac{1}{2}^+ \end{array} \right.$$

$$193 \text{ Au }^*$$

$$79 \text{ } 114$$

$$N=7, M=1$$

$$\tau = 1 \left\{ \begin{array}{l} 558 \text{ } 2^+ \\ 548 \text{ } 4^+ \end{array} \right.$$

$$\tau = 1 \text{ } 316 \text{ } 2^+$$

$$\tau = 1 \text{ } 186 \text{ } 2^+$$

$$\tau = 0 \text{ } 0 \text{ } 0^+$$

$$\tau = 0 \text{ } 0 \text{ } 0^+$$

$$190 \text{ Os }^*$$

$$76 \text{ } 114$$

$$N=9, M=0$$

$$192 \text{ Pt }^*$$

$$78 \text{ } 114$$

$$N=8, M=0$$

U(6|4) SUPERSYMMETRY

3191 $\underline{\quad}$ 6^+	3150 $\underline{\quad}$ 6^+	3330 $\underline{\quad}$ 6^+
2751 $\underline{\quad}$ 4^+	2850 $\underline{\quad}$ 4^+	2673 $\underline{\quad}$ 4^+
1524 $\underline{\quad}$ 2^+	1986 $\underline{\quad}$ 2^+	1554 $\underline{\quad}$ 2^+
	====	
0 $\underline{\quad}$ 0^+	0 $\underline{\quad}$ 0^+	0 $\underline{\quad}$ 0^+
$^{42}_{20}\text{Ca}_{22}$	$^{42}_{21}\text{Sc}_{21}$	$^{42}_{22}\text{Ti}_{20}$
$T_2 = -1$	$T_2 = 0$	$T_2 = +1$

U(2) ISOSPIN SYMMETRY

CONCLUSIONS

⇒ The use of algebraic techniques (interacting boson and boson-fermion models) has led to major advances in nuclear structure physics.

We are now able to predict properties of complex nuclei within 10-20% and do have a better understanding of the physics involved.

⇒ The exploitation of dynamic symmetries (and supersymmetries) has been of crucial importance in this development. We have found that even complex systems can display, in some cases, simple, easily recognizable, patterns.

Similar techniques have been used recently in molecular physics (Vibron Model)

F. Tachello and R. D. Levine, *J. Chem. Phys.* 77, 3066 (1982)

D. S. van Rossum, F. Tachello, R. D. Levine and

A. E. L. Dieperink, *J. Chem. Phys.* 79, 2515 (1983)

- | | |
|--------------------------|--------------------|
| (a) Diatomic molecules | H_2, \dots |
| (b) Triatomic molecules | HCN, CO_2, \dots |
| (c) Polyatomic molecules | H_2O, \dots |

Properties studied :

- (i) Structure (Vibration-Rotation)
- (ii) Transition strengths
- (iii) Electron scattering

It is hoped that the exploitation of dynamic symmetries in this field of physics will be as useful as in nuclear and particle physics.