

### A Brief History of a Big Idea for a Small Thing

#### Calvin W. Johnson, SDSU

"This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics, under Award Number DE-FG02-03ER41272 "





# In the beginning....

#### Discovery of the atomic nucleus 1911







#### Discovery of the atomic nucleus 1911







#### Discovery of the atomic nucleus 1911





#### Discovery of the atomic nucleus 1911











'Engrossing ... I greatly enjoyed it' Michael Frayn

#### THE FLY IN THE CATHEDRAL

How a small group of Cambridge scientists won the race to split the atom

11991

-

#### he atomic nucleus 1911



It's like a tiny fly inside a massive English cathedral!





#### Discovery of the atomic nucleus 1911





1928: Gamow proposes liquid drop model







1928: Gamow proposes liquid drop model





1932: Chadwick discovers neutron





1928: Gamow proposes liquid drop model







1932: Chadwick discovers neutron

1936: Bohr proposes compound nucleus







# 1938: Hahn and Strassmann 'discover' fission (but don't realize it)





<sup>44</sup>56Ba

 $\circ \mathsf{n}$ 

 $\circ$  **n** 

 $O \mathbf{n}$ 

<sup>89</sup><sub>36</sub>Kr



## 1938: Hahn and Strassmann 'discover' fission (but don't realize it)

n

#### 1939: Meitner and Frisch explain fission



<sup>235</sup><sub>92</sub>U

236U



<sup>44</sup>56Ba

 $\circ n$ 

 $\circ$  n

O n

<sup>89</sup><sub>36</sub>Kr

#### 1939: Meitner and Frisch explain fission



1938: Hahn and Strassmann 'discover' fission (but don't realize it)

1944

### 1939: Meitner and Frisch explain fission

n

<sup>235</sup>U

236L



<sup>44</sup>56Ba

 $\circ n$ 

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<sup>89</sup><sub>36</sub>Kr

### PERIODIC TABLE OF ELEMENTS

#### **Chemical Group Block**





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### PERIODIC TABLE OF ELEMENTS

#### Chemical Group Block

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	1	to a	2 24.305 Mg Magnesium aline Earth Me	3	4	5	6	Halogen 7	8	9	10	11	12	13 26.981 Al Aluminum Post-Transition M	14 28.085 Silicon Metalloid	15 30.973 P Phosphorus Nonmetal	16 32.07 Sulfur Nonmetal	17 35.45 Cl Chlorine Halogen	18 39.9 Argon Noble Gas
	1	Alkali Metal	Calcium Alkaline Earth Me	21 44.95591 SC Scandium Transition Metal	22 47.867 <b>Ti</b> Titanium Transition Metal	23 50.9415 V Vanadium Transition Metal	24 51.996 Cr Chromium Transition Metal	25 54.93804 Manganese Transition Metal	26 55.84 Fe Iron Transition Metal	27 58.93319 CO Cobalt Transition Metal	28 58.693 <b>Ni</b> Nickel Transition Metal	29 63.55 Cu Copper Transition Metal	30 65.4 Zn Zinc Transition Metal	31 69.723 Ga Gallium Post-Transition M	32 72.63 Germanium Metalloid	33 74.92159 Ass Arsenic Metalloid	34 78.97 Se Selenium Nonmetal	35 79.90 Br Bromine Halogen	36 83.80 Krypton Noble Gas
	5	37 85.468 Rb Rubidium Alkali Metal	38 87.62 Strontium Alkaline Earth Me	39 88.90584 Y Yttrium Transition Metal	40 91.22 Zr Zirconium Transition Metal	41 92.90637 <b>Nb</b> Niobium Transition Metal	42 95.95 MO Molybdenum Transition Metal	43 96.90636 <b>TC</b> Technetium Transition Metal	44 101.1 Ru Ruthenium Transition Metal	45 102.9055 <b>Rh</b> Rhodium Transition Metal	46 106.42 Pd Palladium Transition Metal	47 107.868 Ag Silver Transition Metal	48 112.41 Cd Cadmium Transition Metal	49 114.818 In Indium Post-Transition M.	50 118.71 Sn Tin Post Transition M	51 121.760 Sb Antimony Metalloid	52 127.6 Te Tellurium Metalloid	53 126.9045 Iodine Halogen	54 131.29 Xee Xenon Noble Gas
1	6	55 132.90 CS Cesium Alkali Metal	56 137.33 Ba Barium Alkaline Earth Me		72 178.49 Hf Hafnium Transition Metal	73 180.9479 <b>Ta</b> Tantalum Transition Metal	74 183.84 W Tungsten Transition Metal	75 186.207 <b>Re</b> Rhenium Transition Metal	76 190.2 OS Osmium Transition Metal	77 192.22 Ir Iridium	78 195.08 Pt Platinum Transition Metal	79 196.96 Au Gold Transition Metal	80 200.59 Hg Mercury Transition Metal	81 204.383 TI Thallium Post-Transition M.			6	5 209.98 At Astatine Halogen	86 222.01 Ran Radon Noble Gas
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#### PERIODIC TABLE OF ELEMENTS

"... a riveting and masterful account of a scientist's devotion to physics." MARCIA BARTUSIAN. Washington Part Back World

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RUTH LEWIN SIME

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PubChem													
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	Pm Promethium Lanthanide	Sm Samarium Lanthanide	Eu Europium Lanthanide	Gd Gadolinium Lanthanide	Tb Terbium Lanthanide	Dysprosium Lanthanide	R			Yb Ytterbium Lanthanide	Lu Lutetium Lanthanide		
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	Np Neptunium Actinide	Pu Plutonium Actinide	Americium Actinide	Cm Curium Actinide	Bk Berkelium Actinide	Cf Californium Actinide			E	No Nobelium Actinide	Lr Lawrencium Actinide		



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Our story so far: by the early 1940s, a lot of nuclear properties seemed well described by the liquid drop model....



....especially fission...



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....especially fission...

....which led to this...





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....especially fission...

....which led to this...



....developed here.





As the movie *Oppenheimer* showed (kind of), many physicists were recruited for the Manhattan project



Shell Model 75 Symposium, July 19, 2024

POST No. 1



One of these was Maria Goeppert Mayer.







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Michael Wiescher







One of these was Maria Goeppert Mayer.

Her Ph.D dissertation (1930, Gottingen) was on two-photon absorption.







One of these was Maria Goeppert Mayer.

Her Ph.D dissertation (1930, Gottingen) was on two-photon absorption.

In 1942 she worked on separation of fissile material at Columbia. In 1945 she joined Teller at Los Alamos to work on opacities.







One of these was Maria Goeppert Mayer.

In 1946, Goeppert Mayer went to the newly formed Argonne National Lab, protesting "I don't know anything about nuclear physics."

Through her work on fission, though, she noticed unusual patterns in binding energies.





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Second Series, Vol. 74, No. 3

AUGUST 1, 1948

#### On Closed Shells in Nuclei\*

MARIA G. MAYER Argonne National Laboratory and Institute for Nuclear Studies, University of Chicago, Chicago, Illinois (Received April 16, 1948)

Experimental facts are summarized to show that nuclei with 20, 50, 82, or 126 neutrons or protons are particularly stable.





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### Magic numbers!







### On Closed Shells in Nuclei. II

MARIA GOEPPERT MAYER Argonne National Laboratory and Department of Physics, University of Chicago, Chicago, Illinois February 4, 1949

Thanks are due to Enrico Fermi for the remark, "Is there any indication of spin-orbit coupling?" which was the origin of this paper.

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PHYSICAL REVIEW

VOLUME 78, NUMBER 1

APRIL 1, 1950

#### Nuclear Configurations in the Spin-Orbit Coupling Model. I. Empirical Evidence

MARIA GOEPPERT MAYER Argonne National Laboratory, Chicago, Illinois (Received December 7, 1949)

An extreme one particle model of the nucleus is proposed. The model is based on the succession of energy levels of a single particle in a potential between that of a three-dimensional harmonic oscillator and a square well. (1) Strong spin orbit coupling leading to inverted doublets is assumed. (2) An even number of identical nucleons are assumed to couple to zero angular momentum, and, (3) an odd number to the angular momentum of the single odd particle. (4) A (negative) pairing energy, increasing with the j value of the orbit is assumed. With these four assumptions all but 2 of the 64 known spins of odd nuclei are satisfactorily explained, and all but 1 of the 46 known magnetic moments. The two spin discrepancies are probably due to failure of rule (3). The magnetic moments of the five known odd-odd nuclei are also in agreement with the model. The existence, and region in the periodic table, of nuclear isomerism is correctly predicted.





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SECOND SERIES, VOL.

Argonne National

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#### PHYSICAL R

#### Nuclear

The red-haired college professor, mother of two, the first woman residing in America to win a Nobe physics prize, the second She received the news in State Dept. at 4 this morning. The caller informed her she had been cited hy the Swedish Royal Academy of Science for her work in determining the na-ture of the shell of the atom's Over 'Leak' Will Share Award Mrs. Mayer will share the WASHINGTON UP - One \$31,158 prize with a West Ger-man scientist, J Hans D Jensen of Heidelberg, who An made a similar but independ- on charges of conduct "un level becoming an officer of the ner of Princeton University. Department of State. who helped lay the groundsquai Otepka, 48, has been unwork for the present advanced study in nuclear physder suspension since Seul of id accused among othe things of giving confiden Wigner will get half the prize. Mrs. Mayer and Jenoformation to the Senat angu Internal Security subcom sen will divide the rest. mittee Second on Campus Here the c A letter removing h Mrs. Mayer is the second Nobel Prize winner on the from the ranks of departfacto university's San Diego cam. ment employes was deliver pus. The other is Dr. Harold, ed today. rus. The other is Dr. Harphe C. Urey of 1890 Tarret Lane professor of chemistry at chief of the department's professor of chemistry at chief of the department's perconnel division. It re plied to Otepka's 12-page of the terminet of the terminet division. prob agree Mother of a married daugh. long letter of Oct. 14, repredi ter and a grown son. Mrs. questing that charges Mayer is the wife of Dr Jo. against him be dismissed aeph E. Mayer, a chemistry and upheld the charges, professor at the University of Otepica Lad been chief ac-California here. They joined eurity risk evaluator for the local faculty in 1960, and department at a salary at 2345 Via Sienna, La \$16,900-a-year.

WORLD RENOWNED-Dr. Maria Goeppert Mayer.

57, holds the slide rule she uses in the study of nu-

clear physics that won her a Nobel Prize today. She

**Nobel Physics Prize** 

Dr. Mayer 1st Woman in U.S.,

Maria Goeppert Mayer, 57, a research physicis

2nd in History So Honored

a 1963 Nobel Prize winner in physics.

By FRANK HOGAN

at the University of California here, today was name

is a University of California professor here.

S.D. Mother Wins

ner leaders inside the personnel gon Friday afternoon. One Diem stronghold after another **Diem Brother** EVENING TRIBUNE **Turned Over To Viet Rebels** U.S. Consulate Phone 234-7111 3 PARTS - 38 PAGES SAN DIEGO, CALIFORNIA, TUESDAY, NOVEMBER 5, 1963 Told Leader Will Get Trial British, Tese View Lawyer, and the rest of as turned over to South Viet ent today after he sought dum at the U.S. consulate U.S. officials said they were ired that Can would not **Gls in Soviet Block** lynched and would receive due process of law There were these other deopments First - The revolutionary overnment named former lice President Nguyen Ngor premier and appointed a 15-man cabinet. Second - The children of Mrs. Ngo Dinh Nhu arrived in Rome today, Mrs. Nhu, in Los Angeles, said she will fly there tomorrow and then may **Convoys Sent** return to the United States. Third-Dr. Tran Van Chu To Join U.S. former South Vietna ambassador to the Unit States and Mrs. Nhu's fa ther, said in Fresno that the In Showdown iew government has the backing of the Vietnamese people and that the United **Red Armored Cars** ates will lose no prestig because of the fall of Dier Box In Yanks and his brother. Nhu. **Trying Break-Out** Fourth-U.S. recognition of he new government is ex-Written From NEWS SERVICES ted quickly, according to BERLIN-The British and Washington officials. Can, who dropped from French sent convoys out to light when the coup over- join a Russian-blockaded U.S. hrew Diem's regime 1 a st Army convoy on the Autobahn weekend went to the U.S. con leading to Berlin today in an ulate last night seeking Allied challenge to the So viet Union. Consular officials notified The Russians allowed the he revolutionary government French and British convoys to and today Can was flown 400 pass a checkpoint outside Ber niles in a U.S. military plane lin en route to their rende Saigon and turned over to yous at the border 110 miles fficials of the military junta, away with the Americans, Buddhist leaders, students Both were halted for 30 to 50 and others in Hue long have minutes before being allowed charged that Can ruled his to proceed. ailiwick as a bloody tyrant . Incident 'Quite Serious' Meantime, Maj. Gen. The Americans have been Duong Van Minh, 47, leader held up since 5 a.m. vester the coup, said in a procla- day at the Russians' Marien-nation that a republican form born checkpoint just across government will be re- from West Germany in a disalthough the junta will pute over clearance proced-NEXT UP-Lt. Baker, left, leader of 56-man U.S. convoy waiting to cross border from West to East the country's final au- ures. The Russians brought Germany at Helmstedt, supervises unloading of Viet Cong War armored cars and 100 armed Minh, who assumed the po-soldiers to hem in the Ameri Reds Warned Early Turnout ion of chief of state, said cans this morning in an inciis committee of generals will dent which the State Departve its chief attention to di- ment has termed "quite seri ction of the war against the ous." **By** Johnson ommunist Viet Cong. Until revision of the 1956 The American convoy at-Points to Record nstitution, Minh said, leg-tempted to run the blockade dative and executive power early this morning but the So-cill center in the junta but victs used the armored cars To Watch Step By RALPH BENNETT | Last night the most inten will be exercised by the pro-to-bead it off and box it in risional government. He ex- in Washington, the White blained that the junta will re-House said today that Presi-EVENING TRIBUNE Painted Writer sive and expensive political The doors to 1,005 politing campaign in the city's history originally forecast for elecplaces in the city swing open came to an end. this morning and the voters. The mayor candidates -

ain active authority over na-dent Kennedy is deeply con-ROTTERDAM, The Netherional defense, security a n d cerned over the blockade and lands (UPI)-Vice President started to file in that officials are trying to re- Johnson warned the Russians under skies of flawless 30, an insurance man, and weak storm front would in a force, in a difficulty of re-i Johnson warried the Russians' Under skies of flawless of an investigation of the skiest of the passe through this lock of the inpasse through this lock of the inflawless of the skiest of the Dinh Thue of Hue, met her in Bonn. three younger children – a Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "can also pro-three younger children – b Kennedy summoned Secre. friendship it "

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Councilman Frank Curran.

Television Debate

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hours. Election officers said



### in Nuclei. II

T MAYER d Department of Physics. Chicago, Illinois 1949

for the remark, "Is there ng?" which was the origin





#### PHYSICAL REVIEW

#### VOLUME 78, NUMBER 1

APRIL 1, 1950

#### Nuclear Configurations in the Spin-Orbit Coupling Model. II. Theoretical Considerations

MARIA GOEPPERT MAYER Argonne National Laboratory, Chicago, Illinois (Received December 7, 1949)

The assumption of short-range attractive forces between identical nucleons in the jj coupling model of nuclear structure is in agreement with the empirically observed spins.

## Pairing!





On the "Magic Numbers" in Nuclear Structure Otto Haxel Max Plenck Institut, Göttingen J. Hans D. Jensen Institut J. theor. Physik, Heidelberg AND Hans E. SUESS Inst. f. phys. Chemie, Hamburg April 18, 1949

A SIMPLE explanation of the "magic numbers" 14, 28, 50, 82, 126 follows at once from the oscillator model of the nucleus,<sup>1</sup> if one assumes that the spin-orbit coupling in the Yukawa field theory of nuclear forces leads to a strong splitting of a term with angular momentum l into two distinct terms  $j=l\pm\frac{1}{2}$ .





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## Notes on the j-j Coupling Shell Model<sup>\*</sup>

EUGENE FEENBERG Washington University, St. Louis, Missouri, and Oak Ridge National Laboratory,\*\* Oak Ridge, Tennessee (Received July 29, 1949)

jj-Coupling in Nuclei

B. H. FLOWERS\* Department of Mathematical Physics, The University, Edgbaston, Birmingham, England (Received February 21, 1952)

Excited states of nuclei in *jj*-coupling

<u>B.H. Flowers</u>\*)

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https://doi.org/10.1016/S0031-8914(52)80179-X 7

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#### Abstract

A brief account is given of the classification of states arising from a configuration  $j^n$  of neutrons and protons in *jj*-coupling with short-range central interactions, and evidence is brought to suggest that the classification has experimental confirmation. On the basis of the new classification it is possible to lay down certain approximate selection rules for radiative transitions. Some of these rules are discussed.

#### Shell Model 75 Symp

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#### PHYSICAL REVIEW

#### VOLUME 99, NUMBER 3

AUGUST 1, 1955

#### Independent Particle Model of the Nucleus. I. Interparticle Forces and Configuration Mixing\*

CARL LEVINSON AND KENNETH W. FORD<sup>†</sup> Indiana University, Bloomington, Indiana (Received March 7, 1955)

A simplified method of obtaining the direct interaction between two identical nucleons in the nuclear shell model is given for the special case of singlet forces. Configuration interaction is included in the method. A semi-empirical analysis of simple two and three particle nuclear spectra is outlined which enables one to determine properties of the two-body perturbing interaction provided many body forces are negligible and coupling to the nuclear surface is weak. Corrections to the singlet force formalism due to triplet central and tensor forces are discussed. Formulas are given for magnetic dipole and quadrupole moments and magnetic dipole transition rates for mixed three-particle configurations. The effect of weak surface coupling on multi-particle configuration is given in paper II of this series. A detailed discussion of the spectra of two isotopes of calcium is given in paper III.

## Early configuration-interaction

PHYSICAL REVIEW

#### VOLUME 101, NUMBER 1

JANUARY 1, 1956

#### Intermediate Coupling in the 1*p*-Shell\*

DIETER KURATH Argonne National Laboratory, Lemont, Illinois (Received August 31, 1955)

The region between He<sup>4</sup> and O<sup>16</sup> is treated for the case of intermediate strength of spin-orbit coupling and central two-body interaction. Energy levels are presented as a function of the relative coupling strength parameter, a/K. Static electromagnetic moments are also computed as functions of a/K. Comparison with experimental results gives a fairly good picture, and determines a definite behavior for a/K as a function of mass number. A possible interpretation of this behavior is suggested.

Shell Model 75 Symposium, July 19, 2024



Independent-particle model: San Diego State UNIVERSITY

A single shell-model 'configuration'

$$|\Psi\rangle = |(0s)^4 (0p_{3/2})^2\rangle$$





Independent-particle model: San Diego State UNIVERSITY

A single shell-model 'configuration'

$$|\Psi\rangle = |(0s)^4 (0p_{3/2})^2\rangle$$

Configuration-interaction:

A superposition of different configurations

 $|\Psi\rangle = c_1 |(0s)^4 (0p_{3/2})^2 \rangle + c_2 |(0s)^4 (0p_{3/2})^1 (0p_{1/2})^1 \rangle + \dots$ 

Model excited states as independent particles moving in mean-field, but one or more particles in a higher orbit = "particle-hole excitation"



original configuration



Model excited states as independent particles moving in mean-field, but one or more particles in a higher orbit = "particle-hole excitation"





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$$|\Psi\rangle = c_1 |(0s)^4 (0p_{3/2})^2 \rangle + c_2 |(0s)^4 (0p_{3/2})^1 (0p_{1/2})^1 \rangle + \dots$$







$$\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$$

$$\begin{split} |\Psi\rangle &= \sum_{\alpha} c_{\alpha} |\alpha\rangle \qquad \qquad H_{\alpha\beta} = \langle \alpha | \hat{\mathbf{H}} |\beta\rangle \\ &\sum_{\beta} H_{\alpha\beta} c_{\beta} = Ec_{\alpha} \end{split}$$



PHYSICAL REVIEW

#### VOLUME 105, NUMBER 5

#### MARCH 1, 1957

#### Shell Model for the Positive-Parity States of $N^{15}$ <sup>†</sup>

E. C. HALBERT\* AND J. B. FRENCH Department of Physics, University of Rochester, Rochester, New York (Received November 16, 1956)



## Edith Halbert

1950's

Energy levels and wave functions arising from the configurations  $s^4p^{10}s$ ,  $s^4p^{10}d$ , and  $s^3p^{12}$  have been calculated using a central plus single-particle spin-orbit interaction. Correlations have been made between theory and experiment for a dozen identified positive parity levels in N<sup>15</sup> (including the 5.31-Mev level). For the seven levels below 9 Mev this has been done mainly by considering N<sup>14</sup>(d,p) l values and reduced widths. In order of increasing energy, the theoretical spin assignments for these levels are 5/2, 1/2, 7/2, 3/2, 5/2, 1/2, 3/2 (the third and fifth could be interchanged); the wave functions derived for these levels give fair agreement for level positions and surprisingly good agreement for reduced widths. For the upper levels correlations are made by means of the experimental spin assignments. The general agreement here is poor; in particular, a state which has been invoked to explain thermal neutron capture and other neutron processes is not predicted, and the C<sup>15</sup>  $\beta$ -decay lifetime is not properly given. In general, the wave functions indicate a small interaction between configurations but, apart from this, are not consistent with the idea that the inequivalent particle is effectively coupled to only one state for A = 14.



## J. Bruce French

#### IV. EIGENVECTORS AND EIGENVALUES

With the basic states and interaction described above, the energy matrices were calculated, transformed to eliminate the spurious states, and then diagonalized to produce the eigenvalues and eigenvectors. The last two steps were carried out with the Univac at New York University.

Shell Model 75 Symposium, July 19, 2024





Nuclear Physics Volume 73, Issue 1, November 1965, Pages 1-24



## Effective interactions for the 1p shell

S. Cohen, D. Kurath









## Two challenges for any configuration-interaction calculation:

N15+

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1950's

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Edith Halbert

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SAN DIEGO STATE **UNIVERSITY** 

## **Edith Halbert**

J. Bruce French

...and finding the eigenvalues and eigenvectors of the matrix pro step Uni



Shell Model 75 Symposium, July 19, 2024

the

elim



## Configuration-interaction method

$$\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$$

$$\begin{split} |\Psi\rangle &= \sum_{\alpha} c_{\alpha} |\alpha\rangle \\ & H_{\alpha\beta} = \left\langle \alpha |\hat{\mathbf{H}}|\beta \right\rangle \\ & \text{Computing this!} \\ & \sum_{\beta} H_{\alpha\beta} c_{\beta} = Ec_{\alpha} \end{split}$$

# Configuration-interaction method



$$\hat{\mathbf{H}} |\Psi\rangle = E |\Psi\rangle$$

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha} |\alpha\rangle \qquad \qquad H_{\alpha\beta} = \langle \alpha | \hat{\mathbf{H}} |\beta\rangle$$

$$\dots \text{and solving this!} \qquad \sum_{\beta} H_{\alpha\beta} c_{\beta} = Ec_{\alpha}$$

# Configuration-interaction method: the early days



Many early calculations relied upon
"coefficients of fractional parentage"
→ think "generalized Clebsch-Gordan coefficients"

$$|(j)^{n}; J\rangle = \sum_{K} c_{K} [|(j)^{n-1}; K\rangle \otimes |j\rangle]_{J}$$

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$$|(j)^{n}; J\rangle = \sum_{K} c_{K} |(j)^{n-1}; K\rangle \otimes |j\rangle]_{J}$$
CFP

## Configuration-interaction method



Today we can find all eigenpairs of a real, symmetric matrix using the Householder algorithm (1958).

But this scales as (dimension)<sup>3</sup>

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha}$$





# Entering the 1970s, the shell-model faced **two challenges**



Shell Model 75 Symposium, July 19, 2024



# Entering the 1970s, the shell-model faced **two challenges**



# Dimensionality and

# Intruders

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# The challenge of dimensionality





Number of many-body states goes like # single-particle

states  $\binom{N_s}{N_p} = \frac{N_s!}{N_p!(N_s - N_p)!}$ # particles

## This exhibits exponential scaling!

(In the fixed- $J_z$ , or M-scheme, the actual dimensions are less because of the selection rule. But the scaling still holds)



# The challenge of dimensionality





Number of many-body states goes like # single-particle states  $\binom{N_s}{N_p} = \frac{N_s!}{N_p!(N_s - N_p)!}$ 

*#* particles

## This exhibits **exponential** scaling!

[8]  $0p_{1/2}$ 2  $0p_{3/2}$ = 84  $0s_{1/2}$ 

*p*-shell: max dim

(In the fixed- $J_z$ , or M-scheme, the actual dimensions are less because of the selection rule. But the scaling still holds)



1d <sub>5/2</sub> The challenge of dimensionality San Diego State		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	shell: max dim billion	University Number of many-body states goes like # single-particle states $\binom{N_s}{N_p} = \frac{N_s!}{N_p!(N_s - N_p)!}$ # particles
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	<i>sd</i> -shell: max d = 93,000	im This exhibits <b>exponential</b> scaling!
$\begin{array}{cccc} 0p_{1/2} & 2 & [8] \\ 0p_{3/2} & 4 \end{array}$	<i>p</i> -shell: max dir = 84	$\mathbf{n}$ (In the fixed-J <sub>z</sub> , or M-scheme, the actual dimensions are
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## The challenge of dimensionality

Not everything scales **exponentially**.

For example, the number of terms in a two-body Hamiltonian has **polynomial** scaling

## Number of many-body states goes like



$$\widehat{H} = \sum_{ijkl} V_{ijkl} \widehat{a}_i^{\dagger} \widehat{a}_j^{\dagger} \widehat{a}_l \widehat{a}_k$$
  
# terms ~  $(N_s)^4$ 

## This exhibits **exponential** scaling!

(In the fixed- $J_z$ , or M-scheme, the actual dimensions are less because of the selection rule. But the scaling still holds)



## The challenge of dimensionality

Not everything scales **exponentially**.

For example, the number of terms in a two-body Hamiltonian has **polynomial** scaling

 $\widehat{H} =$ 

# teri

## Number of many-body states goes like



The **exponential scaling** of the configuration-interaction basis motivates alternate methods, such as coupled clusters, which have **polynomial scaling** 

states

# narticle

## **ntial** scaling!

the actual dimensions are ale. But the scaling still holds)


Not everything scales **exponentially**.

For example, the number of terms in a two-body Hamiltonian has **polynomial** scaling

### But configuration-interaction still has many advantages, such as adaptability and ease in generating excited states



### The **exponential scaling** of the

configuration-interaction basis motivates alternate methods, such as coupled clusters, which have **polynomial scaling** 







 $0g_{9/2}$  10
 [50]

  $1p_{1/2}$  2

  $0f_{5/2}$  6
 *pf*-shell: max dim

  $1p_{3/2}$  4
 = 2 billion

  $0f_{7/2}$  8

With the Householder algorithm, we can diagonalize dimensions of up to a few thousand... how do we handle dimensions of 2 billion?!

$\begin{array}{c} {\rm Od}_{3/2} \ {\rm 1s}_{1/2} \ {\rm 0d}_{5/2} \end{array}$	4 2 6	[20]
0p <sub>1/2</sub> 0p <sub>3/2</sub>	2 4	[8]
$0s_{1/2}$	2	[2]

*sd*-shell: max dim = 93,000

*p*-shell: max dim = 84





### There is another way!



(Cornelius Lanczos)

With the Householder algorithm, we can diagonalize dimensions of up to a few thousand... how do we handle dimensions of 2 billion?!







The Lanczos algorithm (you're welcome) and related power and Arnoldi methods seek to find only the extremal eigenvalues, even in huge dimensions

(Cornelius Lanczos)



### There is another way!

Today we can do dimensions of up to 35 billion! (arXiv:2402.12606)



Anna McCoy

SAN DIEGO STATE

**UNIVERSITY** 



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(Cornelius Lanczos)

The Lanczos algorithm (you're welcome) and related power and Arnoldi methods seek to find only the extremal eigenvalues, even in huge dimensions

Or even more!



Frederic Nowacki



(Cornelius Lanczos)

### The challenge of dimensionality



Whitehead *et al* (Adv. Nucl. Phys 9, 123 (1977)) introduced both the Lanczos algorithm and a simple bit representation of Slater determinants.





Product wavefunction ("Slater Determinant")  $\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3 \dots) = \phi_{(n_1)}(\vec{r}_1)\phi_{(n_2)}(\vec{r}_2)\phi_{(n_3)}(\vec{r}_3)\dots\phi_{(n_N)}(\vec{r}_N)$ 

Each many-body state can be *uniquely* determined by a list of "occupied" single-particle states = "occupation representation"

 $|\alpha\rangle = \hat{a}_{n_1}^+ \hat{a}_{n_2}^+ \hat{a}_{n_3}^+ \dots \hat{a}_{n_N}^+ |0\rangle$ 



Product wavefunction ("Slater Determinant")

 $\Psi(\vec{r}_{1},\vec{r}_{2},\vec{r}_{3}...) = \phi_{n}(\vec{r}_{1})\phi_{n}(\vec{r}_{2})\phi_{n}(\vec{r}_{3})...\phi_{n}(\vec{r}_{N})$ 

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n <sub>i</sub>	1	2	3	4	5	6	7
α=1	1	0	0	1	1	0	1
α=2	1	0	1	0	0	1	1
α=3	0	1	1	1	0	1	0



Product wavefunction ("Slater Determinant")

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α=3	0	1	1	1	0	1	0

$$|\Psi\rangle = \sum_{\mu\nu} c_{\mu\nu} |p_{\mu}\rangle |n_{\nu}\rangle$$

$$01101000...\rangle |10010100...\rangle$$

"bit representation" convenient for digital computers



#### Product wavefunction

 $\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3...) = \phi_{(\vec{r}_1)}(\vec{r}_1)$ 

Each many-body stat by a list of "occupied = "occupation repres

 $|\alpha\rangle = \hat{a}_{n_1}^+ \hat{a}_{n_2}^+ \hat{a}_{n_3}^+ \dots \hat{a}_{n_N}^+ |0\rangle$ 

Working in the M-scheme, one doesn't need coefficients of fractional parentage!

	3	4	5	6	7
	0	1	1	0	1
	1	0	0	1	1
	1	1	0	1	0

"bit representation" convenient for digital computers











Configuration-interaction method ...today

 $\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$ 



$$\Psi \rangle = \sum_{\alpha} c_{\alpha} |\alpha\rangle$$

$$H_{\alpha\beta} = \langle \alpha | \hat{\mathbf{H}} | \beta \rangle$$

$$Can compute quickly using bit manipulation$$
or low the set of the set

... and solve for low eigenstates with Lanczos



What about the other problem...intruders?







# What about the other problem...intruders?















energy

P+Q = 1

Intruders are states predominantly in Q, but low-lying in energy







energy

P+Q = 1

Early calculations worked in the Pspace, but accounted for Q through perturbation theory





1970 Barrett and Kirson, 1972 Schucan and Weidenmuller: intruder states can cause perturbative expansions to ultimately diverge.

This in particular applies to particle-hole states.

This makes expanding beyond the valence space problematic, and **almost** kills the field (except for a stubborn few) for twenty years.







# 1991-1993: Vary and Barrett introduced the **no-core shell model**: Without a core, there is no "particle-hole" expansion.

Around this same time high-precision phase shift data from NN scattering became available.

Fitted to this data, the **Argonne potential** showed one could reproduce nuclear many-body data.

Then chiral EFT gave a systematic way to characterize nuclear forces

The field lurches back to life!



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### The birth of the shell model

Today bases can be a linear combination of simple Slater determinants with fixed total  $J_z/M$  ('M-scheme') or configurations with good total J ('J-scheme') or other group-theory label ('symmetry-adapted')

Configuration-interaction:

A superposition of different configurations

 $|\Psi\rangle = c_1 |(0s)^4 (0p_{3/2})^2 \rangle + c_2 |(0s)^4 (0p_{3/2})^1 (0p_{1/2})^1 \rangle + \dots$ 





## A diversity of approaches Phylogenetic Tree of Life

























It's also important to know:

Computational burden is *not* primarily the dimension but is the # of nonzero Hamiltonian matrix elements.

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha}$$



J-scheme matrices are smaller but much denser than M-scheme, and "symmetry-adapted" (i.e. SU(3)) matrices are smaller (and denser) still.

example:  ${}^{12}C N_{max} = 8$ 

 scheme basis dim

 M
  $6 \ge 10^8$  

 J (J=4)
  $9 \ge 10^7$  

 SU(3)
  $9 \ge 10^6$  

 (truncated)

From Dytrych, et al, Comp Phys Comm 207, 202 (2016)



J-scheme matrices are smaller but much denser than M-scheme, and "symmetry-adapted" (i.e. SU(3)) matrices are smaller (and denser) still.

example:  ${}^{12}C N_{max} = 8$ 

scheme basis dim		basis dim	# of nonzero matrix elements	3
	Μ	$6 \ge 10^8$	$5 \ge 10^{11}$	4 Tb of memory!
	J (J=4)	$9 \ge 10^{7}$	$3 \ge 10^{13}$	240 Tb of memory!
	SU(3)	$9 \ge 10^{6}$	$2 \ge 10^{12}$	16 Tb of memory!
	(truncate	ed)		

From Dytrych, et al, Comp Phys Comm 207, 202 (2016)



J-scheme matrices are smaller but much denser than M-scheme, and "symmetry-adapted" (i.e. SU(3)) matrices are smaller (and denser) still.

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One proton outside a filled shell + filled neutron shell One proton outside a filled shell + neutron 2p-2h



"island of inversion"

Frederic Nowacki















 $\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$ millions or even billions of components (in M-scheme)  $|\Psi\rangle = \sum c_{\alpha} |\alpha\rangle$ α







We can 'x-ray' the wave function using group theory



Jerry Draayer







Grouptheoretical Decomposition

Symplectic Sp(3,R)





<sup>29</sup>F is an analog of <sup>11</sup>Li



One proton outside a filled shell + filled neutron shell One proton outside a filled shell + neutron 2p-2h

#### "island of inversion"

#### CASE STUDY: 29F











Grouptheoretical Decomposition

Symplectic Sp(3,R)









### The future (?) of the shell model





The quantum computing gold rush....











### $|\chi\rangle = a\;|0\rangle + b|1\rangle$



 $|\chi\rangle = a |0\rangle + b|1\rangle$ 



# $\begin{aligned} |\chi\rangle|\chi\rangle|\chi\rangle|\chi\rangle|\chi\rangle|\chi\rangle \dots &= (a |0\rangle + b|1\rangle)(a |0\rangle + b|1\rangle) \dots \\ &= |0000 \dots\rangle + |1000 \dots\rangle + |0100 \dots\rangle \dots\end{aligned}$





### $|\chi\rangle = a |0\rangle + b|1\rangle$

## $|\chi\rangle|\chi\rangle|\chi\rangle|\chi\rangle|\chi\rangle...$ 1 35 qb 'word' = 34.7 *billion* elements in a vector





# This solves the problem of **exponential scaling**!

 $|\chi\rangle|\chi\rangle|\chi\rangle|\chi\rangle|\chi\rangle...$ 

### Yuri Manin

1 35 qb 'word' = 34.7 billion elements in a vector





# So build those quantum computers!

 $|\chi\rangle|\chi\rangle|\chi\rangle|\chi\rangle|\chi\rangle...$ 

Richard Feynman

1 35 qb 'word' = 34.7 billion elements in a vector

### Quantum computing & the shell model









Parrish and McMahon, arXiv:1909.08925 "Quantum Filter Diagonalization"

Key idea of "Quantum Lanczos": take states at different 'times' to form a non-orthogonal **reduced** basis

 $|\psi_n\rangle = e^{-in\Delta t\hat{H}}|\psi_0\rangle \qquad N_{mn} = \langle\psi_m|\psi_n\rangle \quad H_{mn} = \langle\psi_m|\hat{H}|\psi_n\rangle$ 

In this reduced basis, solve generalized eigenvalue problem:

 $\widehat{H}\vec{v} = E \ \widehat{N}\vec{v}$ 



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Amanda Bowman, SDSU M.S. student

in Computational Science

MS thesis: "Nuclear Spectra from Quantum Lanczos Algorithm with Real-Time Evolution and Multiple Reference States" arXiv:2309.00759



Ionel Stetcu,













Figure 8.1. Numerical simulations of the QLanczos algorithm with exact realtime evolution to solve for the lowest five energy states of the valence particles of <sup>8</sup>Be (two protons and two neutrons in the full *p*-shell). The simulation was run using a single reference state; (a) the lowest energy configuration in the spherical basis and (b) the Hartree-Fock state. A fixed number of real-time evolution iterations was used (S = 8) with a time step size of  $\Delta t = 0.1$ .







Figure 8.1. Numerical simulations of the QLanczos algorithm with exact realtime evolution to solve for the lowest five energy states of the valence particles of <sup>8</sup>Be (two protons and two neutrons in the full *p*-shell). The simulation was run using a single reference state; (a) the lowest energy configuration in the spherical basis and (b) the Hartree-Fock state. A fixed number of real-time evolution iterations was used (S = 8) with a time step size of  $\Delta t = 0.1$ .







H requires 975 Pauli strings and ~ 24,000 gates ne QLanczos algorithm with exact realve energy states of the valence particles in the full *p*-shell). The simulation was the lowest energy configuration in the ck state. A fixed number of real-time

evolution iterations was used (S = 8) with a time step size of  $\Delta t = 0.1$ .









Let's look at the data requirements in more detail



Consider <sup>12</sup>C, N<sub>max</sub>=8

*M*-scheme dimension 0.6 billion

55 single-particle orbitals (n1j) 440 single particle states (n1jm) | 011001... > Let's look at the data requirements in more detail



Consider <sup>12</sup>C, N<sub>max</sub>=8

*M*-scheme dimension 0.6 billion

55 single-particle orbitals ( n l j)
440 single particle states (n l j m) | 0 1 1 0 0 1 ... >

= estimate # of qubits needed

Let's look at the data requirements in more detail



Consider <sup>12</sup>C, N<sub>max</sub>=8

*M*-scheme dimension 0.6 billion by superposition

# uncoupled 2-body matrix elements ~ 10 million!  $V_{ijkl}$   $a_i^+ a_j^+ a_l a_k = #$  'Pauli strings'

= # of terms to be evaluated in a quantum circuit
(or, # of separate quantum circuits to be evaluated!)

~ 250,000,000 gates (but **polynomial** scaling)





# Quantum computing **useful** for the shell model is still a ways off!











#### The shell-model has come a long way in 75 years...

and the journey is not yet over!

Enjoy the Symposium!