Lecture 2: MIXING IT UP:
THE INTERACTING SHELL MODEL

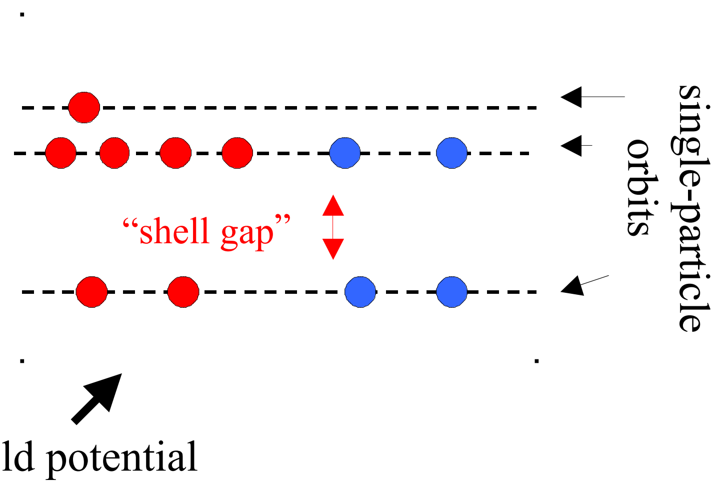
Beyond the mean-field...

We want to:	describe excited states transitions between states include (long-range) correlations

Our story so far: (from lecture 1)

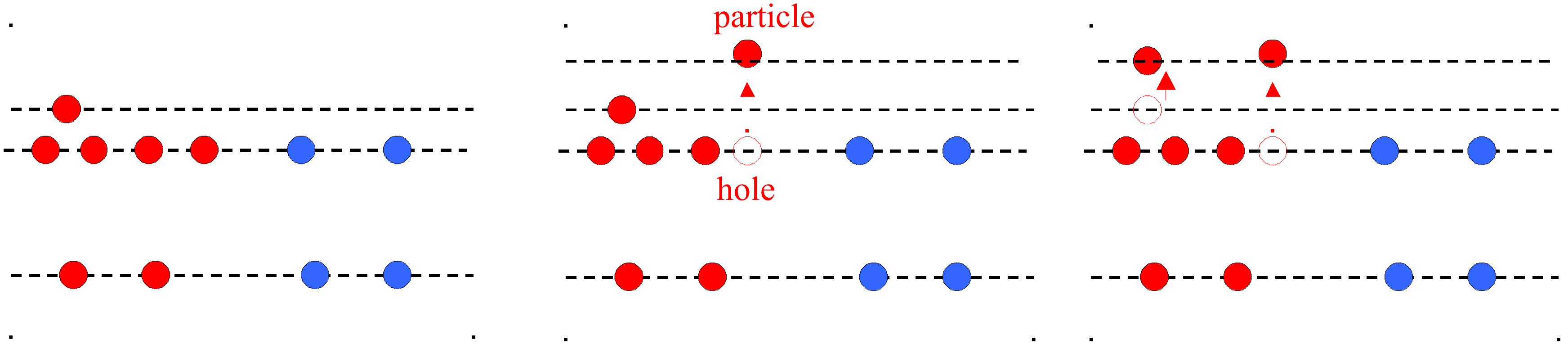
Describe **ground state** as independent nucleons moving in mean-field potential

fill orbits with
lowest single-particle energies first...



SIMPLE MODEL OF EXCITED STATES

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

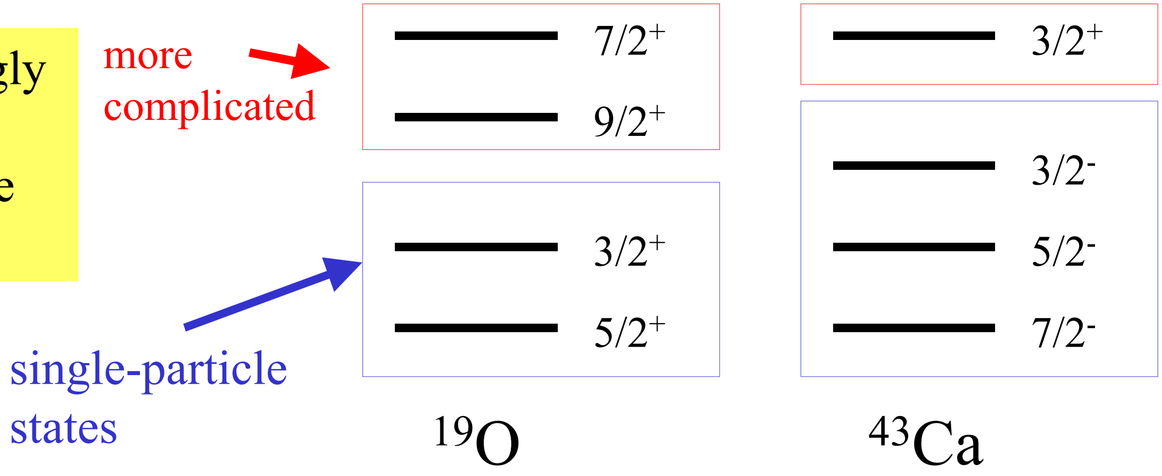


original configuration

one-particle, one-hole (1p1h) excitation

two-particle, two-hole (2p2h) excitation

This works surprisingly well for some nuclei, especially just outside a closed shell:



CONFIGURATION MIXING

In reality, most excited states are an **admixture** of these particle-hole **configurations, including the g.s.**

$$\Psi = c_0 \Psi_{0p0h} + c_1 \Psi_{1p1h} + c_2 \Psi_{2p2h} + \ldots$$

actually many terms for 1p1h, 2p2h, etc.

Particle-hole configurations mixed by **residual interaction:**

$$H = T+V = \underbrace{T+U_{HF}}_{\text{mean field potential}} + \underbrace{V-U_{HF}}_{\text{residual interaction}}$$

(configuration diagonal in this potential)

Basic idea of **interacting shell model:** diagonalize Hamiltonian H in basis of particle-hole configurations

(1) Create many-body basis states
(2) Compute many-body matrix elements
(3) Diagonalize to get eigenvectors, eigenvalues

easy to say,
the details are the key!

BASIS STATES: CREATION OPERATORS

Basis states are Slater determinants, but it is most convenient to use a **completely equivalent** formalism:
second quantization or **creation/annihilation operators**

creation operator $a^\dagger_i$ creates a fermion in the *i*th state
annihilation operator a_i destroys a fermion in the *i*th state
<u>anticommutation relations</u>: $\{a_i , a^\dagger_j\} = a_i \; a^\dagger_j + a_i \, a^\dagger_j = \delta_{ij}$
and $\{a_i^\dagger , a^\dagger_j\} = 0$ so that $a_i^\dagger \, a^\dagger_j = - a^\dagger_j \, a_i^\dagger$ (antisymmetry)

So a Slater determinant can be written as
$|\Psi\rangle = a^\dagger_1 \, a^\dagger_2 \, a^\dagger_3 \ldots a^\dagger_A \, |0\rangle$

particle vacuum

Note (very important): we have suppressed the explicit coordinate-space dependence of the original Slater determinant.
This means we implicitly **assume** we have **already** chosen the form of the **single-particle states**, (i = 1,2,3, ... A) as dictated by some "mean-field"-like potential (HO, WS, HF, etc)

BASIS STATES: OCCUPATION REPRESENTATION

How are many-body basis states **actually** represented in the computer program?

Well, these are fermions, so a single-particle state is either occupied or empty, which in a computer is represented by 1's and 0's

literally $\Psi = 000100110011000110$

state 1 state 4

single-particle states occupied:
4, 7,8,11,12, 16,17

i =	1	2	3	4	5	6
nl_j =	$0s_{1/2}$	$0s_{1/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$	$0p_{3/2}$
m_j =	-1/2	+1/2	-3/2	-1/2	1/2	3/2
occ =	0	1	0	1	0	0

antisymmetry must be programmed in explicitly

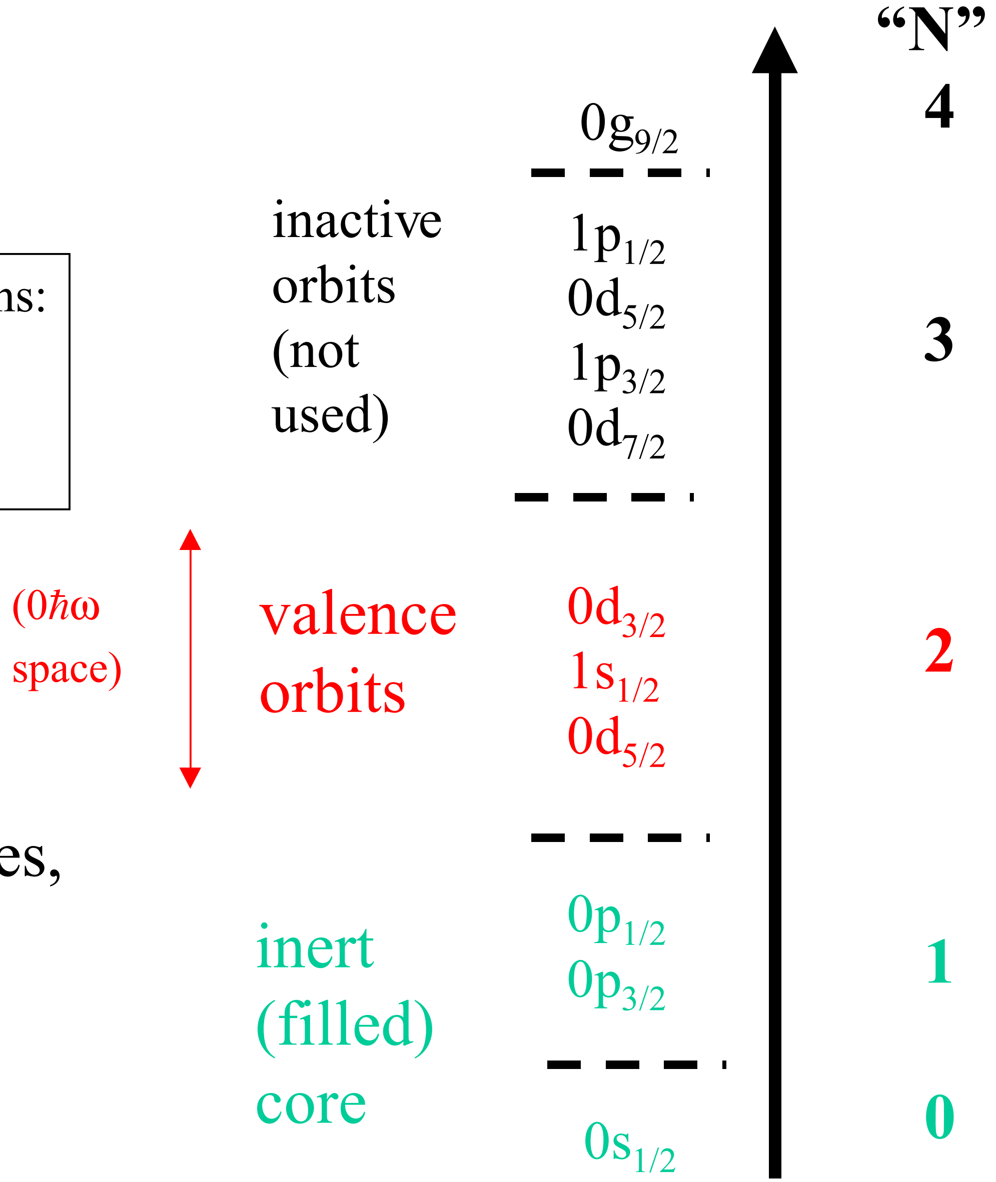
(more about this later)

CHOOSING A (TRACTABLE) MANY-BODY BASIS

Cannot include **all** possible many-body configurations: must truncate

Typical # of many-body configurations:
10,000-100,000 “routine”
1-10 million not unusual
current record: roughly two billion!

First step is to truncate in **single-particle space**. Usually couched in terms of harmonic oscillator states, especially for light nuclei (A < 50) .



“N”

4 — $0g_{9/2}$

3 — inactive orbits (not used): $1p_{1/2}$, $0d_{5/2}$, $1p_{3/2}$, $0d_{7/2}$

2 — ($0\hbar\omega$ space) valence orbits: $0d_{3/2}$, $1s_{1/2}$, $0d_{5/2}$

1 — inert (filled) core: $0p_{1/2}$, $0p_{3/2}$

0 — $0s_{1/2}$

BUILDING THE MANY-BODY BASIS

In principle, we could allow **all** configurations within the valence space...

000111 001101 011001
010011 010101 101001
100011 100101 etc....

$$\text{\# of configurations} = \binom{N_{s.p.states}}{N_{particles}}$$

... but that is neither **necessary** nor always **possible**

Because of rotational invariance, eigenstates will have good J, M .
Can rotate state of J, M to state of J, M' which are physically the same.
Therefore: don't need all M states!! **Choose a fixed M.**

(Later: even of these "M-scheme states" may want to truncate the many-body basis, usually on the basis of **single-particle energies)**

M-SCHEME BASIS STATES

If your mean-field potential (nearly forgotten now) is **spherically symmetric,** then the **single-particle states** will have good **j, m_j.**
Because the third component of ang. mom., J_z, is an additive quantum number, all the many-body basis states will have **good M**= sum of single-particle m_j's

i =	1	2	3	4	5	6	M_{tot} =
nl_j =	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	$0d_{5/2}$	
m_j =	-5/2	-3/2	-1/2	+1/2	3/2	5/2	
occ =	0	1	0	1	0	0	-3/2+1/2 = -1
	1	0	0	0	1	0	-5/2+3/2 = -1
	0	0	1	1	0	0	-1/2+1/2 = 0

Comments: While the many-body states (Slater deteminants) have good M, they do not have good J. States of good J must be a linear combination of Slater determinants. Furthermore, J ≥ |M|, which allows us to separate out and **count** (homework problem!) states of different J.

Summary: for any given calculation, choose ALL states to have the **same** M

MORE ON CONSTRUCTING THE BASIS

Once you have constructed states of good M, you can either start computing the Hamiltonian, **or**, you can project out states of good J (and usually good T) (JT-scheme basis, which is a subset of M-scheme basis).

Often one truncates the basis further, either for reasons of physics (projections of center-of-mass motion) or to further reduce the size of the many-body basis. This is almost always done on the basis of single-particle energies: choose states with Σ(single-particle energies) < E_{max}. Can use either "real" single-particle energies or use harmonic oscillator ($\hbar\omega$) single-particle energies

COMPUTING THE HAMILTONIAN MATRIX

Once we have a set of **many-body basis states** $\{ | \Psi_a \rangle \}$,
we want to compute the matrix elements

$$H_{ab} = \langle \Psi_a | \mathrm{H} | \Psi_b \rangle$$

especially for the two-body interaction V(1,2)

The two-body interaction may have started out life as a funcation in coordinate space, such as $1/|r_1 - r_2|$ or $V\delta(r_1 - r_2)$, but now that we have fixed a single-particle basis, it comes in as an integral:

$$\left\langle ij;J \,|\, V \,|\, kl;J \right\rangle = \quad dr_1 dr_2 \phi_i^*(r_1)\phi_j^*(r_2) V(r_1,r_2)\{\phi_i(r_1)\phi_j(r_2) - \phi_i(r_2)\phi_j(r_1)\}$$

Because we **assume** we know all the ingredients (V, ϕ, etc.), this integral is computed ahead of time and stored as a **number.**

Often in practice we treat the **two-body matrix elements** as numbers alone that are adjusted to data (nuclear spectra) and don't worry about the form of V, ϕ, etc. This is **not** the height of consistency (and in fact can lead to problems) but it **is** common practice.

Many-body matrix elements

Residual interaction in creational/annihilation operators:

$$\hat{V} = {}_{ijkl;J}\frac{1}{4}\langle ij;J|V|kl;J\rangle \hat{a}^*_i \hat{a}^*_j \hat{a}_l \hat{a}_k$$

an integral; but stored as just a number!

creates a fermion in state *i*

destroys a fermion in state *k*

action of $a^\dagger_i\, a^\dagger_j\, a_l\, a_k$ on a basis state = Slater det = 0011000111

(1) see if states *k*,*l* occupied (that is, 1's in locations *k,l*.)

If so, replace by 0 = annihilation of fermions in those states.

(2) see if states *i, j* empty (that is, 0's in locations *i, j*.)

If so, replace by 1 = creation of fermions in those states.

this is a <u>new</u> basis state 0110100011. We have computed the *many-body matrix element* $\langle 0110100011|V|0011000111\rangle$ with the value $\langle ij|V|kl\rangle$ × phases from anticommuting fermions

SOLVING THE MATRIX EIGENVALUE EQUATION

We now have H_{ab}, a very large and very sparse matrix. We want to solve the matrix eigenvalue equation:

$$\underset{a}{} \quad H_{ab} c_b = E c_a$$

Then the wavefunction will be $\Psi = \underset{a}{} \; c_a \Psi_a$

Because *H* can have dimensions up to half a billion, this is not easy!!
Fortunately, we can take a shortcut because: we (almost always) want just a **few,** say 5-10, of the lowest-energy eigenstates.
Industry standard: use the **Lanczos algorithm** which efficiently extracts the extremal eigenstates.

OVERVIEW OF
SHELL-MODEL DIAGONALIZATION PROGRAMS

Input: (1) list of single-particle **valence** states: $0d_{5/2}$ etc.

does not include **any** information whether h.o., w.s. HF, etc

(2) # of valence protons, neutrons; total M; (parity); additional truncations on many-body states if desired

(3) list of single-particle energies and two-body matrix elements *as numbers*

Output: the first few (say, 5-10) eigenstates:

energy E, ang. mom. J, isospin T of those states

and

coefficients c_n for expanding eigenstates in the many-body basis

TYPICAL SHELL MODEL CALCULATIONS

$0p_{1/2}$-$0p_{3/2}$ space (6 s.p. states)
inert $0s_{1/2}$ core (^{4}He)
Interaction: Cohen-Kurath
2 s.p. energies + 15 t.b.m.e's
largest *M*-scheme basis dimension:
3p,3n (^{10}B): 84

$1s_{1/2}$-$0d_{3/2}$-$0d_{5/2}$ space (12 s.p. states)
inert $0s_{1/2}$- $0p_{1/2}$-$0p_{3/2}$ core (^{16}O)
Interaction: Brown-Wildenthal
3 s.p. energies + 63 t.b.m.e's
largest *M*-scheme basis dimension:
6p,6n (^{28}Si): 93,710

$1p_{1/2}$-$1p_{3/2}$-$0f_{5/2}$-$0f_{7/2}$ space (20 s.p. states)
inert $0s_{1/2}$- $0p_{1/2}$-$0p_{3/2}$ $1s_{1/2}$-$0d_{3/2}$-$0d_{5/2}$ core (^{40}Ca)
Interaction: modified Kuo-Brown, Brown-Richter, etc.
4 s.p. energies + 195 t.b.m.e's
largest *M*-scheme basis dimension:
10p,10n (^{60}Zn): 2.3 billion
more common dimensions:
^{48}Cr (4p,4n): 2 million
^{54}Fe (6p, 8n): 500 million

Next time: from wfn, compute transitions (gamma, beta, etc.)