Shell model formalism

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Outline

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Brief Review

- Mesoscopic system- approximate treatment required
- Nuclei exhibit "shell structure" through experimental observables
- Naive mean field description insufficient for correlated many-body problem
- Energy gaps in single particle basis (reproducing magic numbers)
- Select limited model space separated by energy gaps
- Reproduce low-energy nuclear properties

Configuration Interaction Theory

- General theory, applied in quantum chemistry and solid-state physics as well
- Referred to as shell model in nuclear physics
- Main principles discussed already
  - Select a limited model space of valence orbits outside a doubly magic core
  - Core is treated as vacuum
  - Procedure limited by size of model space (by mass in nuclear physics)
  - Determine interaction in reduced model space
  - Solve Schrödinger equation
- Accurate method with limitations
  1. Mass (based on size of necessary model space)
  2. Excitation energy
  3. Interaction
  4. Type of states (intruder, cluster, etc.)
  5. Effective charges (see Lectures IV-VI)
  6. Determination of appropriate model space

Outline

Introduction of notation

$$\begin{aligned} H &= T + V \\ &= (T + V_{mf}) + (V - V_{mf}) \\ &= H_0 + H_1 \end{aligned}$$

where

$$V = V_{NN} + V_{NNN} \qquad (+\ldots)$$

- In coordinate space commonly choose spherically symmetric mean fields

$$T = -\frac{\hbar^2}{2m}\Delta^2$$

$$V_{mf}(r) = V_c(r) + V_{so}(r)\vec{\ell}\cdot\vec{s}$$

- Solution $H_0|\phi_i\rangle = \epsilon_i|\phi_i\rangle$ can be found

Solution to spherical mean field

- In coordinate space,

$$\phi_{n\ell jm}(\vec{r}) = \frac{R_{nlj}(r)}{r}\left[Y^{\ell}\otimes\chi^{\frac{1}{2}}\right]^{j}_{m}$$

$$\left[Y^{\ell}\otimes\chi^{\frac{1}{2}}\right]^{j}_{m} \equiv \sum_{m_\ell m_s}\langle \ell m_\ell \frac{1}{2} m_s | jm\rangle\, Y_{\ell m_\ell}(\hat{r})\chi_{\frac{1}{2}m_s}$$

- Intrinsic spin wavefunctions are orthonormal

$$\langle \chi_{\frac{1}{2}m_s} | \chi_{\frac{1}{2}m'_s}\rangle = \delta_{m_s m'_s}$$

- Harmonic oscillator potential $V_{mf} = \frac{1}{2}m\omega^2 r^2$
  1. Typically employed in nuclear structure theory
  2. Strength (given in energy scale $\hbar\omega$) determined empirically
  3. Properties, especially deficiencies, affect calculations

Harmonic oscillator basis

- Important to consider whether spin-orbit is included explicitly
- No spin-orbit
  1. Degenerate orbits with same main oscillator quantum number

$$N = 2n + \ell$$

  2. Simpler radial wavefunctions[1]

$$R_{nl}(r) = \sqrt{\frac{2^{2+\ell-n}(2\ell+2n+1)!}{\sqrt{\pi}n!b^{2\ell+3}[(2\ell+1)!!]^2}} r^{\ell+1} e^{-r^2/2b^2} \times \sum_{k=0}^{n} \frac{(-2)^k n!(2\ell+1)!!}{k!(n-k)!(2\ell+2k+1)!!} \left(\frac{r}{b}\right)^{2k}$$

$$\text{where} \qquad b = \sqrt{\frac{\hbar}{m\omega}} = \sqrt{\frac{41.4\text{MeV fm}^2}{\hbar\omega}} \tag{1}$$

- Including spin-orbit
  1. Non-degenerate orbits (important for deriving effective interactions)
  2. More complicated orbits (not reproduced here)
- In the end, $\langle\Phi|V_{ms}|\Phi\rangle$ are quantities of interest
- Wavefunction can be written in any basis
- Modifies the interpretation of V_{ms}

[1] Courtesy of Alex Brown

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Conserved quantities

- In A-body system, conserved quantity O relates to

$$[H, O] = 0$$

- Simultaneously conserved quantities
  - Commute with Hamiltonian
  - Commute with each other
  - Produced by a set of Casimir operators
- Set provides symmetry quantum numbers labeling A-body states
  - Angular momentum J and projection M (in space-fixed frame)
  - Energy E (and therefore mass)
  - Momentum $\vec{P} = 0$ in center-of-mass frame
  - Electric charge Q and baryon charge B
- Approximately conserved quantities
  - Isospin T only approximately conserved by strong interaction
  - Parity π only approximately conserved by weak interaction
  - Will treat both as conserved quantities throughout these lectures

Outline

Many-body problem

- Schrödinger equation is hard to solve- start with simpler problem
  - For now, solving system of A independent identical nucleons
  - Protons and neutrons not distinguished

A-body Schrödinger equation

$$H_0|\Phi_a\rangle = E_a|\Phi_a\rangle$$

- Build from one particle solution $H_0|\phi_i\rangle = \epsilon_i|\phi_i\rangle$

$$E_a = \sum_{i=1}^{A} \epsilon_{a_i}$$

$$|\Phi_a\rangle = \prod_{i=1}^{A} a^\dagger_{a_i}|0\rangle$$

- Single particle wavefunctions are orthonormal $\langle\phi_i|\phi_j\rangle = \delta_{ij}$
- Label a refers to a particular choice of the A single particle orbits
- For lowest energy state, $E_0 = \sum_{i=1}^{A} \epsilon_i$
- Basis $\{|\Phi_a\rangle\}$ spans the Hilbert space of the A-body problem
- Can write $|\Psi_k\rangle = \sum_a c_a^k|\Phi_a\rangle$

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Many-body problem

Perturbation theory focusing on ground state

- $|\Psi_0\rangle = |\Psi_0^{(0)}\rangle + |\Psi_0^{(1)}\rangle + \dots$
  - $|\Psi_0^{(0)}\rangle = |\Phi_0\rangle$
  - $|\Psi_0^{(1)}\rangle = \sum_{a\neq 0} \frac{\langle\Phi_0|H_1|\Phi_a\rangle}{E_0^{(0)} - E_a^{(0)}}|\Phi_a\rangle$
- $E = E_0^{(0)} + E_0^{(1)} + \dots$
  - $E_0^{(0)} = \langle\Phi_0|H_0|\Phi_0\rangle$
  - $E_0^{(1)} = \langle\Phi_0|H_1|\Phi_0\rangle$

Configuration interaction theory

$$|\Psi_k\rangle = \sum_a c_a^k |\Phi_a\rangle \qquad \rightarrow \qquad \sum_a c_a^k H|\Phi_a\rangle = \sum_b c_b^k E_k|\Phi_b\rangle$$

- Multiply from left by arbitrary $\langle\Phi_b|$ to get line b of matrix equation

$$\sum_a \langle\Phi_b|H|\Phi_a\rangle c_a^k = E_k c_b^k$$

- Either way, matrix elements of H are ingredients of the calculation

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- $E = E_0^{(0)} + E_0^{(1)} + \dots$
  - $E_0^{(0)} = \langle\Phi_0|H_0|\Phi_0\rangle$
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CI matrix formulation

$$\begin{pmatrix} \langle\Phi_0|V_{ms}|\Phi_0\rangle & \langle\Phi_0|V_{ms}|\Phi_1\rangle & \cdots & \langle\Phi_0|V_{ms}|\Phi_{basis}\rangle \\ \langle\Phi_1|V_{ms}|\Phi_0\rangle & \langle\Phi_1|V_{ms}|\Phi_1\rangle & \cdots & \langle\Phi_1|V_{ms}|\Phi_{basis}\rangle \\ \langle\Phi_2|V_{ms}|\Phi_0\rangle & \langle\Phi_2|V_{ms}|\Phi_1\rangle & \cdots & \langle\Phi_2|V_{ms}|\Phi_{basis}\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle\Phi_{basis}|V_{ms}|\Phi_0\rangle & \langle\Phi_{basis}|V_{ms}|\Phi_1\rangle & \cdots & \langle\Phi_{basis}|V_{ms}|\Phi_{basis}\rangle \end{pmatrix} \begin{pmatrix} c_0^k \\ c_1^k \\ c_2^k \\ \vdots \\ c_{basis} \end{pmatrix} = E_k \begin{pmatrix} c_0^k \\ c_1^k \\ c_2^k \\ \vdots \\ c_{basis} \end{pmatrix}$$

- Example (diagonal)

$$\begin{aligned} \langle\Phi_a|T|\Phi_a\rangle &= \sum_{i,j=1}^{basis} \langle\Phi_a|t_{ij}a_i^\dagger a_j|\Phi_a\rangle \\ &= \sum_{i=1}^{basis} \langle\Phi_a|t_{ii}a_i^\dagger a_i|\Phi_a\rangle \\ &= \sum_{i=1}^{A} t_{ii} \end{aligned}$$

- Still impossible to solve without truncation

CI matrix formulation

$$\begin{pmatrix} \langle\Phi_0|V_{ms}|\Phi_0\rangle & \langle\Phi_0|V_{ms}|\Phi_1\rangle & \cdots & \langle\Phi_0|V_{ms}|\Phi_{basis}\rangle \\ \langle\Phi_1|V_{ms}|\Phi_0\rangle & \langle\Phi_1|V_{ms}|\Phi_1\rangle & \cdots & \langle\Phi_1|V_{ms}|\Phi_{basis}\rangle \\ \langle\Phi_2|V_{ms}|\Phi_0\rangle & \langle\Phi_2|V_{ms}|\Phi_1\rangle & \cdots & \langle\Phi_2|V_{ms}|\Phi_{basis}\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle\Phi_{basis}|V_{ms}|\Phi_0\rangle & \langle\Phi_{basis}|V_{ms}|\Phi_1\rangle & \cdots & \langle\Phi_{basis}|V_{ms}|\Phi_{basis}\rangle \end{pmatrix} \begin{pmatrix} c_0^k \\ c_1^k \\ c_2^k \\ \vdots \\ c_{basis} \end{pmatrix} = E_k \begin{pmatrix} c_0^k \\ c_1^k \\ c_2^k \\ \vdots \\ c_{basis} \end{pmatrix}$$

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- Still impossible to solve without truncation

Center of mass motion

- Interested only in internal structure of nucleus
- Rewrite Hamiltonian $H = H_{cm} + H_{int}$ (separate out center of mass)
- For $T = \frac{1}{2m}\sum_{i=1}^{A} p_i^2$
  - Introduce $\vec{Q} \equiv \sum_{i=1}^{A} \vec{p}_i$ and $\vec{q}_i = \vec{p}_i - \frac{\vec{Q}}{A}$
  - $T_{cm} = \frac{1}{2mA} Q^2$
  - $T_{int} = \frac{1}{2m}\sum_{i=1}^{A} q_i^2$
- In general: hard to separate potential into similar components V_{cm} and V_{int}
- Can be done algebraically for harmonic oscillator potential
- Introducing $\vec{R} \equiv \frac{1}{A}\sum_{i}^{A} \vec{r}_i$
  - $H_{cm} = \frac{1}{2mA} Q^2 + \frac{1}{2} A m \omega^2 R^2$
  - $|\Psi\rangle = |\Psi_{int}\rangle|\Psi_{cm}\rangle$, $E = E_{int} + E_{cm}$
  - In the ground state, $\langle\Psi|H_{cm}|\Psi\rangle = \frac{3}{2}\hbar\omega$
- Must account for this contribution to determine internal energies

Spurious States

- Solutions to the Schrödinger equation which do not describe internal structure
- Especially problematic in large model spaces (multiple oscillator shells)
- Excitations of center of mass wavefunction result in spurious states
- Ground state of even-even nucleus with $J^\pi = 0^+$
  - Spurious state $J^\pi = 1^-$ from excited center of mass
  - Infinite number of states (to high energy)

Angular momentum coupling

- Coupling of angular momentum $\vec{J}_1$ and $\vec{J}_2$ to $\vec{J}$
  - Triangle condition leads to $J_{min} = |J_1 - J_2|$ and $J_{max} = J_1 + J_2$
  - Wavefunction associated with coupled J written in terms of $|J_1 M_1 J_2 M_2\rangle$

$$|J_1 J_2 JM\rangle = \sum_{M_1 M_2} \langle J_1 M_1 J_2 M_2 | JM\rangle |J_1 M_1 J_2 M_2\rangle$$

  - Clebsch-Gordan coefficients $\langle J_1 M_1 J_2 M_2 | JM\rangle$

- Can employ Clebsch-Gordan coefficients to couple many-body wavefunctions

  Require $M_1 + M_2 = M$ for non-zero coupling

- Can write in terms of $3j$ symbols
- Coupling three angular momenta requires $6j$, four requires $9j$, etc.

Many-body wavefunctions

- *m*-scheme

$$M = \sum_{i=1}^{A} m_i$$

  - Hamiltonian is diagonal in M since M is conserved quantity
  - Use basis $\{|\Phi\rangle\}$ with good M value (but not necessarily good J)
  - Determine J from $\hat{J}^2|\Psi\rangle = J(J+1)|\Psi\rangle$
  - All values of J with $J \geq M$ are found in one calculation
  - Infinite basis can be truncated

- *J*-scheme
  - Reduce the dimension of the problem by limiting to states with good J
  - Calculation performed for each J value
  - More advantageous for lower J values

- In both cases, determine T from $\hat{T}^2|\Psi\rangle = T(T+1)|\Psi\rangle$

Outline

Partitions

- Complicated many-body wavefunction: sum over simple Slater determinants
- Each Slater determinant is one configuration in reduced model space
- Configuration corresponds to a partition of valence nucleons into available orbits
- Number of partitions determined by number of valence protons and neutrons
- Truncations possible by limiting partitions in the calculation
  1. Explicitly done through the use of restrictions in 'lpe' option of 'shell'
  2. See Lecture III and Tutorial III for more details

Simple example

- Two neutrons in *sd* shell (^{18}O)
- Six possible partitions:

$n\ell(2j)$	$0d5$	$0d3$	$1s1$
	2	0	0
	1	1	0
	1	0	1
	0	2	0
	0	1	1
	0	0	2

- Can determine m-scheme dimension $D(M)$ and J-scheme dimension $\mathcal{D}(J)$
- Each partition P has its own values $D^P(M)$ and $\mathcal{D}^P(J)$

$$\mathcal{D}^P(J) = D^P(M = J) - D^P(M = J + 1)$$

- Model space dimensions given by sum over partitions

$$D(M) = \sum_P D^P(M)$$

$$\mathcal{D}(J) = \sum_P \mathcal{D}^P(J)$$

Counting possibilities to determine dimensions

- For partition with both neutrons in $0d_{5/2}$ orbit, $P = (0d_{5/2})^2 \equiv 5_2$

$$M = \sum_i m_i$$

- Ways to produce $M = 0$

$2m$	+5	+3	+1	-1	-3	-5
	1	0	0	0	0	1
	0	1	0	0	1	0
	0	0	1	1	0	0

- Ways to produce $M = 1$

$2m$	+5	+3	+1	-1	-3	-5
	1	0	0	0	1	0
	0	1	0	1	0	0

Counting possibilities to determine dimensions

- For partition with both neutrons in $0d_{5/2}$ orbit, $P = (0d_{5/2})^2 \equiv 5_2$

M	$D^{5_2}(M)$
0	3
1	2
2	2
3	1
4	1
-4	1
-3	1
-2	2
-1	2

- In general, don't need to calculate both M and $-M$ since $D^P(M) = D^P(-M)$
- Check all configurations are accounted for

$$\binom{6}{2} = 15 = \sum_M D^{5_2}(M)$$

Counting possibilities to determine dimensions

- For partition with both neutrons in $0d_{5/2}$ orbit, $P = (0d_{5/2})^2 \equiv 5_2$

M	$D^{5_2}(M)$
0	3
1	2
2	2
3	1
4	1
-4	1
-3	1
-2	2
-1	2

- $\mathcal{D}^{5_2}(J) = D^{5_2}(M = J) - D^{5_2}(M = J + 1)$
- Only nonzero values: $\mathcal{D}^{5_2}(J = 0) = \mathcal{D}^{5_2}(J = 2) = \mathcal{D}^{5_2}(J = 4) = 1$
- Significant reduction in dimension for J-scheme

Counting possibilities to determine dimensions

- Determine dimension for all partitions, sum over to find

M	$D(M)$
0	14
1	11
2	9
3	4
4	2
-4	2
-3	4
-2	9
-1	11

J	$\mathcal{D}(J)$
0	3
1	2
2	5
3	2
4	2

- $\sum_M D(M)$ corresponds to $\binom{12}{2} = 66$ as expected
- Full CI calculation for ^{18}O produces 14 states from $\sum_J \mathcal{D}(J)$
- In agreement with result shown in Lecture I

Realistic example

- ^{48}Cr in *pf* model space (four protons and four neutrons)
- 31 partitions for each type of nucleon
- Can determine $\mathcal{D}_p(J)$ and $\mathcal{D}_n(J)$ as shown previously
- Of course, $\mathcal{D}_p(J) = \mathcal{D}_n(J)$ in this case
- Must include all possibilities $\vec{J} = \vec{J}_p + \vec{J}_n$
- For simplest $J = 0$ example[2]:

$$\mathcal{D}(J=0) = \sum_{J_i} \mathcal{D}_p(J_i)\mathcal{D}_n(J_i)$$

J	0	1	2	3	4	5	6	7	8	9	10
$\mathcal{D}_p(J)$	28	54	94	91	99	75	59	33	22	7	3
$\mathcal{D}_n(J)$	28	54	94	91	99	75	59	33	22	7	3

- $\mathcal{D}(J=0) = 41,355$ in total

[2] Courtesy of Alex Brown

^{48}Cr (continued)

- Performing similar steps while accounting for coupling of $\vec{J}_p$ and $\vec{J}_n$

$$\mathcal{D}(J=0) = 41,355$$
$$\mathcal{D}(J=1) = 118,269$$
$$\mathcal{D}(J=2) = 182,242$$
$$\vdots$$

- $D(M) = \sum_{J \geq M} \mathcal{D}(J)$
- $D(M=0) = 1,963,461$
- Dimension of the problem $\approx 2 \cdot 10^6$
  - Diagonalize H to get eigenvalues E
  - H is a sparse matrix $\rightarrow$ algorithms available
  - Matrix multiplication $u = Hv$
  - In m-scheme, u, v have 1,963,461 components for ^{48}Cr
  - In J-scheme, u, v have 41,355 components for $J = 0$ states of ^{48}Cr
- NUSHELLX solves ten lowest $J = 0$ states in ≈ 1 minute (standard laptop)

Approximate matrix dimensions

- *sd* shell: 10^5
- *pf* shell: 10^9
- *jj*44 model space $(1p_{3/2}, 1p_{1/2}, 0f_{5/2}, 0g_{9/2})$: 10^{11}

- Approximate time corresponding to longest calculation
  - Level scheme for ^{28}Si in about an hour
  - Level scheme for ^{56}Ni in days
  - Level scheme for ^{78}Y in weeks
- Need parallelization or patience
- Also exceed memory requirements as mass and model space increase
- Need truncations or other alternatives

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