15thNational Nuclear Physics Summer School

June 15-27, 2003





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Nuclear Structure

Erich Ormand N-Division, Physics and Adv. Technologies Directorate Lawrence Livermore National Laboratory

Lecture #2

This work was carried out under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.



We want an accurate description of low-lying states



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Low-lying structure – The interacting Shell Model

The interacting shell model is one of the most powerful tools

- Calculate Hamiltonian matrix $H_{ij} = \langle \phi_j | H | \phi_i \rangle$ ٠
 - Diagonalize to obtain eigenvalues

 $\begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1N} \\ H_{21} & H_{22} & & \\ \vdots & & \ddots & \\ H_{N1} & & \dots & H_{NN} \end{pmatrix}$





Nuclear structure with NN-interaction

- NN-interaction determined from scattering and the deuteron
 - Argonne, Bonn, Paris, Reid, etc.

Phase shift and potential in ¹S₀ channel



Problem: Repulsion in strong interaction \rightarrow **Infinite space!**



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Can we get around this problem? Effective interactions



- Choose subspace of ϕ_n for a calculation (*P*-space)
 - Include most of the relevant physics
 - Q -space (excluded infinite)
- Effective interaction:

$$H_{eff}\hat{\mathbf{P}}\Psi_i = E_i\hat{\mathbf{P}}\Psi_i$$

- Two approaches:
 - Bloch-Horowitz



$$H_{eff} = \hat{P}H + \hat{P}H \frac{1}{E_i - \hat{Q}H} \hat{Q}H\hat{P}$$
- Lee-Suzuki:

$$H_{eff} = \mathbf{PXHX^{-1}I}$$





Effective interactions permit first-principles shell-model applications



- Impossible problem \rightarrow Difficult problem
 - Two, three, four, ... A-body operators



- Compromise between size of P-space and number of clusters
 - Three-body clusters





The general idea behind effective interactions





- Ideally, we would like to use these fundamental interactions in our theory calculations
- In most cases this is not really practical as the the NN-interaction has a very strong repulsive core at short distances
 - This means that in many-body applications an infinite number of states are needed as states can be scattered to high-energy intermediate states
- We need to use effective interactions
 - Derived from some formal theory
 - This is in principle possible and is difficult. But it is becoming practical now for light nuclei
 - Assume they exist as the formal theory stipulates and determine it empirically to reproduce data
 - This has permitted many studies in nuclear structure to go forward





- The practical Shell Model
 - 1. Choose a model space to be used for a range of nuclei
 - E.g., the 0d and 1s orbits (sd-shell) for ¹⁶O to ⁴⁰Ca or the 0f and 1p orbits for ⁴⁰Ca to ¹²⁰Nd
 - 2. We start from the premise that the effective interaction exists
 - 3. We use effective interaction theory to make a first approximation (G-matrix)
 - 4. Then tune specific matrix elements to reproduce known experimental levels
 - 5. With this empirical interaction, then extrapolate to all nuclei within the chosen model space
 - 6. Note that radial wave functions are explicitly not included, so we add them in later

The empirical shell model works well! But be careful to know the limitations! More on exact treatments later.





We write the Hamiltonian as

- Start with closed inner core, e.g., for ²⁴Mg, close the p-shell
- Active valence particles in a computationally viable model space, e.g., the 0d_{5/2}, 0d_{3/2}, 1s_{1/2} orbits for ²⁴Mg



- •Single-particle energy ε_i
- Two-body residual interactions

Energy is relative to ¹⁶O core







Building the shell-model basis states



- Choose states with definite parity, J_z and T_z and let the Hamiltonian do the rest
 - A very useful approach is a bitrepresentation known as the M-scheme



uclear Theory 8



A single integer represents a complicated Slater Determinant





Basis states - How many are there?

- To do a calculation we need states with fixed J_z
 - All J-values are contained in $J_z=0$ or $J_z=1/2$
- Counting the number of basis states
 - Order-of-magnitude estimate
 - *n* particles, and N_{sps} single-particle states
 - N_{sps} in the sd-shell = 12 (0d_{5/2}=6, 0d_{3/2}=4, 1s_{1/2}=2)
 - N_{sps} in the fp-shell = 20 (0f_{7/2}=8, 0f_{5/2}=6, 1p_{3/2}=4, 1p_{1/2}=2)

- Includes states of all J and J_z
 - Number of J_z =0 divide by a factor of ten
- Number of states with a given J





- Setup Hamiltonian matrix (j|H|i) and diagonalize
- Lanczos algorithm
 - Bring matrix to tri-diagonal form

$$\hat{H}\mathbf{v}_{1} = \alpha_{1}\mathbf{v}_{1} + \beta_{1}\mathbf{v}_{2}$$

$$\hat{H}\mathbf{v}_{2} = \beta_{1}\mathbf{v}_{1} + \alpha_{2}\mathbf{v}_{2} + \beta_{2}\mathbf{v}_{3}$$

$$\hat{H}\mathbf{v}_{3} = \beta_{2}\mathbf{v}_{2} + \alpha_{3}\mathbf{v}_{3} + \beta_{3}\mathbf{v}_{4}$$

$$\hat{H}\mathbf{v}_{4} = \beta_{3}\mathbf{v}_{3} + \alpha_{4}\mathbf{v}_{4} + \beta_{4}\mathbf{v}_{5}$$

- nth iteration computes 2nth moment



Note that after each iteration,

we need to re-orthogonalize!

- But you can't find eigenvalues with calculated moments
- Eigenvalues converge to extreme (largest and smallest) values
- ~ 100-200 iterations needed for 10 eigenvalues (even for 10^8 states)



N Division





- Oak Ridge (1969)
 - Coefficients of Fractional parentage (CFP)
- Glasgow (1977)
 - Good J_z (M-scheme)
 - J restored in diagonalization
- OXBASH (1985)
 - J-projected M-scheme
 - Smaller matrices
- RITSSCHIL (1985)
 - CFP

- DUSM (1989)
 - Permutation groups
- ANTOINE (1991 & 1999)
 - M-scheme
 - Apply matrix on-the-fly
 - Large dimensions
- NATHAN (1998)
 - J-projected similar to ANTOINE
 - "Hybrid" M-scheme-CFP code
- REDSTICK (now)
 - Similar to ANTOINE
 - M-scheme
 - Three-body interactions
 - Parallel architecture





REDSTICK – basis state ordering

- **Ordering of basis states** speeds up the calculation
- Need a *FAST* lookup scheme ٠
- **Construct proton and** neutron many-body Slater determinants
 - Order by Parity, J, and $\hbar\Omega$





For each proton SD store start in Lanczos vector: pos(*i*) For each neutron SD store relative position in Jz, parity list: pos(j) Position in Lanczos vector determined by summing two integers k = pos(i) + pos(j)Same algorithm can be used to sort and find two-body matrix elements

- Limits truncations •
 - Partition truncations not possible
- Much faster!
- Lanczos vector points to p & n SD's (less memory)



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REDSTICK – Applying the Hamiltonian – pn part On-the-fly



$$\hat{H}\mathbf{v} = \hat{H}\sum_{i} c_{i} |\Phi_{i}\rangle = \sum_{j} \sum_{i} c_{i} \langle \Phi_{i} | H | \Phi_{i} \rangle |\Phi_{j}\rangle = \sum_{j} c_{j}' |\Phi_{j}\rangle$$

- With large dimensions, it may be better not to pre-calculate and store the Hamiltonian matrix
- Find states connected by one-body proton or neutron operator
- pn-part is the hardest
 - Product of two one-body operators

$$\hat{H}^{pn} = \sum_{ijkl} v_{ijkl}^{pn} \pi_i^+ \pi_j v_k^+ v_l$$

- Pre-sort connections by one-body operators; store operator and phase
- Loop over all initial proton-neutron SD's $\Phi_i = \phi_k^p \phi_l^n$
 - For each ϕ_k^p loop over all ϕ_m^p connected by one-body operator
 - For each ϕ^n_l loop over all ϕ^n_n connected by onebody operator but limited in J_z , parity, and $\hbar\Omega$ by final proton state ϕ^p_m
 - Update Lanczos vector: Position=pos(m)+pos(n)









REDSTICK – Applying the Hamiltonian



•
$$\mathbf{v}_j = \mathbf{v}_j - \sum_{i < j} \mathbf{v}_i \cdot \mathbf{v}_j$$

- Not that trivial (but also not the main bottleneck in the calculation)
- Let each processor be responsible for a sub set of Lanczos vectors written to disk
- Each processor has a copy of the current vector
- Accumulate sum overlaps $\mathbf{a}_n = \sum_{i \le j} \mathbf{v}_i \cdot \mathbf{v}_j$ on each node, *n*
- Global sum $\mathbf{a} = \sum_{n} \mathbf{a}_{n}$ then $\mathbf{v}_{j} = \mathbf{v}_{j} \mathbf{a}$ and normalize
- Not quite the same as sequential reorthogonalization, but seems to work fine (also used in MFD).



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REDSTICK or ANTOINE





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Simple application of the shell model

- A=18, two-particle problem with ¹⁶O core
 - Two protons: ¹⁸Ne (T=1)
 - One Proton and one neutron: ¹⁸F (T=0 and T=1)
 - Two neutrons: ¹⁸O (T=1)

Example: ¹⁸O

Question # 1?

- How many states for each J_z ? How many states of each J?
 - There are 14 states with J_z=0
 - N(J=0)=3
 - N(J=1)=2
 - N(J=2)=5
 - N(J=3)=2
 - N(J=4)=2







Simple application of the shell model, cont.



Example:

Question #2

What are the energies of the three 0⁺ states in ¹⁸O?
 — Use the Universal SD-shell interaction (Wildenthal)

$$\varepsilon_{0d_{5/2}} = -3.94780$$

 $\varepsilon_{1s_{1/2}} = -3.16354$
 $\varepsilon_{0d_{3/2}} = 1.64658$

Measured relative to 16 O core Note $0d_{3/2}$ is unbound

$$\begin{array}{l} \left\langle 0d_{5/2}0d_{5/2}; J=0, T=1 \middle| V \middle| 0d_{5/2}0d_{5/2}; J=0, T=1 \right\rangle = -2.8197 \\ \left\langle 0d_{5/2}0d_{5/2}; J=0, T=1 \middle| V \middle| 0d_{3/2}0d_{3/2}; J=0, T=1 \right\rangle = -3.1856 \\ \left\langle 0d_{5/2}0d_{5/2}; J=0, T=1 \middle| V \middle| 1s_{1/2}1s_{1/2}; J=0, T=1 \right\rangle = -1.0835 \\ \left\langle 1s_{1/2}1s_{1/2}; J=0, T=1 \middle| V \middle| 1s_{1/2}1s_{1/2}; J=0, T=1 \right\rangle = -2.1246 \\ \left\langle 1s_{1/2}1s_{1/2}; J=0, T=1 \middle| V \middle| 0d_{3/2}0d_{3/2}; J=0, T=1 \right\rangle = -1.3247 \\ \left\langle 0d_{3/2}0d_{3/2}; J=0, T=1 \middle| V \middle| 0d_{3/2}0d_{3/2}; J=0, T=1 \right\rangle = -2.1845 \end{array}$$



Simple application of the shell model, cont.



Example:

Finding the eigenvalues

- Set up the Hamiltonian matrix
 - We can use all 14 J_{z} =0 states, and we'll recover all 14 J-states
 - But for this example, we'll use the two-particle J=0 states





3.522

1.964

-0.830

-1.243

-1.348

-1.616

-2.706

3.522

1.964

11.341

10.928

0.823

9.465

8.750





Effective interactions with the Lee-Suzuki method

- Choose P-space for A-body calculation, with dimension d_p
 - P-space basis states: and Q-space basis states:
 - Need d_p solutions, $|k\rangle$, in the "infinite" space, i.e.,
 - Write X=e^{-w}



For an *n*-body cluster in H_{eff} , we must first solve the *n*-body problem!



- Find *H_{n-eff}* iteratively

 n-particles bound in oscillator potential
- Steps:
 - $A=2 \\ \Rightarrow H_{2-eff}$
 - Use H_{2-eff} for A=3 $\Rightarrow H_{3-eff}$ - Use H_{3-eff} for A=4





• ⁴He with the effective-field theory Idaho-A potential



•Effective interactions improve convergence! •Are EFT potentials useful for nuclear-structure studies?



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- Complex computational problem!
- Example: ¹⁰B, *N_{max}*=4
- *H*_{3-eff}
 - 39,523,066 3-particle matrix elements
- $\langle \phi_j | H | \phi_i \rangle$ matrix dimension: 581,740 × 581,740 = 1.7 × 10¹¹
 - Easy for $H_{2-eff} \sim 1-2$ CPU-hr for lowest ten states
 - $-H_{3-eff}$:
 - $-~\langle \varphi_j | \textbf{\textit{H}} | \varphi_i \rangle$ has 2.2 \times 10 9 non-zero elements!
 - > 100 CPU-hr
- Three-body effective interaction takes 24-48 hours
- True three-body interaction ~ 1 week
- The future:
 - H_{3-eff} with N_{max} =6
 - $H_{4-\text{eff}}$ with N_{max} =4





Results with three-body effective interactions



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Excitation spectra with NN-interactions



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Excitation spectrum of 8Be

- Experiments hint at a new excited state in ⁸Be
 - Excitation energy ~10-30
 MeV
- Previous theory studies were unable to predict the existence of such a state
- In large model spaces we find an intruder band
 - $10\hbar\Omega \text{ model space} \\ \text{ and } \mathbf{2\times10^8 \text{ basis states!}} \\$
 - No-core ANTIONE







Excitation spectrum of 8Be



- What is the nature of this state?
 - Is it real?
 - Stable 0⁺, 2⁺, 4⁺ rotational band
 - $I \sim 1 1.1 \hbar \,\mathrm{MeV^{-1}}$
 - E_x appears to be stabilizing
 ~10-15 MeV
 - Beta-vibration of the ground-state α - α cluster?
 - Excitation energy seems too high
 - Super-deformed prolate shape?



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The NN-interaction clearly has problems





The NN-interaction by itself does not describe nuclear structure Also true for A=11



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Three-body interaction in a nucleus





The three-nucleon interaction plays a *critical* role in determining the structure of nuclei





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More on three-body interactions in a nucleus

- Gamow-Teller and M1
 transitions
 - Sensitive to spin-orbit force
 - Because στ is a generator of SU(4) and transitions in different representations are forbidden, i.e., B(GT)=0!!
 - NN-interaction tends to preserve SU(4)
 - Spin-orbit breaks SU(4)







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- Significant progress towards an exact understanding of nuclear structure is being made!
- These are exciting times!!
- Extensions and improvements:
 - Determine the form of the NNN-interaction
 - Implementation of effective operators for transitions
 - Four-body effective interactions
 - Effective field-theory potentials; are they any good for structure?
 - Integrate the structure into some reaction models (R-matrix)
- Questions and open problems to be addressed:
 - Is it possible to improve the mean field?
 - Can we improve the convergence of the higher $\,\hbar\Omega\,$ states?
 - Unbound states. Can we use a continuum shell model?
 - How high in A can we go?
 - Can we use this method to derive effective interactions for conventional nuclear structure studies?



