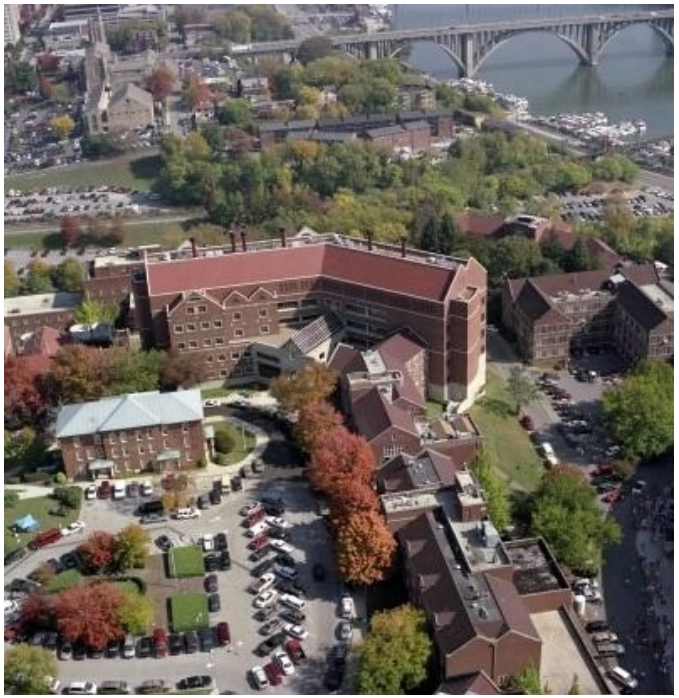
15thNational Nuclear Physics Summer School

June 15-27, 2003



OAK RIDGE NATIONAL LABORATORY

Nuclear Structure

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Lecture #2

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Physics & Advanced Technologies
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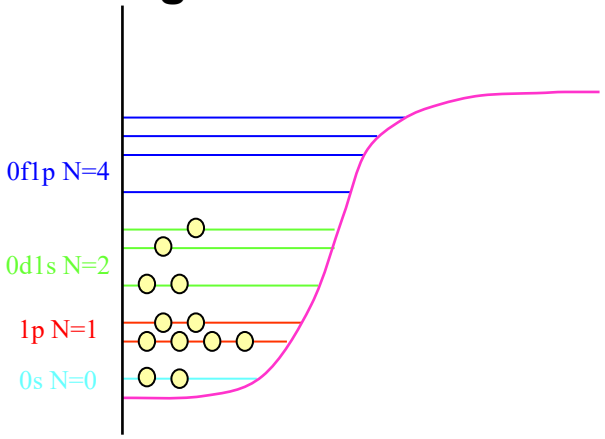
Low-lying structure – The interacting Shell Model

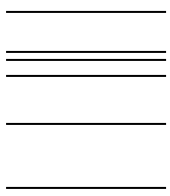
- The interacting shell model is one of the most powerful tools available too us to describe the low-lying structure of light nuclei
- We start at the usual place:

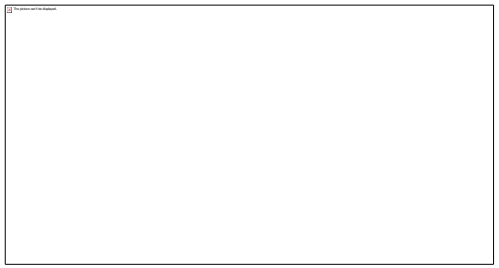


- Construct many-body states $|\phi_i\rangle$ so that

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

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



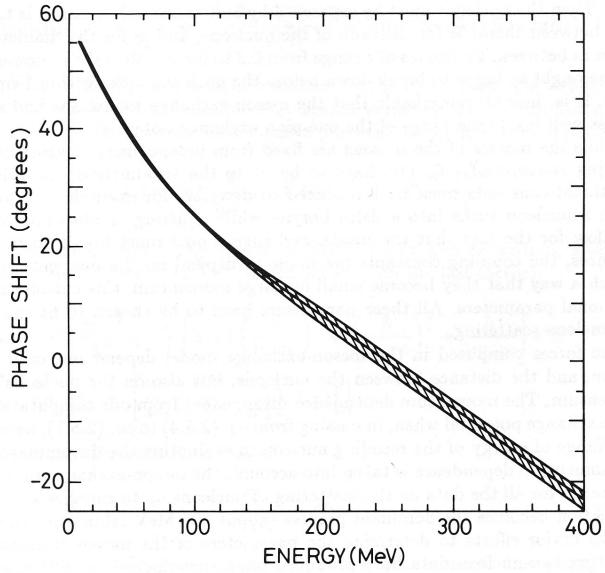


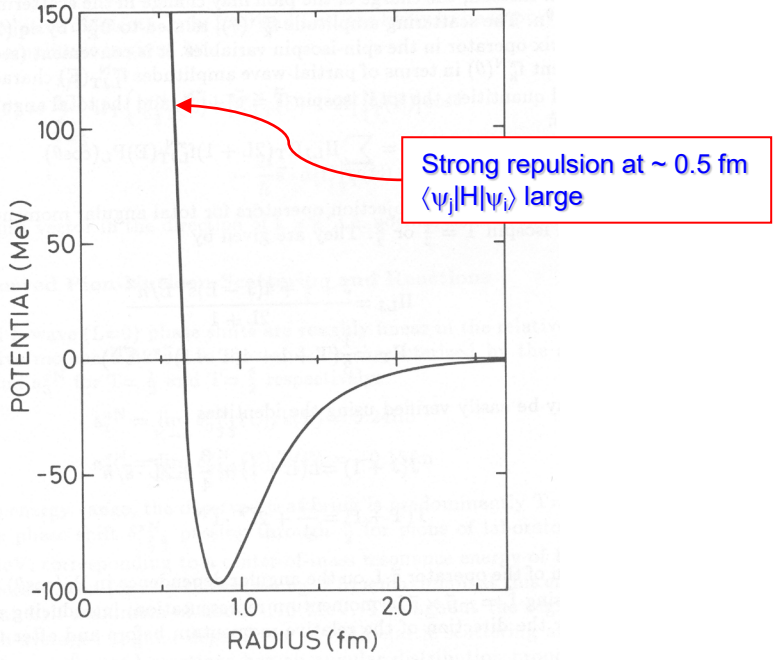
We want an accurate description of low-lying states

Nuclear structure with *NN*-interaction

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

Phase shift and potential in $^1S_0$ channel

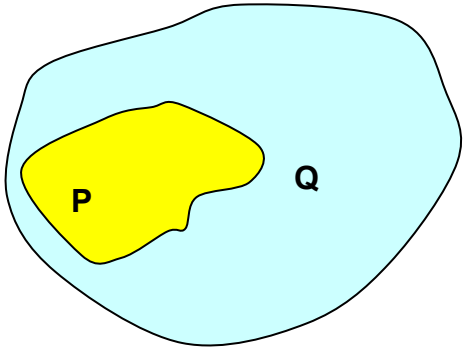




Problem: Repulsion in strong interaction → Infinite space!

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)



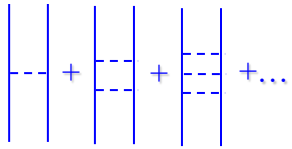
- Effective interaction:

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

  - Two approaches:
    - Bloch-Horowitz

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

$$\langle ij|G|kl\rangle \Rightarrow$$



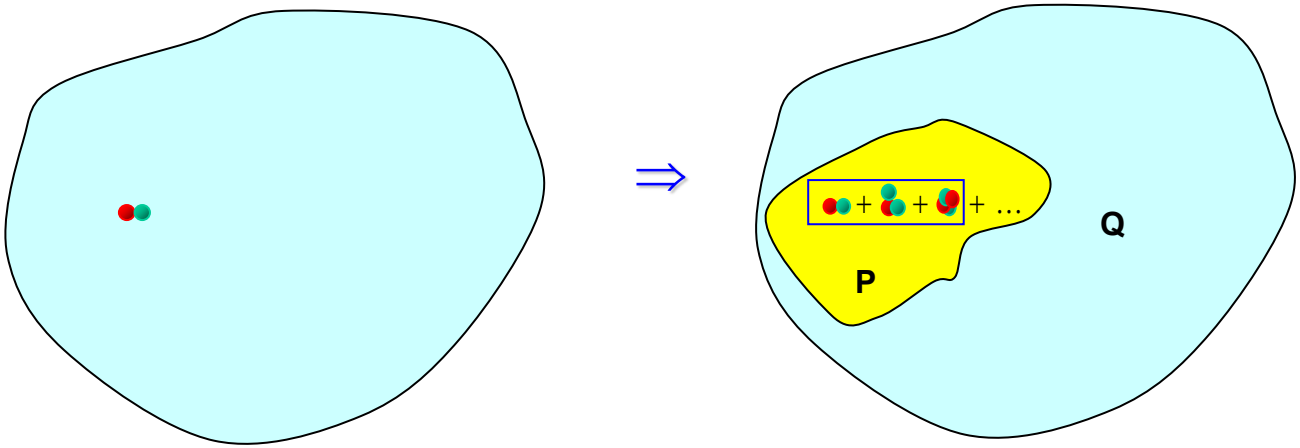
    - Lee-Suzuki:

$$H_{eff}=PXHX^{-1}P$$

$$QXHX^{-1}P=0$$

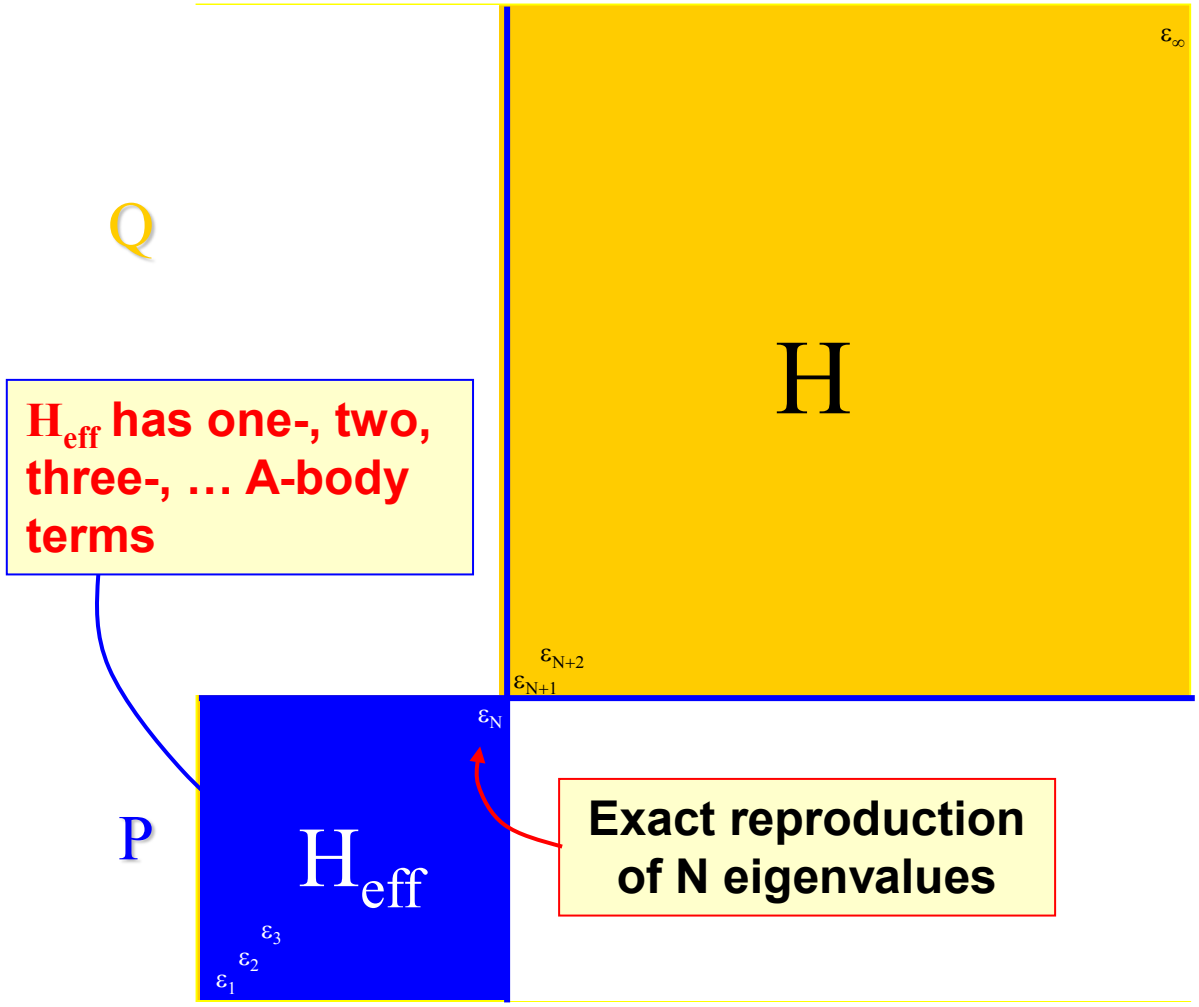
Effective interactions permit first-principles shell-model applications

- **Impossible problem → 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



P-space defined by $N_{\max}\hbar\Omega$

Interactions in real-world applications

- 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

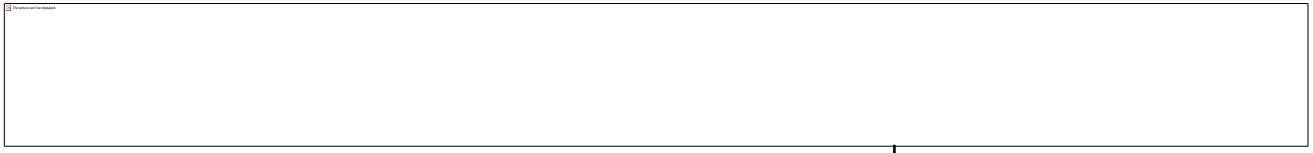
Shell model applications

- **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 ^{16}O to ^{40}Ca or the 0f and 1p orbits for ^{40}Ca to ^{120}Nd**
  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**

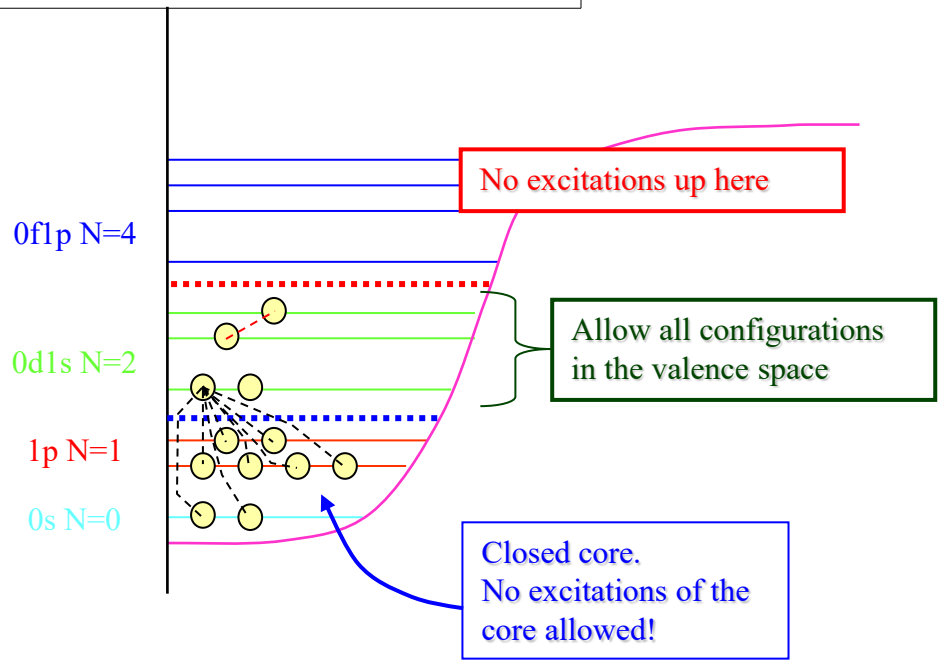
The empirical shell model works well!
But be careful to know the limitations!
More on exact treatments later.

The Shell Model

- We write the Hamiltonian as



- Start with closed inner core, e.g., for ^{24}Mg, 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 ^{24}Mg

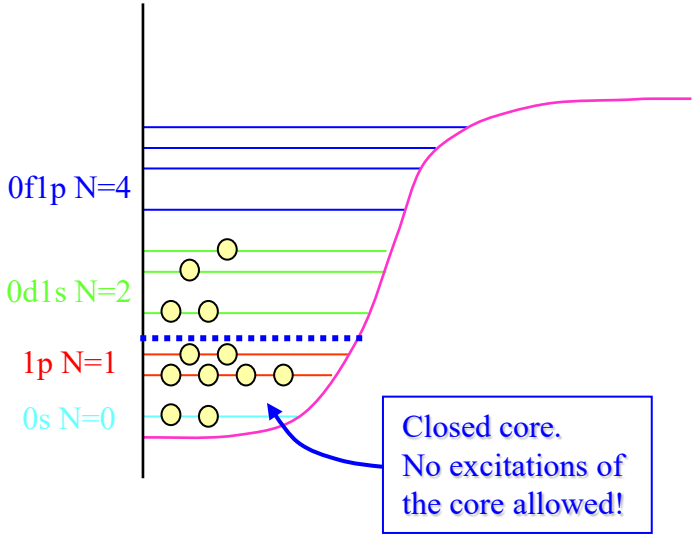


- Single-particle energy ε_i
- Two-body residual interactions

Energy is relative to ^{16}O core

Building the shell-model basis states

- Need to construct the many-body basis states to calculate matrix elements of H
- Choose states with definite parity, J_z and T_z and let the Hamiltonian do the rest
  - A very useful approach is a bit-representation known as the M-scheme



$$a^{+}_{\frac{5}{2},-\frac{1}{2}} a^{+}_{\frac{5}{2},\frac{3}{2}} a^{+}_{\frac{3}{2},-\frac{1}{2}} a^{+}_{\frac{1}{2},-\frac{1}{2}} |0\rangle =$$

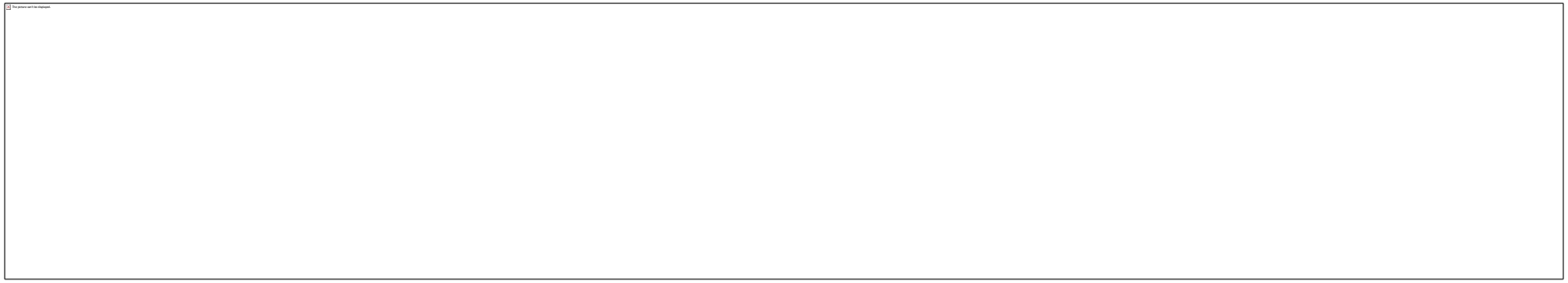
	0	0	1	0	1	0	0	1	0	0	1	0
$2j_z$	-5	-3	-1	1	3	5	-3	-1	1	3	-1	1
						$0d_{5/2}$				$0d_{3/2}$		$1s_{1/2}$

$$= 2^2 + 2^4 + 2^7 + 2^{10} = 1172$$

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

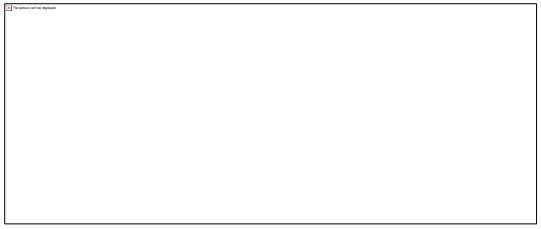
Tools of the trade - Lanczos

- Setup Hamiltonian matrix $\langle j|H|i\rangle$ and diagonalize
- Lanczos algorithm
  - Bring matrix to tri-diagonal form

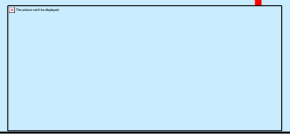
$$\hat{H}\mathbf{v}_1 = \alpha_1\mathbf{v}_1 + \beta_1\mathbf{v}_2$$
$$\hat{H}\mathbf{v}_2 = \beta_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2 + \beta_2\mathbf{v}_3$$
$$\hat{H}\mathbf{v}_3 = \beta_2\mathbf{v}_2 + \alpha_3\mathbf{v}_3 + \beta_3\mathbf{v}_4$$
$$\hat{H}\mathbf{v}_4 = \beta_3\mathbf{v}_3 + \alpha_4\mathbf{v}_4 + \beta_4\mathbf{v}_5$$

Note that after each iteration, we need to re-orthogonalize!

  - n^{th} iteration computes $2n^{th}$ moment



Prove that Lanczos computes moments -



    - 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)

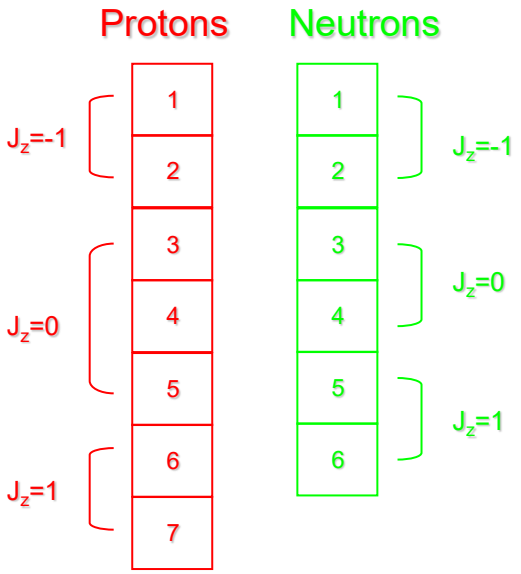
Shell-model codes

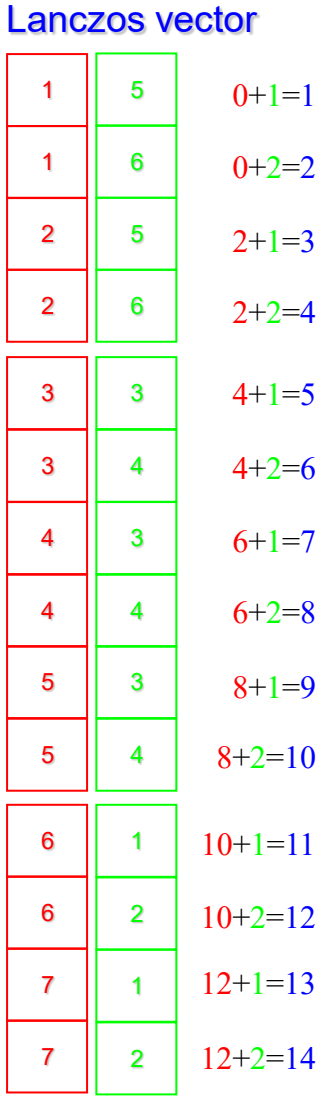
- Oak Ridge (1969)
  - Coefficients of Fractional parentage (CFP)

- 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
- Construct proton and neutron many-body Slater determinants
  - Order by Parity, J_z 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)

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

$$\hat{H}\mathbf{v} = \hat{H}\sum_i c_i \left|\Phi_i\right\rangle = \sum_j \sum_i c_i \left\langle \Phi_i \left| H \right| \Phi_i \right\rangle \left|\Phi_j\right\rangle = \sum_j c'_j \left|\Phi_j\right\rangle$$

- 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

$$\hat{H}^{pn} = \sum_{ijkl} v_{ijkl}^{pn} \pi_i^+ \pi_j \nu_k^+ \nu_l$$

    - Pre-sort connections by one-body operators; store operator and phase

- Loop over all initial proton-neutron SD's $\Phi_i = \phi^p_k \, \phi^n_l$
  - For each ϕ^p_k loop over all ϕ^p_m connected by one-body operator
    - For each ϕ^n_l loop over all ϕ^n_n connected by one-body 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)

Initial PN-SD

$$\left\langle \Phi^p_m \left| \pi^+_\alpha \pi_\beta \right| \Phi^p_k \right\rangle \left\langle \Phi^n_n \left| \nu^+_\gamma \nu_\delta \right| \Phi^n_l \right\rangle v^{pn}_{\alpha\beta\gamma\delta}$$

Jump List #1 Jump List #2

REDSTICK – Applying the Hamiltonian Parallel execution

- **Note loop over N_{dim} states**
  - **Divide loop over N_{CPU} independent processors**
    - **For load balance use do i=1,N_{dim},N_{CPU}**
    - **Creates updated Lanczos vector on each processor**
    - **Total Lanczos vector with Global sum**

- Loop over all initial proton-neutron SD's $\Phi_i=\phi^p_k\phi^n_l$ steps of N_{CPU}
  - For each ϕ^p_k loop over all ϕ^p_m connected by one-body operator
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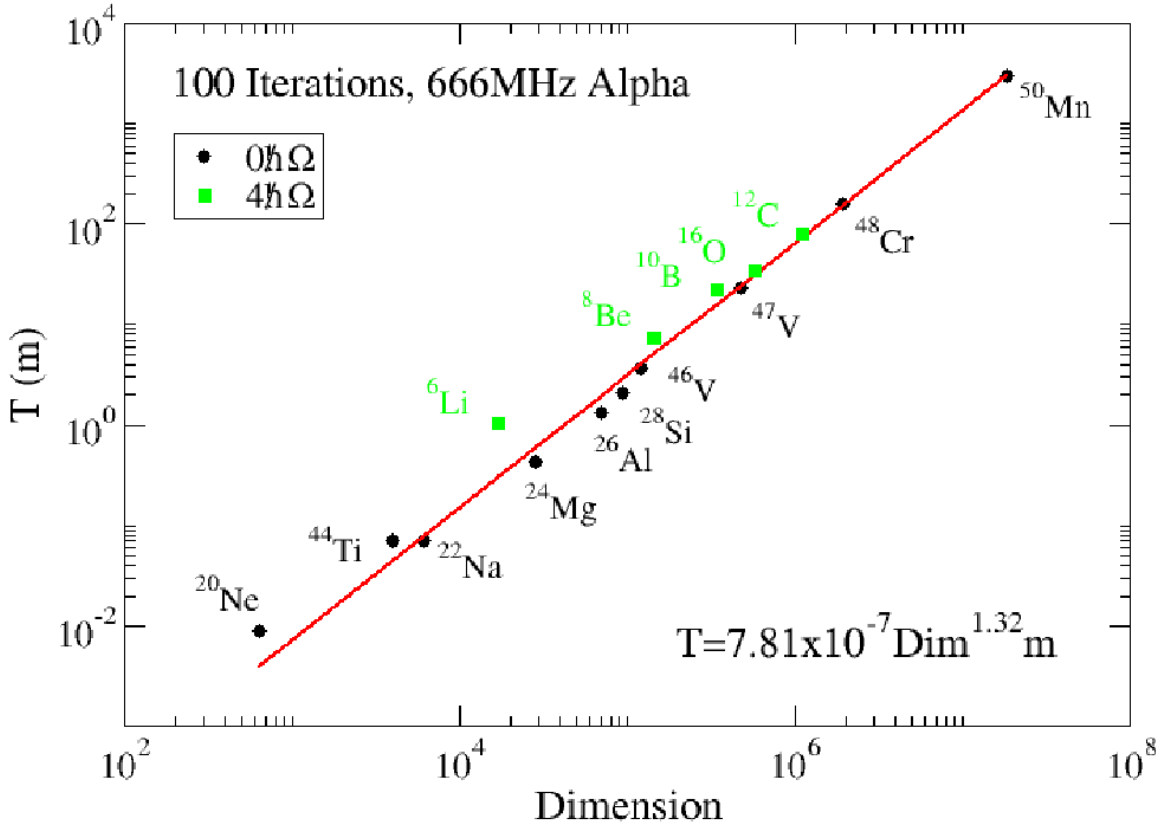
Global Sum ~ N_{CPU} speed up

REDSTICK – Reorthogonalization
Parallel execution

- $\mathbf{v}_j = \mathbf{v}_j - \sum_{i<j} \mathbf{v}_i \cdot \mathbf{v}_j$
- **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** $\mathbf{a}_n = \sum_{i<j} \mathbf{v}_i \cdot \mathbf{v}_j$ **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).**

Shell-model codes - Performance

REDSTICK or ANTOINE



Simple application of the shell model

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

Example: ^{18}O

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 ^{18}O?**
  - **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

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

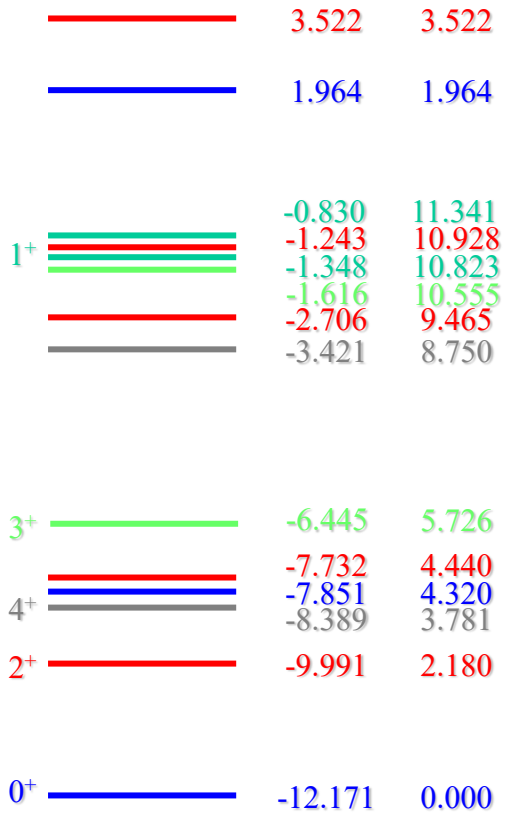
Simple application of the shell model, cont.

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

$|(0d_{5/2})^2\rangle_{J=0}$ $|(1s_{1/2})^2\rangle_{J=0}$ $|(0d_{3/2})^2\rangle_{J=0}$



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 $X=e^{-\omega}$

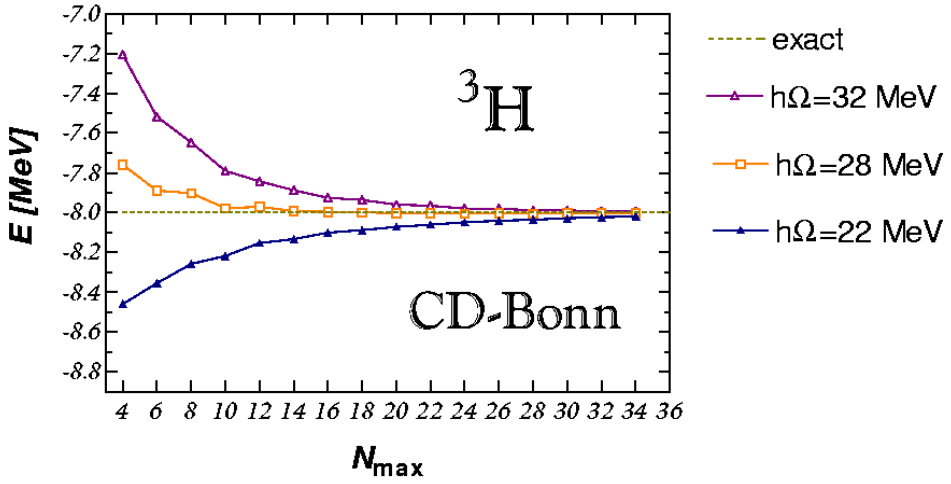
[ ]

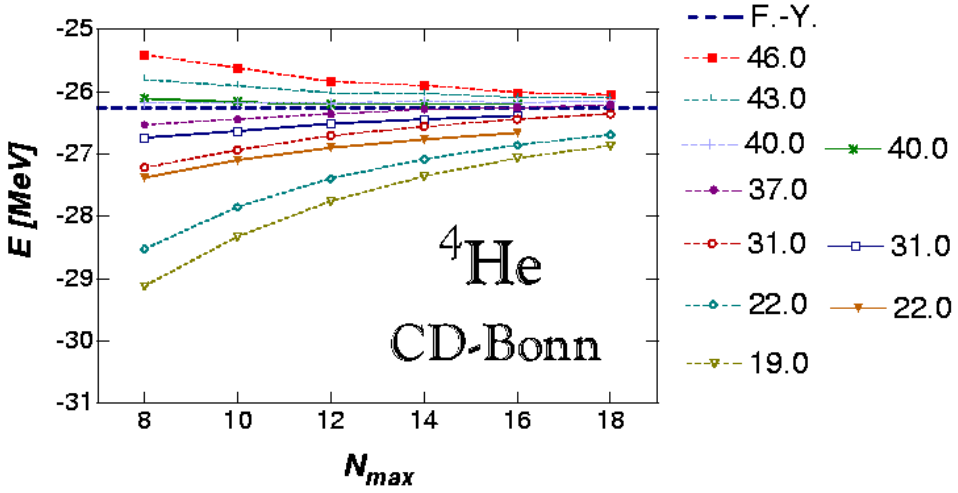
Hermitian effective interaction

The matrix $\langle\beta_P|H_{eff}|\alpha_P\rangle$ exactly reproduces d_p solutions of the full problem

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

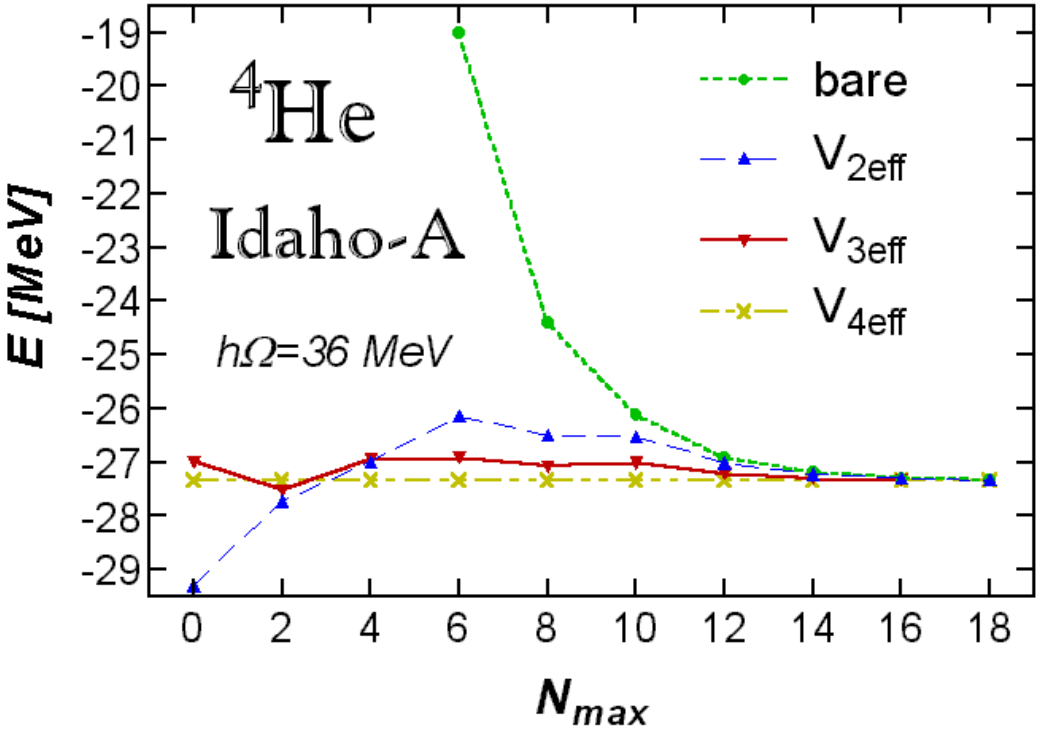
- Find $H_{n\text{-}eff}$ iteratively
  - n-particles bound in oscillator potential
- Steps:
  - A=2
    - $\Rightarrow H_{2\text{-}eff}$
  - Use $H_{2\text{-}eff}$ for A=3
    - $\Rightarrow H_{3\text{-}eff}$
  - Use $H_{3\text{-}eff}$ for A=4
    - $\Rightarrow H_{4\text{-}eff}$





Effective interactions really work

- ^{4}He with the effective-field theory Idaho-A potential



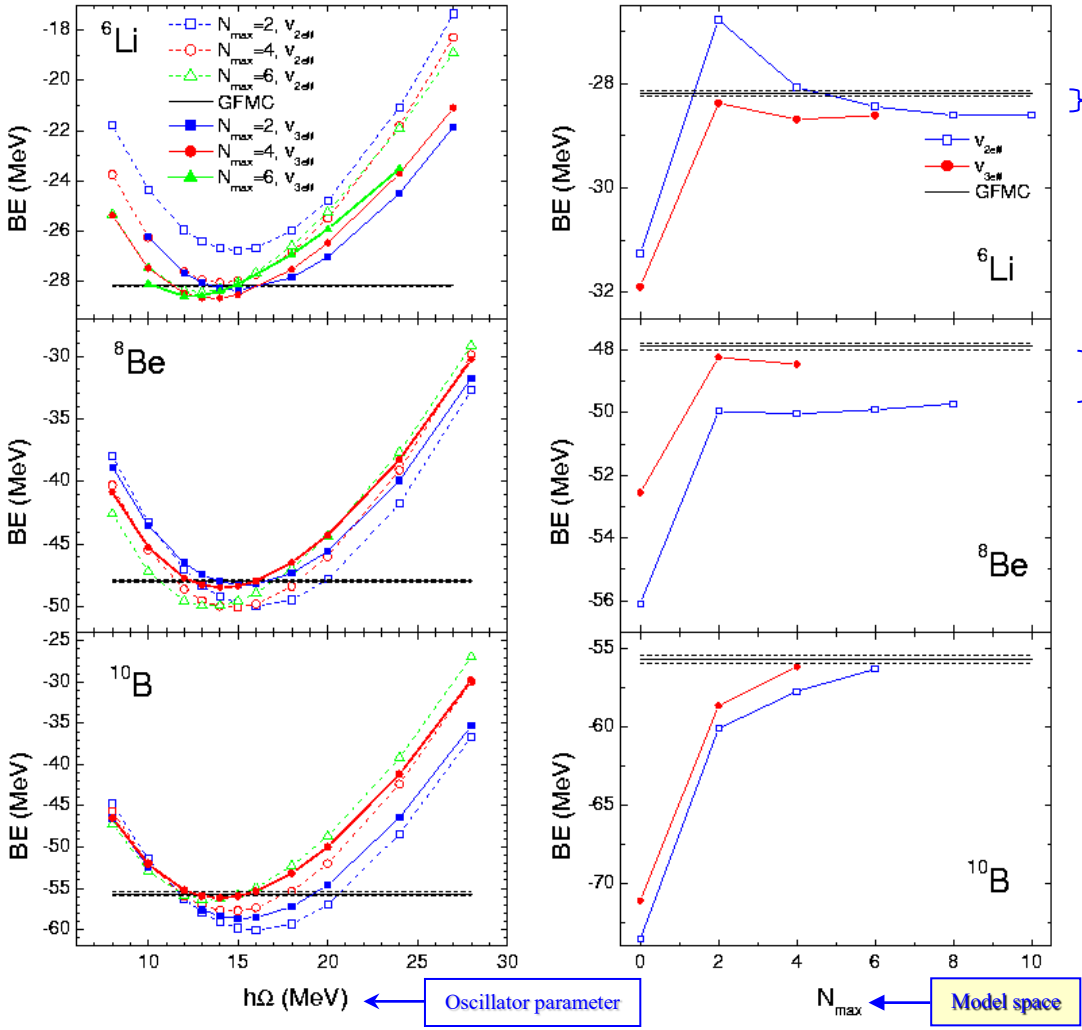
- Effective interactions improve convergence!
- Are EFT potentials useful for nuclear-structure studies?

But, we do need to use big computers

- **Complex computational problem!**
- **Example: ^{10}B, N_{max}=4**
- **$H_{3\text{-}eff}$**
  - ***39,523,066* 3-particle matrix elements**
- **$\langle\phi_j|H|\phi_i\rangle$ matrix dimension: *581,740* × *581,740* =1.7 × 10^{11}**
  - **Easy for $H_{2\text{-}eff}$ ~ 1-2 CPU-hr for lowest ten states**
  - **$H_{3\text{-}eff}$:**
    - **$\langle\phi_j|H|\phi_i\rangle$ has 2.2 × 10^9 non-zero elements!**
    - **> 100 CPU-hr**
- **Three-body effective interaction takes 24-48 hours**
- **True three-body interaction ~ 1 week**
- **The future:**
  - **$H_{3\text{-}eff}$ with N_{max}=6**
  - **$H_{4\text{-}eff}$ with N_{max}=4**

Results with three-body effective interactions

Binding energies with Av8'

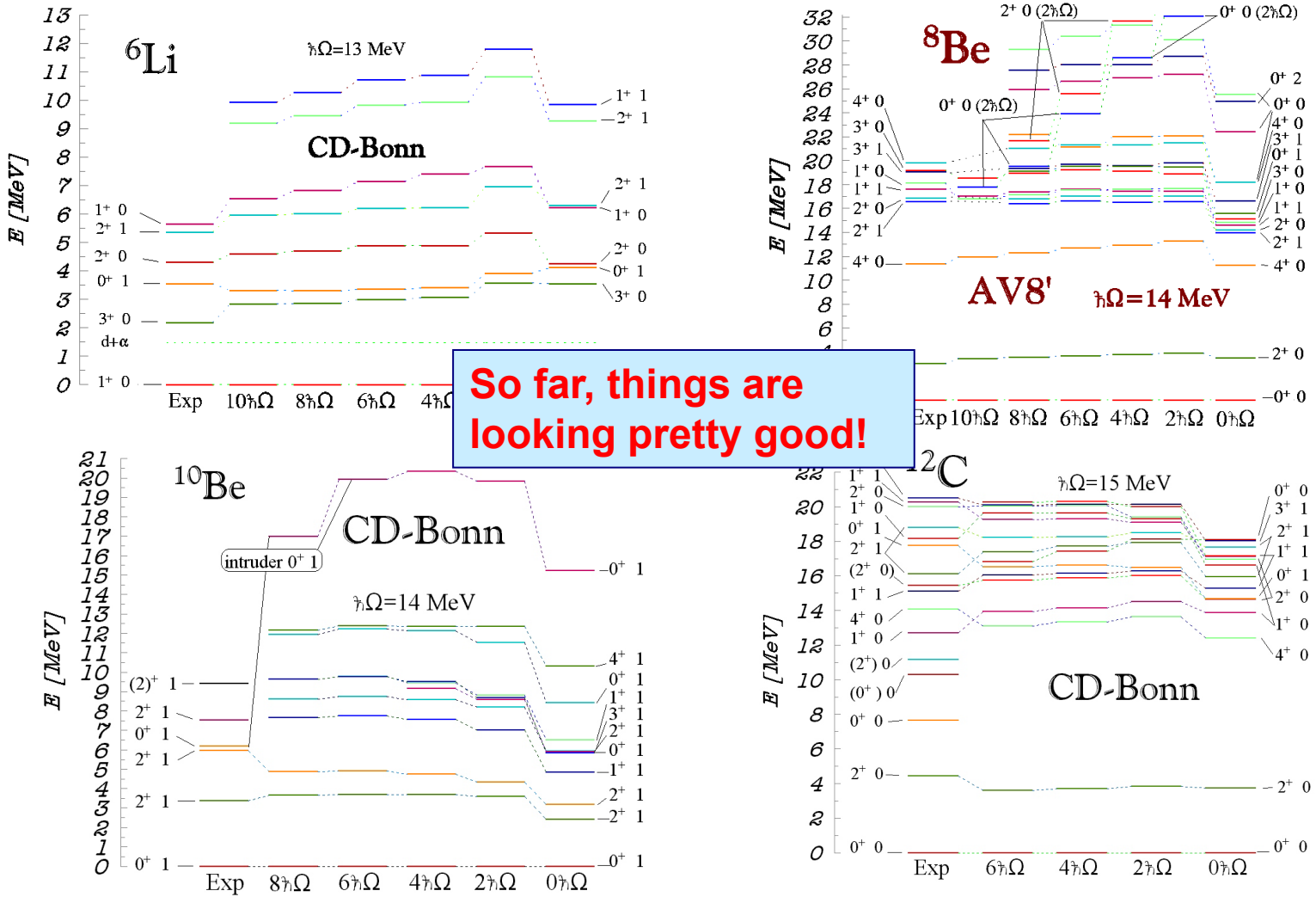


400 keV

1.8 MeV, Clustering?

Three-body effective interactions represent a significant improvement and give results within 400 keV of the GFMC

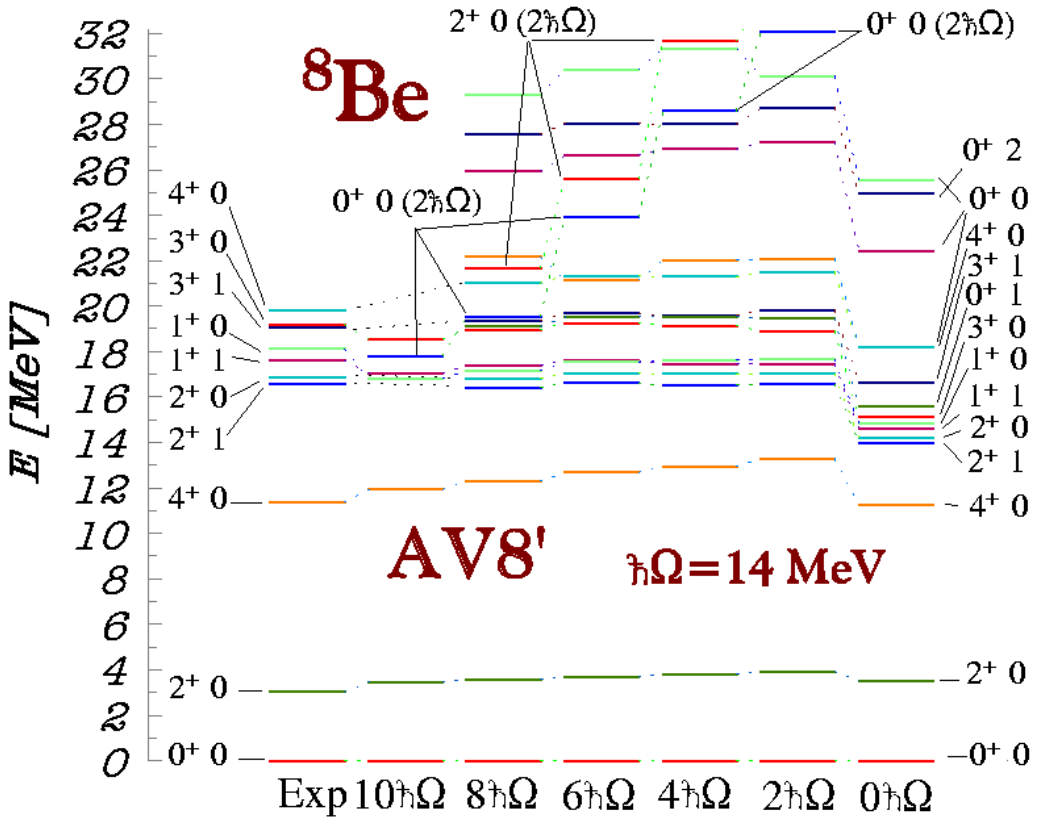
Excitation spectra with NN-interactions



So far, things are looking pretty good!

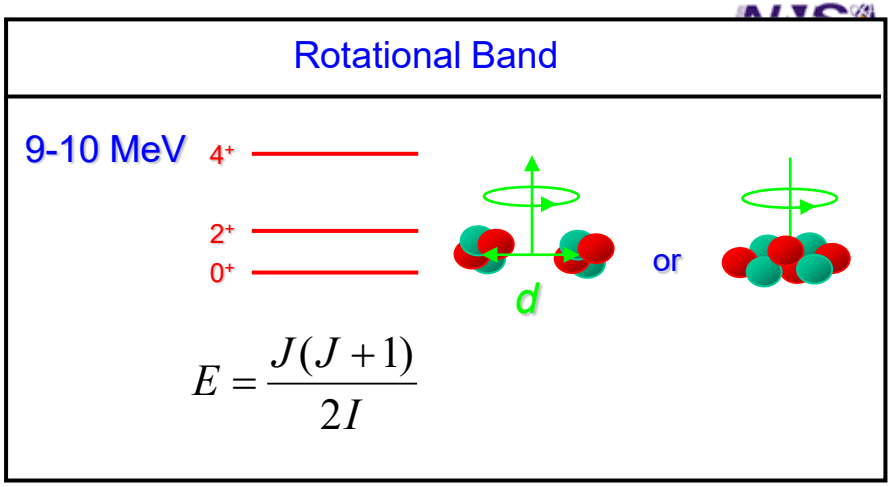
Excitation spectrum of ^{8}Be

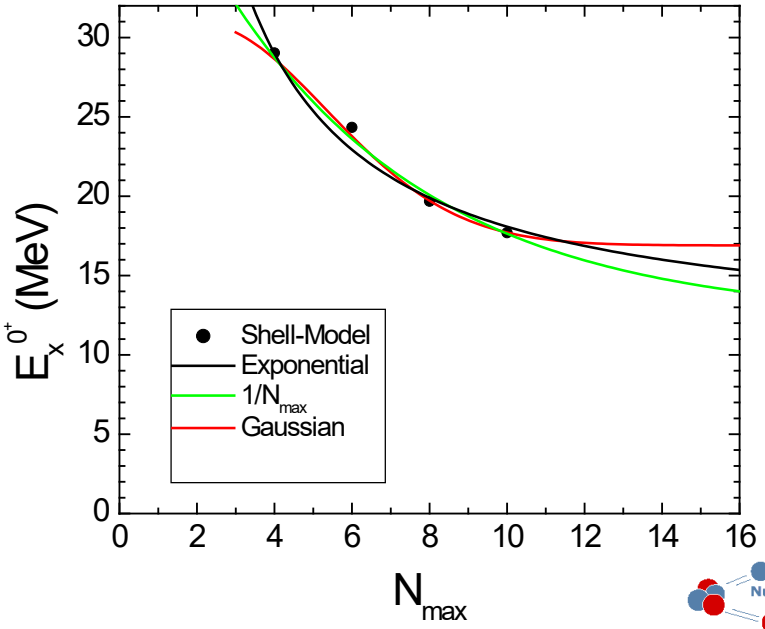
- Experiments hint at a new excited state in ^{8}Be
  - Excitation energy ~10-30 MeV
- Previous theory studies were unable to predict the existence of such a state
- In large model spaces we find an intruder band
  - $10\hbar\Omega$ model space and 2×10^{8} basis states!
  - No-core ANTIONE



Excitation spectrum of ^{8}Be

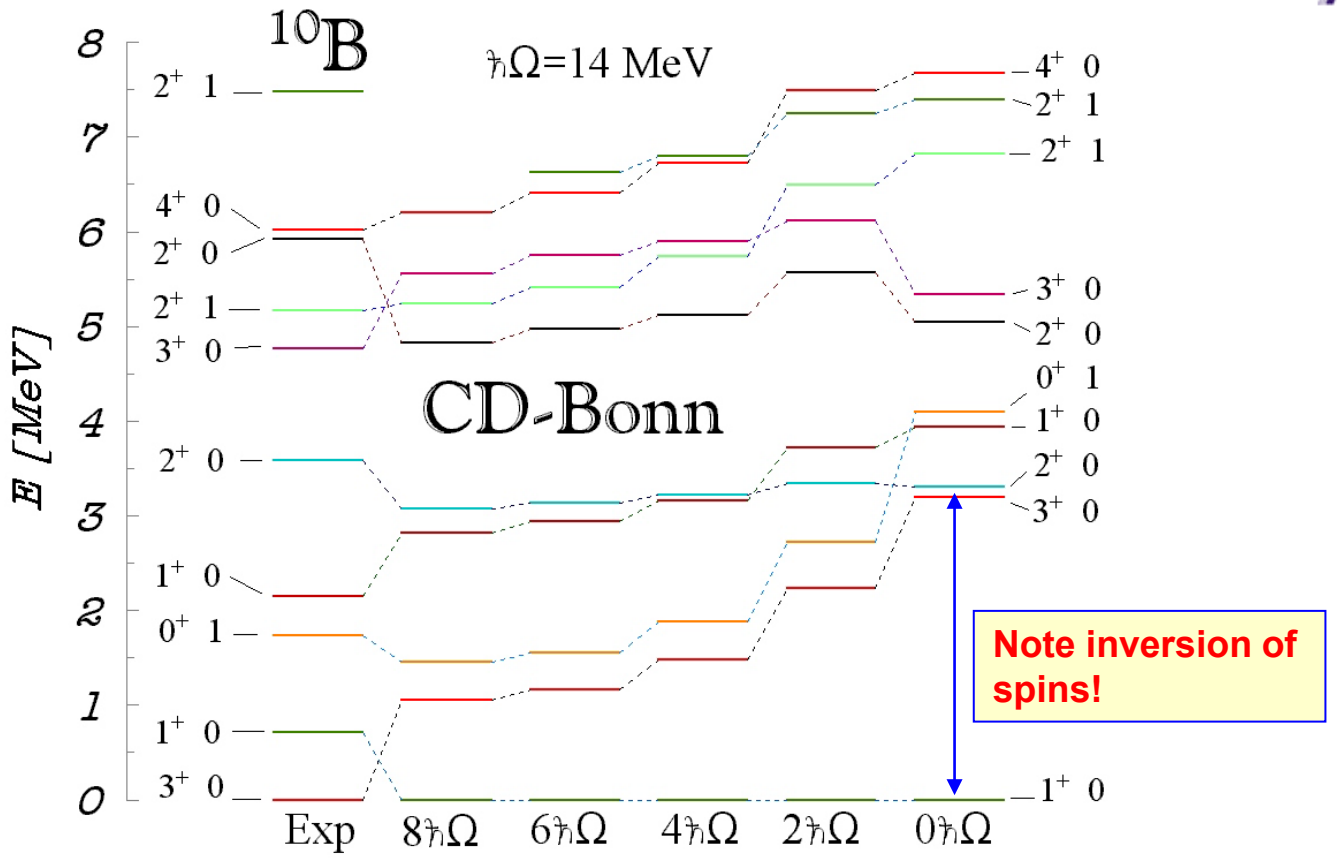
- **What is the nature of this state?**
  - **Is it real?**
    - **Stable 0^+, 2^+, 4^+ rotational band**
      - $I \sim 1 - 1.1\,\hbar\,\mathrm{MeV}^{-1}$
    - **E_x appears to be stabilizing**
      - **~10-15 MeV**
  - **Beta-vibration of the ground-state α–α cluster?**
    - **Excitation energy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





Nuclear Theory & Modeling Group

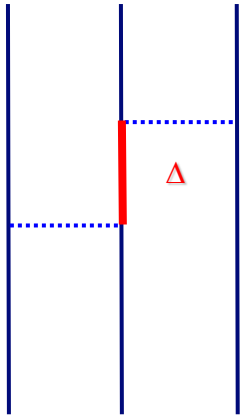
The NN-interaction clearly has problems

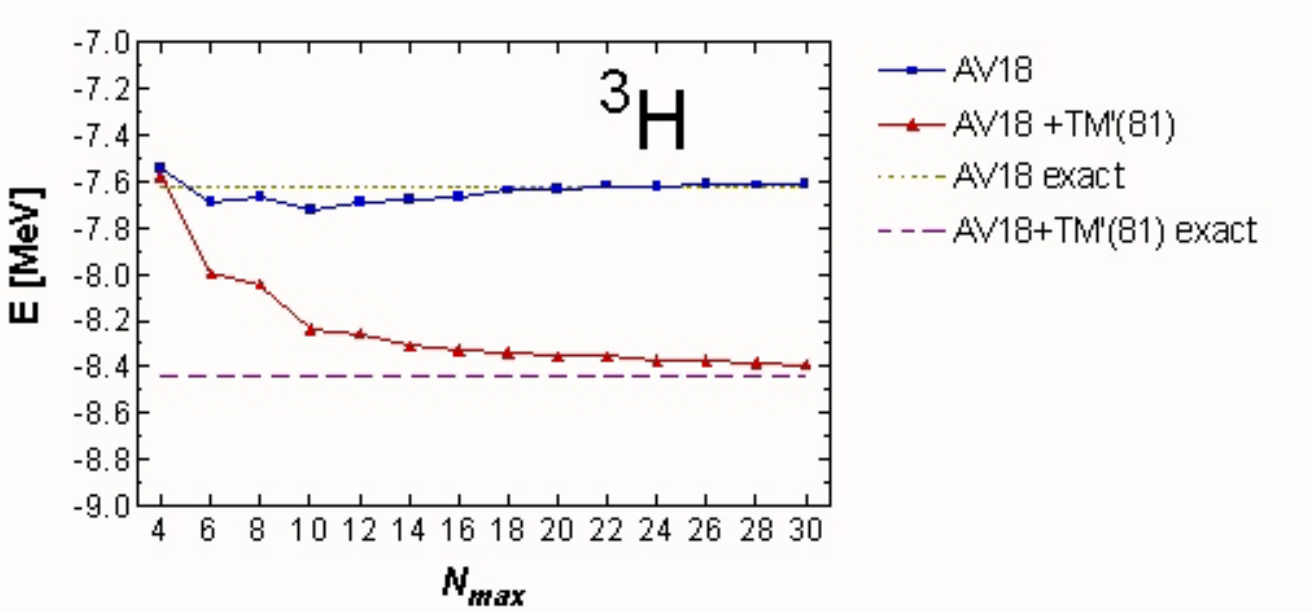


- The NN-interaction by itself does not describe nuclear structure
- Also true for A=11

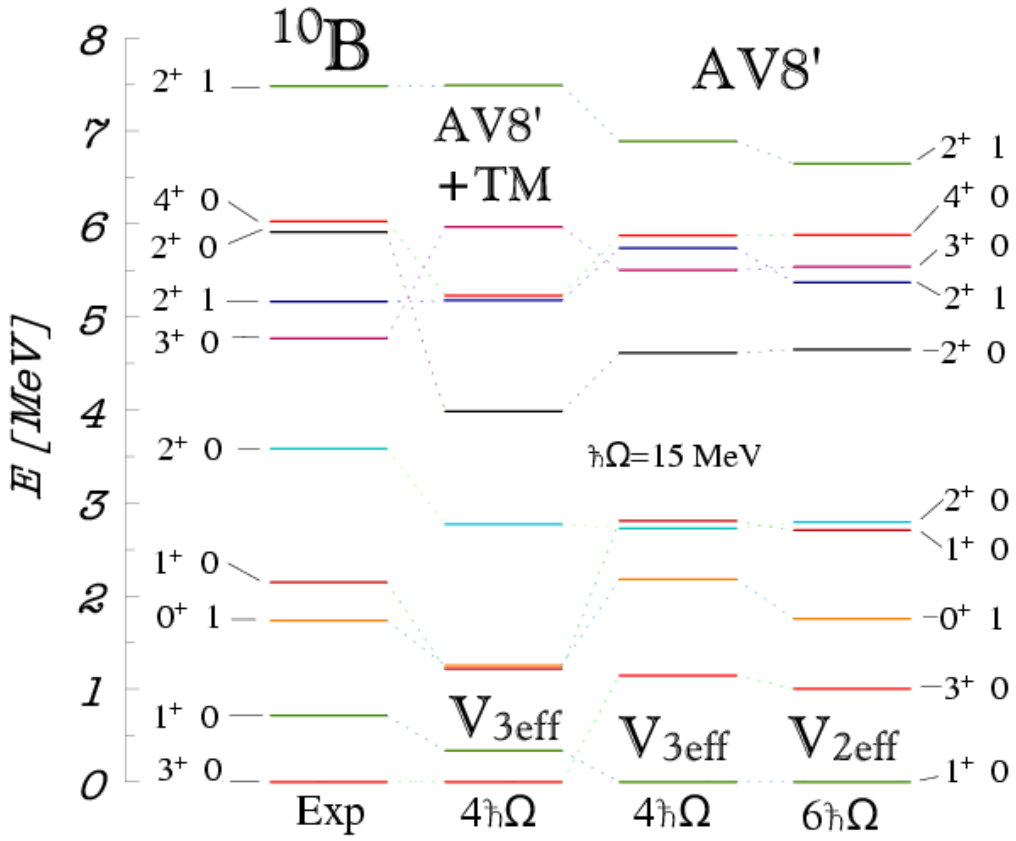
How about the three-body interaction?

- **Tucson-Melbourne**





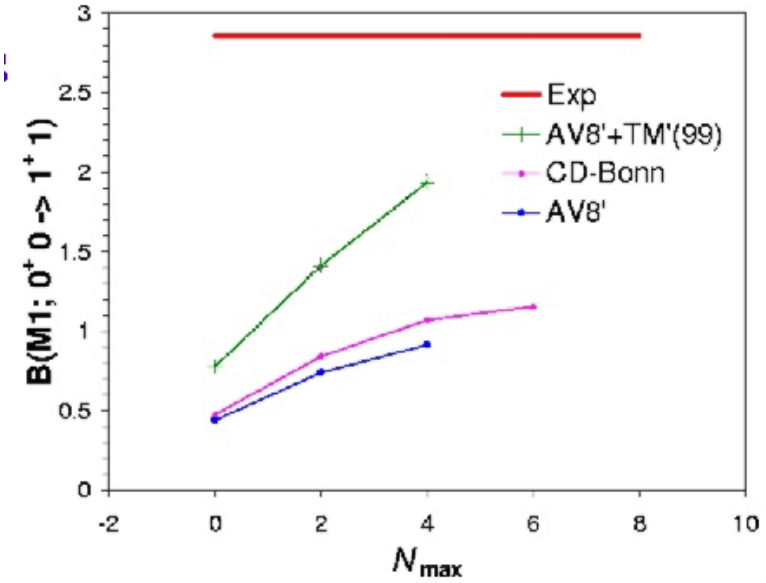
Three-body interaction in a nucleus



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

More on three-body interactions in a nucleus

- **Gamow-Teller and M1 transitions**
  - **Sensitive to spin-orbit force**
  - **Because $\sigma\tau$ 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)**



The three-nucleon interaction has a strong spin-orbit component

Summary of ab initio studies

- **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?**