Introduction to NUSHELLX

Angelo Signoracci

CEA/Saclay

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Outline

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1. NUSHELLX shell model code
2. Inputs for calculation
3. Practical Implementation

Brief Review

1. Full CI calculations are exact solutions in reduced model space
   - Diagonalization of matrix is required
   - Dimension depends on angular momentum coupling
   - Computational limits typically around $A \sim 70$, but depends on model space
2. Select model space to account for low-energy degrees of freedom
3. Effective interaction required
   - Accounts for dynamics associated with excluded orbits

Shell model codes by Bill Rae

- Bill Rae wrote NuShell and NuShellX codes in previous decade
- NuShell
    - Replaces old shell model code OXBASH
    - JT-projected M-scheme
    - Stores complete matrix, which limits the size of calculations
- NuShellX
    - Calculates Hamiltonian "on the fly"
    - Utilizes NuShell modules for protons and neutrons
    - J-scheme built on coupling between protons and neutrons
- Not identical codes- some advantages for each
- Neither is user friendly

NUSHELLX@MSU - Alex Brown

- NuShellX refers to the shell model package written by Bill Rae
- Alex Brown has written a "wrapper" code to simplify input
  - Provides more consistency with I/O of OXBASH
  - NuShellX with the wrapper is called NUSHELLX@MSU
  - Generally will refer to it simply as NUSHELLX
  - Most common NuShellX options available from the "shell" interface
- See manuals in help folder for more information
- Any resulting publications should cite appropriate code and effective interaction
- For examples, see NUSHELLX manual

Treatment of center of mass motion

- Recall that spurious states from center of mass motion must be eliminated
- Only internal structure is desired
- In harmonic oscillator basis

$$H_{cm} = \frac{1}{2mA} Q^2 + \frac{1}{2} Am\omega^2 R^2$$

- In ground state, $E_{cm} = \frac{3}{2}\hbar\omega$
- NUSHELLX adds a fictitious Hamiltonian

$$H'_{cm} = \beta \left\{ \frac{1}{2mA} Q^2 + \frac{1}{2} Am\omega^2 R^2 - \frac{3}{2}\hbar\omega \right\}$$

- Large β by construction
  1. Excitations of center of mass occur at high energy
  2. Higher energy than intrinsic excitations of interest
- Center of mass always in ground state
- Fictitious Hamiltonian does not add energy

Technicalities

1. Conventions
   - Wavefunction is undetermined up to a phase
   - Defined as real and positive at the origin
   - Does not affect observables
   - If used in reaction calculations, definition of phase must be consistent
2. Diagonalization
   - Most time-consuming step in CI calculation is diagonalization
   - OpenMP utilized efficiently, extension to MPI developed
   - Standard linear algebra techniques (e.g. LAPACK) exhaust computing resources
   - Lanczos procedure
     - Iterative technique to convert a sparse matrix into tridiagonal form
     - Tridiagonal matrix can be diagonalized quickly to obtain eigenvalues
     - Approximate technique that can produce spurious states
     - Most typically, spurious states appear for large model spaces

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Directory structure

- sps folder
  - Contains predefined (standard) model space and interaction files
  - Listed in label.dat file
    1. Available model spaces listed at top of file
    2. Each model space is then listed below with available interactions
    3. NUSHELLX naming scheme provided for each combination
    4. Provides references for majority of interactions
    5. Some mistakes present in label.dat (not for most common files)
- rsh folder
  - Suggested location to run calculations (create yourself)
  - Output of calculations all written to working directory
    - Old files in the directory can be written over by new calculations
    - Safest to create new subdirectory for each calculation
- Most common output files
  1. responses to shell prompts *.ans (can modify to run new calculation)
  2. wavefunction information *.lpe
  3. level scheme *.lpt
  4. plot comparing experimental data to calculations *.eps
  5. γ decay scheme *.deo
  6. spectroscopic factors *.lsf
- Executable 'cleanup' eliminates large binary files used internally by NUSHELLX
  - All important output files remain afterwards
  - Only run 'cleanup' after all calculations in the directory are complete

Model Space

- Two formats: isospin formalism (t) and proton-neutron formalism (pn)

Input for sd.sp file

Description	File variables	Explanation for *sd* case
comment line	! sd.sp	
format	t	isospin formalism
$A_c Z_c$	16 8	core is ^{16}O
number of orbits n_o	3	$0d_{5/2}, 0d_{3/2}, 1s_{1/2}$
k,n(k);	1 3	for t format, k=1 n(1)=n_o
index, $n', \ell, 2j$	1 1 2 3	index starts with 1, $n' = n + 1, 0d_{3/2}$
index, $n', \ell, 2j$	2 1 2 5	$0d_{5/2}$
index, $n', \ell, 2j$	3 2 0 1	$1s_{1/2}$

- Most NUSHELLX files can start with (any number of) lines commented out by '!'
- Isospin formalism
  - Protons and neutrons identical by construction
  - Occupation of orbit is $2(2j+1)$
- Results in reduced number of TBME relative to proton-neutron formalism

Model Space

- Two formats: isospin formalism (t) and proton-neutron formalism (pn)
- Proton-neutron formalism

Input for ppn.sp file

Description	values in file	Explanation for *ppn* case
comment line	! ppn.sp	
format	pn	proton-neutron formalism
$A_c Z_c$	4 2	core is ^{4}He
number of orbits n_o	4	$\pi 0p_{3/2}, \pi 0p_{1/2}, \nu 0p_{3/2}, \nu 0p_{1/2}$
k,n(k);	2 2 2	for pn format, k=2 n(1)=n_p n(2)=n_n
index, $n', \ell, 2j$	1 1 1 3	index starts with 1, $n' = n + 1, 0p_{3/2}$
index, $n', \ell, 2j$	2 1 1 1	$0p_{1/2}$
index, $n', \ell, 2j$	3 1 1 3	$0p_{3/2}$
index, $n', \ell, 2j$	4 1 1 1	$0p_{1/2}$

- Most NUSHELLX files can start with (any number of) lines commented out by '!'

Effective interaction

- List of single particle energies and two-body matrix elements
- Must use indices consistent with *.sp file
- Example in isospin formalism: USD interaction

63 1.64658 -3.9478 -3.16354

1	1	1	1	0	1	-2.1845
1	1	1	1	1	0	-1.4151
1	1	1	1	2	1	-0.0665
1	1	1	1	3	0	-2.8842
2	1	1	1	1	0	0.5647
2	1	1	1	2	1	-0.6149
2	1	1	1	3	0	2.0337
2	1	2	1	1	0	-6.5058

⋮

Effective interaction

- List of single particle energies and two-body matrix elements
- Must use indices consistent with *.sp file

- For proton-neutron interactions:
  - Can produce from isospin interactions (see NUSHELLX manual)
  - Must use unnormalized matrix elements
  - Normalized TBME typically obtained from microscopic interactions
  - 'ham' executable automatically converts to unnormalized TBME

$$\langle (ab)J|V_{ms}|(cd)J\rangle_{unnorm} = 2^{[1-\frac{1}{2}(\delta_{ab}+\delta_{cd})]}\langle (ab)J|V_{ms}|(cd)J\rangle_{norm}$$

Outline

Command line

- 'shell' executable
  - Initialize NUSHELLX@MSU wrapper code with executable 'shell'
  - Calculate level schemes with option 'lpe'
    1. Energies
    2. Wavefunctions
  - Calculate transitions with option 'den'
    1. One-body transition densities (OBTD)
    2. One-nucleon transfer (spectroscopic factors)
    3. Two-nucleon transfer
  - Respond to prompts
    - Most questions are self-explanatory
    - Refer to manual and problem sessions for examples
  - Terminate 'shell' with option 'st'
  - Run batch file as instructed by output of shell
- 'toi' executable
  - Access experimental data from table of isotopes
  - Binding energies, excitation energies, thresholds, etc.
- 'dens' executable
  - Capable of calculating more than we have time to discuss
  - One example: $B(E2)$ from OBTD
  - Somewhat detailed instructions in help option
- 'ham' executable
  - Creates interactions (more information in final slide of Lecture VII)

Level schemes

Refer to NUSHELLX manual help.pdf for more detailed description
Explicit examples given at beginning of Tutorial I

- Necessary inputs for 'lpe' option of 'shell'
  - Model space
  - Effective interaction
  - Nucleus of interest (charge and mass)
  - States of interest (J^π values)
- Optional input to truncate model space to speed up diagonalization
  1. Answer yes (y) to prompt 'any restrictions (y/n)'
  2. Choose subshell (s) restrictions
  3. Select minimum and maximum number of particles in each model space orbit

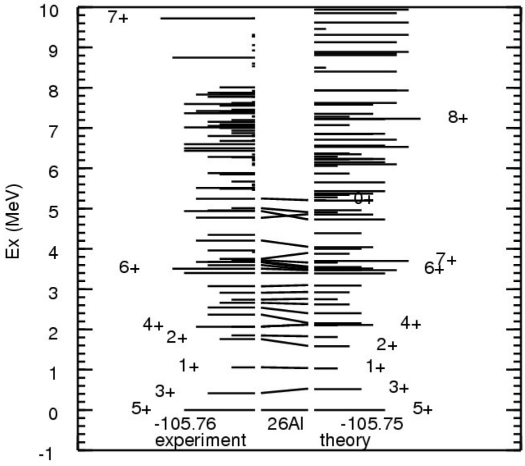
  Not consistent with derivation of effective interaction!

- Produce level schemes for comparison to experimental data

  Examples: $A = 26$ nuclei with USDB interaction

Level schemes

- Only positive-parity experimental states included in the plots
- Plots obtained from http://www.nscl.msu.edu/∼brown/resources/resources.html



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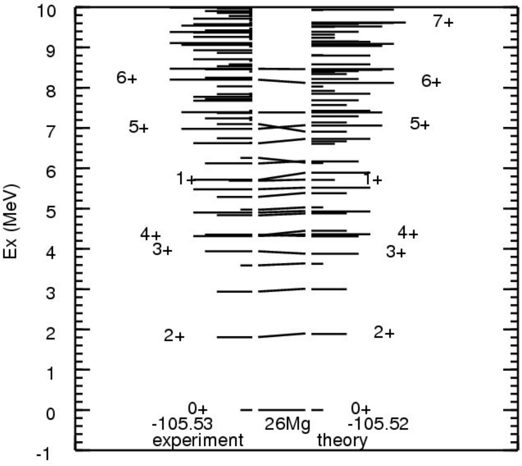

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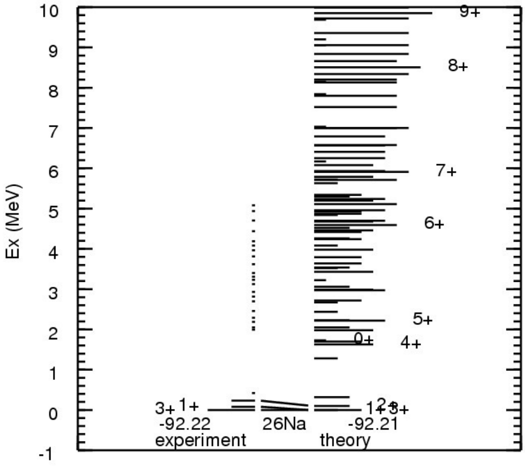

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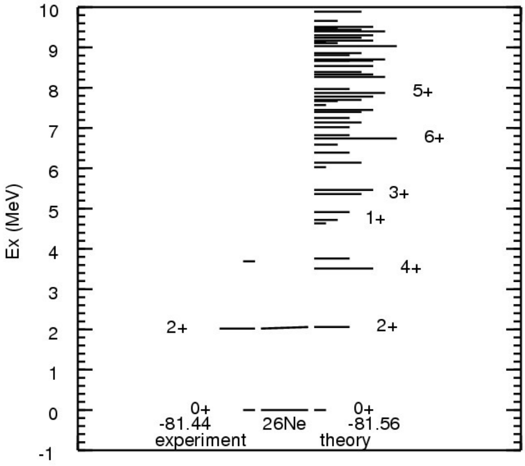

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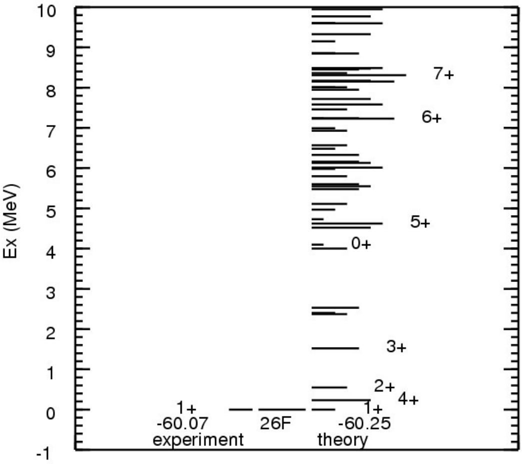

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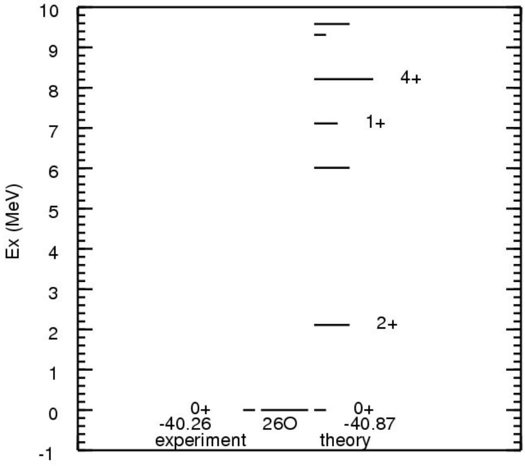

Transitions

Refer to NUSHELLX manual help.pdf for more detailed description
Explicit examples given at beginning of Tutorial I

- Necessary inputs for 'den' option of 'shell'
  - Initial and final state wavefunctions must first be calculated with 'lpe' option
    - Lighter mass must always be initial state
    - Only cleanup directory after performing all calculations
    - Nomenclature for wavefunctions can be found in help manual
    - Can also find wavefunction by searching for *.lpe/*.lph files
  - Number of eigenfunctions for each value of J^π
    - Prompt 'max number for given J'
    - Reply with number up to amount calculated by 'lpe' (or -1 for all)
  - J-values (parity taken from name of wavefunction)
- Optional input to truncate angular momentum coupling to shorten calculation
  - Prompt 'restrict coupling for operator'
  - Only use for calculations of transition densities (option 't' of 'den')

Comparison to experiment for various transitions undertaken in Lecture IV