

The Shell-Model Code NuShellX@MSU

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Use of the code NuShellX@MSU is outlined. It connects to the ENSDF data files for automatic comparisons to energy level data. Operator overlaps provide predictions for spectroscopic factors, two-nucleon transfer amplitudes, nuclear moments, gamma decay and beta decay.

I. INTRODUCTION

NuShellX is a set of computer codes written by Bill Rae [1] that are used to obtain exact energies, eigenvectors and spectroscopic overlaps for low-lying states in shell-model Hamiltonian matrix calculations with very large basis dimensions. It uses a J -coupled proton-neutron basis, and J -scheme matrix dimensions of up to the order of 100 million can be considered.

NuShellX@MSU is a set of wrapper codes written by Alex Brown [2] that use data files for model spaces and Hamiltonians to generate input for NuShellX. The wrapper codes also convert the NuShellX output into figures and tables for energy levels, gamma decay and beta decay.

II. FORMALISM

The NuShellX code uses a proton-neutron basis and a technique similar to that used for the code NATHAN [3]. The Hamiltonian is written as a sum of three terms

$$H = H_{nn} + H_{pp} + H_{pn}. \quad (1)$$

The second quantized form for H_{pn} is

$$H_{pn} = \sum_{pn p' n', J_o} \{ [a_p^+ a_n^+]^{J_o} \otimes [\tilde{a}_{p'} \tilde{a}_{n'}]^{J_o} \}^{(0)}. \quad (2)$$

We can recouple the operators to

$$\begin{aligned} & \{ [a_p^+ a_n^+]^{J_o} \otimes [\tilde{a}_{p'} \tilde{a}_{n'}]^{J_o} \}^{(0)} = \\ & - \sum_{\lambda} \sqrt{(2\lambda + 1)(2J_o + 1)} (-1)^{j_n + j_{p'} - \lambda - J_o} \\ & \times \left\{ \begin{matrix} j_p & j_n & J_o \\ j_{n'} & j_{p'} & \lambda \end{matrix} \right\} \times \{ [a_p^+ \tilde{a}_{p'}]^\lambda \otimes [a_n^+ \tilde{a}_{n'}]^\lambda \}^{(0)}, \quad (3) \end{aligned}$$

where, for example, p stands for the single-particle wavefunction (n_p, ℓ_p, j_p) . H_{pn} can thus be written in the particle-hole form

$$H_{pn} = \sum_{pp' nn' \lambda} F_\lambda(pp' nn') \{ [a_p^+ \tilde{a}_{p'}]^\lambda \otimes [a_n^+ \tilde{a}_{n'}]^\lambda \}^{(0)}, \quad (4)$$

where

$$\begin{aligned} F_\lambda(pp' nn') = & \\ - \sum_{J_o} \sqrt{(2\lambda + 1)(2J + 1)} (-1)^{n+p'-\lambda-J_o} & \left\{ \begin{matrix} p & n & J_o \\ n' & p' & \lambda \end{matrix} \right\}. \quad (5) \end{aligned}$$

The NuShellX basis states have the form

$$|B, J\rangle = [(J_p, \alpha_p) \otimes (J_n, \alpha_n)] J. \quad (6)$$

For the Lanczos multiplications we need the matrix elements of H_{pp} as

$$\delta_{J_{n_f}, J_{n_i}} \delta_{\alpha_{n_f}, \alpha_{n_i}} \delta_{J_{p_f}, J_{p_i}} \langle (J_{p_f}, \alpha_{p_f}) | H_{pp} | (J_{p_i}, \alpha_{p_i}) \rangle,$$

with a similar expression of H_{nn} , and

$$\begin{aligned} & \sum_{pp' nn' \lambda} F_\lambda(pp' nn') \times \\ & \langle B_f, J | \{ [a_p^+ \tilde{a}_{p'}]^\lambda \otimes [a_n^+ \tilde{a}_{n'}]^\lambda \}^{(0)} | B_i, J \rangle = \\ & \sum_{\lambda} \Gamma_{\lambda} \sum_{pp' nn'} F_\lambda(pp' nn') \times \\ & \text{RDM}(p_f, p_i, p, p', \lambda) \text{RDM}(n_f, n_i, n, n', \lambda) \quad (7) \end{aligned}$$

where, for example, p_f , stands for labels (J_{p_f}, α_{p_f}) ,

$$\Gamma_{\lambda} = \left\{ \begin{matrix} J_{p_f} & J_{p_i} & \lambda \\ J_{n_f} & J_{n_i} & \lambda \\ J & J & 0 \end{matrix} \right\}, \quad (8)$$

and RDM are the reduced density matrices (for protons)

$$\begin{aligned} & \text{RDM}(p_f, p_i, p, p', \lambda) = \\ & \langle (J_{p_f}, \alpha_{p_f}) | [a_p^+ \tilde{a}_{p'}]^\lambda | (J_{p_i}, \alpha_{p_i}) \rangle. \quad (9) \end{aligned}$$

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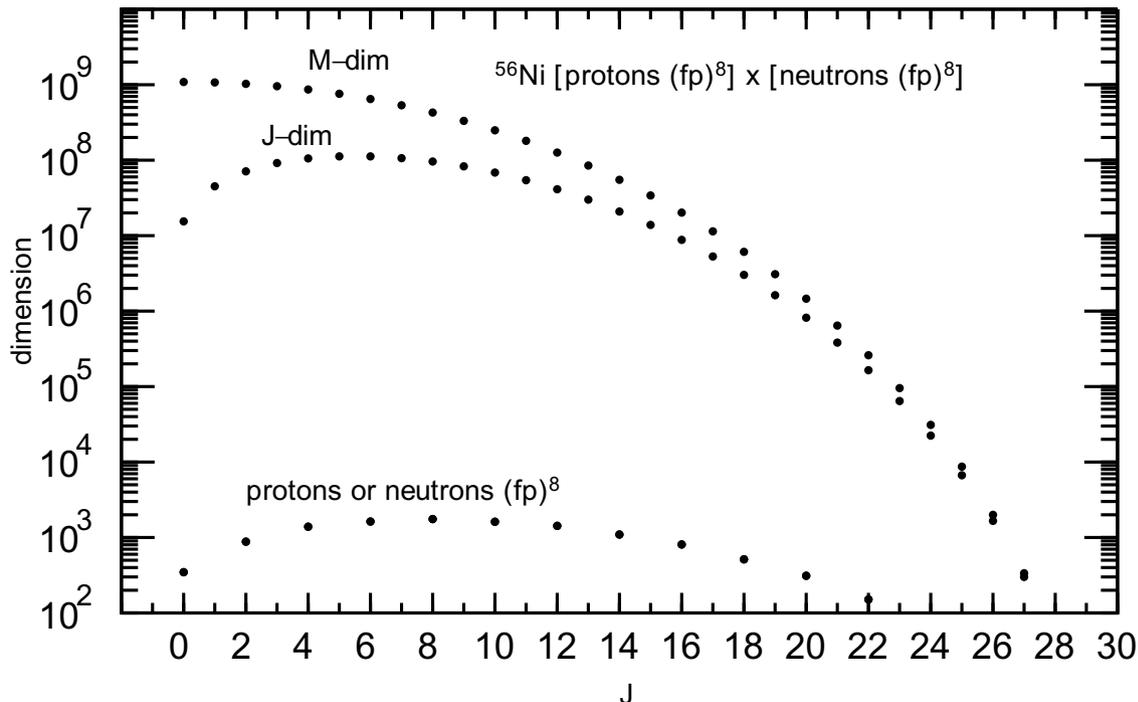


FIG. 1. Basis dimensions for the 8 protons or 8 neutrons in the pf model space (bottom). The combined proton-neutron J -scheme and M -scheme dimensions are shown at the top.

Successive Lanczos multiplications produce vectors

$$|\omega, J\rangle = \sum_{J_p \alpha_p} \sum_{J_n \alpha_n} A(J_p, \alpha_p, J_n, \alpha_n, J) \times |[(J_p, \alpha_p) \otimes (J_n, \alpha_n)]J\rangle. \quad (10)$$

Multiplying H_{pn} on $|\omega_i, J\rangle$ gives

$$H_{pn}|\omega_i, J\rangle = |\omega_f, J\rangle = \sum_{J_p \alpha_p} \sum_{J_n \alpha_n} A'(J_p, \alpha_p, J_n, \alpha_n, J) |[(J_p, \alpha_p) \otimes (J_n, \alpha_n)]J\rangle, \quad (11)$$

with

$$A'(J_p, \alpha_p, J_n, \alpha_n, J) = \sum_{\lambda} \Gamma_{\lambda} \sum_{pp'nn'} F_{\lambda}(pp'nn') \times \sum_{J_{p_i} \alpha_{p_i}} \sum_{J_{n_i} \alpha_{n_i}} \text{RDM}(p_f, p_i, p, p', \lambda) \text{RDM}(n_f, n_i, n, n', \lambda) \times A(J_{p_i}, \alpha_{p_i}, J_{n_i}, \alpha_{n_i}, J). \quad (12)$$

The Hamiltonian matrix elements are calculated “on-the-fly.” The amount of storage associated with the separate proton and neutron basis and the combined proton-neutron vectors is modest. NuShellX makes use of OpenMP to use many cores with high efficiency for the Lanczos iterations. The power of this method is illustrated in Fig. 1 where the J -scheme and M -scheme dimensions for 8 protons and 8 neutrons in the pf model space are shown. The eigenvectors associated with the

very large J -scheme combined dimensions are generated from the pre-calculated information on the separate proton and neutron basis states that each have relative small dimensions. The proton and neutron basis states are obtained by J -projection on M -states with the code NuShell. NuShell is a modern Fortran replacement for the original JT projection code Oxbash. Truncations can be made in terms of the allowed partitions, the range of J_p and J_n values and range of λ values.

The layout of NuShellX@MSU is shown in Fig. 2. At the center is NuShellX. It is surrounded by wrapper codes that bring in information from a library of previously derived Hamiltonians (bottom left). Or the Hamiltonians may be obtained from ab-initio approaches such as those available from the from Ref. [4] (top left). At the end, the wrapper combines the theoretical energies with the information from the ENSDF files to produce a figure for the comparison between experiment and theory. NuShellX takes the overlaps for the operators a^+ , a^+a^+ and a^+a . The wrapper converts these into spectroscopic factors, two-nucleon transfer amplitudes and one-body transition densities, respectively. The one-body transition densities are then used together with the program DENS to calculate the matrix elements for $M\lambda$, $E\lambda$ and Gamow-Teller (GT) operators. The $M1$ and $E2$ results are used to obtain a gamma-ray decay scheme together with the magnetic and quadrupole moments for all states in the calculation. The GT matrix elements are used to obtain an

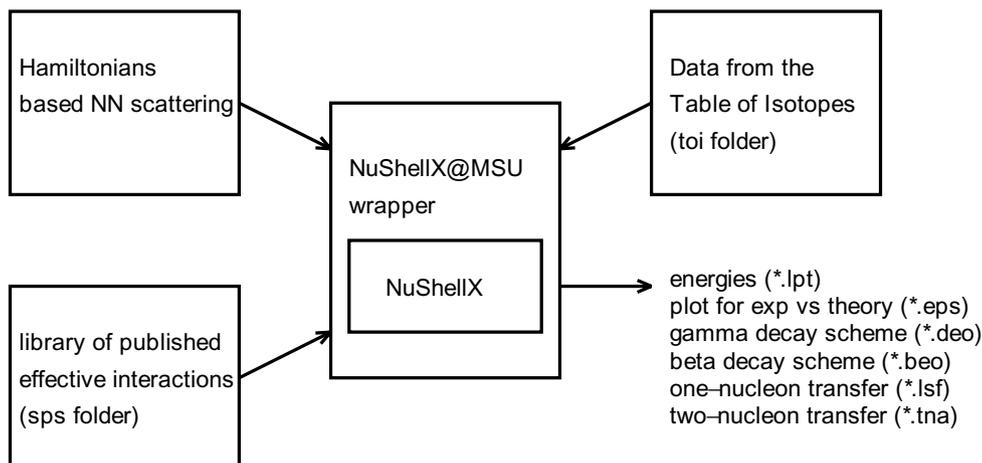


FIG. 2. Schematic layout of the NuShellX@MSU codes.

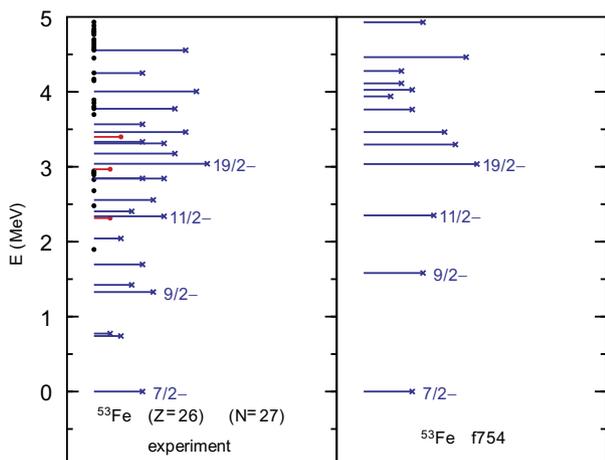


FIG. 3. Energy levels for ^{53}Fe . The experimental values are plotted on the left-hand side with the length of the line proportional to the J value. If the J value is not certain it is indicated by a point on the y-axis. The lines end in crosses for negative parity and filled circles for positive parity states. The theoretical results for negative parity states obtained in the $f_{7/2}$ model space are shown on the right-hand side.

allowed beta-decay scheme. The program DENS allows one to use radial wavefunctions from harmonic-oscillator, Woods-Saxon or Skyrme energy-density functions methods for the matrix elements. DENS can also be used to obtain electron scattering form factors.

III. SOME EXAMPLES

A review of the shell-model method and references for many of the Hamiltonians that have been used is given in Ref. [5]. As an example for energy levels, the results

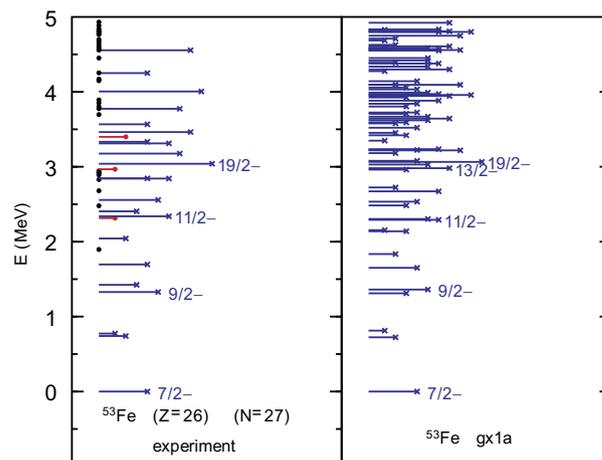


FIG. 4. Same as Fig. 3 except that the calculation is carried out in the full pf model space with the GPFX1A Hamiltonian.

for ^{53}Fe are shown in Figs. 3 and 4. Fig. 3 shows a comparison of experiment with a calculation in the model space consisting of just one orbital, the $0f_{7/2}$. This is the type of calculation that was possible in the 1960's. The spectrum is shown by energy levels (lines) with lengths that are proportional to their J value. For guidance some of these are labeled. If the experimental J value is not known it is indicated by a point on the y-axis. For the $0f_{7/2}$ model space the effective Hamiltonian based upon the spectrum for three holes in ^{56}Ni reproduces the experimental high-spin levels. This case was of early interest because of the isomeric property of the $19/2^-$ level that leads to a rare E6 gamma decay to the ground state. But it is obvious that there many lower J states that are not described by the $0f_{7/2}$ model space. With the NuShellX code it is relatively easy to consider ^{53}Fe in the full pf

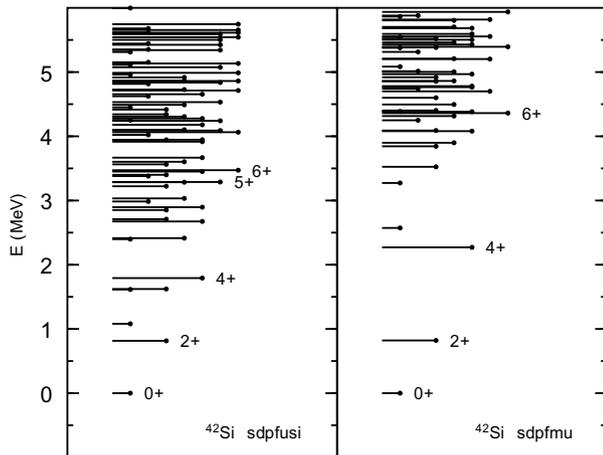


FIG. 5. Spectrum of ^{42}Si predicted by the (left) *sdpfusi* [6] and (right) *sdpfmu* [7] Hamiltonians.

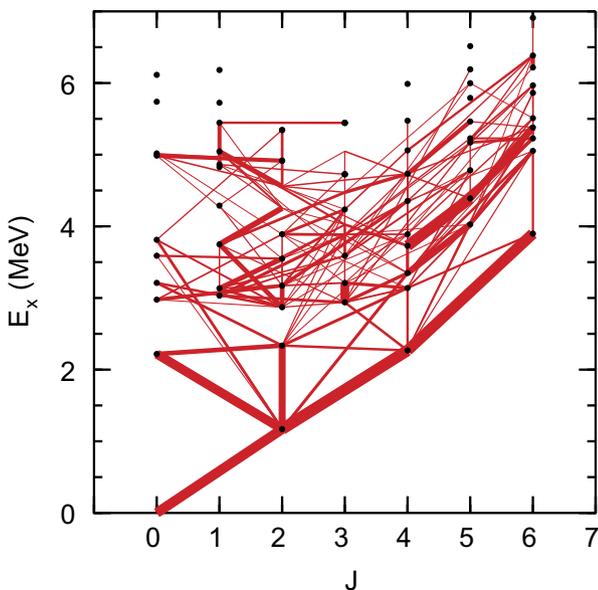


FIG. 6. Energies in ^{62}Ni are plotted vs J on the x-axis and the excitation energy the y-axis. The states are connected by red bands whose width is proportional to the $B(E2)$ value.

model space where the $M=1/2$ dimension is 214,688,113. The results are compared to experiment in Fig. 4. The theoretical spectrum is now much more complete with the first “intruder” states outside of the pf model space starting with the $1/2^+$ state at 2.31 MeV. Starting around 3 MeV many of the predicted theoretical levels have not yet been observed in experiment.

A more current example is shown in Fig. 5 where the predicted levels for the neutron-rich nucleus ^{42}Si are compared for two proposed Hamiltonians. The energies of the first 2^+ states are the same for the two Hamiltonians, but above that they are very different. Over the next decade one will be able to obtain experimental information with the new facilities such as RIBF, FAIR and FRIB that will test these two models. Two-nucleon knockout from ^{44}S has been proposed as a way of doing this [8].

The gamma-decay spectra are complex and are difficult to compare graphically with experimental data. Fig. 6 shows the theoretical “E2-map” for ^{62}Ni . This type of plot immediately shows the complex bands that are obtained theoretically. In this case, the energy spectrum for the low-lying states looks like that expected for one and two E2 phonons and there are strong E2 connections between these states. But there is no evidence in the calculation for a three-phonon structure connected by strong E2 transitions, except for the yrast line. This is consistent with the experimental data [9].

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