Introduction of our theoretical framework

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INTRODUCTION

We investigate the structural changes of the $^{18-28}$O isotopes, both even and odd isotopes, by examining the energies of their low-lying states. This is done by developing our own shell model program and comparing the energies it generates to the NushellX@MSU program [1]. We use a frozen ^{16}O core, having 8 protons and 8 neutron at the *sp*-shell $(0s_{1/2}, 0p_{3/2}, 0p_{1/2})$. More neutrons are then excited in the *sd*-shell $(0d_{5/2}, 1s_{1/2}, 0d_{3/2})$, which serves as our model space. We use all possible configurations in these orbits and work in a harmonic oscillator basis with spin-orbit splitting. The model space Hamiltonian reads

$$\hat{H} = \hat{H}_0 + \hat{H}_I, \tag{1}$$

where $\hat{H}_0$ is the unperturbed one-body Hamiltonian

$$\hat{H}_0 = \sum_{p,q} \langle p|h_0|q\rangle\, \hat{a}_p^\dagger \hat{a}_q, \tag{2}$$

and $\hat{H}_I$ is the pair breaking interaction

$$\hat{H}_I = \sum_{p,q,r,s} \langle p,q|V|r,s\rangle\, \hat{P}^+_{p,q}\hat{P}^-_{r,s}, \tag{3}$$

with

$$\hat{P}^+_{p,q} = \sum_{p,q} \hat{a}_p^\dagger \hat{a}_q^\dagger, \qquad \hat{P}^-_{r,s} = \sum_{r,s} \hat{a}_r \hat{a}_s, \tag{4}$$

where p,q,r,s represent all possible single-particle states (SPS) quantum numbers. The Hamiltonian is rotationally invariant

For the two-body matrix elements (TBME) **(define them as in [2])** in Eq. (3) we use the USDB interaction TBME [2] (Tables I and II in [2], given in J-scheme, for $T = 1, 0$ respectively), and the single-particle energies (SPE) $(1s_{1/2}, 0d_{3/2}, 0d_{5/2})$ are $(-3.2079, 2.1117, -3.9257)$. We work in M-scheme, where the SPS are ordered as given in Table I.

The transformation from J-scheme reads?

Using the SPS we construct the appropriate slater determinants, $|\psi\rangle$, according to the number of particles (even or odd) which we place in the *sd*-shell.

TABLE I. Single particle energies of the *sd*-shell in the M-scheme basis with their corresponding quantum numbers: N, the principle quantum number; ℓ, the orbital angular momentum; J, the total angular momentum; M_j, the total angular momentum projection to the z axis..

index	N	ℓ	J	M_j	SPE
1	1	0	1	$-1/2$	-3.20790
2	1	0	1	$+1/2$	-3.20790
3	0	2	3	$-3/2$	2.11170
4	0	2	3	$-1/2$	2.11170
5	0	2	3	$+1/2$	2.11170
6	0	2	3	$+3/2$	2.11170
7	0	2	5	$-5/2$	-3.92570
8	0	2	5	$-3/2$	-3.92570
9	0	2	5	$-1/2$	-3.92570
10	0	2	5	$+1/2$	-3.92570
11	0	2	5	$+3/2$	-3.92570
12	0	2	5	$+5/2$	-3.92570

My TOC

Background

1. Description for the Oxygen isotopes - the physical phenomenon we investigate.

2. The $1s0d$-shell model space.

3. Pairing Hamiltonian and pair breaking Hamiltonian (We use second quantization. Is this only in m-scheme?).

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{5}$$

$$\hat{H}_0 = \xi \sum_{p,\sigma} (p-1)\hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}, \tag{6}$$

$$\hat{V} = \sum_{p\le q} \langle p|V|q\rangle\, \hat{P}^+_p \hat{P}^-_q, \tag{7}$$

$$\hat{P}^+_p = \sum_{\sigma_p,\ge 0} \hat{a}^\dagger_{p,\sigma_p}\hat{a}^\dagger_{p,-\sigma_p}, \qquad \hat{P}^-_p = \sum_{\sigma_p,\ge 0} \hat{a}_{p,-\sigma_p}\hat{a}_{p,\sigma_p}. \tag{8}$$

Aren't we using

$$\hat{V} = \sum_{p \leq q} \langle pq|V|rs\rangle \, \hat{P}^{+}_{p,q} \hat{P}^{-}_{r,s}? \tag{9}$$

$$\hat{P}^{+}_{p,q} = \sum_{\sigma_p, \sigma_q, \geq 0} \hat{a}^{\dagger}_{p,\sigma_p} \hat{a}^{\dagger}_{q,-\sigma_q}, \qquad \hat{P}^{-}_{r,s} = \sum_{\sigma_r, \sigma_s, \geq 0} \hat{a}_{r,-\sigma_r} \hat{a}_{s,\sigma_s} ?? \tag{10}$$

Introduction of our theoretical framework

1. The *sd*-shell serves as our model space.
2. The Hamiltonian we are using.
   (a) Few words on the pair breaking interaction.
   (b) The Hamiltonian is rotationally invariant.
3. SPS coupling to M_{tot}. For $M_{tot} = 0$ ($M_{tot} = 1/2$) we obtain all possible J values for even (odd) nuclei. Explain this when comparing our results to NushellX.
4. Matrix elements in m-scheme.
   (a) Translate Eq. (19) in [2] to M-scheme?
   (b) The USD Hamiltonian is defined by 63 sd-shell TBME and three SPE given in Table I of [1]. This is converted to the M-scheme and was given to us by Morten in the sdshellint.dat file. To this we added the refinement of Eq. (19) in [2].
5. Slater determinants.
6. We solve the many-body Schrodinger eq.
7. The different NushellX interactions:
   (a) USD (the original, by Winldenthal)
   (b) USDB.
   (c) USDA.
   (d) CCEI (Gustav's).

[1] B. A. Brown and W. Rae, Nucl. Data Sheets **120**, 115 (2014).
[2] B. A. Brown and W. A. Richter, Phys. Rev. C **74**, 034315 (2006).