Nuclear Structure: Final Exam

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Project

- Project A: shell model code
- Goals:
 - 1. Write a shell model code
 - 2. Calculate levels for ¹⁸O through ²⁸O
 - 3. Compare to NuShellX and experiment

Outline of code

- Written in Python
- Represents Slater determinants as lists
- M-scheme basis

States & interaction

- Read from file
- USDB interaction
- 1s0d shell states

```
def load_interaction(filename):
    let states be an empty list
    let mels be an empty dictionary

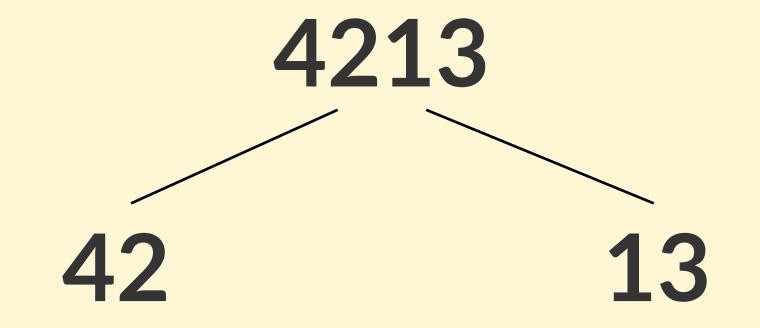
open file called filename
    for line in file:
        if line starts with '#':
            ignore and continue
        else if line has 6 numbers:
            append list of numbers to states
        else if line has 5 numbers:
            let indices be a tuple of the first 4 numbers
            add entry {indices: last number in line} to mels
    return states, mels
```

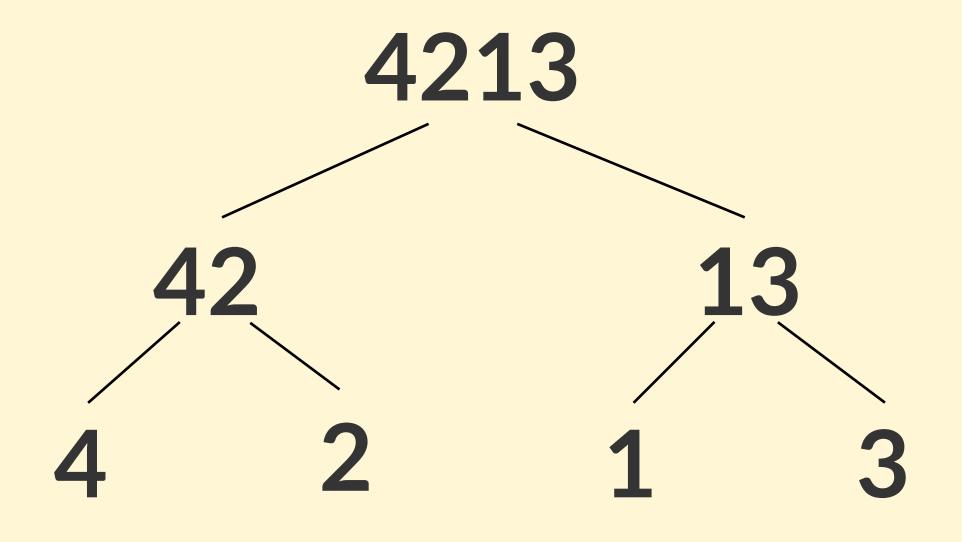
Slater determinants

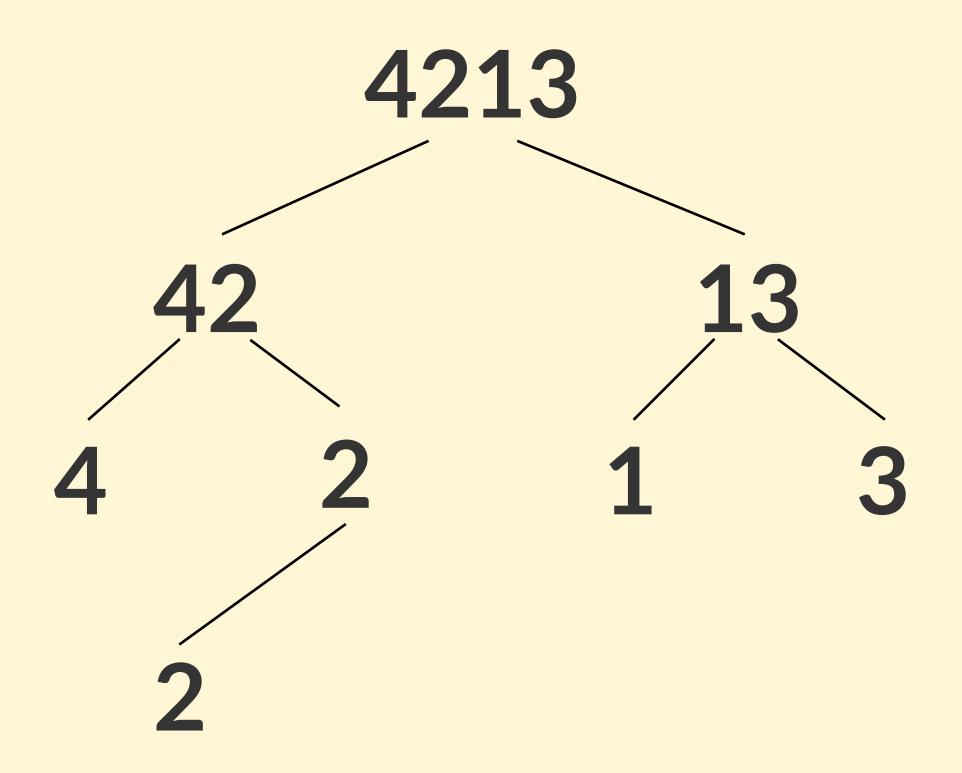
- Find all combinations of indices
 - [0, 1, 2, 3], [0, 1, 2, 4], ...
- Store only those with the chosen total angular momentum projection

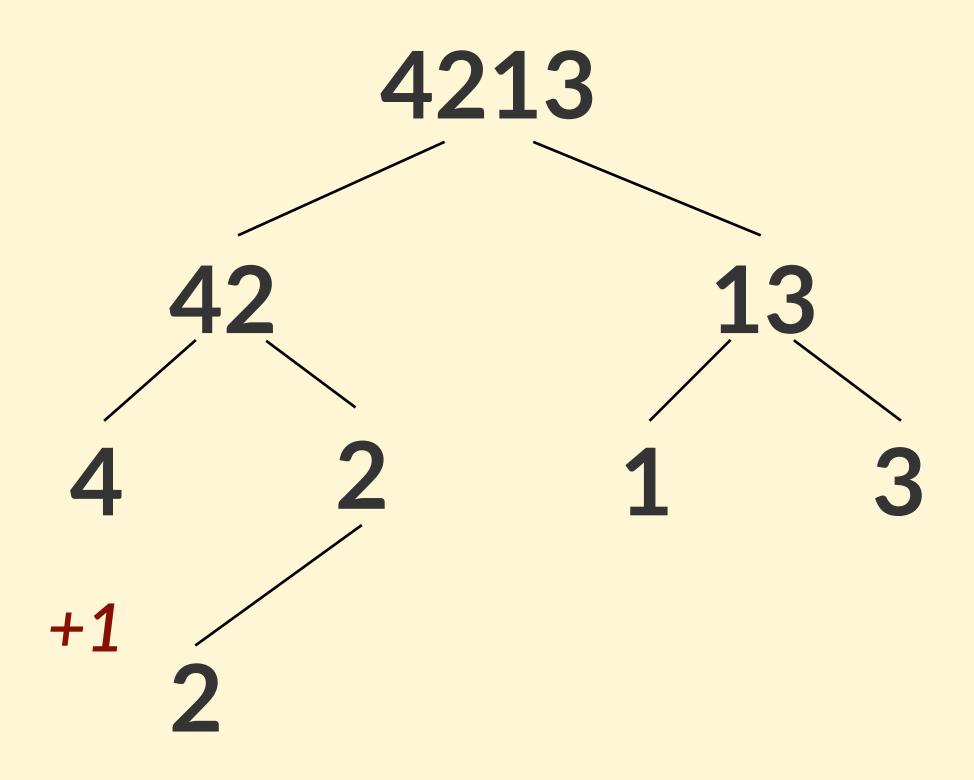
```
def slater(n, states, m):
    label the states by index
    let sds be an empty list
    for each unique combination of n states:
        find total M for these states
        if this M == m:
            add indices to sds
    return sds
```

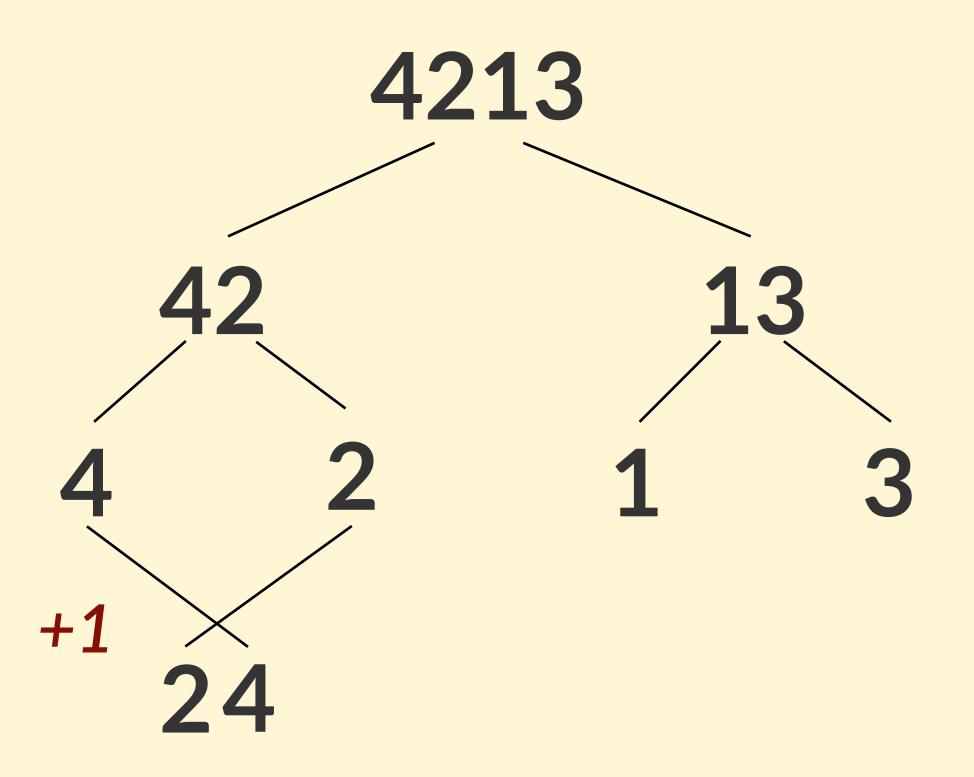
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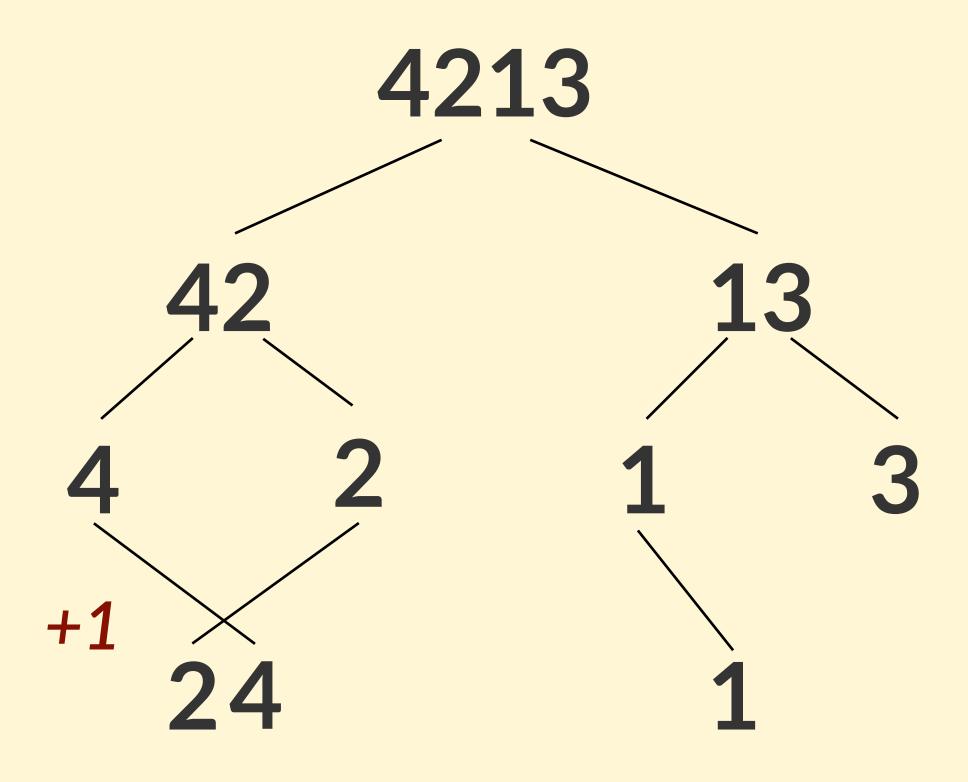


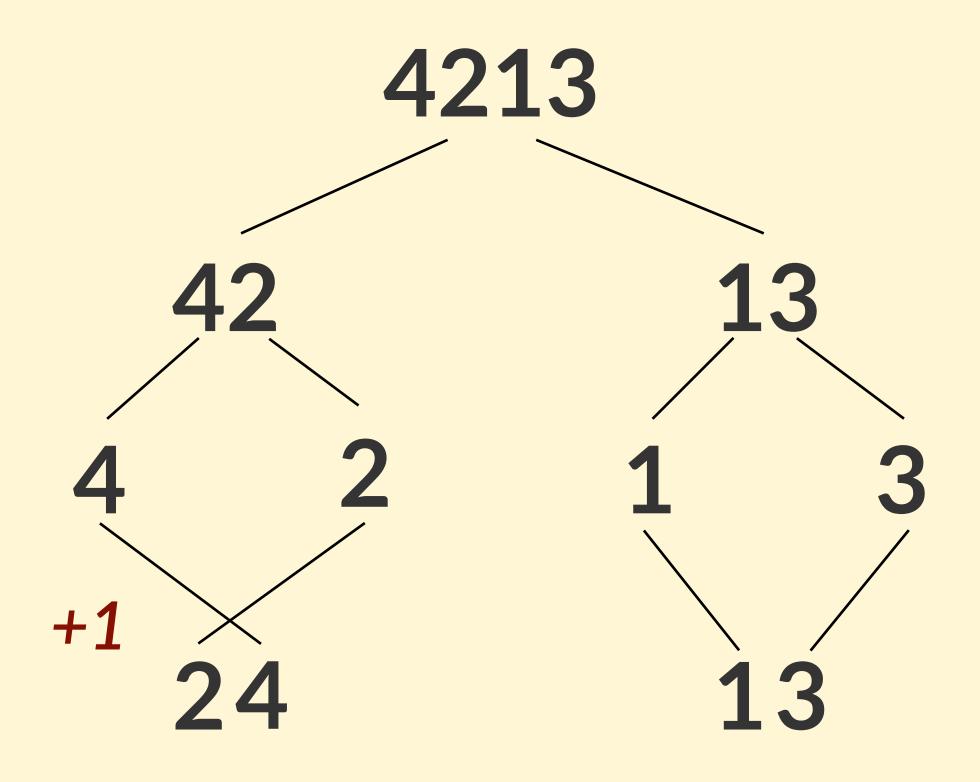


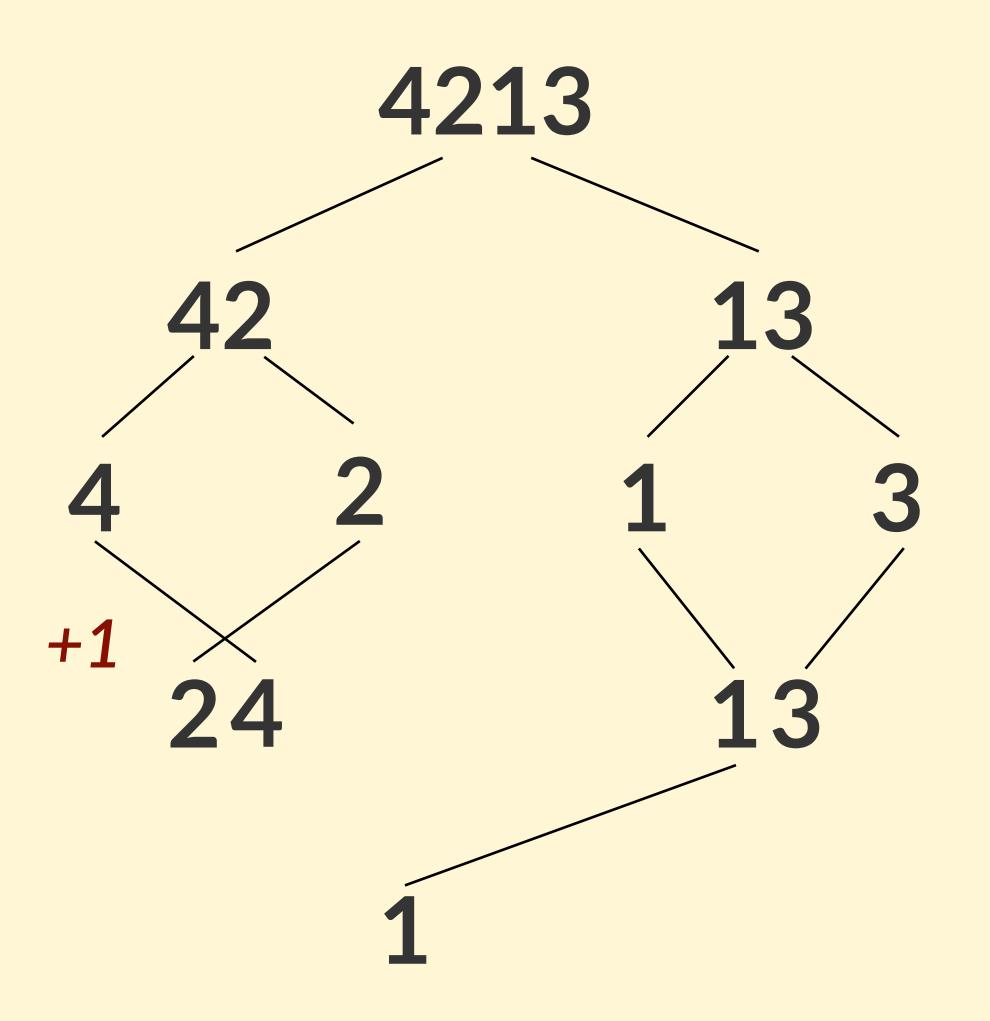


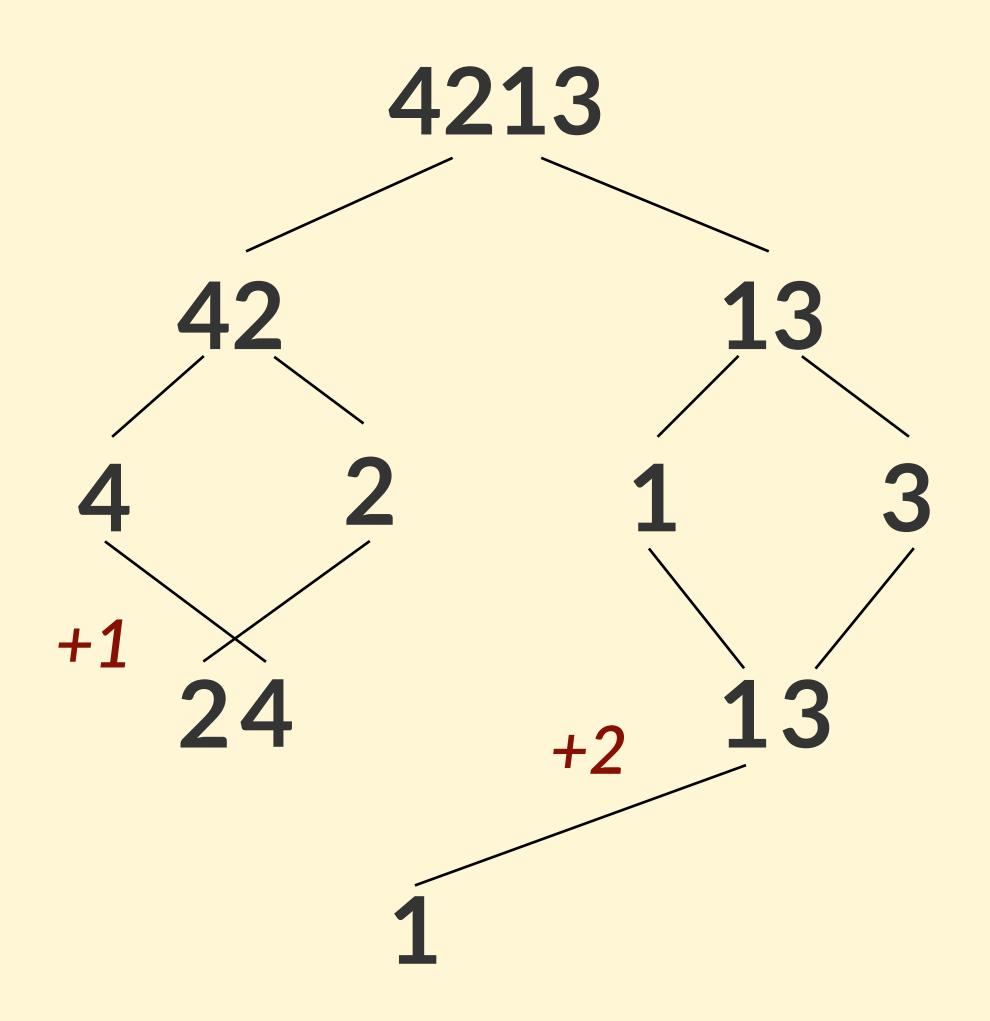


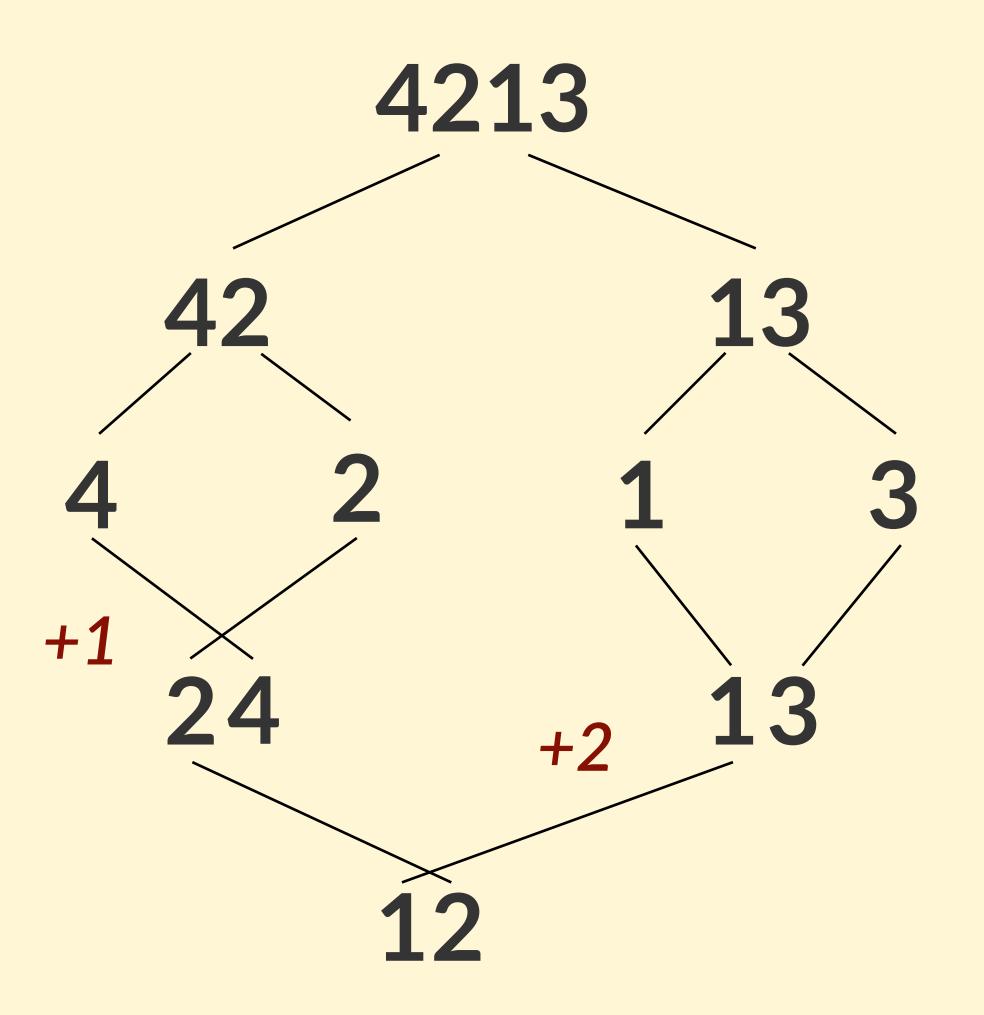


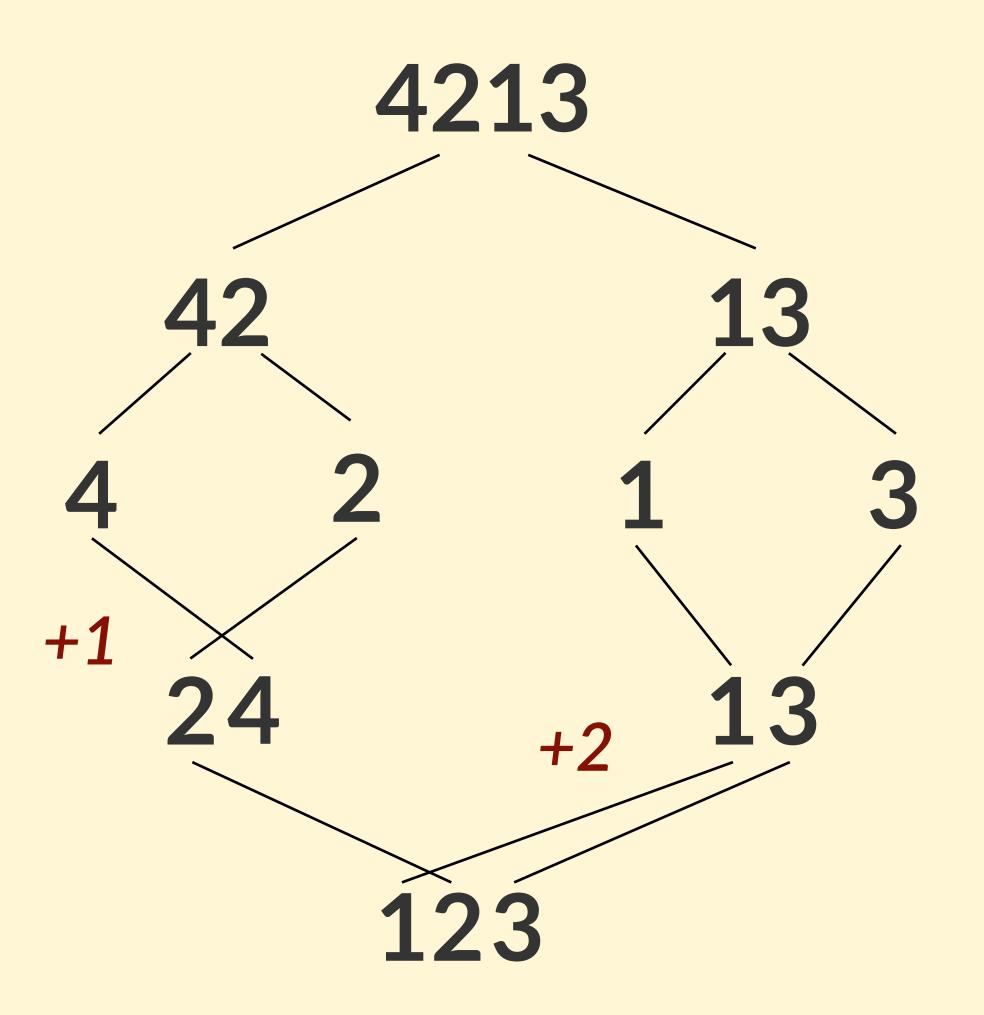


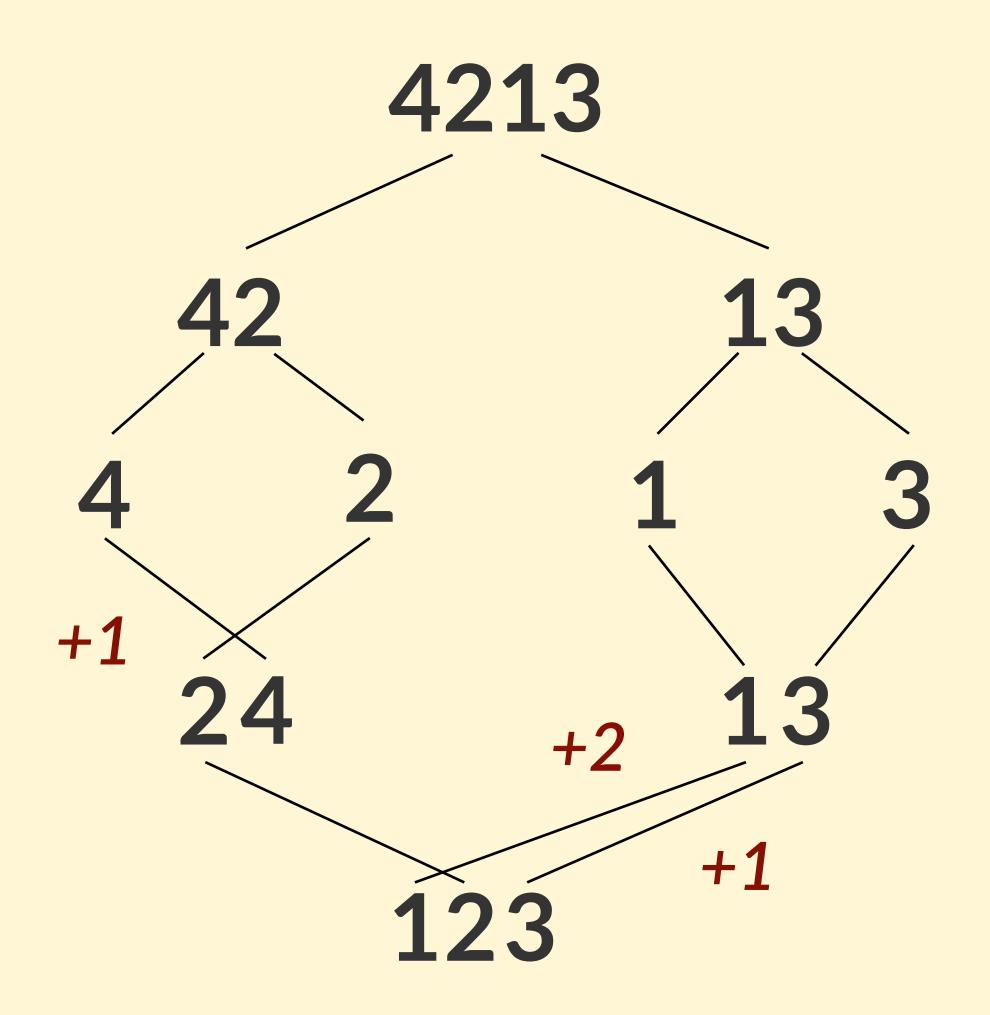


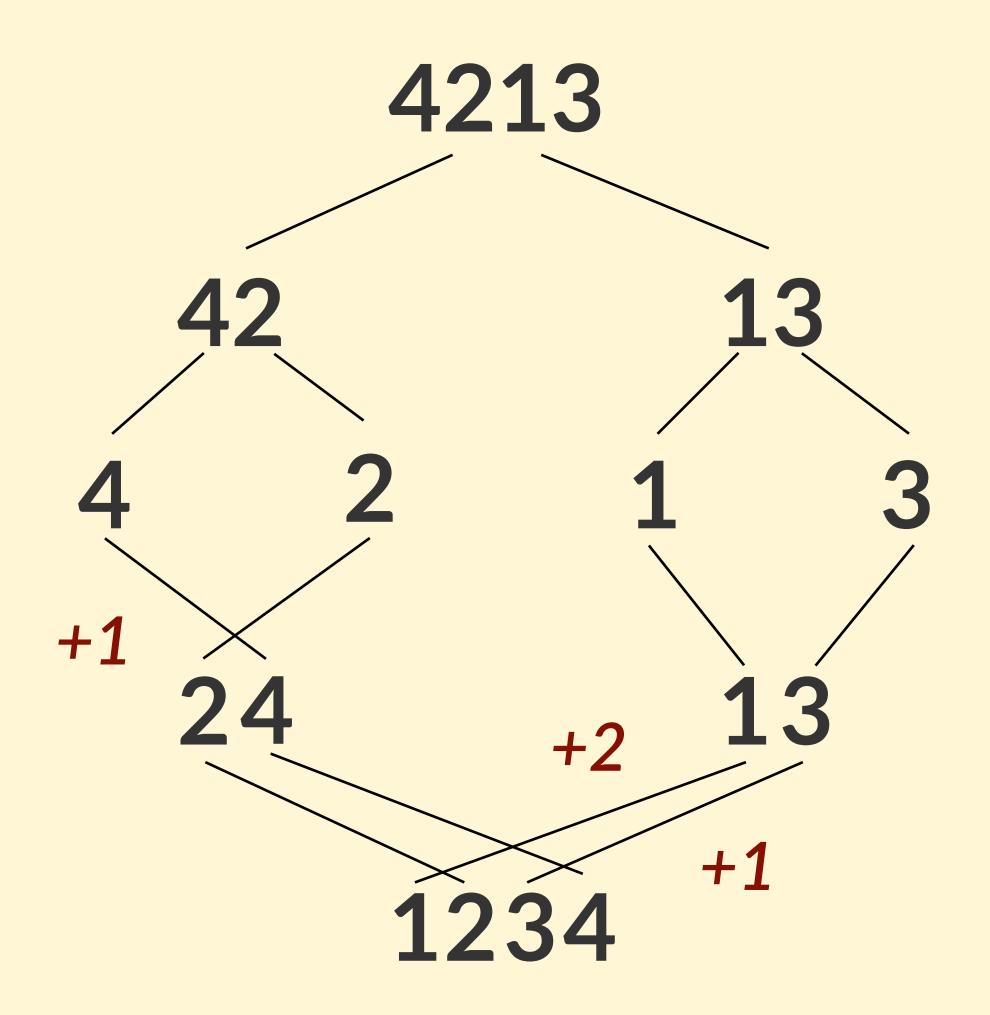


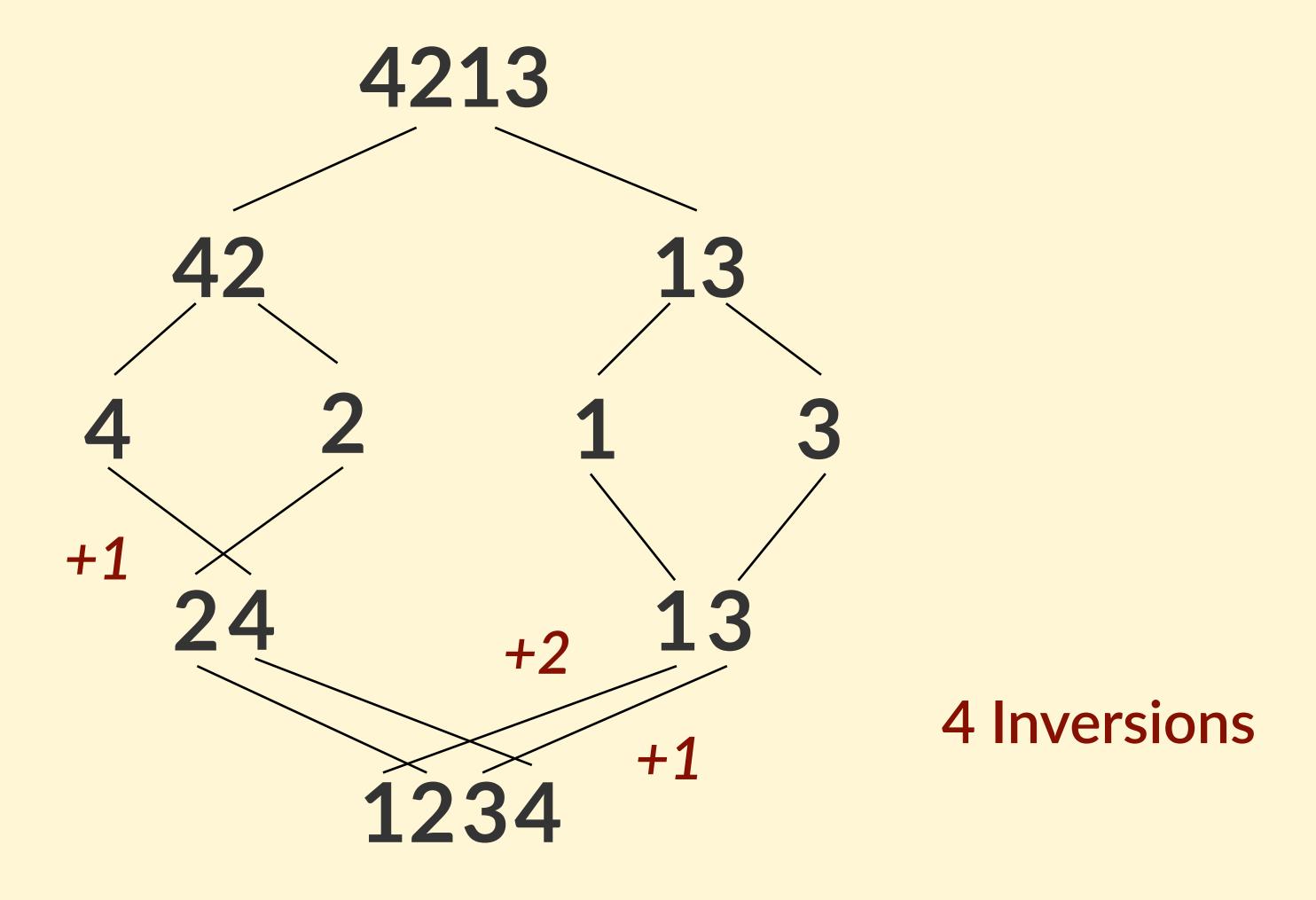


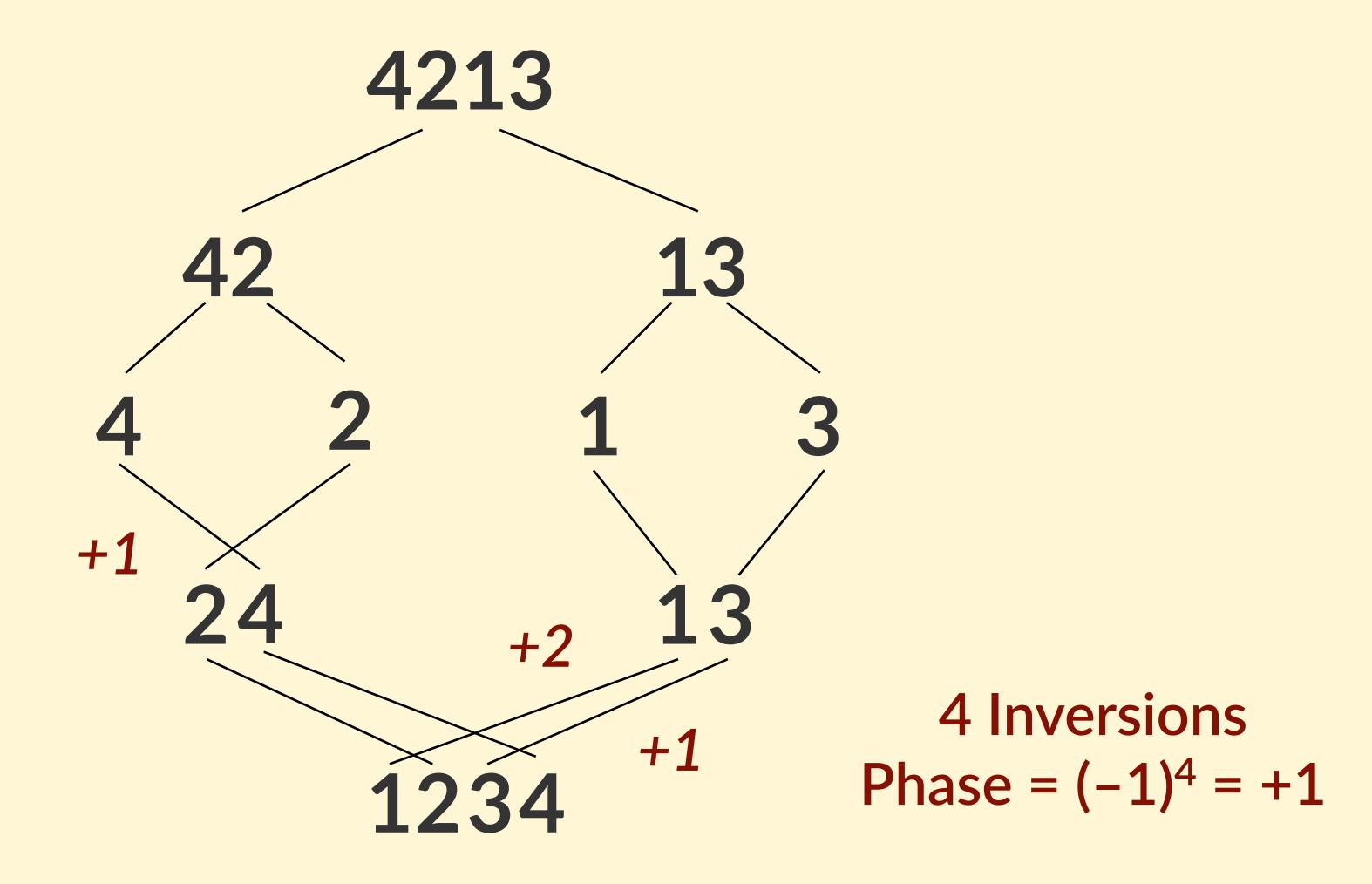










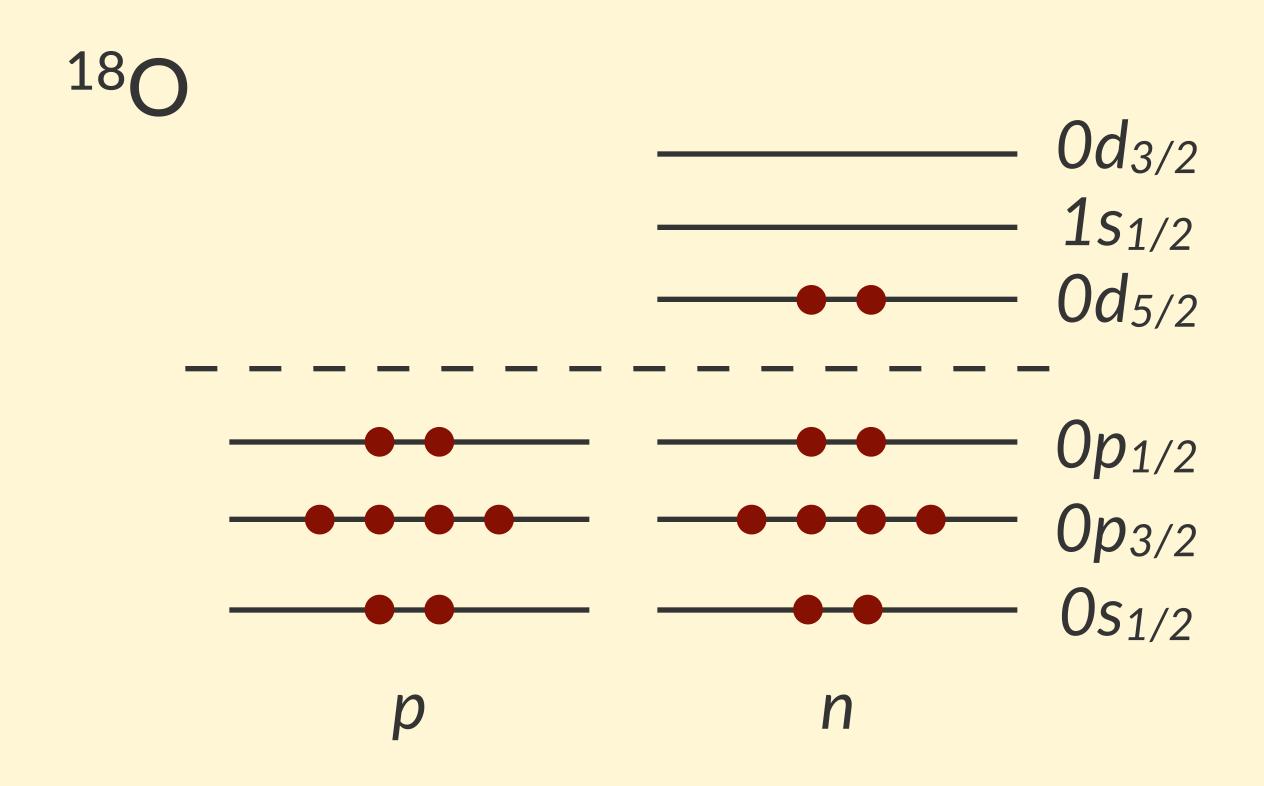


Hamiltonian

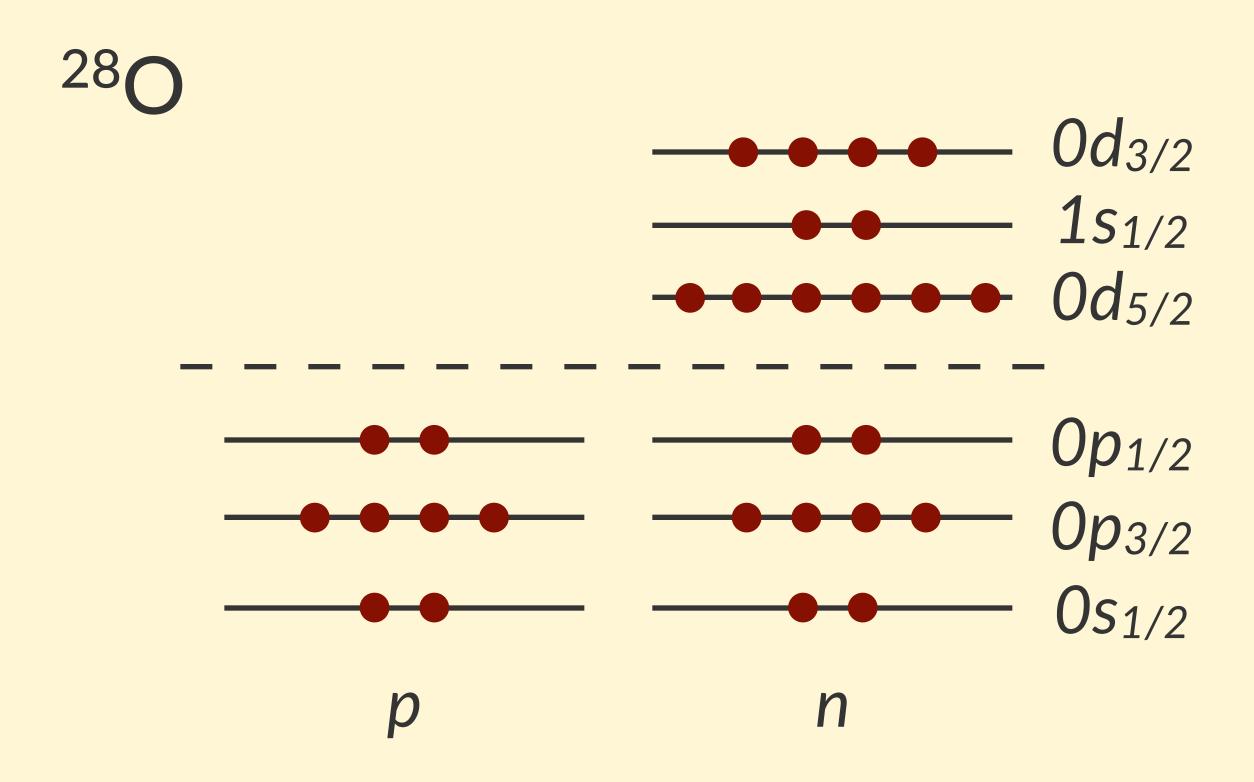
- Iterate over each ket
- Maintain Pauli principle and rules from second quantization
- Find phase using merge sort
- Use matrix elements from USDB file
- Diagonalize with built-in eigenvalue solver from NumPy

```
def find_hamiltonian_matrix(sds, states, interaction):
    let hmat be a square matrix with dim of sds
    fill hmat with 0.0
    for each ket in sds:
        for each p, q, r, s, energy in interaction:
            if r not in ket or s not in ket:
                skip and continue
            if p in ket and (p != r \text{ and } p != s):
                skip and continue
            if q in ket and (q != r \text{ and } q != s):
                skip and continue
            copy ket to new_ket
            replace s with q in new_ket
            replace r with p in new_ket
            sort new_ket and find number of inversions
            let i be the matrix row for ket
            let j be the matrix column for new_ket
            hmat[i, j] += energy * (-1)^{(number of inversions)}
            hmat[j, i] = hmat[i, j]
    for each diagonal element:
        hmat[i, i] += sum(single particle energies)
    return hmat
```

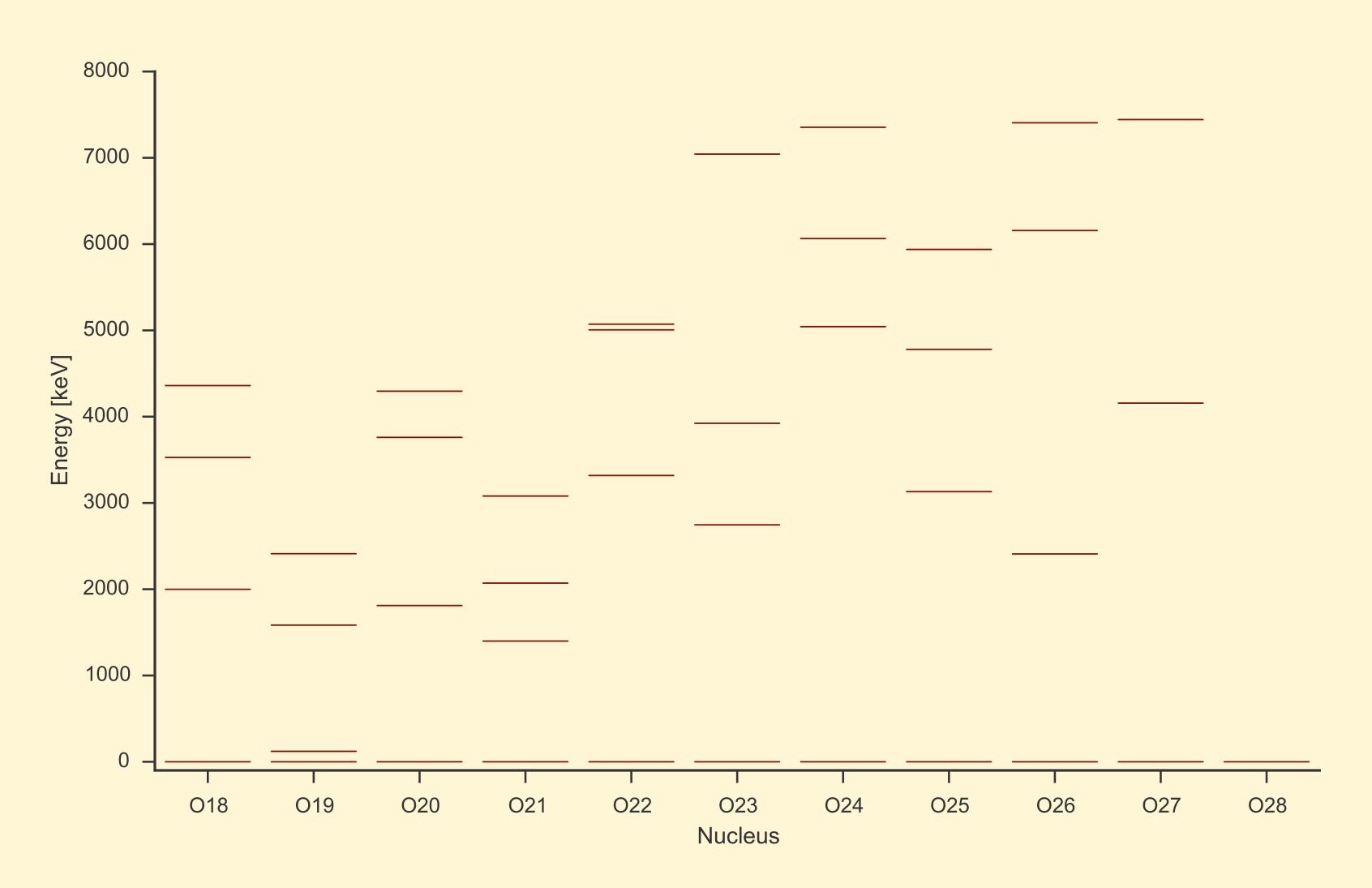
Test: Oxygen isotopes



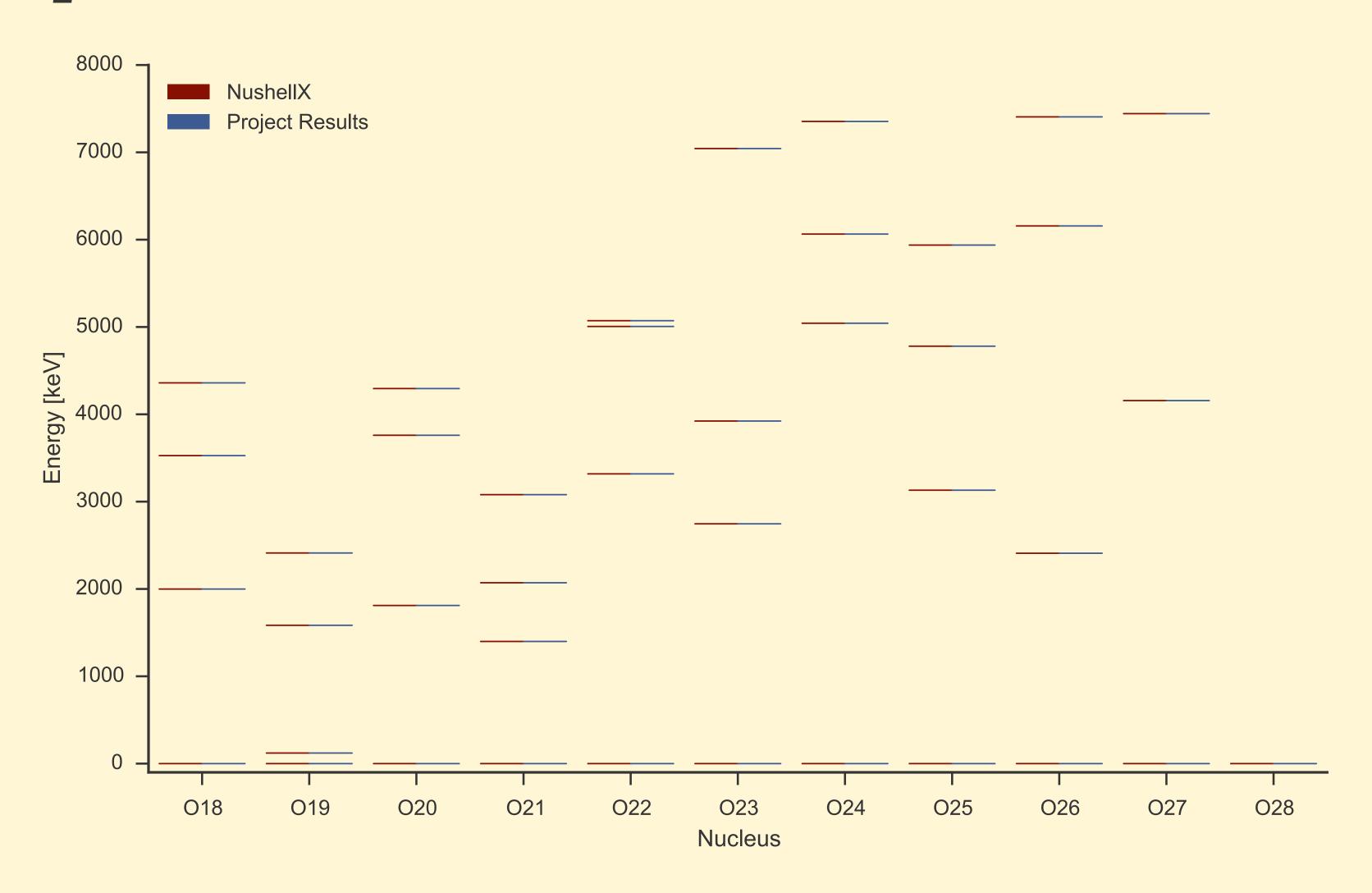
Test: Oxygen isotopes



Levels



Compared to NuShellX



Compared to experiment

