Visualization of nuclear many-body correlations with the most probable nucleon arrangement

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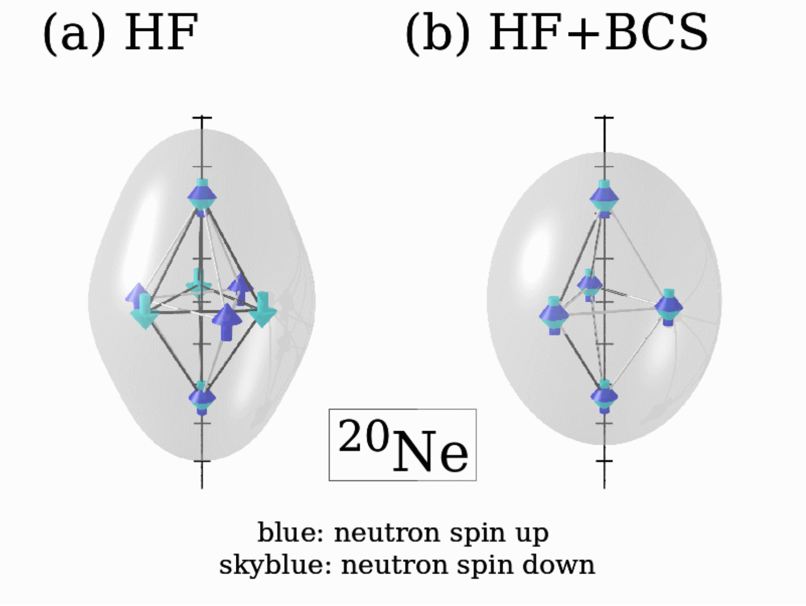

← Most probable arrangements of neutrons in ^{20}Ne

M. Matsumoto and YT, PRC**106**, 014317 ('22)

2022/12/12 DFT2022, YITP

Many-body theory

- Solution of Schrödinger eq. $H\Psi = E\Psi$
  → $\Psi(\boldsymbol{r}_1\sigma_1,\boldsymbol{r}_2\sigma_2,\ldots,\boldsymbol{r}_A\sigma_A)$

- Structure, observables, …
  - ✓ $\langle\Psi|O^{(1)}|\Psi\rangle = \mathrm{Tr}[\rho^{(1)}O^{(1)}]$ -- ex. size, EM moment, EM transitions, …
  - ✓ $\langle\Psi|O^{(2)}|\Psi\rangle = \mathrm{Tr}[\rho^{(2)}O^{(2)}]$ -- ex. binding energy, 2-body correlation, …

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- **Method to visualize many-body correlations based on the full information of wave function**
- **Structure of light nuclei**
  - ✓ **Hartree-Fock**
  - ✓ **Hartree-Fock + BCS**

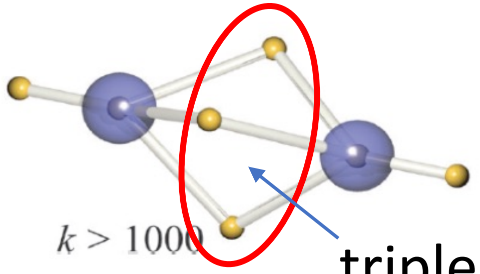
How to extract information out of a many-body wave function?

In quantum chemistry:

"Likely" arrangement of electrons in molecule
(N-body correlation in N-body system)

Liu et al., Phys. Chem. Chem. Phys. **18**, 13385 ('16).
Liu et al., Nat. Commun. **11**, 1210 ('20).
…

N_2 molecule (HF)



$$\langle \boldsymbol{X} \rangle = \int d\boldsymbol{X}\ \boldsymbol{X} |\Psi(\boldsymbol{X})|^2$$

$$\boldsymbol{X} = (\boldsymbol{r}_1\sigma_1, \ldots, \boldsymbol{r}_N\sigma_N)$$

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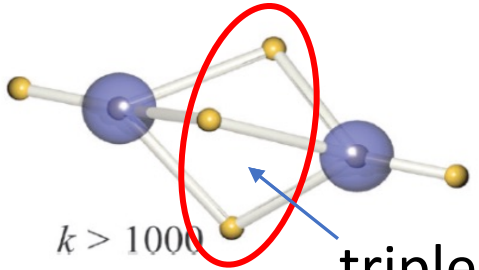

triple-bond structure

spin-up e^-
N nuclei

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$$\boldsymbol{X} = (\boldsymbol{r}_1\sigma_1, \ldots, \boldsymbol{r}_N\sigma_N)$$

Similar analysis can be made for nuclear wave functions?
→ Simple $|\Psi|^2$ maximization as the 1st step

$|\Psi|^2$ maximization

M. Matsumoto and YT, PRC**106**, 014317 ('22).

System of N (= even) identical Fermions

Probability density of finding the particles simultaneously at ($r_1\sigma_1,\ldots,r_N\sigma_N$):

to be maximized

$$\rho^{(N)}(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2, \ldots, \boldsymbol{r}_N\sigma_N) = \left|\Psi(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2, \ldots, \boldsymbol{r}_N\sigma_N)\right|^2$$

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Spins fixed

#up = #down

$$\rho_0^{(N)}(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) = \left|\Psi(\boldsymbol{r}_1\uparrow, \ldots, \boldsymbol{r}_{N/2}\uparrow, \boldsymbol{r}_{N/2+1}\downarrow, \ldots, \boldsymbol{r}_N\downarrow)\right|^2$$

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Short-range & attractive nature of nuclear force

→ max($\rho_0^{(N)}$) is the global maximum of $|\Psi|^2$

Set up

α-cluster (and other possible) **correlations**
in N=Z light nuclei

- Hartree-Fock calculation
  - ✓SLy4 interaction
  - ✓Time-reversal symmetry
  - ✓Axial and reflection symmetries
  - ✓HF+BCS: constant-gap approx.

- Maximization
  - ✓$\rho^{(N)}{}_0(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)$ is maximized with conjugate-gradient method
  - ✓initial $(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_A)$ is generated randomly

$$\rho_0^{(N)}(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N) = \left|\Psi(\boldsymbol{r}_1\uparrow,\ldots,\boldsymbol{r}_{N/2}\uparrow,\boldsymbol{r}_{N/2+1}\downarrow,\ldots,\boldsymbol{r}_N\downarrow)\right|^2$$

E. Chabanat et al., Nucl. Phys. **A635**, 231 (1998).
Vautherin, Phys. Rev. C**7**, 296 (1973).

Remarks: symmetries

- Due to axial symmetry, **$|\Psi|^2$ is invariant under rotation about z axis.**

- Hartree-Fock wave function

$$\langle x_1, \ldots, .x_A | \Psi \rangle = \det B_n \det B_p$$ = (neutron determinant)*(proton determinant)

$$(B_q)_{ij} = \langle x_i | \varphi_j^{(q)} \rangle$$ q = p or n

→No explicit correlation between neutrons and protons
→**$|\Psi|^2$ does not depend on relative angle between n and p about z axis**.

- The same applies to reflection symmetry

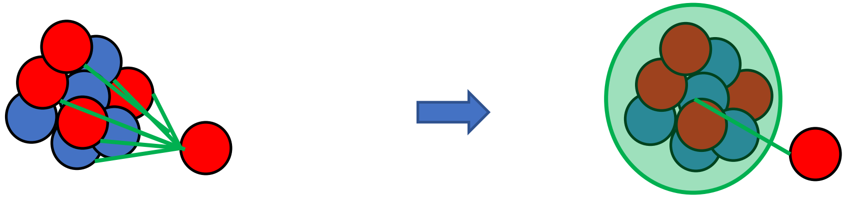
Remarks: correlations in Hartree-Fock

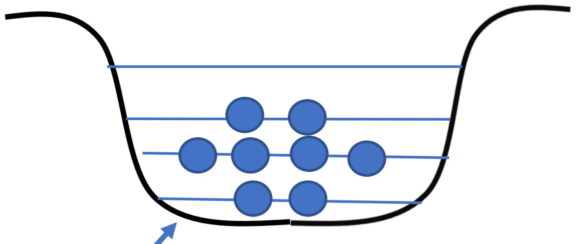
Mean-field (Hartree-Fock) theory

$$H = \sum_{i=1}^{A} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{i>j}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j) \Rightarrow \sum_{i=1}^{A} h(i) = \sum_{i=1}^{A} \left[\frac{\boldsymbol{p}_i^2}{2m} + v_{\mathrm{MF}}(\boldsymbol{r}_i) \right]$$

2-body int.

"Mean field"





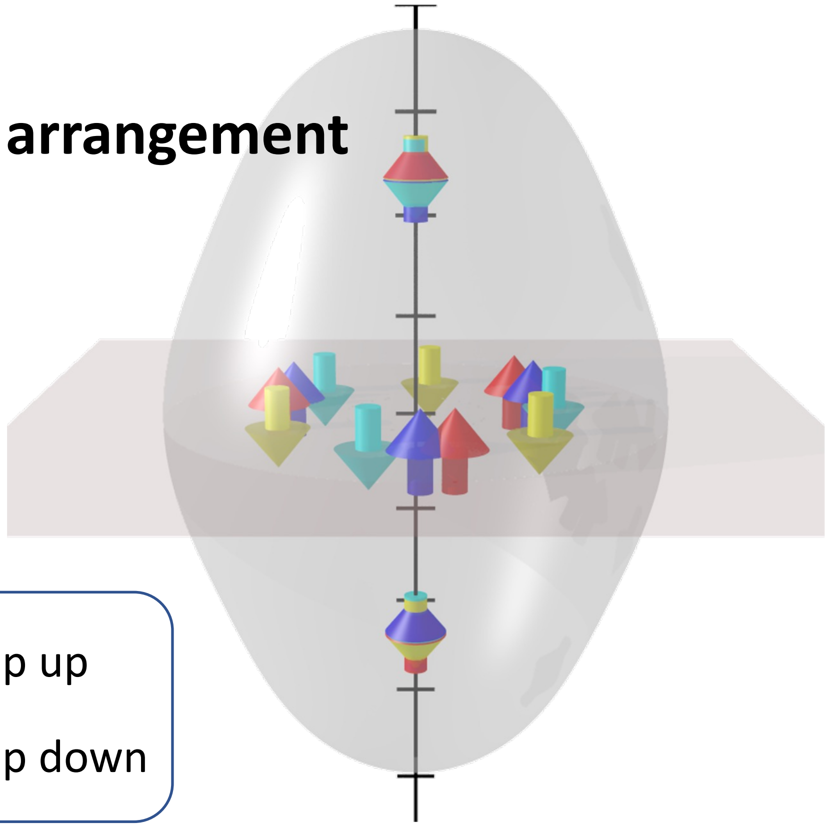
$$v_{\mathrm{MF}}(\boldsymbol{r}) \sim \int d^3r' \; v(\boldsymbol{r}, \boldsymbol{r}')\rho(\boldsymbol{r}')$$

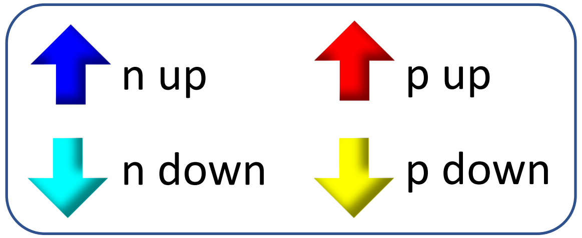
Correlations in HF

- Explicit: Pauli principle
- **Implicit/explicit: interaction through the mean field** ("long-range correlation")
  - → **size**
  - → **deformation (symmetry breaking)**

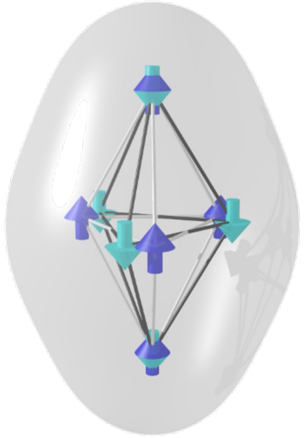
Result: HF ground state of ^{20}Ne

most probable arrangement of all nucleons





neutrons →



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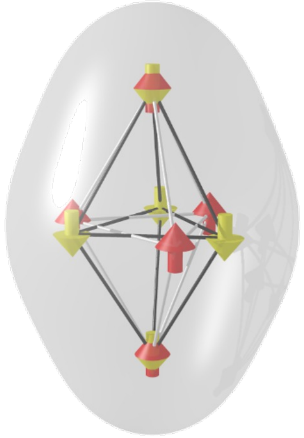

protons ≈ neutrons

Result: HF ground state of ^{20}Ne

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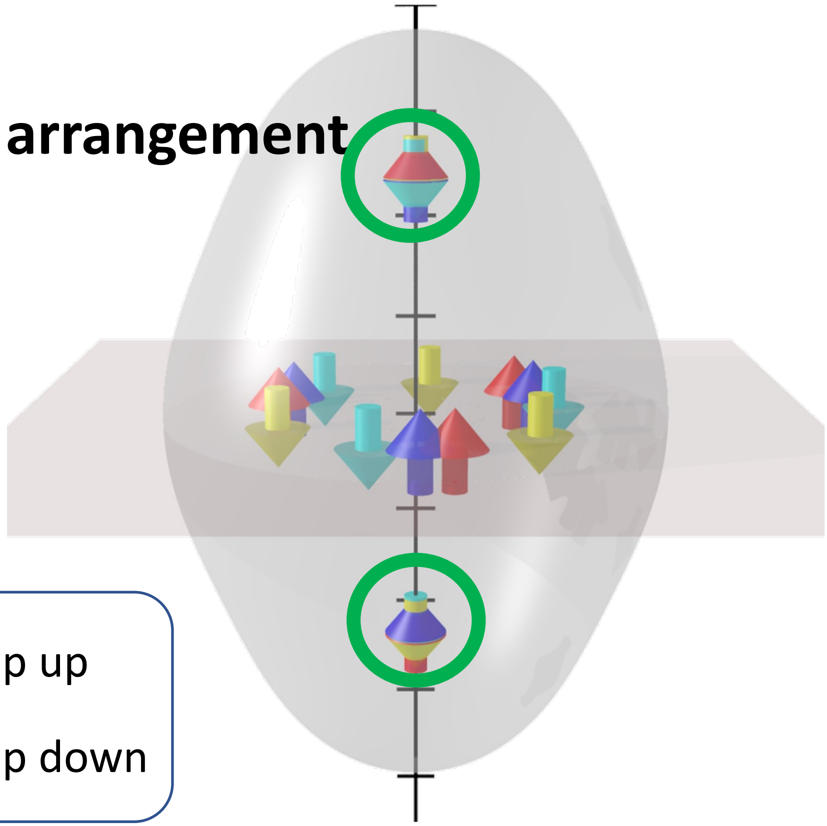

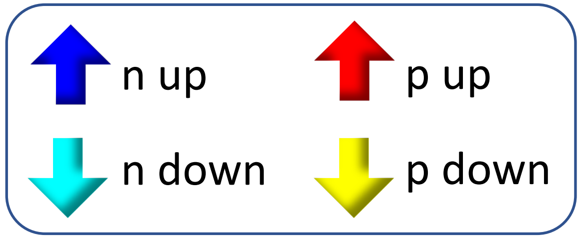

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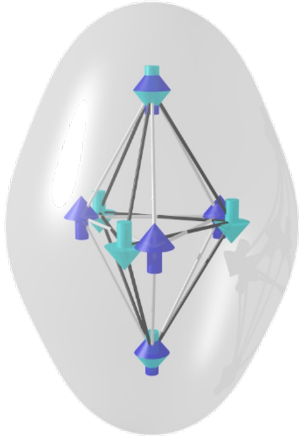

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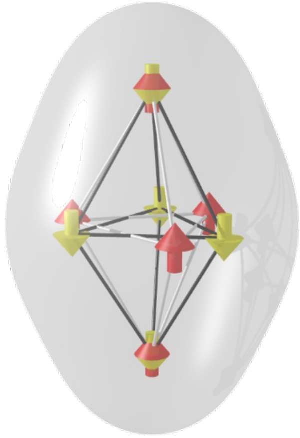
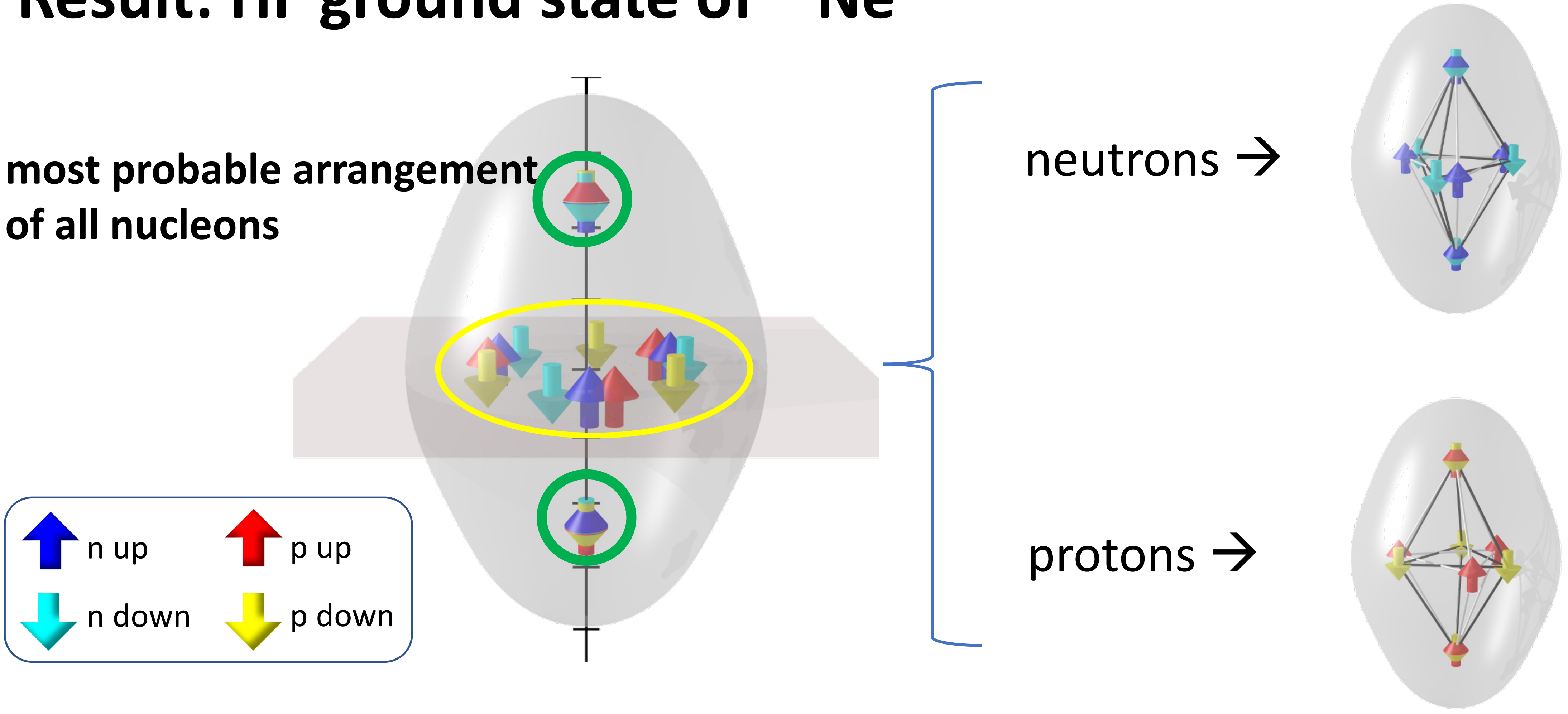


- α clusters at top/bottom

protons ≈ neutrons

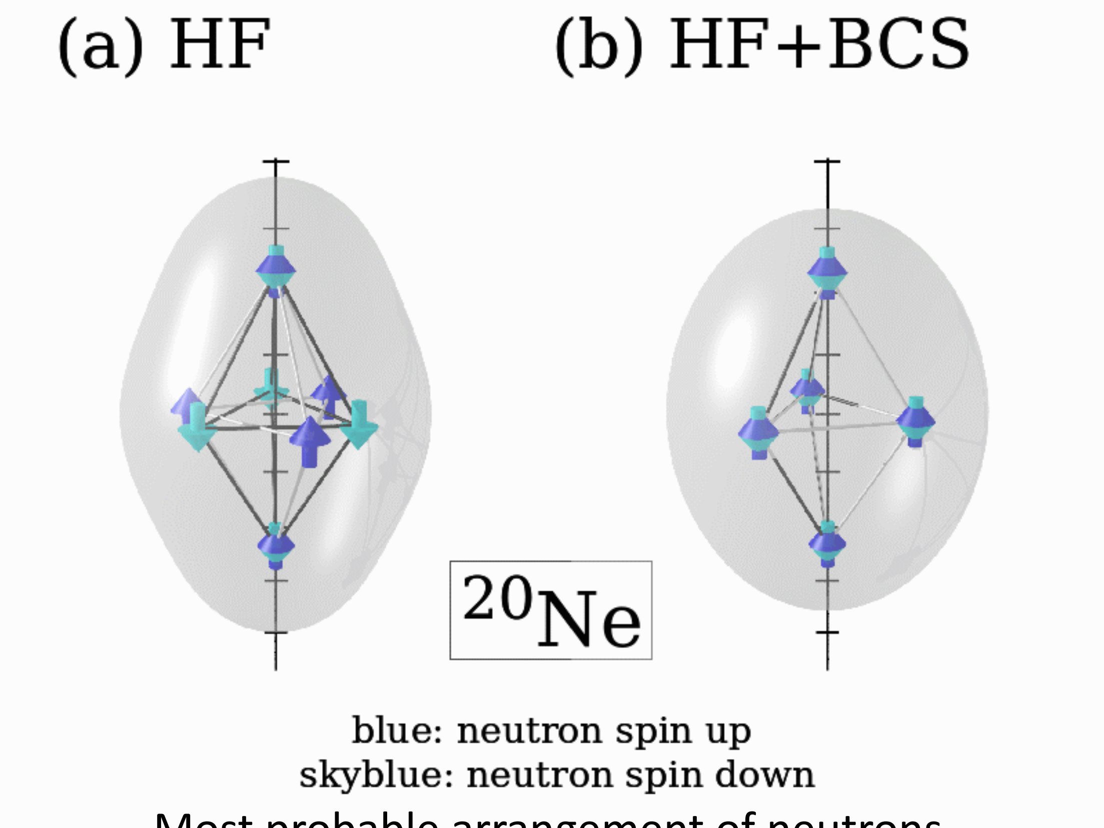
Result: HF ground state of ^{20}Ne



- **α clusters at top/bottom**
- **12 nucleons on xy plane**

protons ≈ neutrons

Results: HF+BCS g.s. of ^{20}Ne



Most probable arrangement of neutrons

Protons ≈ neutrons

Attractive correlation between spin-up and -down

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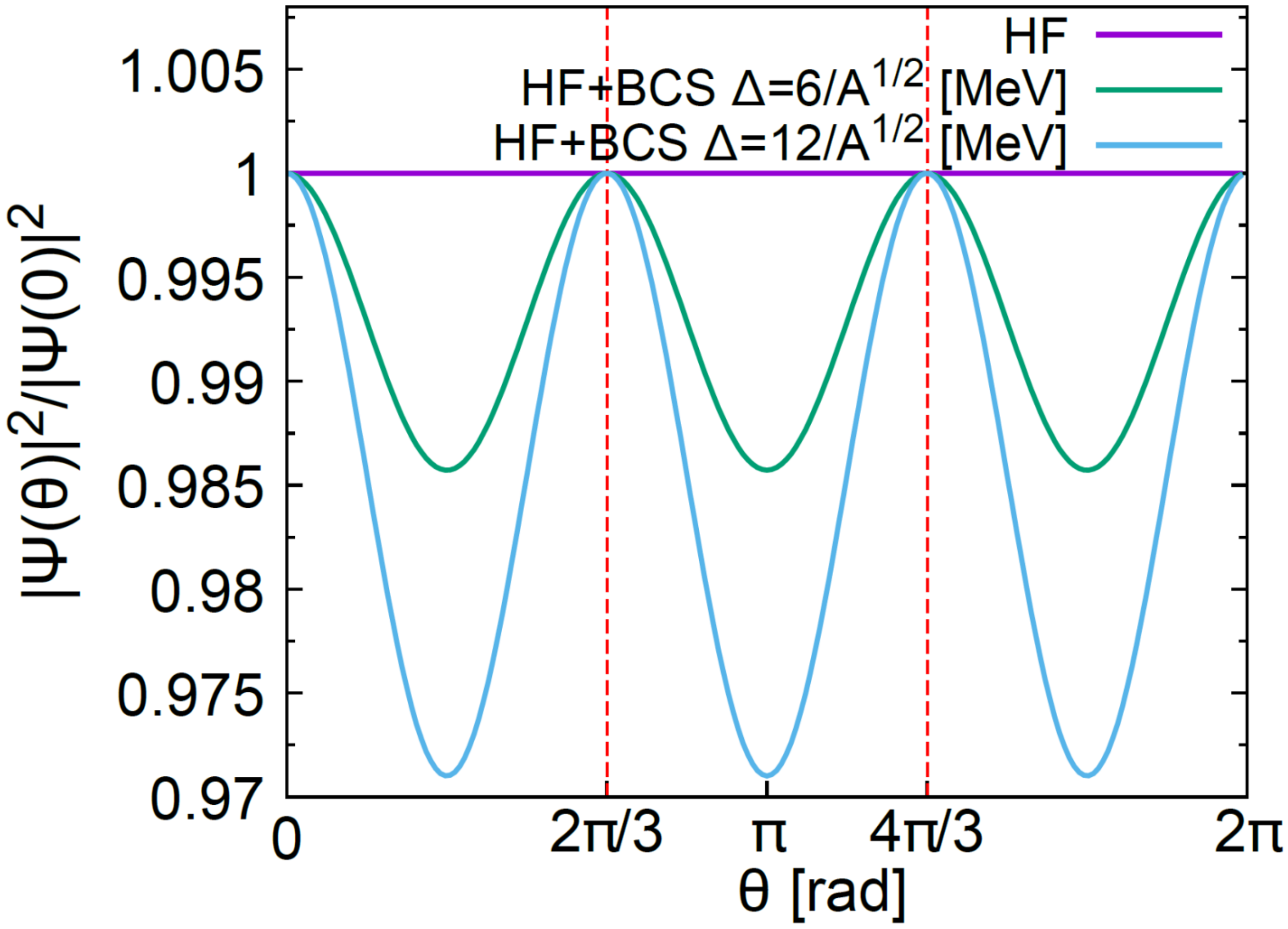
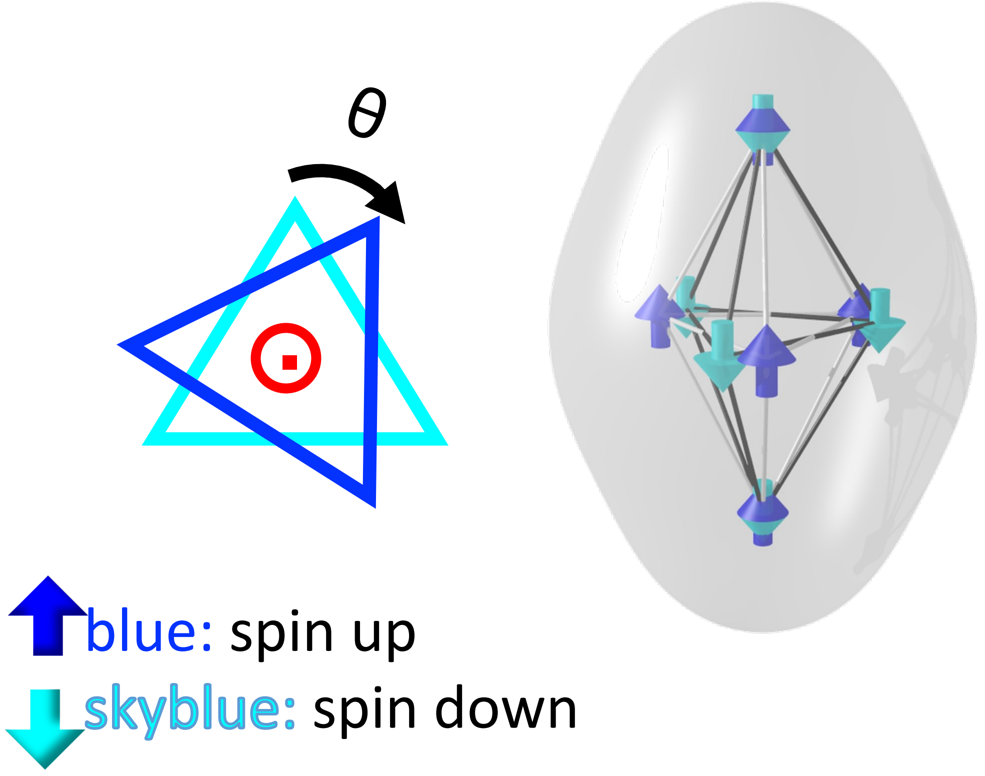
Result (1) ^{20}Ne

Probability variation as a function of the relative angle (θ) around the z axis between spin-up and –down neutrons





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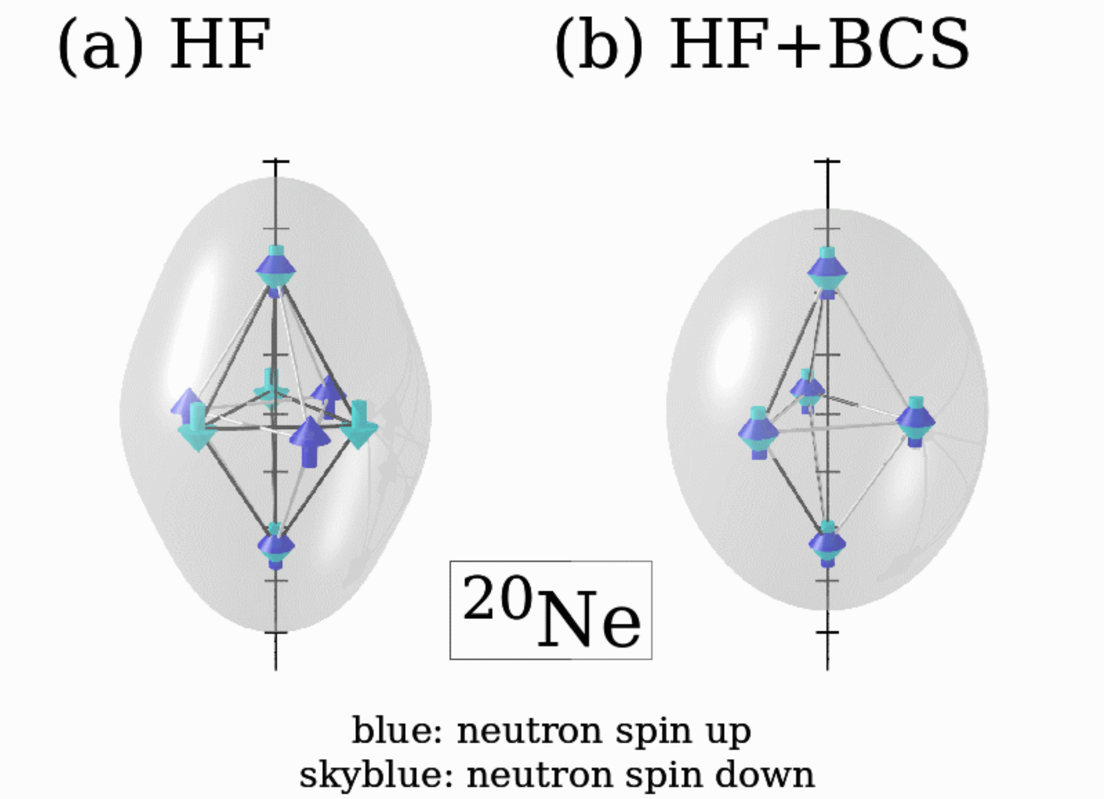

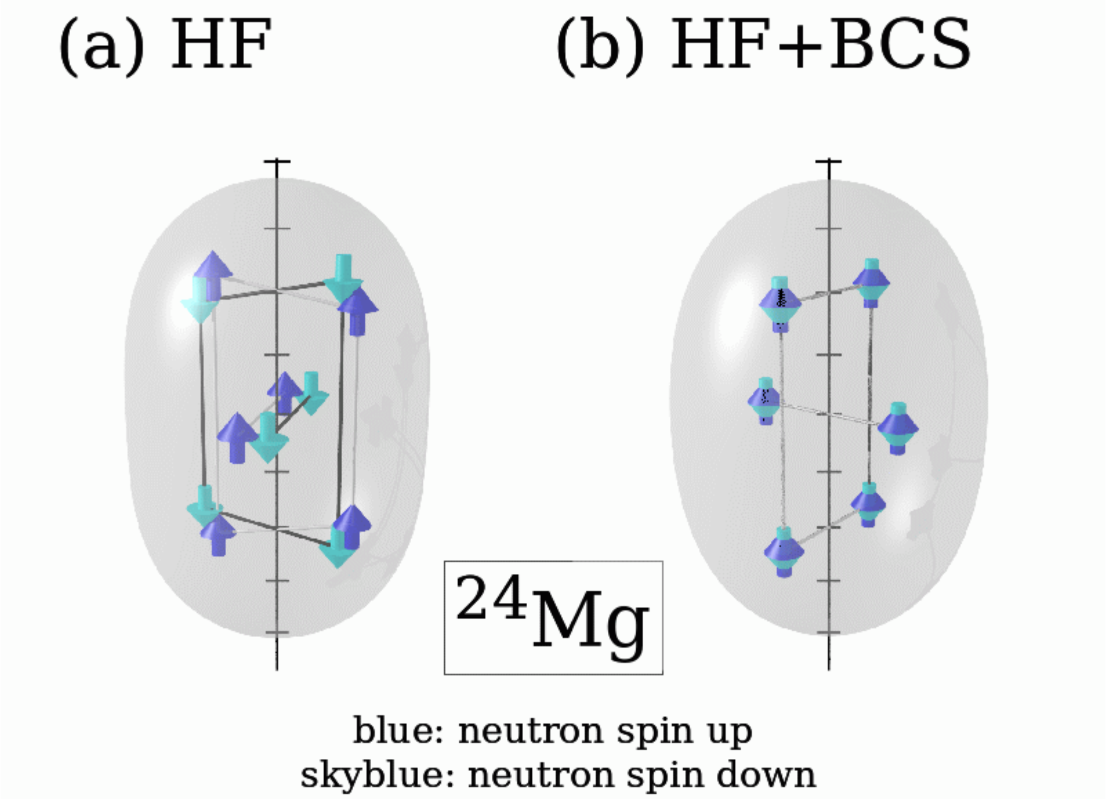

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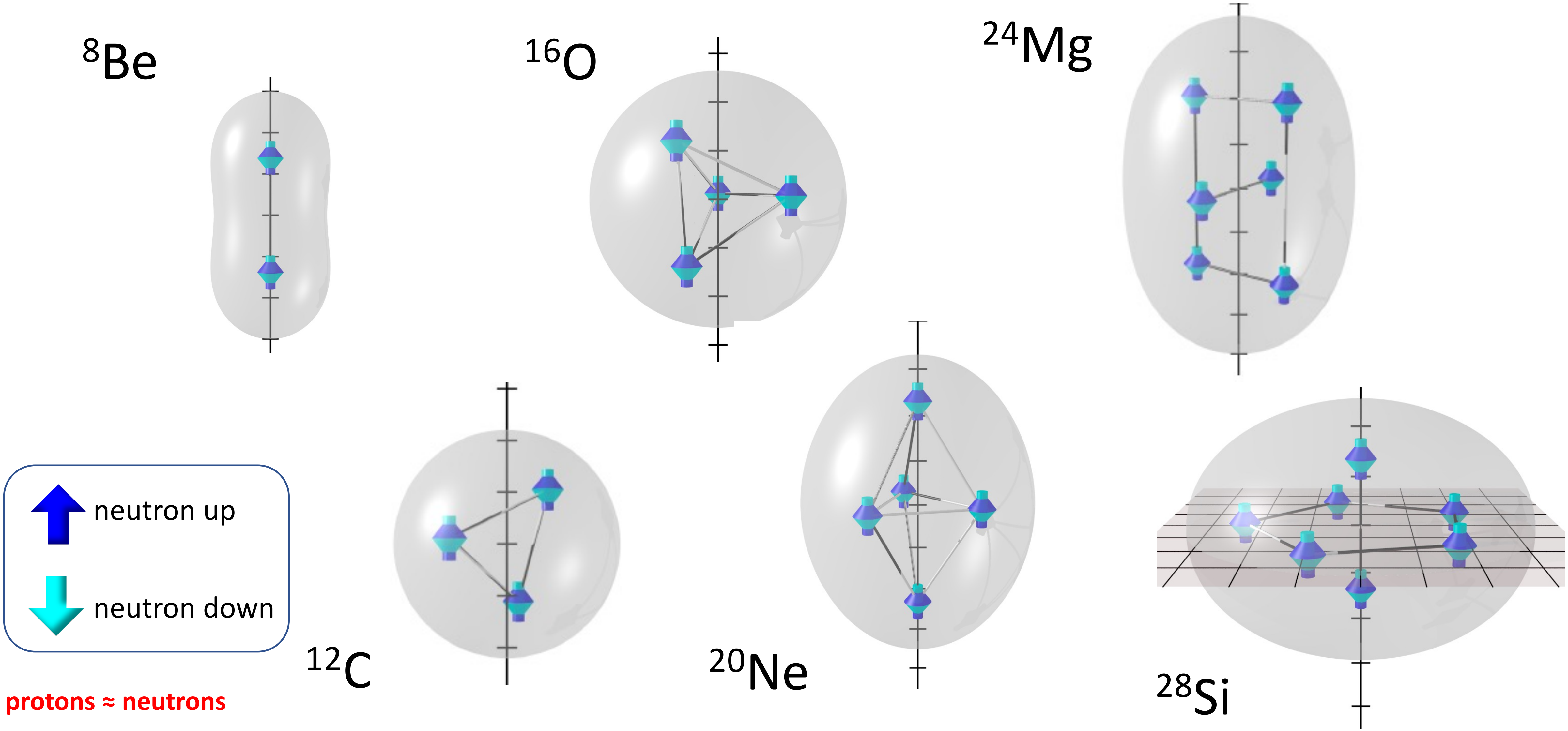
Ground states of ^{8}Be, ^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg, and ^{28}Si



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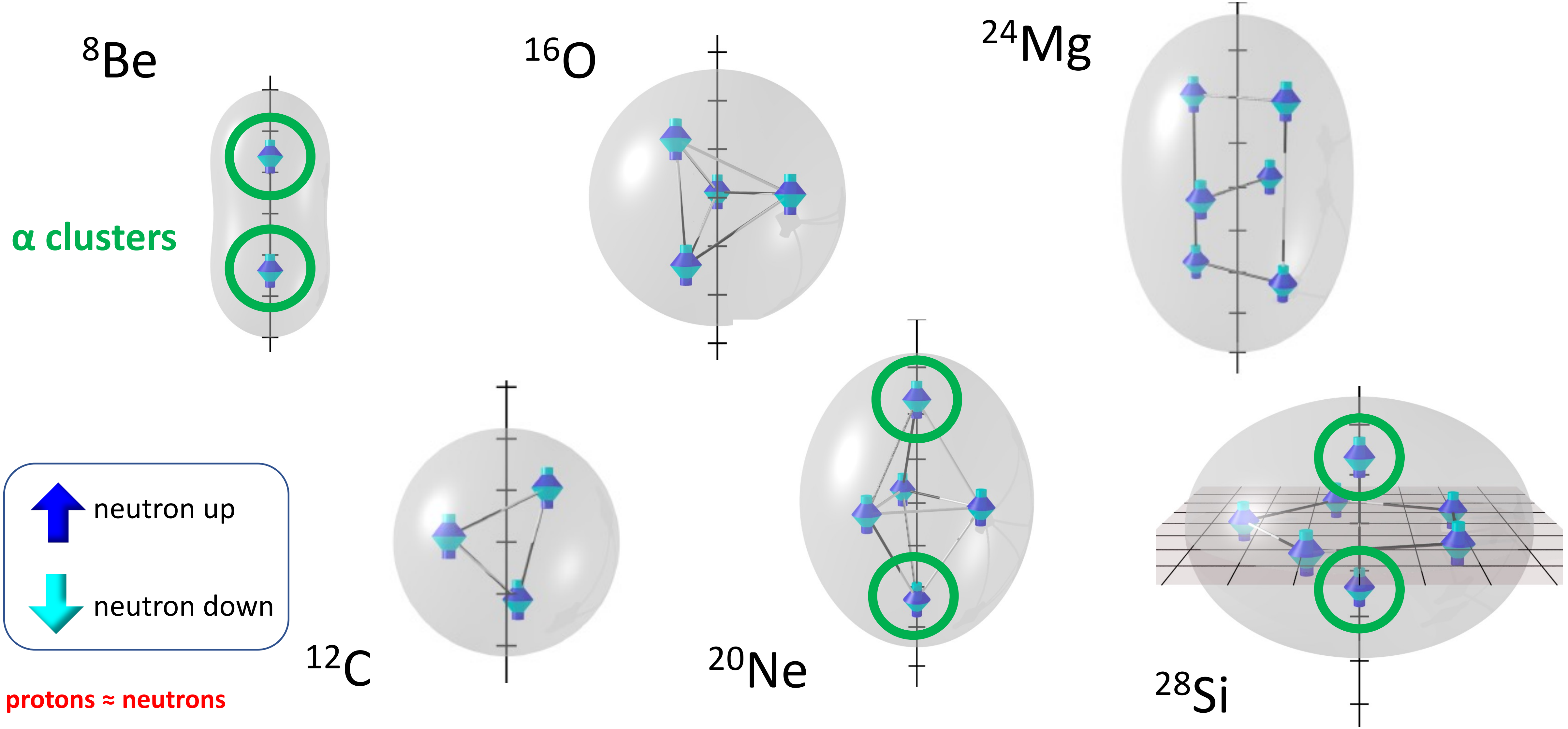


Results:
Deformed states of ^{16}O

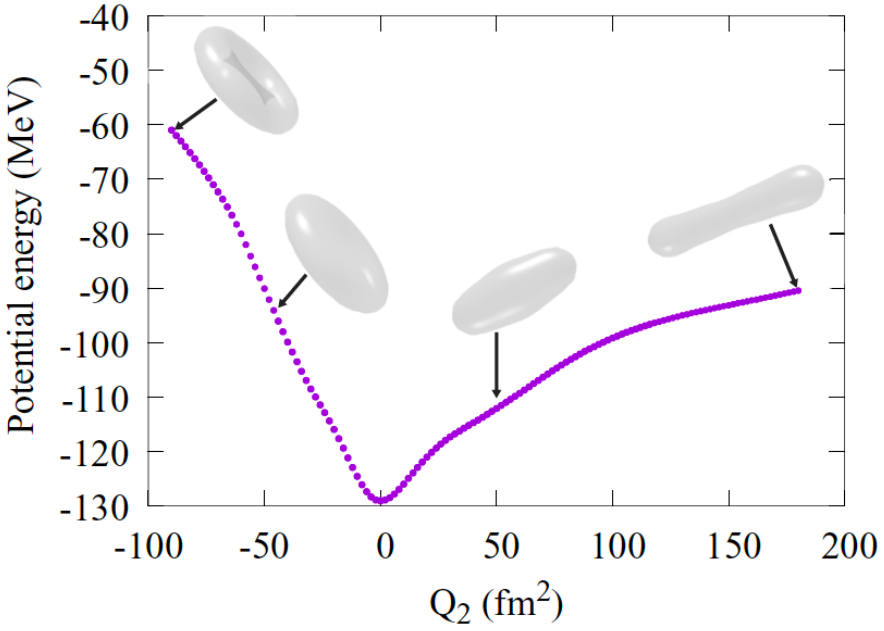


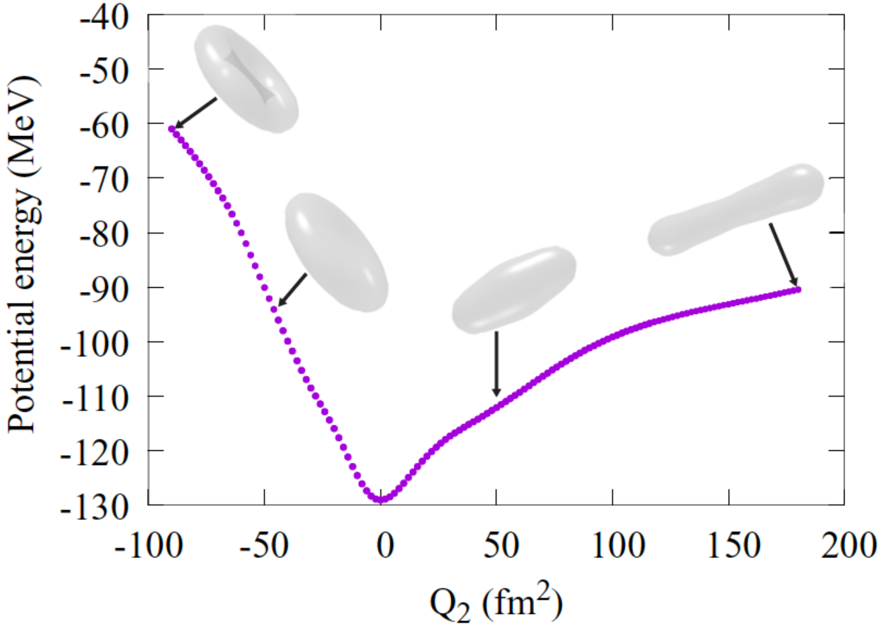
FIG. 9. The HF+BCS potential-energy curve of the ^{16}O nucleus as a function of the quadrupole moment Q_2. The HF + BCS result

← Potential energies obtained with Q_2-constrained HF + BCS

$$Q_2 = \int d^3r\, r^2 Y_{20}(\hat{\boldsymbol{r}})\rho(\boldsymbol{r})$$

Results:
Deformed states of ^{16}O

proton arrangement ≈ neutron arrangement



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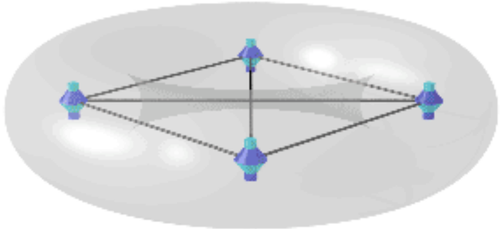

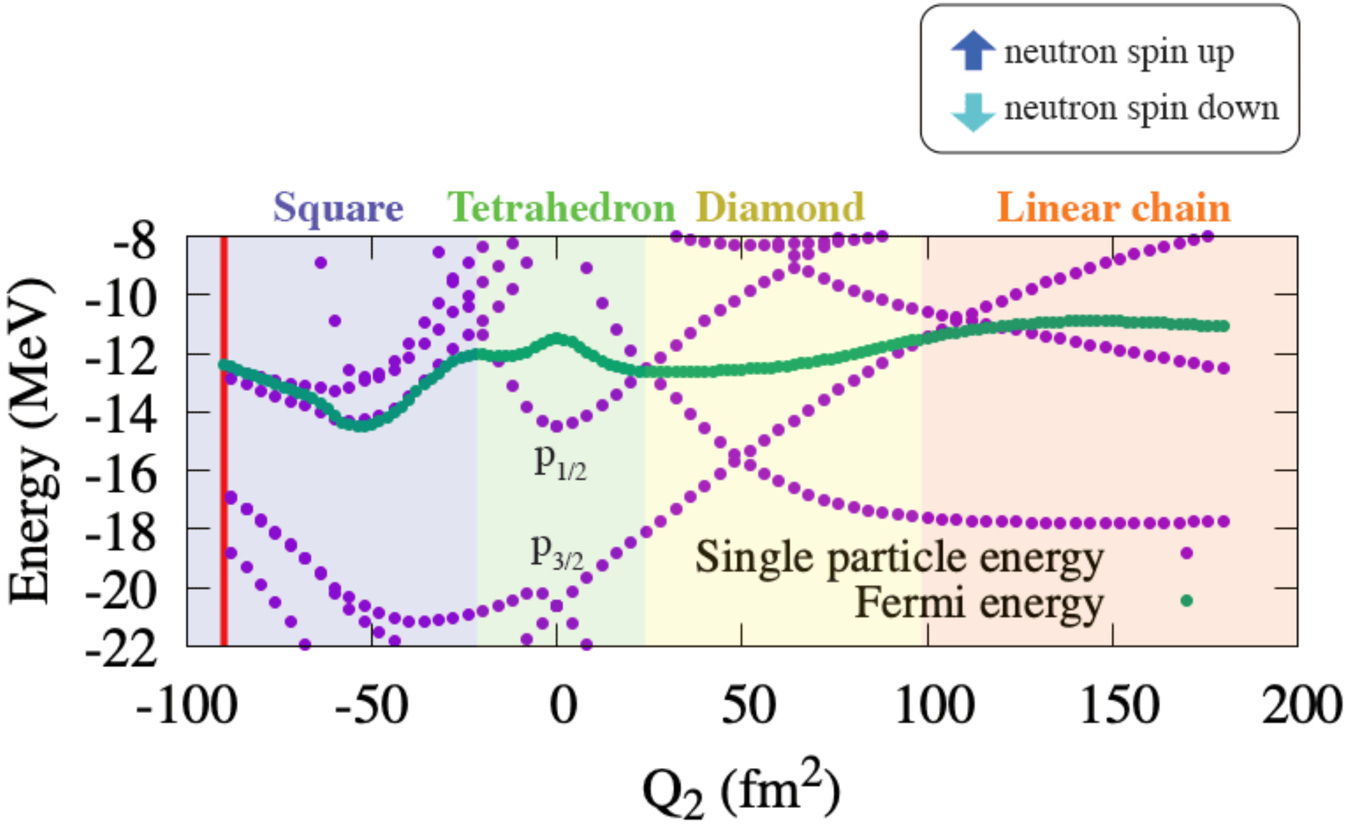

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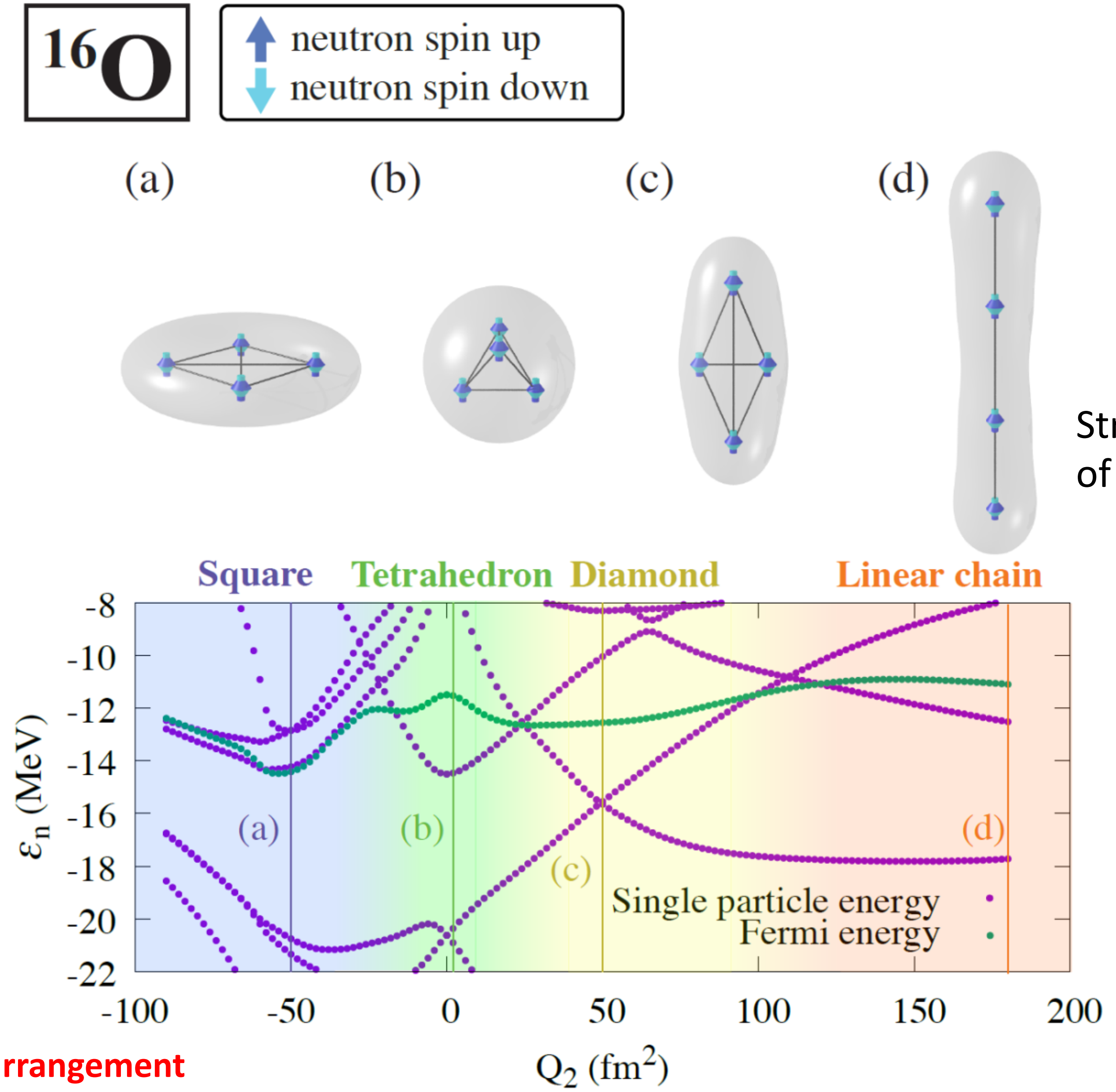

Structure changes at alternations of the Fermi level

proton arrangement ≈ neutron arrangement

Summary and perspectives

- **$|\psi|^2$-maximization method**
  - **✓cluster correlations in mean-field wave functions in light nuclei**
  - **✓Intuitive picture on correlations embedded in many-body state**
  - **✓New viewpoint to a nuclear many-body wave function**

Summary and perspectives

- **$|\psi|^2$-maximization method**
  - ✓ **cluster correlations in mean-field wave functions in light nuclei**
  - ✓ **Intuitive picture on correlations embedded in many-body state:**
    New viewpoint to a nuclear many-body wave function

- Global behaviors of $|\psi|^2$ with Markov-chain Monte-Carlo sampling?
  - ✓ fluctuation around the maximum
  - ✓ local maxima
- More correlated states
  - n-p mixing (explicit n-p correlation)
    - ✓ (semi-)magic core/cluster appears?
  - RPA, GCM (collective motion/fluctuation)
- Other phenomena
  - ✓ molecular-bond structure
  - ✓ valence neutrons in n-rich nuclei
  - ✓ nucleon motions in reactions