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# From Gogny force to shell-model calculations…

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**I. Introduction**

**How to calculate TBMEs is a big issue for shell-model calculations !**

**Realistic vs empirical potentials**

**II. SM calculations based on Gogny force**

***a)*** ***sd*-shell, no *NNN* force, modify Gogny parameters, calculate spectra…**

**b) With *NNN*, but use existing MF Gogny parameters, calculate spectra…**

**All results are preliminary!**

**III. From realistic interaction to HF-type calculations with higher order corrections "Many-Body Perturbation Theory (MBPT)"**

***ab-initio*, but our calculations are preliminary yet.**

**IV. Summary**

# I. Introduction (our motivations)

**From realistic nuclear forces:**

**Nijmegen; Bonn; Argonne; JISP;**

**Chiral perturbation theory (ChPT, Chiral EFT), e.g., $N^2LO$, $N^3LO$…**

**others**

**1) Renormalization from bare to effective form**

**G- matrix, SRG, $V_{low\text{-}k}$, Okubo-Lee-Suzuki (OLS) , UCOM…**

**2) No-core shell-model calculations, but limited to light nuclei**

**3) With-core calculations, further renormalization needed to include excluded space (including core polarization), e.g., folded diagrams (Q-box)…**

**How good quantitatively?**

**From empirical TBMEs (with-core calculations)**

***p*-shell: CK…**

***sd*-shell: USD, WBP…**

***pf*-shell: KB3, GFPX…**

***sd*+*pf*-shell: SDPF-U…**

**Well quantitative, BUT too many parameters (TBMEs) needed to be determined by fitting data.**

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**From empirical potentials to calculate TBMEs ?**

- **Skyrme and Gogny, for example, have been successful in mean-field (MF) calculations.**

  **≈ 10 model parameters involved**

- **Do these potentials work well also for SM calculations?**
- **Can we use the same MF parameters for SM calculations?**

  **or need readjustment specially for SM calculations?**

- **Can we find "universal" parameters working for any mass regions, as in MF calculations?**

## Why do we choose the Gogny force?

**1) Somebodies else have tested the Skyrme force (but this is not a reason)**

**H. Sagawa *et al.*, PLB 159 (1985) 228: *sd*-shell $^{18}$O and $^{36}$Ar**

**J.M.G. Gomez *et al.*, NPA 551 (1993) 451: *p*-shell nuclei**

**Adopted existing parameters and results are sensitive to parameter used!**

**2) Compared with Skyrme, the Gogny force is finite-range,**

**which is more reasonable in physics!**

**3) Only about 5 sets of Gogny parameters existing, while more than 240**

**sets of Skyrme parameters existing.**

# Our motivations

**Search possibility to use Gogny to calculate TBMEs for with-core SM calculations of any mass regions!**

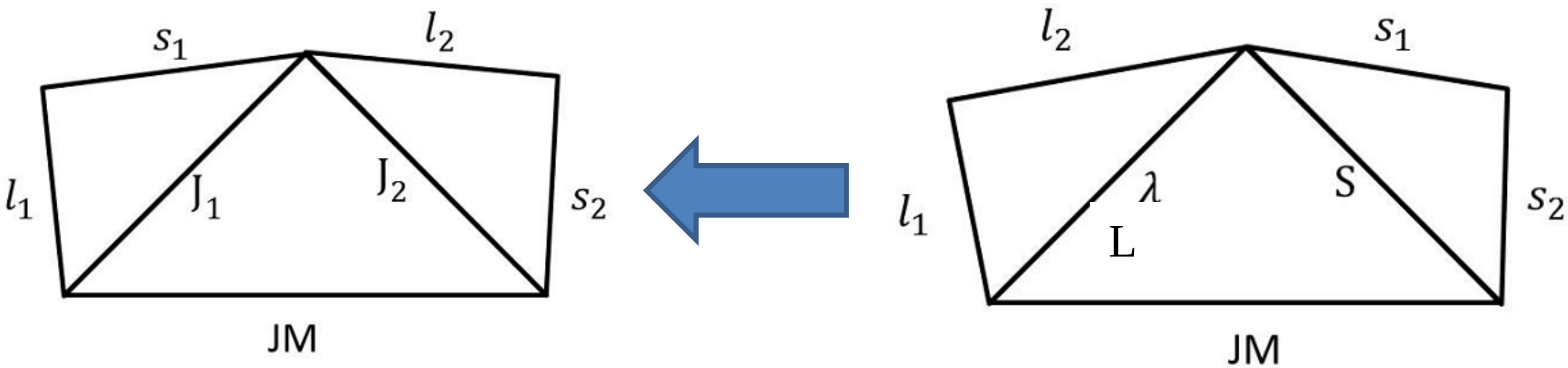
- **Empirical TBMEs, too many parameters needed to be fitted!**
- **Realistic forces, quantitatively good?**

# II. Our SM calculations based on Gogny force

$$V(1,2) = \sum_{j=1,2} e^{-\frac{(\vec{r}_1-\vec{r}_2)^2}{\mu_j^2}} (W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau)$$
$$+ t_0(1 + x_0 P_\sigma)\delta(\vec{r}_1 - \vec{r}_2)\left[\rho\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)\right]^\alpha$$
$$+ iW_{LS}\overleftarrow{\nabla}_{12}\delta(\vec{r}_1 - \vec{r}_2) \times \overrightarrow{\nabla}_{12}.(\vec{\sigma}_1 + \vec{\sigma}_2).$$

***sd* shell**

1) **We test how important the *NNN* force is**




**But in shell mode code (e.g., NushellX), use *l s* coupling**

**To calculate Gogny TBMEs, we need to seperate wavefunction into spatial and spin components.**

$$\delta(\vec{r}_1 - \vec{r}_2) \quad (\vec{\sigma}_1 + \vec{\sigma}_2)$$

# TBMEs calculations:

$$iW_{LS}\overleftarrow{\nabla}_{12}\delta(\vec{r}_1 - \vec{r}_2) \times \overrightarrow{\nabla}_{12}.(\vec{\sigma}_1 + \vec{\sigma}_2)$$

$$\{ \, |n_1 l_1 j_1(1)\rangle \otimes |n_2 l_2 j_2(2)\rangle \, \}_{JM}$$

$$= \sum_{\lambda S} \sqrt{2j_1+1}\sqrt{2j_2+1}\sqrt{2S+1}\sqrt{2\lambda+1} \begin{Bmatrix} l_1 & 1/2 & j_1 \\ l_2 & 1/2 & j_2 \\ \lambda & S & J \end{Bmatrix} \cdot \{|n_1 l_1(1), n_2 l_2(2); \lambda\mu\rangle \otimes |\chi_S\rangle\}_{JM}$$

$$= \sum_{\lambda s} \gamma^{(I)}_{\lambda s}(j_1 l_1; j_2 l_2) \; \{ \, |n_1 l_1(1), n_2 l_2(2); \lambda\mu\rangle \otimes |\chi_S\rangle \, \}_{JM} \tag{8}$$

## HO basis in the relative coordinate space (for Gaussians finite-range and NNN)

$$|nlm_l\rangle = R_{nl} \cdot Y_{lm}(\theta,\phi)$$
$$= \sqrt{\frac{2^{l-n+2}(2\nu)^{l+1.5}(2l+2n+1)!!}{\sqrt{\pi}[(2l+1)!!]^2 n!}} \cdot r^l e^{-\nu r^2}$$
$$\sum_{m=0}^{n}(-1)^m 2^m \frac{n!(2l+1)!!}{m!(n-m)!(2l+2m+1)!!}(2\nu r^2)^m \cdot Y_{lm}(\theta,\phi)$$

$$\mathrm{r} = r_1 - r_2 \qquad \nu_r = \frac{\mu\omega}{2\hbar}$$

## HO basis in the relative momentum (*k*) space (for spin-orbit coupling term)

$$|nlm_l\rangle = R_{nl} \cdot Y_{lm}(\theta,\phi)$$
$$= \sqrt{\frac{2^{l-n+2}(2\nu)^{l+1.5}(2l+2n+1)!!}{\sqrt{\pi}[(2l+1)!!]^2 n!}} \cdot k^l e^{-\nu k^2}$$
$$\sum_{m=0}^{n}(-1)^m 2^m \frac{n!(2l+1)!!}{m!(n-m)!(2l+2m+1)!!}(2\nu k^2)^m(-i)^{2n+l} \cdot Y_{lm}(\theta,\phi)$$

# TBME calculations

$$\langle n_1 l_1 j_1, n_2 l_2 j_2; J M_J T | V_{NN,12} | n_3 l_3 j_3, n_4 l_4 j_4; J M_J T \rangle$$

$$= \sum_{\lambda=J-1}^{J+1} \sum_{S=0}^{1} \sum_{nlNL} \sum_{\mu=-\lambda}^{\lambda} \sum_{M_S=-S}^{S} \sum_{m_l=-l}^{l} \sum_{M_L=-L}^{L} \sum_{\lambda'=J-1}^{J+1} \sum_{S'=0}^{1} \sum_{n'l'N'L'} \sum_{\mu'=-\lambda'}^{\lambda'} \sum_{M'_S=-S'}^{S'} \sum_{m'_l=-l'}^{l'} \sum_{M'_L=-L'}^{L'}$$

$$\frac{1-(-1)^{S+T+l}}{\sqrt{2(1+\delta_{n_1 n_2}\delta_{l_1 l_2}\delta_{j_1 j_2})}} \frac{1-(-1)^{S+T+l'}}{\sqrt{2(1+\delta_{n_3 n_4}\delta_{l_3 l_4}\delta_{j_3 j_4})}}$$

$$\sqrt{2j_1+1}\sqrt{2j_2+1}\sqrt{2S+1}\sqrt{2\lambda+1}\sqrt{2j_3+1}\sqrt{2j_4+1}\sqrt{2S'+1}\sqrt{2\lambda'+1}$$

$$\begin{Bmatrix} l_1 & 1/2 & j_1 \\ l_2 & 1/2 & j_2 \\ \lambda & S & J \end{Bmatrix} \begin{Bmatrix} l_3 & 1/2 & j_3 \\ l_4 & 1/2 & j_4 \\ \lambda' & S' & J' \end{Bmatrix} M_\lambda(nlNL; n_1 l_1 n_2 l_2) M_{\lambda'}(n'l'N'L'; n_3 l_3 n_4 l_4)$$

$$\langle \lambda \mu S M_S | J M_J \rangle \langle \lambda' \mu' S' M'_S | J M_J \rangle \langle l m_l L M_L | \lambda \mu \rangle \langle l' m'_l L' M'_L | \lambda' \mu' \rangle$$

$$\langle n l m_l | \otimes \langle \chi_{S M_S} | \otimes \langle N L M_L | \quad V_{NN,12} \quad | n' l' m'_l \rangle \otimes | \chi_{S' M'_S} \rangle \otimes | N' L' M'_L \rangle$$

$$= C \cdot \langle n l m_l | \otimes \langle \chi_{S M_S} | \otimes \langle N L M_L | \quad V_{NN,12} \quad | n' l' m'_l \rangle \otimes | \chi_{S' M'_S} \rangle \otimes | N' L' M'_L \rangle$$

$|nlm_l\rangle$ **in relative coordinate space;** $|NLM_L\rangle$ **for the center-of-mass space**

**We found: the results are not good if we take existing parameters with no *NNN* force included.**

**1. We refit Gogny parameters BUT still no *NNN* force, to test NNN.**

a) **We choose the five nuclei: $^{18}$O, $^{18}$F, $^{20}$Ne, $^{22}$Na, $^{24}$Mg, fit the lowest level at each given spin, using Monte Carlo simulated annealing algorithm.**

b) **Take USDB s.p. energies: $d_{5/2}$= -3.9257; $s_{1/2}$= -3.2079; $d_{3/2}$= 2.1117 MeV**

a) **Adopt** $\hbar\omega \approx 45A^{-1/3} - 25A^{-2/3}$ **(USDB)**

# Preliminary fitting

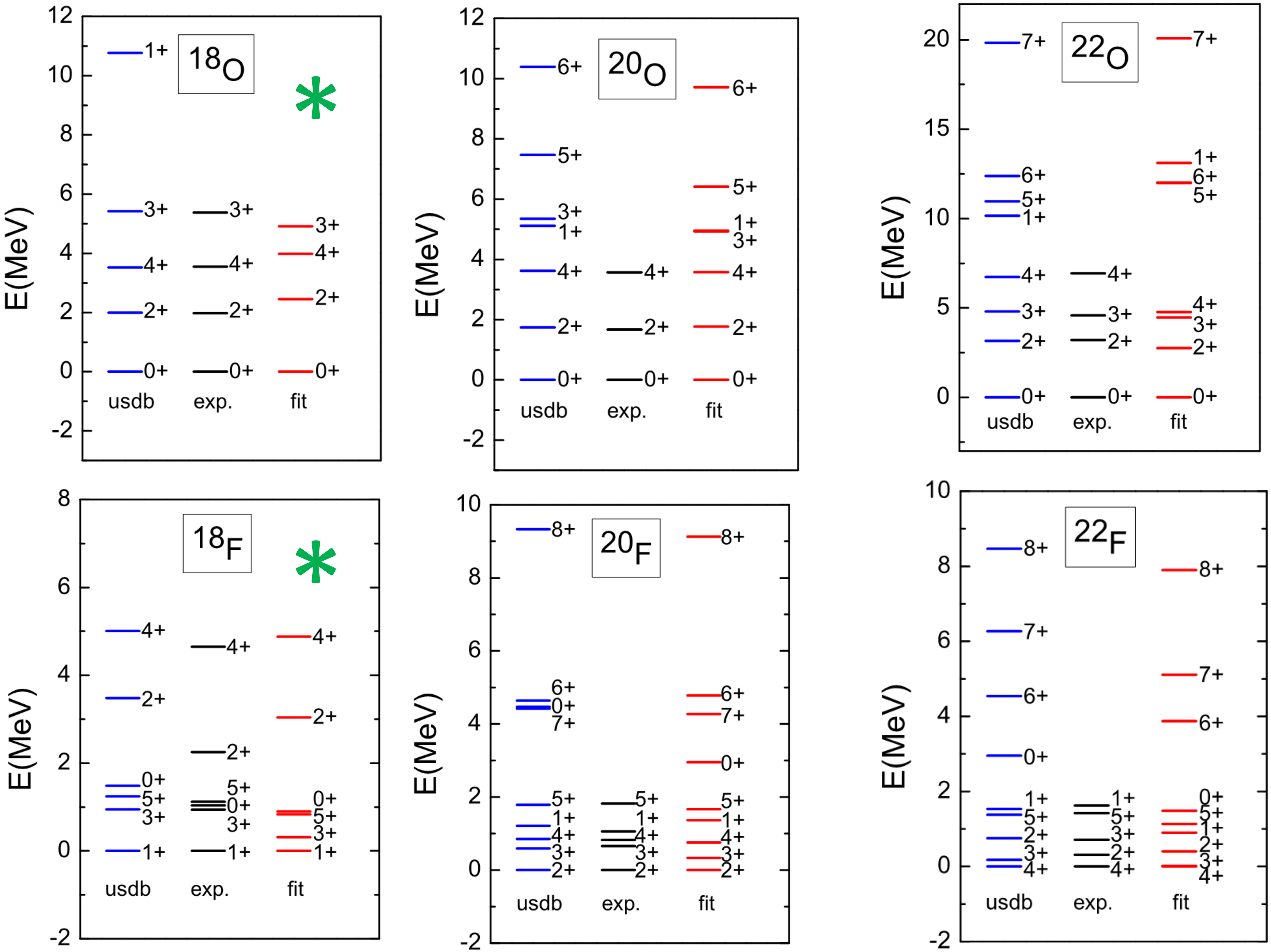
TABLE I. The parameters of different Gogny interactions.

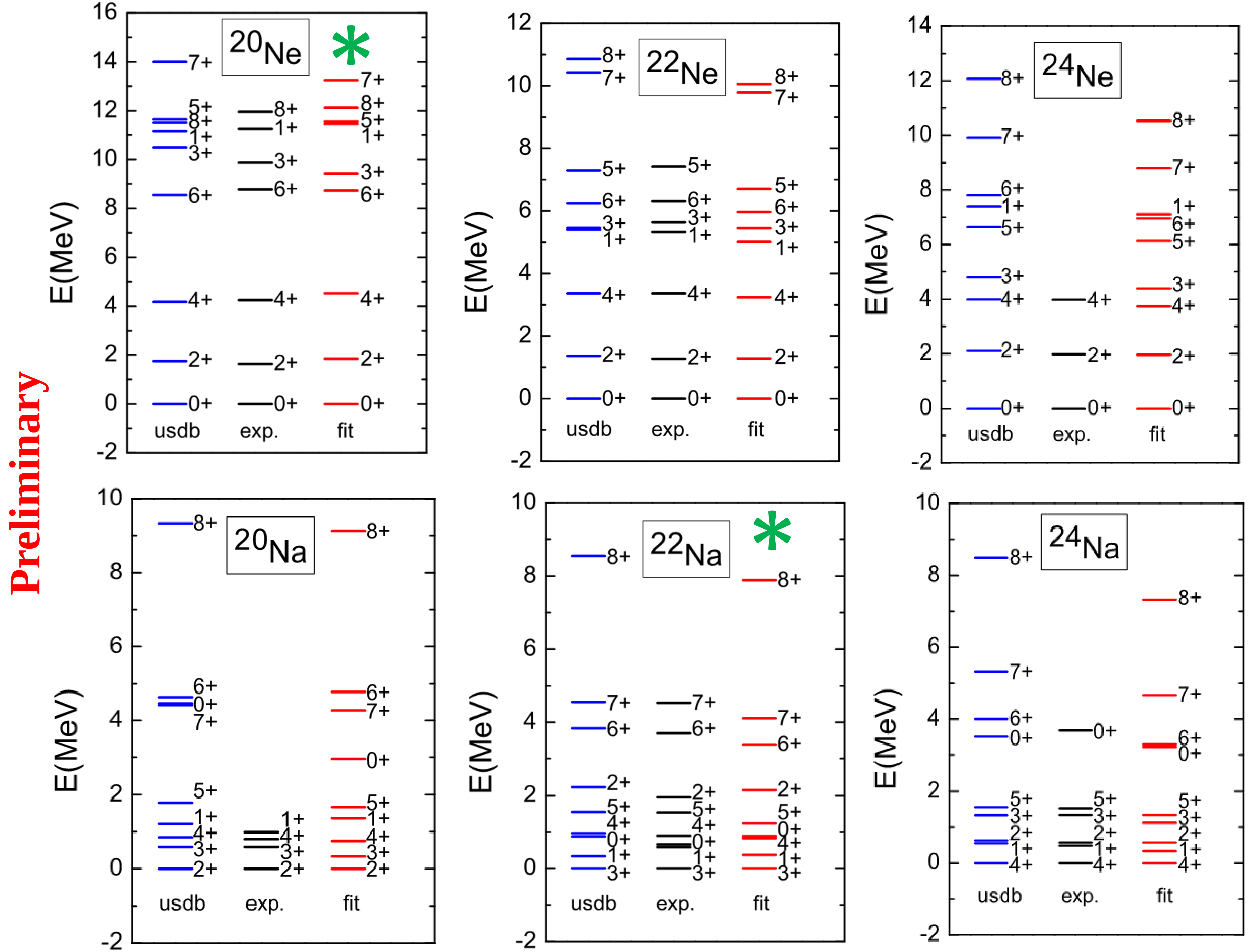
| | D1'[1] | D1[1] | D1M[2] | D1N[3] | D1S[4] | FIT |
|---|---|---|---|---|---|---|
| $\mu_1$ | 0.7000 | 0.7000 | 0.5000 | 0.8000 | 0.7000 | 0.6537 |
| $\mu_2$ | 1.2000 | 1.2000 | 1.0000 | 1.2000 | 1.2000 | 0.9837 |
| $w_1$ | −402.40 | −402.40 | −12797.57 | −2047.61 | −1720.30 | −1951.8104 |
| $w_2$ | −21.30 | −21.30 | 490.95 | 293.02 | 103.64 | 272.4556 |
| $b_1$ | −100.00 | −100.00 | 14048.85 | 1700.00 | 1300.00 | 3280.8417 |
| $b_2$ | −11.77 | −11.77 | −752.27 | −300.78 | −163.48 | −607.9833 |
| $h_1$ | −496.20 | −496.20 | −15144.43 | −2414.93 | −1813.53 | −2433.3474 |
| $h_2$ | 37.27 | 37.27 | 675.12 | 414.59 | 162.81 | 273.1813 |
| $m_1$ | −23.56 | −23.56 | 11963.89 | 1519.35 | 1397.60 | 2562.6194 |
| $m_2$ | −68.81 | −68.81 | −693.57 | −316.84 | −223.93 | −647.3149 |
| $W_0$ | 130.00 | 115.00 | 115.36 | 115.00 | −130.00 | −460.8928 |


[1] J. Dechargé and D. Gogny, Phys. Rev. C **21**, 1568 (1980).
[2] S. Goriely, S. Hilaire, M. Girod, and S. Péru, Phys. Rev. Lett. **102**, 242501 (2009).
[3] F. Chappert, M. Girod, and S. Hilaire, Physics Letters B **668**, 420 (2008).
[4] J. Berger, M. Girod, and D. Gogny, Computer Physics Communications **63**, 365 (1991).


**11 Gogny parameters fitted, while in USDB: 63 TBMEs fitted**

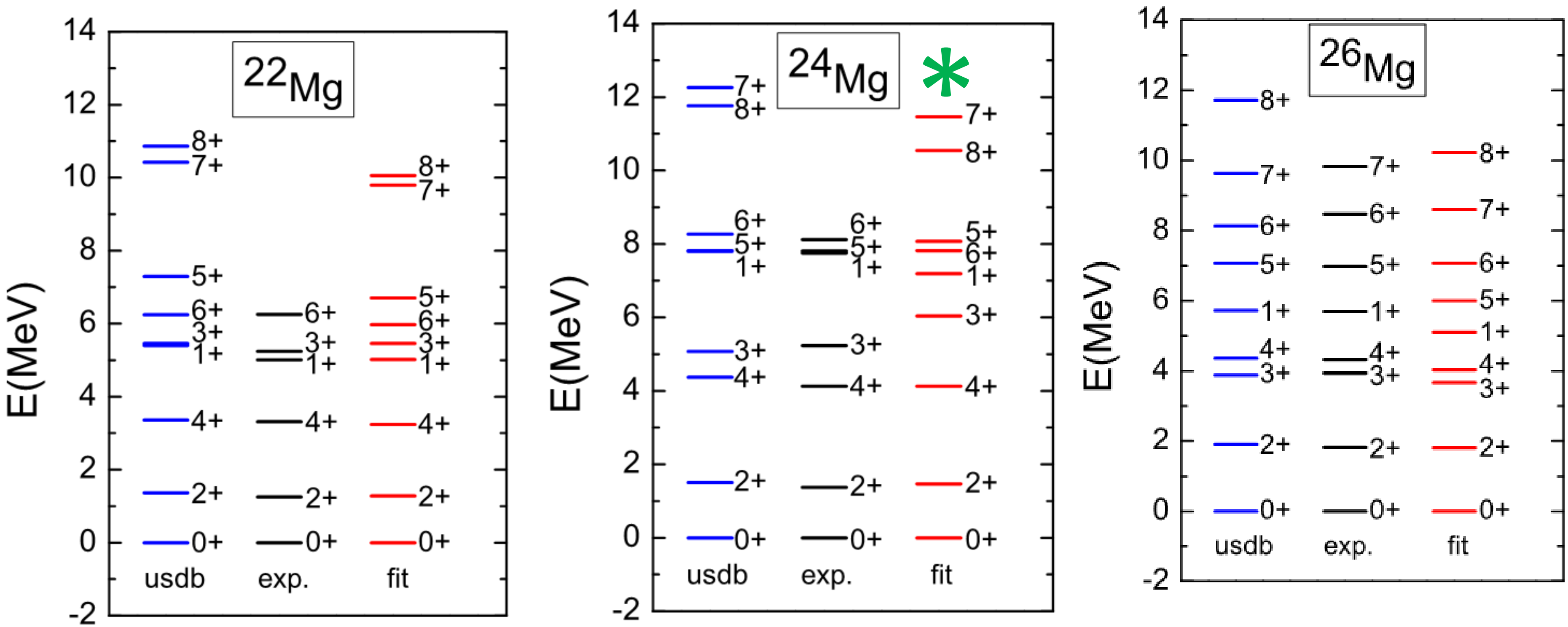
# Preliminary





Preliminary
20Ne
22Ne
24Ne
20Na
22Na
24Na
E(MeV)
usdb
exp.
fit

# Preliminary




**Indication:** **one may obtain reasonable results with no *NNN*, BUT one has to refit the Gogny parameters.**

**2) *NNN* force included, BUT no parameter modified, i.e., take existing Gogny parameters.**

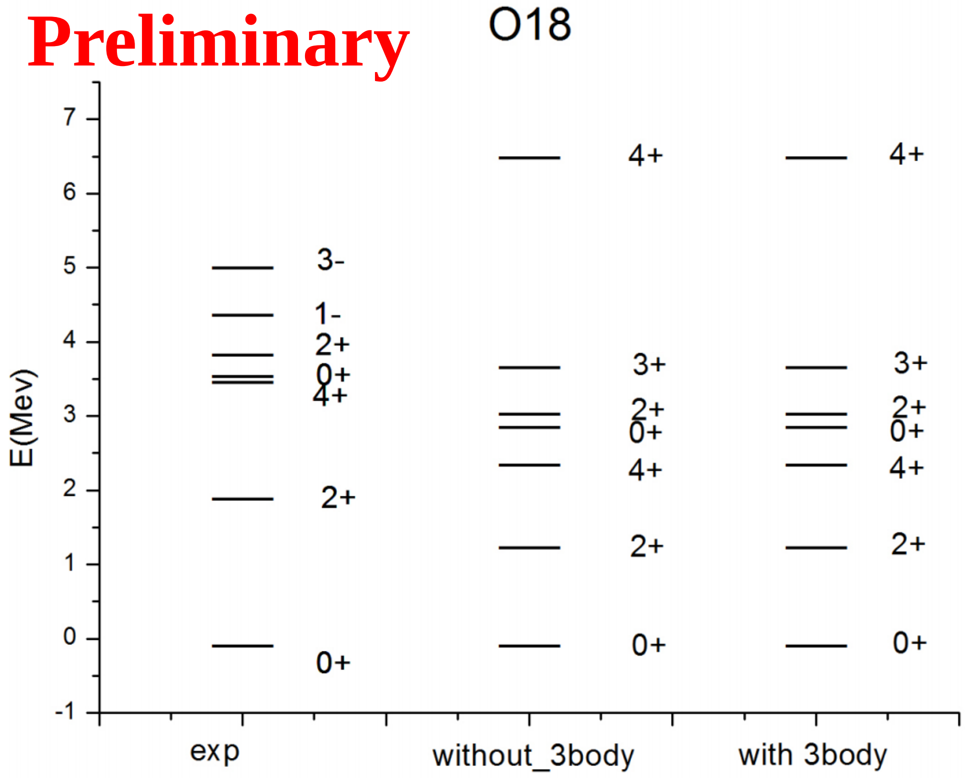
$$t_0(1+x_0P_\sigma)\delta(\vec{r}_1-\vec{r}_2)\left[\rho\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)\right]^\alpha$$

**The density is calculated using HO basis wavefunctions, which is mass-dependent.**

**In existing Gogny parameters: $\chi_0$=1 and $\alpha$=1/3**

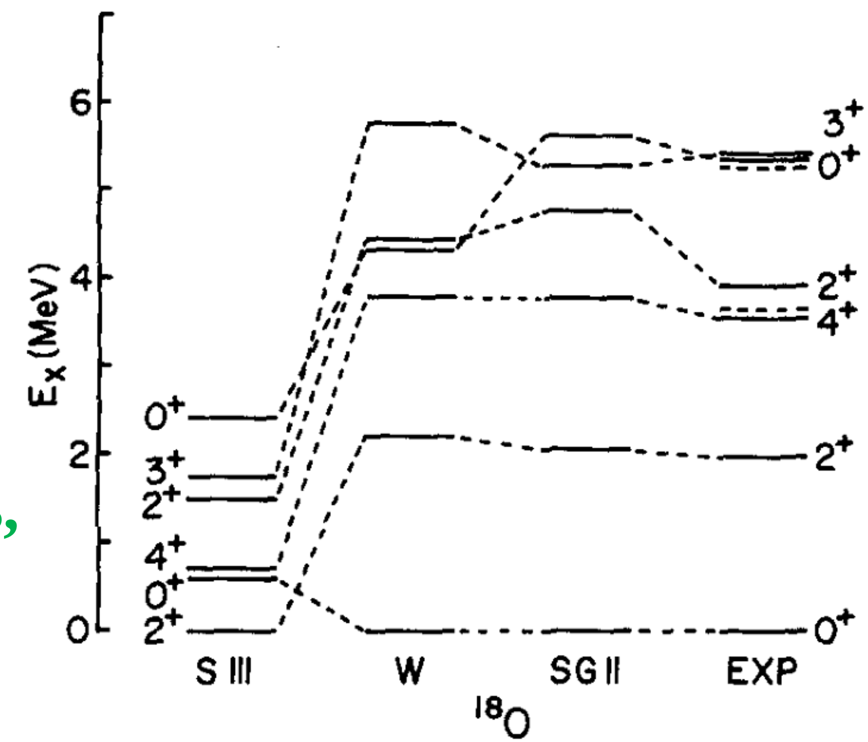
**We take D1S Gogny: for *sd*-shell**

**Preliminary**

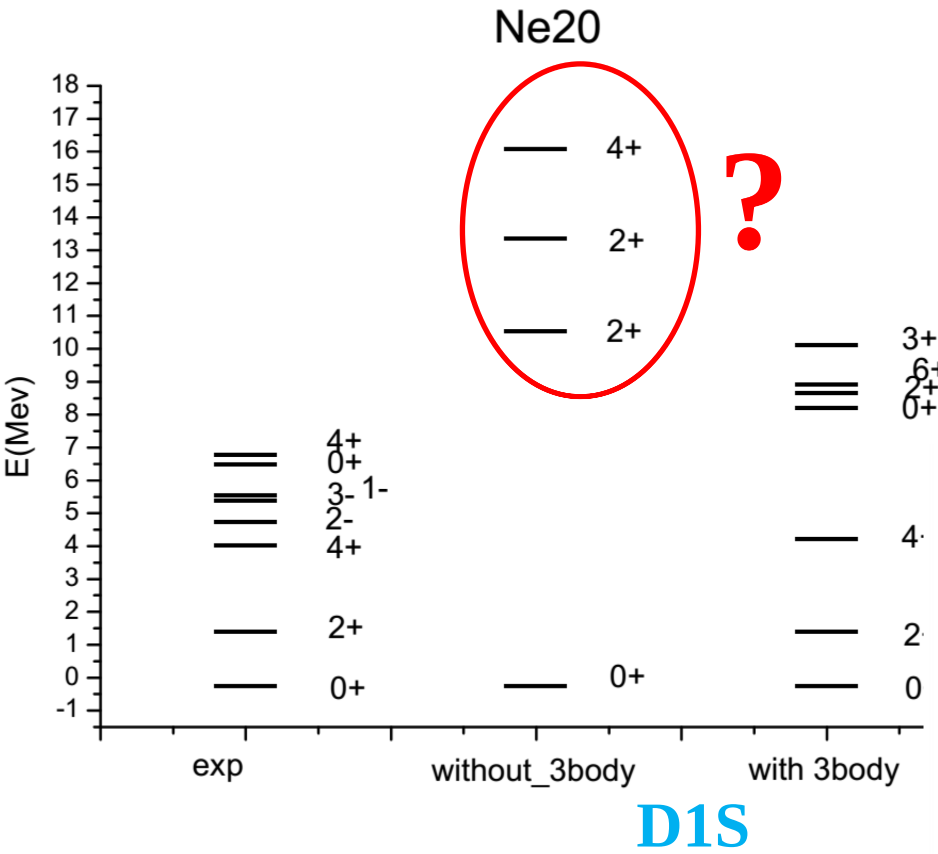


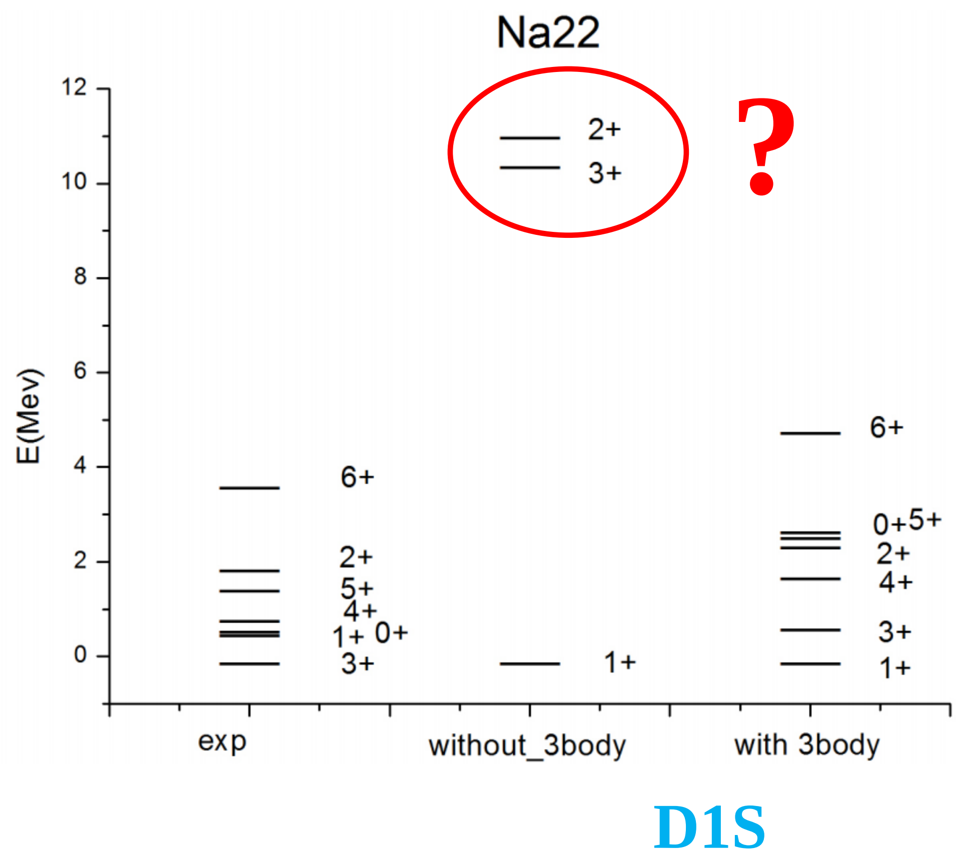

**D1S**

**For $^{18}$O, only two valence neutrons, hence no *NNN***




H. Sagawa *et al.*, PLB 159 (1985) 228

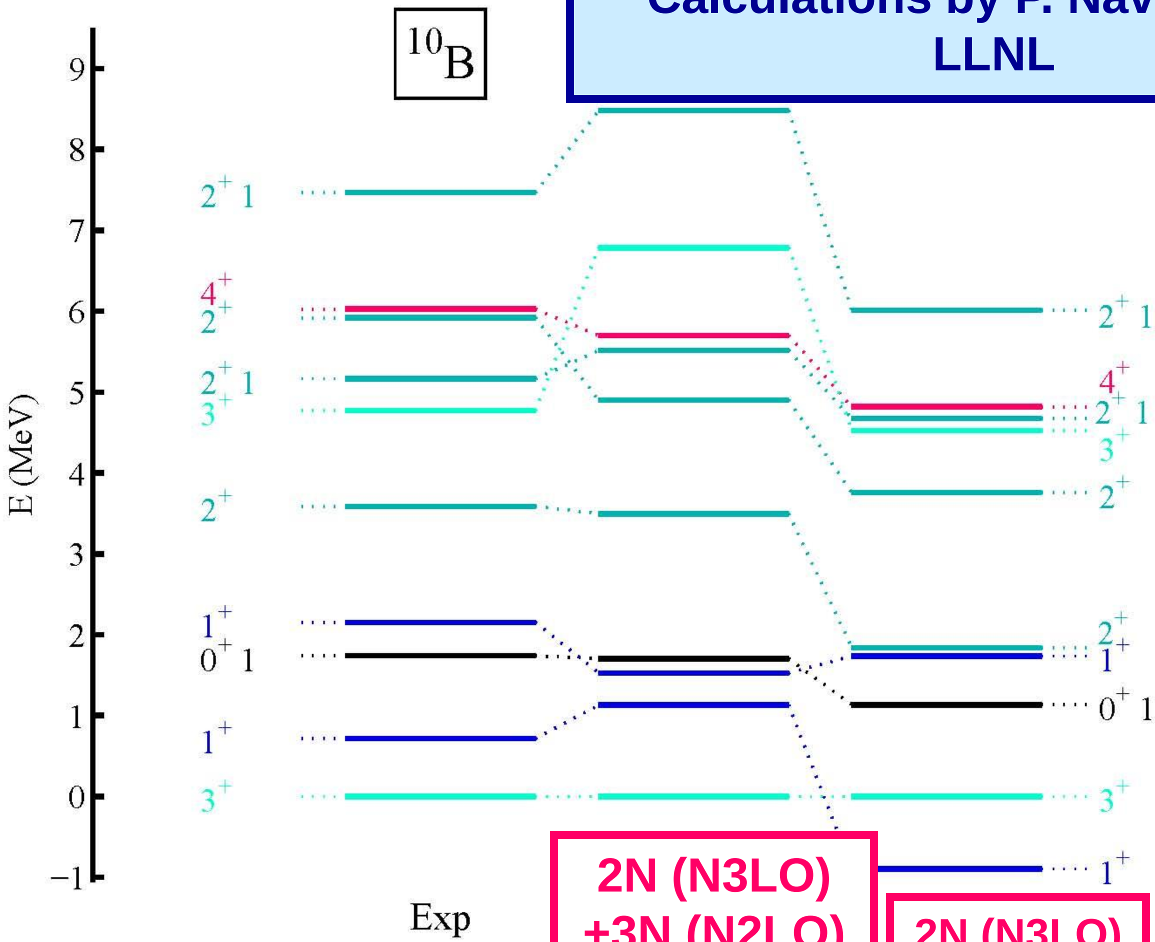



***NNN*** **has to be included for SM calculations if one wants to use the existing Gogny parameters which were determined in MF calculations!**

# Calculating the properties of light nuclei using chiral 2N and 3N forces

**“No-Core Shell Model “ Calculations by P. Navratil et al., LLNL**




**2N (N3LO) +3N (N2LO) forces**

**2N (N3LO) force only**

Nuclear NF from EFT (CNSSS13)

**From R. Machleidt**

# III. Realistic force for HF-type calculations with higher-order corrections using Many-Body Perturbation Theory (MBPT)

**Renormalization of realistic nuclear force**

**G- matrix, SRG, $V_{low\text{-}k}$, OLS, UCOM**

**M.A. Hasan, J.P. Vary, P. Navratil (2004), PRC 69, 034332**

**CD-Bonn, OLS: "HF + MBPT", corrections to 2nd order**

TABLE I. Experimental and calculated observables for the ground state of $^4$He with an $N_{max}$=10 effective Hamiltonian based on the 1996 CD-Bonn [25] and using $\hbar\Omega$=22 MeV. Experimental and calculated ground state energy (in MeV) and rms radii (in fm). The (negative) correction for spurious center-of-mass motion [Δ spur(c.m.)] is described in the text. For the experimental rms radius, we take the measured charge radius and correct for the contribution of the proton charge rms radius (0.8 fm).

| Observable | Experiment | SHF<br>Δ SHF<br>Δ spur(c.m.) | SHF+ΔSHF<br>+Δ spur(c.m.) | NCSM |
|---|---|---|---|---|
| $E_{g.s.}$ | −28.296 | −14.156<br>−10.835 | −24.991 | −27.913 |
| $n$-rms | | 1.584 | | 1.411 |
| $p$-rms | 1.450 | 1.590 | | 1.416 |
| rms | | 1.587<br>0.118<br>−0.145 | 1.560 | 1.413 |

TABLE IV. Experimental and calculated observables for the ground state of $^{16}$O with an $N_{max}$=6 effective Hamiltonian based on the 2000 CD-Bonn [26] and using $\hbar\Omega$=15 MeV. Experimental and calculated ground state energy (in MeV) and rms radii (in fm). The (negative) correction for spurious center-of-mass motion [Δ spur(c.m.)] is described in the text. For the experimental rms radius, we take the measured charge radius and correct for the contribution of the proton charge rms radius (0.8 fm). SHF results are presented for four-shell-, five-shell-, and six-shell-model spaces.

| Observable<br>[Experiment] | four-shell SHF<br>Δ SHF<br>Δ spur(c.m.)<br>Total | five-shell SHF<br>Δ SHF<br>Δ spur(c.m.)<br>Total | six-shell SHF<br>Δ SHF<br>Δ spur(c.m.)<br>Total | NCSM |
|---|---|---|---|---|
| $E_{g.s.}$<br>[−127.62] | −107.46<br>−31.46<br>−138.92 | −109.83<br>−49.88<br>−159.71 | −126.00<br>−38.21<br>−164.21 | −132.87 |
| $n$-rms | 2.093 | 2.071 | 1.954 | 2.209 |
| $p$-rms<br>[2.58] | 2.101 | 2.080 | 1.968 | 2.223 |
| rms | 2.097<br>0.072<br>−0.040<br>2.129 | 2.076<br>0.112<br>−0.040<br>2.148 | 1.961<br>0.117<br>−0.042<br>2.036 | 2.216 |

**L. Coraggio *et al*. (2003) PRC 68, 034320**

$N^3LO$, $V_{low-k}$: corrections to $3^{rd}$ order

TABLE I. Comparison of the calculated binding energy per nucleon (MeV/nucleon) and rms charge radius (fm) with the experimental data for $^{16}O$ and $^{40}Ca$.

| Nucleus | | HF | HF+2nd | HF+2nd +3rd | Expt. |
|---|---|---|---|---|---|
| $^{16}O$ | | | | | |
| | $B/A$ | 3.23 | 7.22 | 7.52 | 7.98 |
| | $\langle r_c \rangle$ | 2.30 | 2.52 | 2.65 | $2.73 \pm 0.02$ |
| $^{40}Ca$ | | | | | |
| | $B/A$ | 6.19 | 9.10 | 9.19 | 8.55 |
| | $\langle r_c \rangle$ | 2.610 | 3.302 | 3.444 | $3.485 \pm 0.003$ |

# R. Roth *et al*. (2006) PRC 73, 044312

## AV18, UCOM: corrections to 3rd order for energy, 2nd order to radius

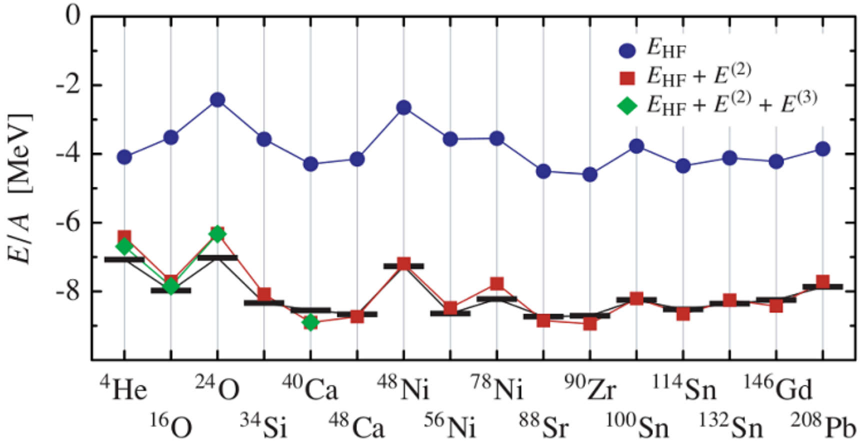



FIG. 5. (Color online) Ground-state energies for selected closed-shell nuclei in HF approximation and with added second- and third-order MBPT corrections. The correlated AV18 potential with $I_{\vartheta} = 0.09\,\text{fm}^3$ was used. The bars indicate the experimental binding energies [31].

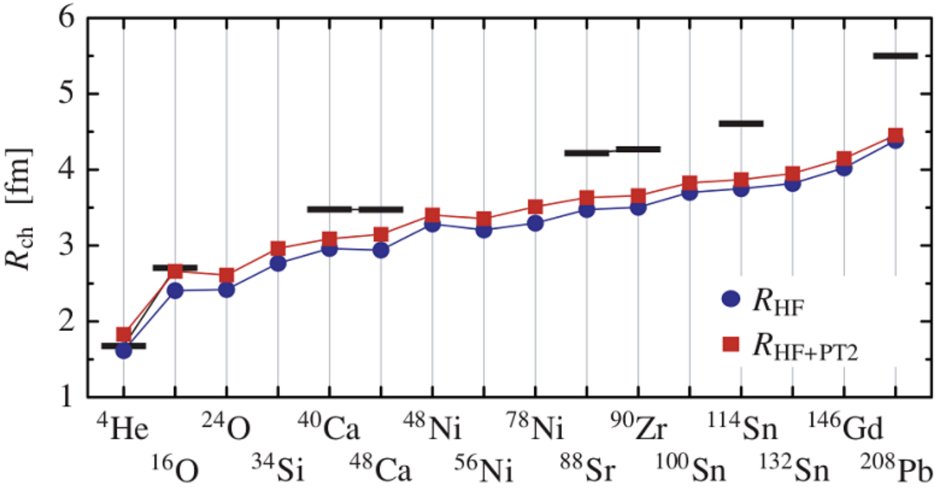



FIG. 8. (Color online) Charge radii for selected closed-shell nuclei in the HF approximation and with added second-order MBPT corrections. The correlated AV18 potential with $I_{\vartheta} = 0.09\,\text{fm}^3$ was used. The bars indicate experimental charge radii [32].

# Our calculations

1. **From realistic nuclear force ($N^3LO$, JISP16)**
2. **SRG renormalization**
3. **Spherical Hartree-Fock firstly (which leads to the 1st order term) for closed-shell nuclei**
4. **Using MBPT to make higher-order corrections: 2nd and 3rd orders to energy, and 2nd order to radius.**

$$\hat{H}_{int} = \sum_{i<j}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \sum_{i<j}^{A} V_{NN,ij}$$

We can separate the A-nucleon Hamiltonian into a zero-order part and a perturbation,

$$\hat{H} = \hat{H}_0 + (\hat{H} - \hat{H}_0) = \hat{H}_0 + \hat{V}$$

The exact solutions of the A-nucleon system are,

$$\hat{H}\Psi_n = E_n\Psi_n, \qquad n = 0, 1, 2, ...$$

The zero-order part is,

$$\hat{H}_0 \Phi_n = E_n^{(0)} \Phi_n, \qquad n = 0, 1, 2, \ldots$$

**For the ground state:**

$$\chi_0 = \Psi_0 - \Phi_0$$

$$\Delta E = E_0 - E_0^{(0)}$$

**Perturbation (MBPT)**

$$\Psi_0 = \sum_{m=0}^{\infty} \left[\hat{R}_0(E_0^{(0)})(\hat{V} - \Delta E)\right]^m \Phi_0$$

$$\Delta E = \sum_{m=0}^{\infty} \langle \Phi_0 | \hat{V} \left[\hat{R}_0(E_0^{(0)})(\hat{V} - \Delta E)\right]^m | \Phi_0 \rangle$$

where $\hat{R}_0 = \sum_{i \neq 0} \frac{|\Phi_i\rangle\langle\Phi_i|}{E_0^{(0)} - E_i^{(0)}}$ is called the resolvent of $\hat{H}_0$

**Rayleigh-Schrodinger perturbation theory**

$$E_0 = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} + E_0^{(3)} + \dots$$

$$E_0^{(1)} = \langle \Phi_0 | \hat{V} | \Phi_0 \rangle$$

$$E_0^{(2)} = \langle \Phi_0 | \hat{V} \hat{R}_0 \hat{V} | \Phi_0 \rangle$$

$$E_0^{(3)} = \langle \Phi_0 | \hat{V} \hat{R}_0 (\hat{V} - \langle \Phi_0 | \hat{V} | \Phi_0 \rangle) \hat{R}_0 \hat{V} | \Phi_0 \rangle$$

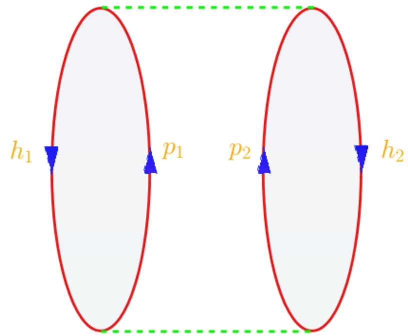
$$\Psi_0 = \Phi_0 + \Psi_0^{(1)} + \Psi_0^{(2)} + \dots$$

$$\Psi_0^{(1)} = \hat{R}_0 \hat{V} | \Phi_0 \rangle$$

$$\Psi_0^{(2)} = \hat{R}_0 (\hat{V} - E_0^{(1)}) \hat{R}_0 \hat{V} | \Phi_0 \rangle$$

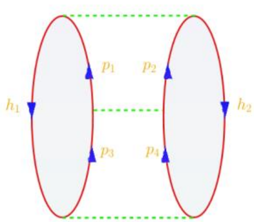
# Anti-Symmetrized Goldstone (ASG) diagram expansion:

## $\mathbf{E^{(2)}}$

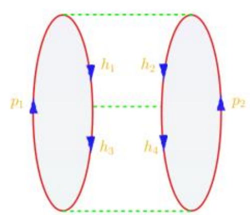



$$\frac{1}{4} \sum_{h_1, h_2 < \varepsilon_F} \sum_{p_1, p_2 > \varepsilon_F} \frac{|\langle p_1 p_2 | \hat{\mathrm{H}} | h_1 h_2 \rangle|^2}{\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_1} - \varepsilon_{p_2}}$$

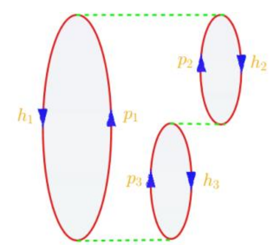
## $\mathbf{E^{(3)}}$




$$\frac{1}{8} \sum_{h_1, h_2 < \varepsilon_F} \sum_{p_1, p_2, p_3, p_4 > \varepsilon_F} \frac{\langle p_3 p_4 | \hat{\mathrm{H}} | h_1 h_2 \rangle \langle p_1 p_2 | \hat{\mathrm{H}} | p_3 p_4 \rangle \langle h_1 h_2 | \hat{\mathrm{H}} | p_1 p_2 \rangle}{(\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_1} - \varepsilon_{p_2})(\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_3} - \varepsilon_{p_4})}$$



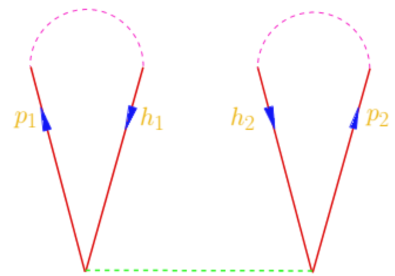

$$\frac{1}{8} \sum_{h_1, h_2, h_3, h_4 < \varepsilon_F} \sum_{p_1, p_2 > \varepsilon_F} \frac{\langle p_1 p_2 | \hat{\mathrm{H}} | h_3 h_4 \rangle \langle h_3 h_4 | \hat{\mathrm{H}} | h_1 h_2 \rangle \langle h_1 h_2 | \hat{\mathrm{H}} | p_1 p_2 \rangle}{(\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_1} - \varepsilon_{p_2})(\varepsilon_{h_3} + \varepsilon_{h_4} - \varepsilon_{p_1} - \varepsilon_{p_2})}$$



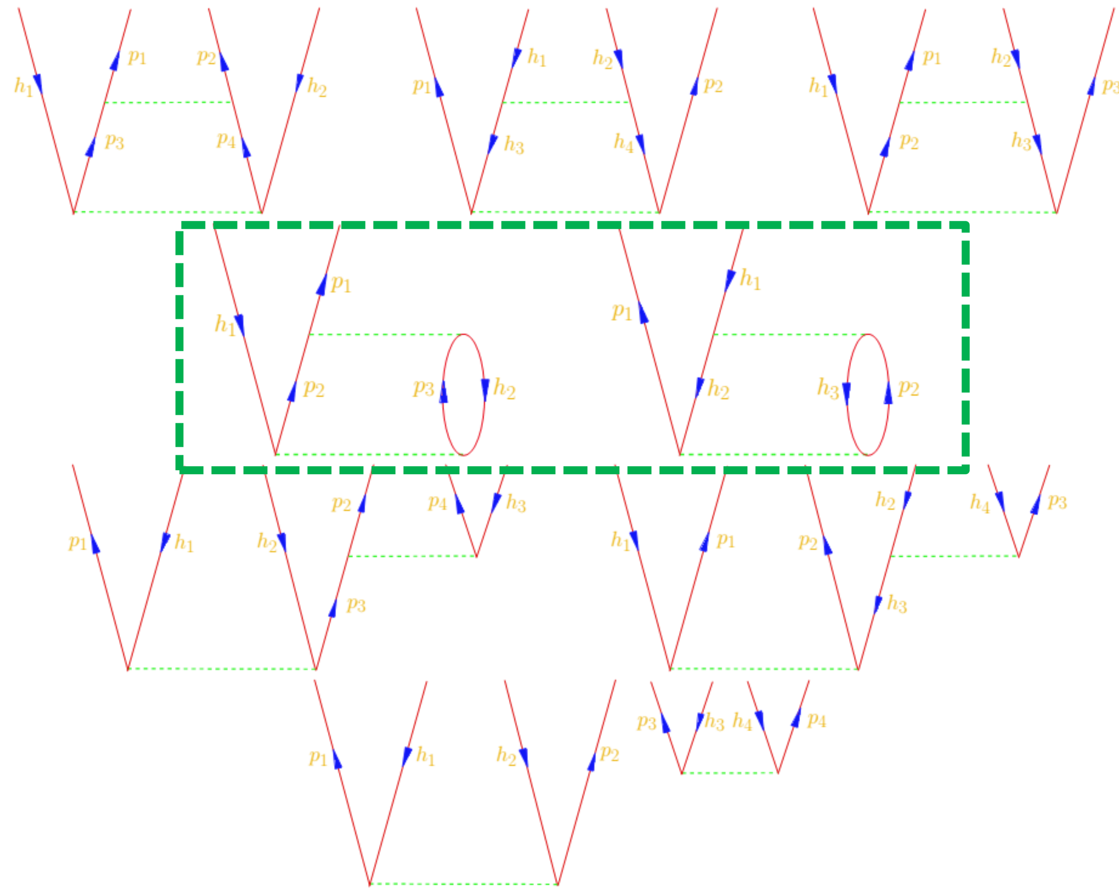

$$\sum_{h_1, h_2, h_3 < \varepsilon_F} \sum_{p_1, p_2, p_3 > \varepsilon_F} \frac{\langle p_1 p_3 | \hat{\mathrm{H}} | h_1 h_3 \rangle \langle h_3 p_2 | \hat{\mathrm{H}} | p_3 h_2 \rangle \langle h_1 h_2 | \hat{\mathrm{H}} | p_1 p_2 \rangle}{(\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_1} - \varepsilon_{p_2})(\varepsilon_{h_1} + \varepsilon_{h_3} - \varepsilon_{p_1} - \varepsilon_{p_3})}$$

# ASG diagrams for wave functions

$\psi^{(1)}$




$\psi^{(2)}$



# Density

$$\rho(\vec{r}) = \sum_{k=1}^{A} \delta^3(\vec{r} - \vec{r}_k) = \sum_{k=1}^{A} \frac{\delta(r - r_k)}{r^2} \sum_{lm} Y^*_{lm}(\hat{r}_k) Y_{lm}(\hat{r})$$

For spherically symmetric system(K=0), we can get a more simple form,

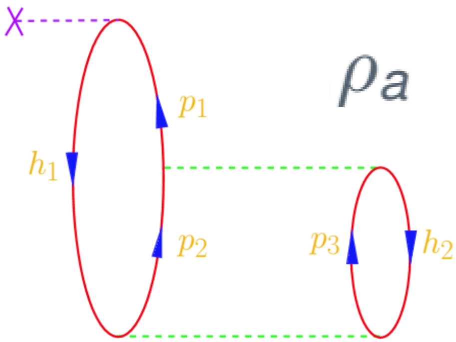
$$\rho(\vec{r}) = \sum_{n_1, n_2} \sum_{l, j, m_j} \left[ \frac{R_{n_1, l}(r) R_{n_2, l}(r)}{4\pi} \right] a^\dagger_{n_1, l, j, m_j} a_{n_2, l, j, m_j}$$

**For ground state, the 2nd order to density includes only the 4th and 5th ASG diagrams of the 2nd-order wavefunction, others belong to higher order corrections, i.e.,**

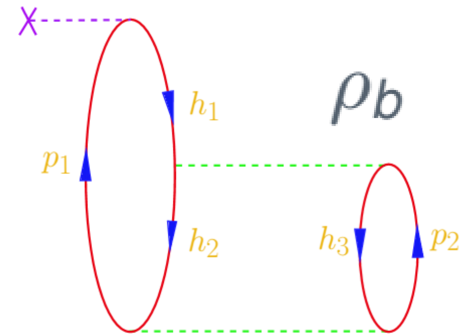
$$\Psi'_0 = \Phi_0 + \Psi_0^{(1)} + \Psi_{0,4}^{(2)} + \Psi_{0,5}^{(2)}$$

$$\rho(\vec{r}) = \langle\Phi_0|\rho(\vec{r})|\Phi_0\rangle + \langle\Phi_0|\rho(\vec{r})|\Phi_0\rangle\langle\Psi_0^{(1)}|\Psi_0^{(1)}\rangle + \underline{2\rho_a + 2\rho_b + \rho_{c1} + \rho_{c2}} + \ldots$$

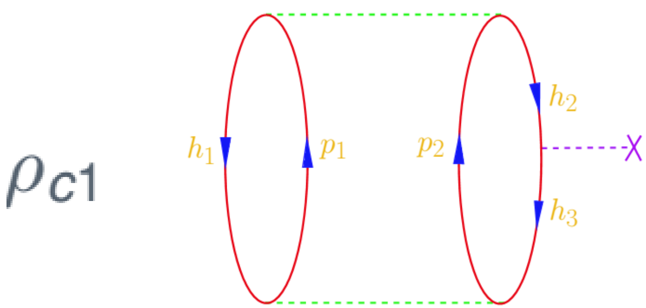
**2nd order terms**



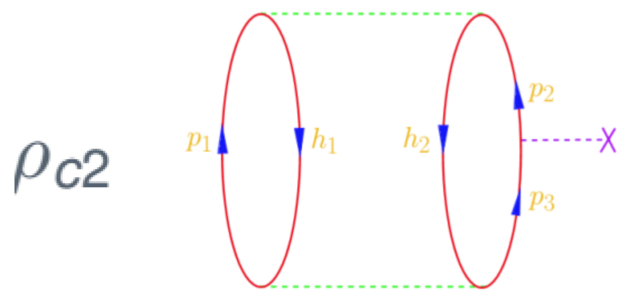

$$\frac{1}{2}\sum_{h_1,h_2<\varepsilon_F}\sum_{p_1,p_2,p_3>\varepsilon_F}\frac{\langle h_1h_2|\hat{H}|p_2p_3\rangle\langle p_2p_3|\hat{H}|p_1h_2\rangle\langle h_1|\rho|p_1\rangle}{(\varepsilon_{h_1}-\varepsilon_{p_1})(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_2}-\varepsilon_{p_3})}$$




$$-\frac{1}{2}\sum_{h_1,h_2,h_3<\varepsilon_F}\sum_{p_1,p_2>\varepsilon_F}\frac{\langle p_1p_2|\hat{H}|h_2h_3\rangle\langle h_2h_3|\hat{H}|h_1p_2\rangle\langle h_1|\rho|p_1\rangle}{(\varepsilon_{h_1}-\varepsilon_{p_1})(\varepsilon_{h_2}+\varepsilon_{h_3}-\varepsilon_{p_1}-\varepsilon_{p_2})}$$




$$-\frac{1}{2}\sum_{h_1,h_2,h_3<\varepsilon_F}\sum_{p_1,p_2>\varepsilon_F}\frac{\langle h_1h_2|\hat{H}|p_1p_2\rangle\langle p_1p_2|\hat{H}|h_1h_3\rangle\langle h_3|\rho|h_2\rangle}{(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_2})(\varepsilon_{h_1}+\varepsilon_{h_3}-\varepsilon_{p_1}-\varepsilon_{p_2})}$$




$$\frac{1}{2}\sum_{h_1,h_2<\varepsilon_F}\sum_{p_1,p_2,p_3>\varepsilon_F}\frac{\langle p_1p_3|\hat{H}|h_1h_2\rangle\langle h_1h_2|\hat{H}|p_1p_2\rangle\langle p_2|\rho|p_3\rangle}{(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_3})(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p_1}-\varepsilon_{p_2})}$$

$$\langle {r_{pp}}^2 \rangle = \frac{\int r^2 \rho_p(\vec{r}) d^3 r}{\int \rho_p(\vec{r}) d^3 r} \qquad \langle {r_{nn}}^2 \rangle = \frac{\int r^2 \rho_n(\vec{r}) d^3 r}{\int \rho_n(\vec{r}) d^3 r}$$

**The correction for the spurious center-of-mass motion**

$$r_{COM} = [r^2_{SHF} - \frac{b^2}{A}]^{1/2} \qquad b^2 = \frac{\hbar}{m\Omega}$$

$$\langle {r_{ch}}^2 \rangle = \langle {r_{pp}}^2 \rangle + {\langle R \rangle_p}^2 \qquad (\langle R \rangle_p = 0.8 fm)$$

# NCSM with $N^3LO$+SRG

**S.K. Bogner *et al.*, arXiv0708.3754v2 (2007)**

Both calculations without NNN

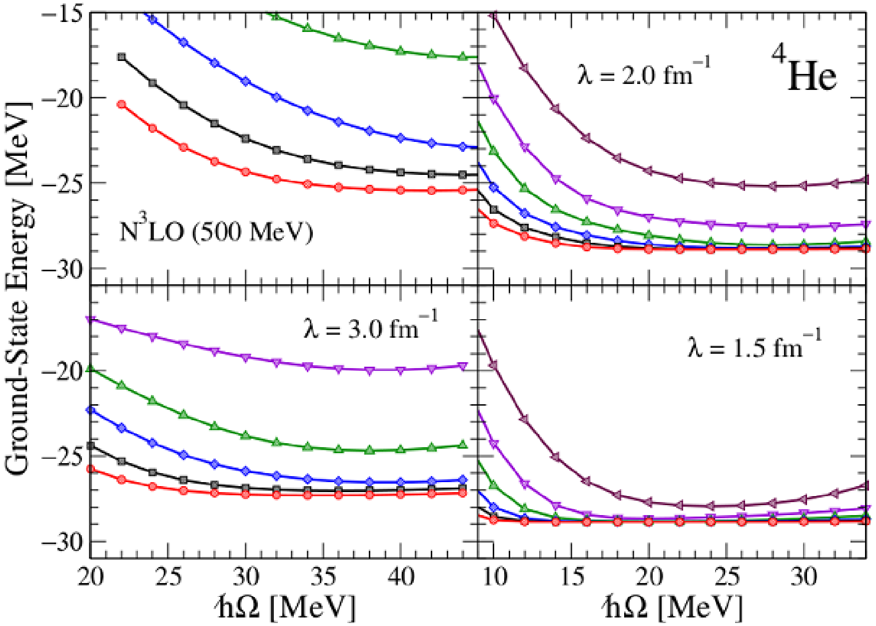
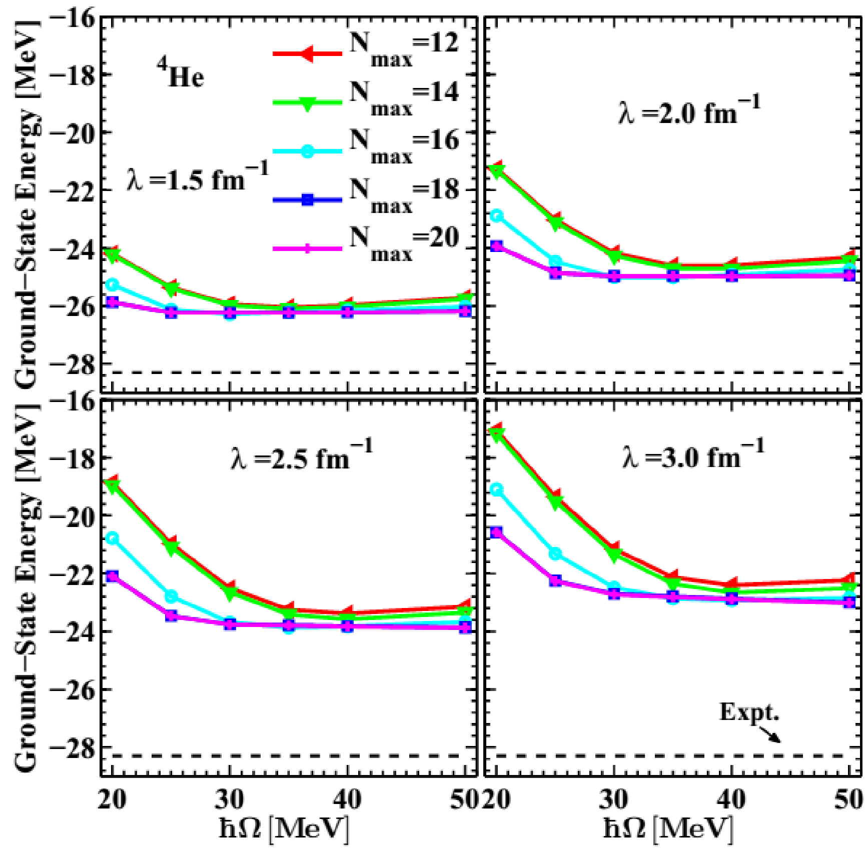



Fig. 3. Ground-state energy of $^4$He as a function of $\hbar\Omega$ at four different values of $\lambda$ ($\infty$, 3, 2, 1.5 $\mathrm{fm}^{-1}$). The initial potential is the 500 MeV $N^3LO$ NN-only potential from Ref. [13]. The legend from Fig. 1 applies here.

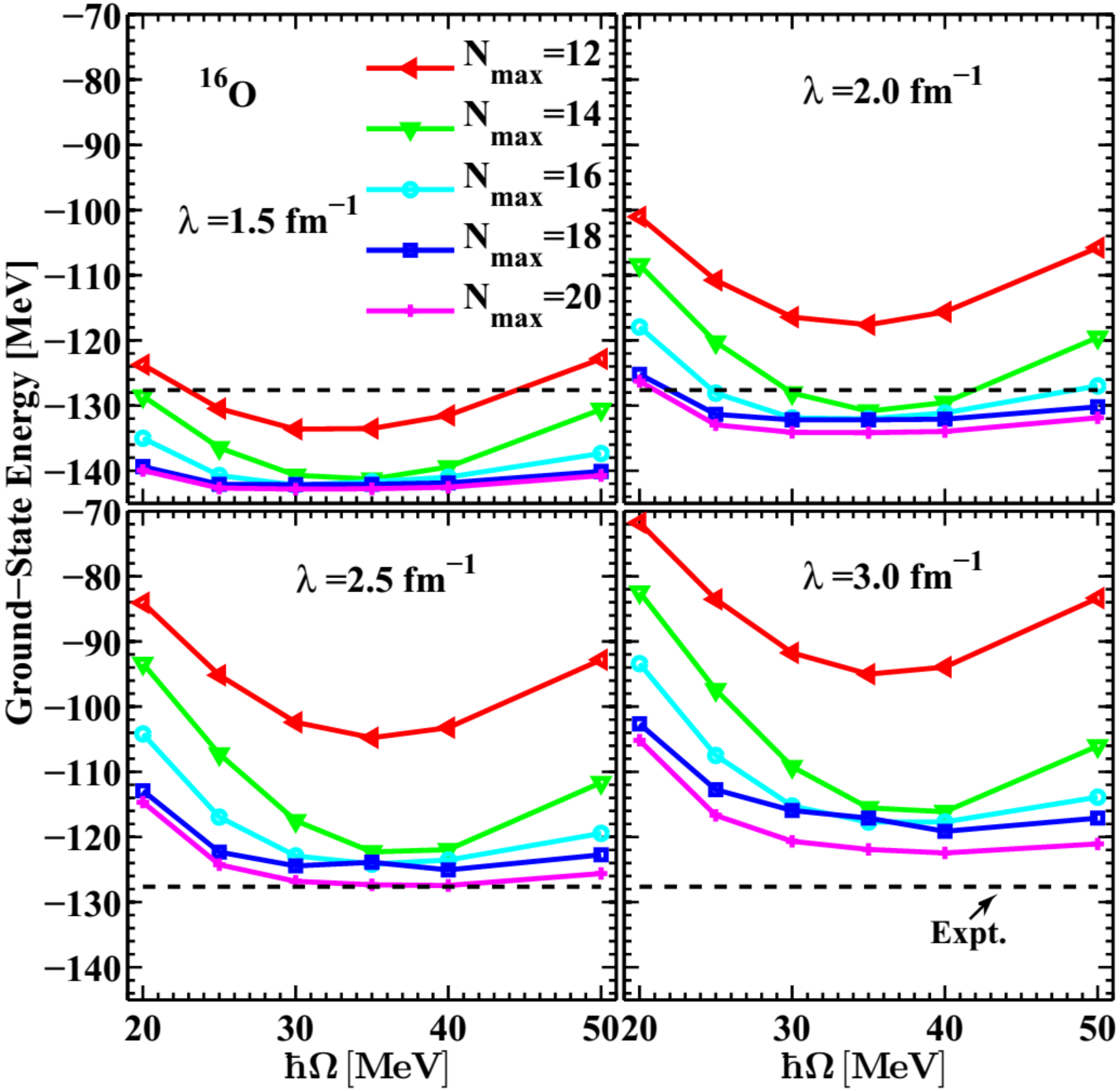
## $^4$He

## Our MBPT with $N^3LO$+SRG



# Our calculations

$^{16}$O



# Our calculations and compared to data

$N^3LO[4]$ with SRG for $^4He$ ($N_{max} = 20$, $\hbar\Omega = 35MeV$ and $\lambda = 2.0fm^{-1}$)

| Observable | p-rms(fm) | $E_{g.s.}$(MeV) |
|---|---|---|
| Expreiment | 1.450 | -28.296 |
| SHF | 1.8380 | -9.1657 |
| Second-order correction | -0.0622 | -13.7430 |
| Third-order correction | – | -2.0587 |
| C.M. motion correction | -0.0854 | – |
| MBPT | 1.6903 | -24.9675 |

**[4] Entem and Machleidt, (2003) PRC 68, 041001**

**$^4$He**

**JISP16 is better, because it reduces *NNN* effects, while our present calculations do not include *NNN*. NNN makes MBPT to be much complicated and much computing time consuming!**

**Shirokov, Vary, Mazur, Weber, PLB 644 (2007) 33**

Bare JISP16[10–12] for $^4He$ ($N_{max} = 14$ and $\hbar\Omega = 10MeV$)

| Observable | p-rms(fm) | $E_{g.s.}$(MeV) |
|---|---|---|
| Expreiment | 1.450 | -28.296 |
| NCSH | – | -28.297 |
| SHF | 1.5714 | -22.4143 |
| Second-order correction | 0.0160 | -4.3126 |
| Third-order correction | – | -0.8031 |
| C.M. motion correction | -0.3695 | – |
| MBPT | 1.2179 | -27.5301 |

$N^3LO[4]$ with SRG for $^{16}O$ ($N_{max} = 20$, $\hbar\Omega = 35MeV$ and $\lambda = 2.0 fm^{-1}$)

| Observable | p-rms(fm) | $E_{g.s.}$(MeV) |
|---|---|---|
| Expreiment | 2.58 | -127.62 |
| SHF | 2.3874 | -36.6856 |
| Second-order correction | -0.0504 | -90.0375 |
| Third-order correction | – | -7.4287 |
| C.M. motion correction | -0.0158 | – |
| MBPT | 2.3211 | -134.1518 |

**$^{16}$O**

Bare JISP16[10–12] for $^{16}O$ ($N_{max} = 10$ and $\hbar\Omega = 15MeV$)

| Observable | p-rms(fm) | $E_{g.s.}$(MeV) |
|---|---|---|
| Expreiment | 2.58 | -127.62 |
| NCSH($N_{max} = 6$) | – | -126.2 |
| SHF | 1.8693 | -70.8461 |
| Second-order correction | 0.0618 | -51.7671 |
| Third-order correction | – | -3.2451 |
| C.M. motion correction | -0.0453 | – |
| MBPT | 1.8858 | -125.8583 |

**JISP 16 vs N3LO: better in energy, worse in radius.**

**JISP16 gives smaller radii at least in $^4$He and $^{16}$O**

**JISP16 more reasonable?**

# IV. Summary

## 1. Apply Gogny to SM calculations

**i) Without NNN, one has to refit Gogny parameters, indicating NNN may be largely included by readjusting NN parameters in empirical calculations?**

**ii) With NNN, existing Gogny parameters work roughly for SM calculations, giving chance to calculate shell-model TBMEs using Gogny.**

**NNN is important in Gogny, which has been well approved in MF models.**

## 2. *ab-initio* MBPT calculations with realistic interactions in spherical HF basis

**i) $2^{nd}$ and $3^{rd}$ order corrections for energy; $2^{nd}$ order for radius.**

**We have calculated $^4$He and $^{16}$O with quite reasonable results obtained.**

**ii) Open questions: NNN in MBPT? Open-shell nuclei (much challenging)?**

## Group members involved

**B.H. Hu, W.G. Jiang, W.J. Chen, Z.H. Sun, L.F. Jiao, Z.X. Xu, J.C. Pei**

## Thanks for collaboration

**James Vary**

# Thank you for your attention

**Peking University Campus**

**Khabarovsk, June 23-27, 2014**