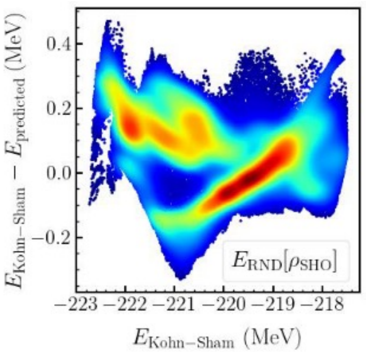
Orbital Free DFT in nuclear physics



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1. Introduction 1: Orbital-based DFT in nuclear physics
2. Introduction 2: Orbital-free DFT in nuclear physics
3. Comparisons between nuclear and electronic systems
4. Applications of machine learning to OF-DFT
5. Summary

- G. Colo and K. Hagino, PTEP 2023, 103D01 (2023).
- N. Hizawa, K. Hagino, and K. Yoshida, PRC108, 034311 (2023).

Second Workshop on Fundamentals in Density Functional Theory (DFT2024), RIKEN Kobe, 2024.2.20-22.

Introduction 1: Orbital-based DFT in nuclear physics

Density Functional Theory

$$E = E[\rho] = \int d\boldsymbol{r} \mathcal{E}[\rho(\boldsymbol{r})]$$

Kohn-Sham scheme ("orbital-based" DFT)

$$E = \int d\boldsymbol{r} \left(\frac{\hbar^2}{2m} \tau(\boldsymbol{r}) + \mathcal{E}_{\text{int}}[\rho(\boldsymbol{r})] \right)$$

$$\tau(\boldsymbol{r}) = \sum_i |\boldsymbol{\nabla} \varphi_i(\boldsymbol{r})|^2, \quad \rho(\boldsymbol{r}) = \sum_i |\varphi_i(\boldsymbol{r})|^2$$

$$\rightarrow \left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 + \frac{\delta \mathcal{E}_{\text{int}}}{\delta \rho} \right) \varphi_i(\boldsymbol{r}) = \epsilon_i \varphi_i(\boldsymbol{r})$$

Skyrme energy functional

T.H.R. Skyrme, Phil. Mag. 1, 1043 (1956).
D. Vautherin and D.M. Brink, PRC5, 626 (1972).

for N=Z nuclei (with x_2=0)

$$\mathcal{E}_{\rm int} = \frac{3}{8}t_0\rho(\boldsymbol{r})^2 + \frac{t_3}{16}\rho(\boldsymbol{r})^{\alpha+2} + \frac{1}{16}(3t_1+5t_2)\rho(\boldsymbol{r})\tau(\boldsymbol{r}) + \frac{1}{64}(9t_1-5t_2)(\boldsymbol{\nabla}\rho(\boldsymbol{r}))^2 - \frac{3}{4}W_0\rho(\boldsymbol{r})\boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{r})$$

$$\tau(\boldsymbol{r}) = \sum_i |\boldsymbol{\nabla}\varphi_i(\boldsymbol{r})|^2$$ kinetic energy density

$$\rho(\boldsymbol{r}) = \sum_i |\varphi_i(\boldsymbol{r})|^2$$ particle number density

$$\boldsymbol{J}(\boldsymbol{r}) = -i\sum_i \varphi_i^*(\boldsymbol{r})(\boldsymbol{\nabla}\times\boldsymbol{\sigma})\varphi_i(\boldsymbol{r})$$ spin-orbit density

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cf. Skyrme interaction (for t_0, t_3, and W_0 parts):

$$v(\boldsymbol{r},\boldsymbol{r}') = \underbrace{t_0\delta(\boldsymbol{r}-\boldsymbol{r}')}_{\text{short-range attraction}} + \underbrace{\frac{1}{6}t_3\delta(\boldsymbol{r}-\boldsymbol{r}')\rho^\alpha(\boldsymbol{r})}_{\text{repulsion to avoid collapse}}$$

$$\underbrace{+iW_0(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot\boldsymbol{k}\times\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k}}_{\text{spin-orbit interaction}}$$

Skyrme energy functional

$$\mathcal{E}_{\rm int} = \frac{3}{8}t_0\rho(\boldsymbol{r})^2 + \frac{t_3}{16}\rho(\boldsymbol{r})^{\alpha+2} + \frac{1}{16}(3t_1+5t_2)\rho(\boldsymbol{r})\tau(\boldsymbol{r}) + \frac{1}{64}(9t_1-5t_2)(\boldsymbol{\nabla}\rho(\boldsymbol{r}))^2 - \frac{3}{4}W_0\rho(\boldsymbol{r})\boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{r})$$

$$\rightarrow \left[-\boldsymbol{\nabla}\cdot\frac{\hbar^2}{2m^*(\boldsymbol{r})}\boldsymbol{\nabla} + V(\boldsymbol{r}) + \boldsymbol{W}(\boldsymbol{r})\cdot(-i)(\boldsymbol{\nabla}\times\boldsymbol{\sigma})\right]\varphi_i = e_i\varphi_i$$

$$\frac{\hbar^2}{2m^*(\boldsymbol{r})} = \frac{\hbar^2}{2m} + \frac{1}{16}(3t_1+5t_2)\rho$$

$$V(\boldsymbol{r}) = \frac{3}{4}t_0\rho + \frac{\alpha+2}{16}t_3\rho^{\alpha+1} + \frac{1}{16}(3t_1+5t_2)\tau - \frac{1}{32}(9t_1-5t_2)\boldsymbol{\nabla}^2\rho - \frac{3}{4}W_0\boldsymbol{\nabla}\cdot\boldsymbol{J}$$

$$\boldsymbol{W}(\boldsymbol{r}) = \frac{3}{4}W_0\boldsymbol{\nabla}\rho$$

Skyrme energy functional

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10 parameters ← fitting to experimental data:

B.E. and $r_{\rm rms}$: ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{208}Pb,…..
infinite nuclear matter: E/A, $\rho_{\rm eq}$,….

Parameter sets:

SIII, SkM*, SGII, SLy4,…….

Skyrme energy functional

T.H.R. Skyrme, Phil. Mag. 1, 1043 (1956).
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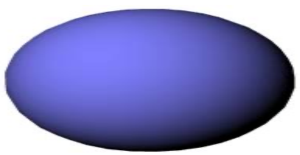
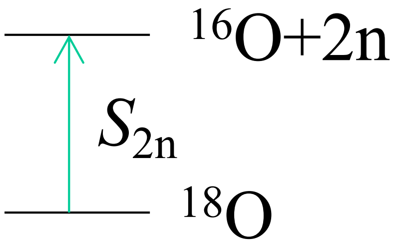
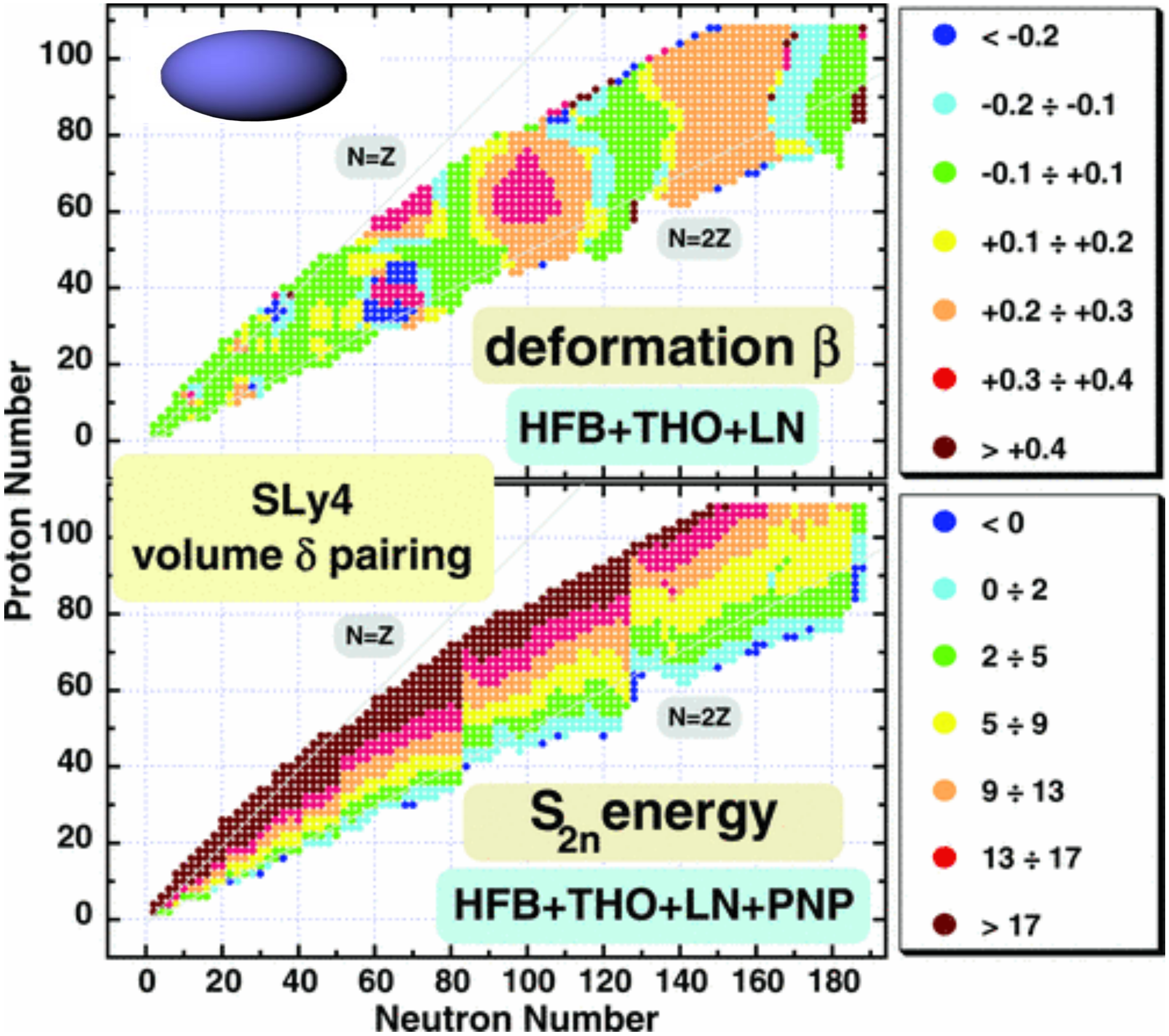
- ✓ a more complicated form for N $\neq$ Z
- ✓ Coulomb: direct + Slater approximation for exchange
- ✓ an additional pairing functional for Bogoliubov-de-Gennes
- ✓ nuclear systems $\longrightarrow$ self-bound systems



◆ deformed density for open shell nuclei

a global calculations: deformation and two-neutron separation energy





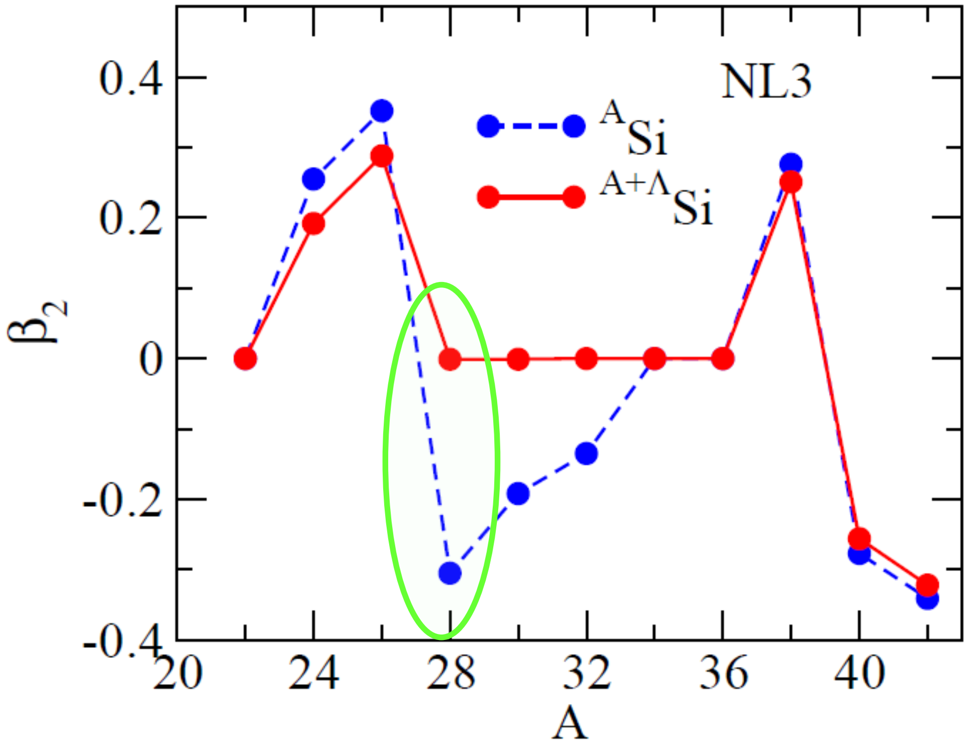
M.V. Stoitsov et al., PRC68('03)054312

deformation of hypernuclei

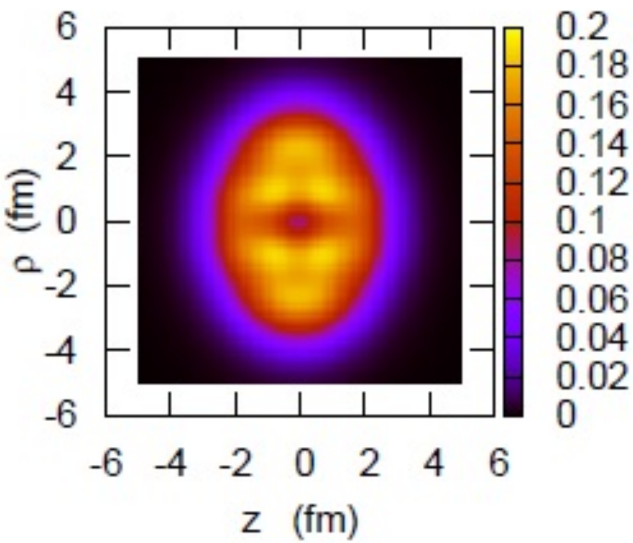
^{28}Si = 14 protons + 14 neutrons
$^{29}{}_{\Lambda}Si$ = 14 protons + 14 neutrons + Λ particle

n = (udd)
p = (uud)
Λ = (uds)

Si isotopes (covariant DFT)

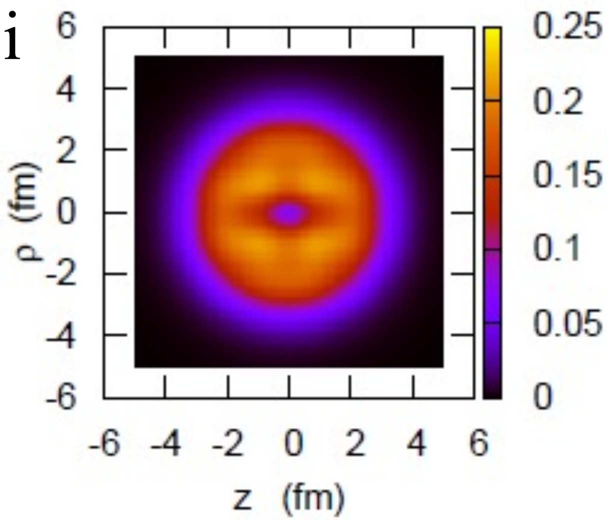


^{28}Si



Λ →

$^{29}{}_{\Lambda}Si$



Myaing Thi Win and K.Hagino, PRC78('08)054311

Introduction 2: Orbital-free DFT in nuclear physics

$$E = \int d\boldsymbol{r} \left(\frac{\hbar^2}{2m} \tau(\boldsymbol{r}) + \mathcal{E}[\rho(\boldsymbol{r})] \right)$$

Kohn-Sham scheme ("orbital-based" DFT)

$$\tau(\boldsymbol{r}) = \sum_i |\boldsymbol{\nabla}\varphi_i(\boldsymbol{r})|^2, \quad \rho(\boldsymbol{r}) = \sum_i |\varphi_i(\boldsymbol{r})|^2$$

$$\rightarrow \left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 + \frac{\delta \mathcal{E}}{\delta \rho} \right) \varphi_i(\boldsymbol{r}) = \epsilon_i \varphi_i(\boldsymbol{r})$$

A simpler approach: orbital-free DFT

M. Levy, J.P. Perdew, and V. Sahni, PRA30 ('84) 2745

$$\left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 + V_{\rm eff}(\boldsymbol{r}) \right) \sqrt{\rho(\boldsymbol{r})} = \mu \sqrt{\rho(\boldsymbol{r})}$$

(note) $\rho(\boldsymbol{r}) = N|\varphi(\boldsymbol{r})|^2 \rightarrow \varphi(\boldsymbol{r}) \propto \sqrt{\rho(\boldsymbol{r})}$

Density Functional Theory

Kohn-Sham scheme ("orbital-based" DFT)

$$\tau(\boldsymbol{r}) = \sum_i |\boldsymbol{\nabla}\varphi_i(\boldsymbol{r})|^2, \quad \rho(\boldsymbol{r}) = \sum_i |\varphi_i(\boldsymbol{r})|^2$$

interacting many-fermion systems
→a mapping to non-interacting many-Fermion systems

A simpler approach: orbital-free DFT

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(note) $\rho(\boldsymbol{r}) = N|\varphi(\boldsymbol{r})|^2 \to \varphi(\boldsymbol{r}) \propto \sqrt{\rho(\boldsymbol{r})}$

interacting many-fermion systems
→a mapping to non-interacting many-Boson systems

the extended Thomas-Fermi approximation

$$\tau_{\mathrm{TF}}(\boldsymbol{r}) = \alpha\rho^{5/3} + \frac{\beta}{4}\frac{(\boldsymbol{\nabla}\rho)^2}{\rho} \qquad \alpha = \frac{3}{5}(3\pi^2)^{2/3}, \quad \beta = \frac{1}{9}$$

$$\frac{\delta}{\delta\rho}\left(E - \mu\int\rho(\boldsymbol{r})d\boldsymbol{r}\right) = 0$$

$$\rightarrow \frac{\hbar^2}{2m}\left(\frac{5}{3}\alpha\rho^{2/3} + \frac{\beta}{4}\frac{(\boldsymbol{\nabla}\rho)^2}{\rho^2} - \frac{\beta}{2}\frac{\boldsymbol{\nabla}^2\rho}{\rho}\right) + \frac{\delta\mathcal{E}}{\delta\rho} - \mu = 0$$

$$= -\frac{\beta}{\sqrt{\rho}}\boldsymbol{\nabla}^2\sqrt{\rho}$$

$$\rightarrow \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \underbrace{\frac{1}{\beta}\frac{\delta\mathcal{E}}{\delta\rho} + \frac{5\alpha}{3\beta}\frac{\hbar^2}{2m}\rho(\boldsymbol{r})^{2/3}}_{V_{\mathrm{eff}}}\right)\sqrt{\rho(\boldsymbol{r})} = \frac{\mu}{\beta}\sqrt{\rho(\boldsymbol{r})}$$

the extended Thomas-Fermi approximation

$$\tau_{\rm TF}(\boldsymbol{r}) = \alpha\rho^{5/3} + \frac{\beta}{4}\frac{(\boldsymbol{\nabla}\rho)^2}{\rho} \qquad \alpha = \frac{3}{5}(3\pi^2)^{2/3}, \quad \beta = \frac{1}{9}$$

$$\frac{\delta}{\delta\rho}\left(E - \mu\int\rho(\boldsymbol{r})d\boldsymbol{r}\right) = 0$$

$$\rightarrow \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \underbrace{\frac{1}{\beta}\frac{\delta\mathcal{E}}{\delta\rho} + \frac{5\alpha}{3\beta}\frac{\hbar^2}{2m}\rho(\boldsymbol{r})^{2/3}}_{V_{\rm eff}}\right)\sqrt{\rho(\boldsymbol{r})} = \frac{\mu}{\beta}\sqrt{\rho(\boldsymbol{r})}$$

electron systems: β ⟶ a free parameter

popular choices: β = 1/9, 1/5, 1

- 1/9 ← semi-classical
- 1/5 ← empirical fit
- 1 ← original Weizsacker

$$\tau_{\mathrm{TF}}(\boldsymbol{r}) = \alpha\rho^{5/3} + \frac{\beta}{4}\frac{(\boldsymbol{\nabla}\rho)^2}{\rho}$$

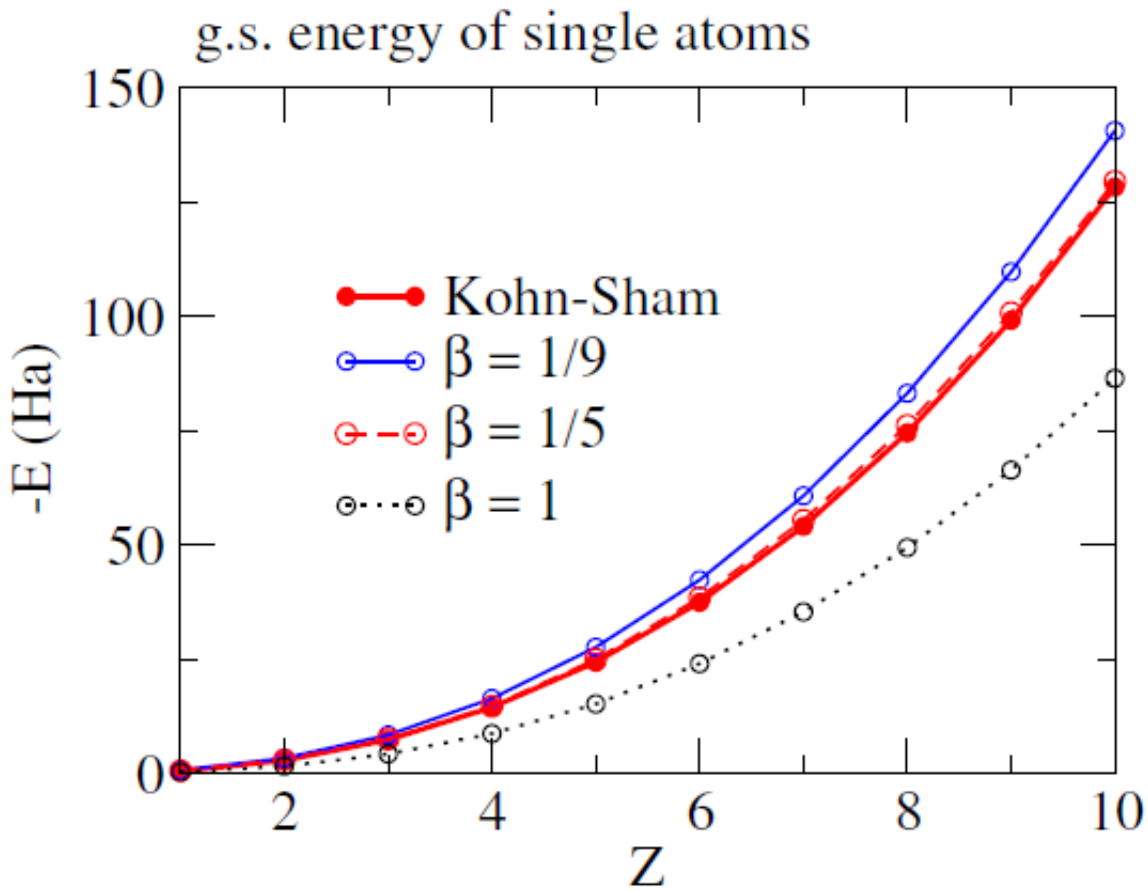
semi-classical

empirical fit

electron systems: β → a free parameter

popular choices: β = 1/9, 1/5, 1

original Weizsacker



V.V. Karasiev and S.B. Trickey, CPC183 ('12) 2519, table 3

Nuclear systems:

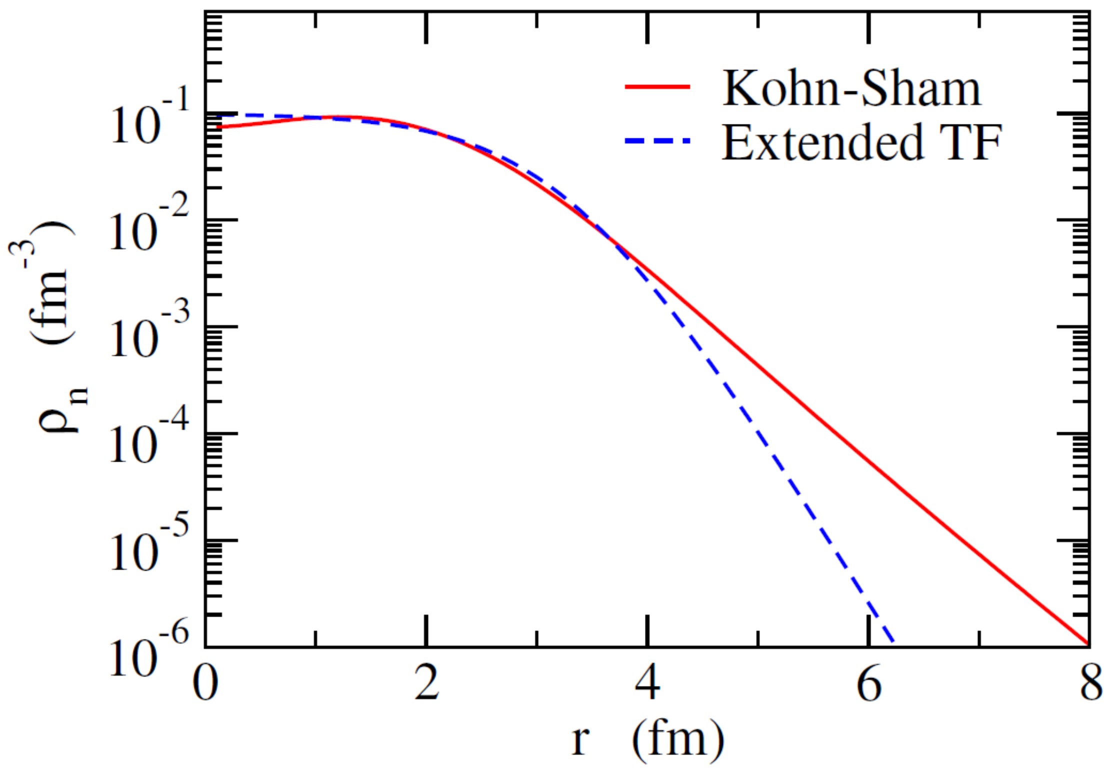
A long history of a method based on the Extended TF approximation

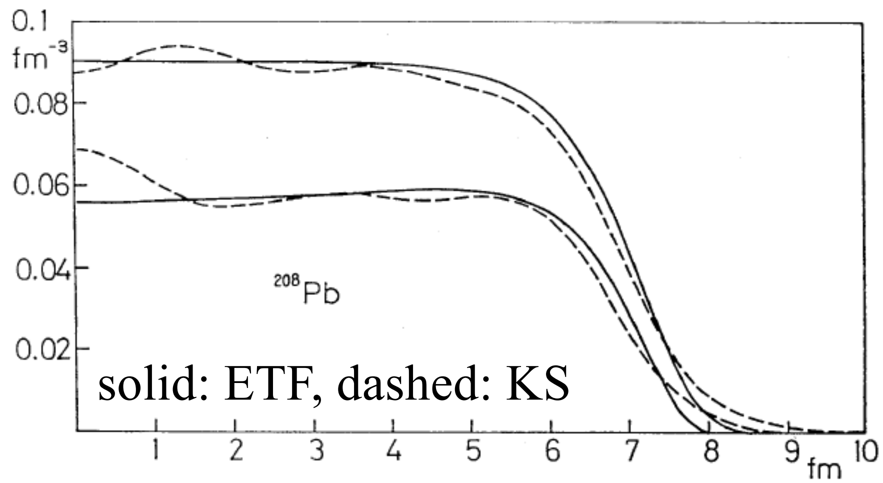
M. Brack et al., Phys. Rep. 123 (1985) 275

cf. ETF-SI (Strutinsky Integral) mass formula,
A.K. Dutta et al., Nucl. Phys. A458, 77 (1986)

→ the extended TF: E_{tot} is reasonable, but a wrong tail in ρ

a potential model, ^{16}O





cf. H. Sagawa and G. Holzwarth,
PTP59, 1213 (1978).

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M. Brack et al., Phys. Rep. 123 (1985) 275

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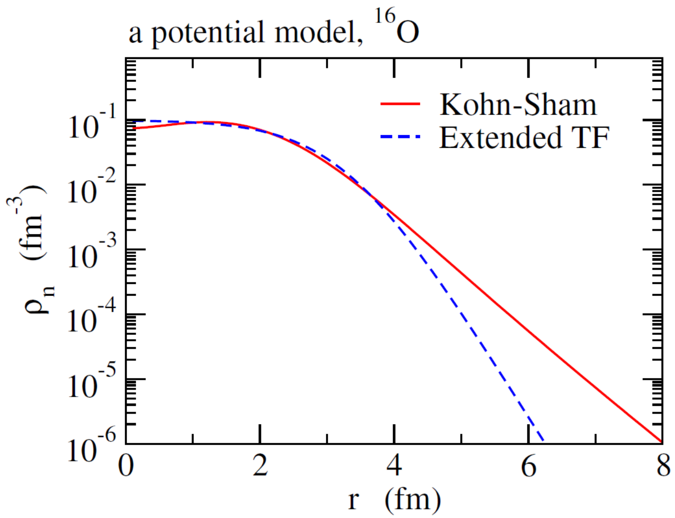


H. Krivine and J. Treiner, Phys. Lett. 88B, 212 (1979):

$$\tau_{\mathrm{TF}}(\boldsymbol{r}) = \alpha\rho^{5/3} + \frac{\beta}{4}\frac{(\boldsymbol{\nabla}\rho)^2}{\rho}$$

good *E* and ρ by adjusting α and β → but a strong system dependence

"a dilemma between *E* and ρ"

Nuclear systems:

the extended TF: E_{tot} is reasonable, but a wrong tail in ρ

M. Brack et al., Phys. Rep. 123 (1985) 275

Our Questions: G. Colo and K. Hagino, PTEP 2023, 103D01 (2023)

- How does this statement hold for beta = 1/9, 1/5, and 1, which have been often employed in electronic systems?
- Is there any way to cure this problem?

- To what extent is the OF-DFT useful for nuclear systems?
- Does the tail matter in electron systems?
- What are similarities and differences between nuclear and electron systems?

Comparisons between nuclear and electric systems

A simple potential model

$$E = \int d\boldsymbol{r} \left(\frac{\hbar^2}{2m} \tau(\boldsymbol{r}) + V(\boldsymbol{r})\rho(\boldsymbol{r}) \right) = \sum_i \epsilon_i$$

V(r): a Woods-Saxon potential (with no ls)
or a pure Coulomb potential

$$\left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 + V(\boldsymbol{r}) \right) \varphi_i(\boldsymbol{r}) = \epsilon_i \varphi_i(\boldsymbol{r})$$

Comparisons between nuclear and electric systems

A simple potential model

$$E = \int d\boldsymbol{r} \left(\frac{\hbar^2}{2m} \tau(\boldsymbol{r}) + V(\boldsymbol{r}) \rho(\boldsymbol{r}) \right) = \sum_i \epsilon_i$$

$$\left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 + V(\boldsymbol{r}) \right) \varphi_i(\boldsymbol{r}) = \epsilon_i \varphi_i(\boldsymbol{r})$$

Exact: $$E_{\text{exact}} = \sum_i \epsilon_i, \quad \rho_{\text{exact}}(\boldsymbol{r}) = \sum_i |\varphi_i(\boldsymbol{r})|^2$$

OF-DFT: $$\tau_{\text{TF}}(\boldsymbol{r}) = \alpha \rho^{5/3} + \frac{\beta}{4} \frac{(\boldsymbol{\nabla} \rho)^2}{\rho}$$

$$\left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 + \frac{1}{\beta} \frac{\delta \mathcal{E}}{\delta \rho} + \frac{5\alpha}{3\beta} \frac{\hbar^2}{2m} \rho(\boldsymbol{r})^{2/3} \right) \sqrt{\rho(\boldsymbol{r})} = \frac{\mu}{\beta} \sqrt{\rho(\boldsymbol{r})} \rightarrow \rho_{\text{OF}-\text{DFT}}$$

$$\rightarrow E = \int d\boldsymbol{r} \left(\frac{\hbar^2}{2m} \tau[\rho(\boldsymbol{r})] + V(\boldsymbol{r}) \rho(\boldsymbol{r}) \right)$$

Comparisons between nuclear and electric systems

(a) Nuclear System

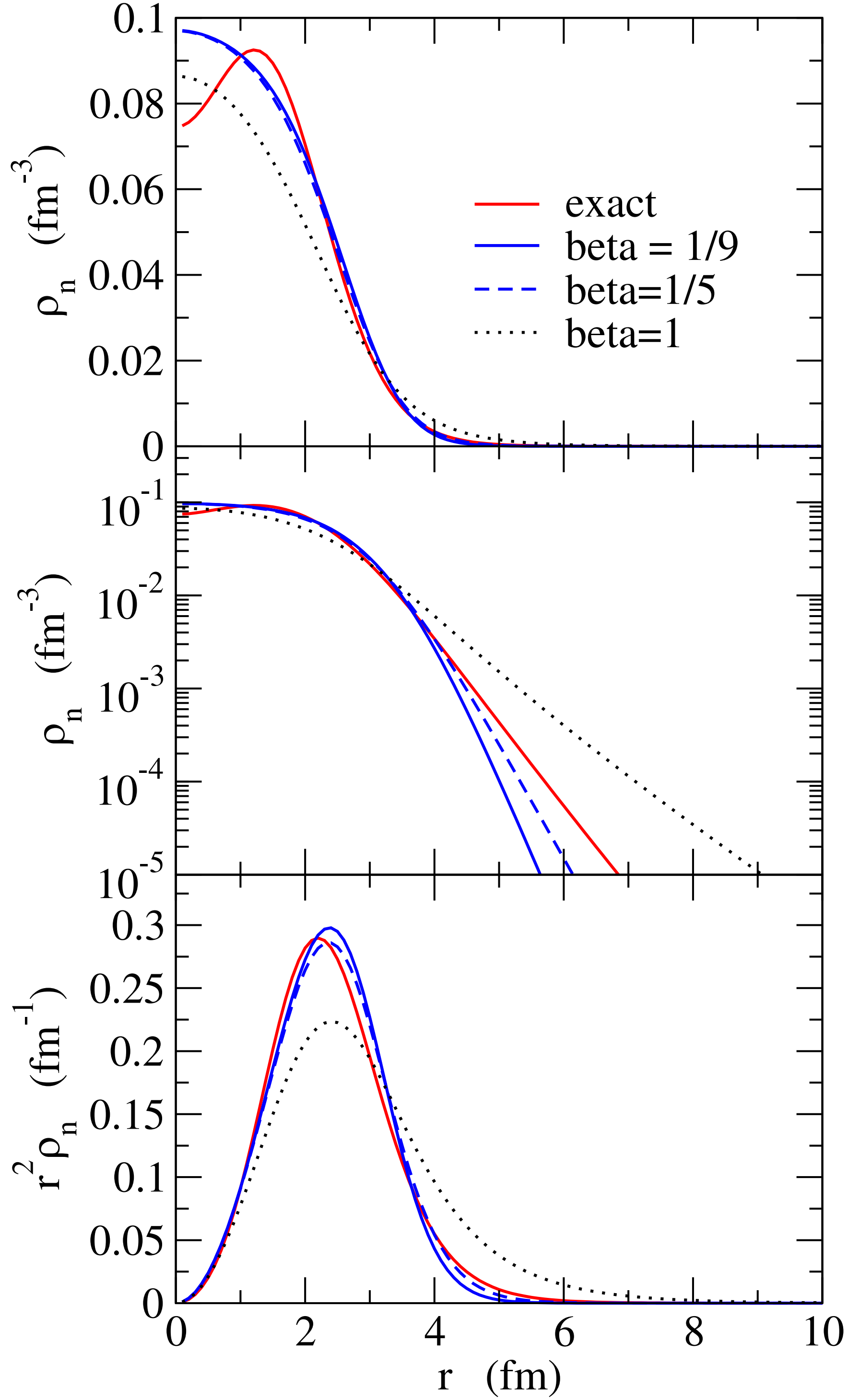
$$V(r) = -\frac{V_0}{1+\exp[(r-R_0)/a]}$$

$V_0 = 50$ MeV, $R_0 = 1.2 \times 16^{1/3}$ fm, $a = 0.65$ fm

neutrons only with N=8

$e(1s_{1/2}) = -32.6$ MeV, $e(1p_{3/2}) = e(1p_{1/2}) = -16.8$ MeV

	E_{tot} (MeV)	Rms radius (fm)
exact	-142.27	2.575
OF-DFT (β = 1/9)	-140.85	2.500
OF-DFT (β = 1/5)	-135.19	2.562
OF-DFT (β = 1)	-96.31	3.12



	E_{tot} (MeV)	Rms radius (fm)
exact	-142.27	2.575
β = 1/9	-140.85	2.500
β = 1/5	-135.19	2.562
β = 1	-96.31	3.12

- ✓ the choice of β=1 is not good
- ✓ the choice of β=1/5 and 1/9 are both reasonable

$E_{tot} \rightarrow$ β=1/9 is better
$r \rightarrow$ β=1/5 is slightly better

Comparisons between nuclear and electric systems

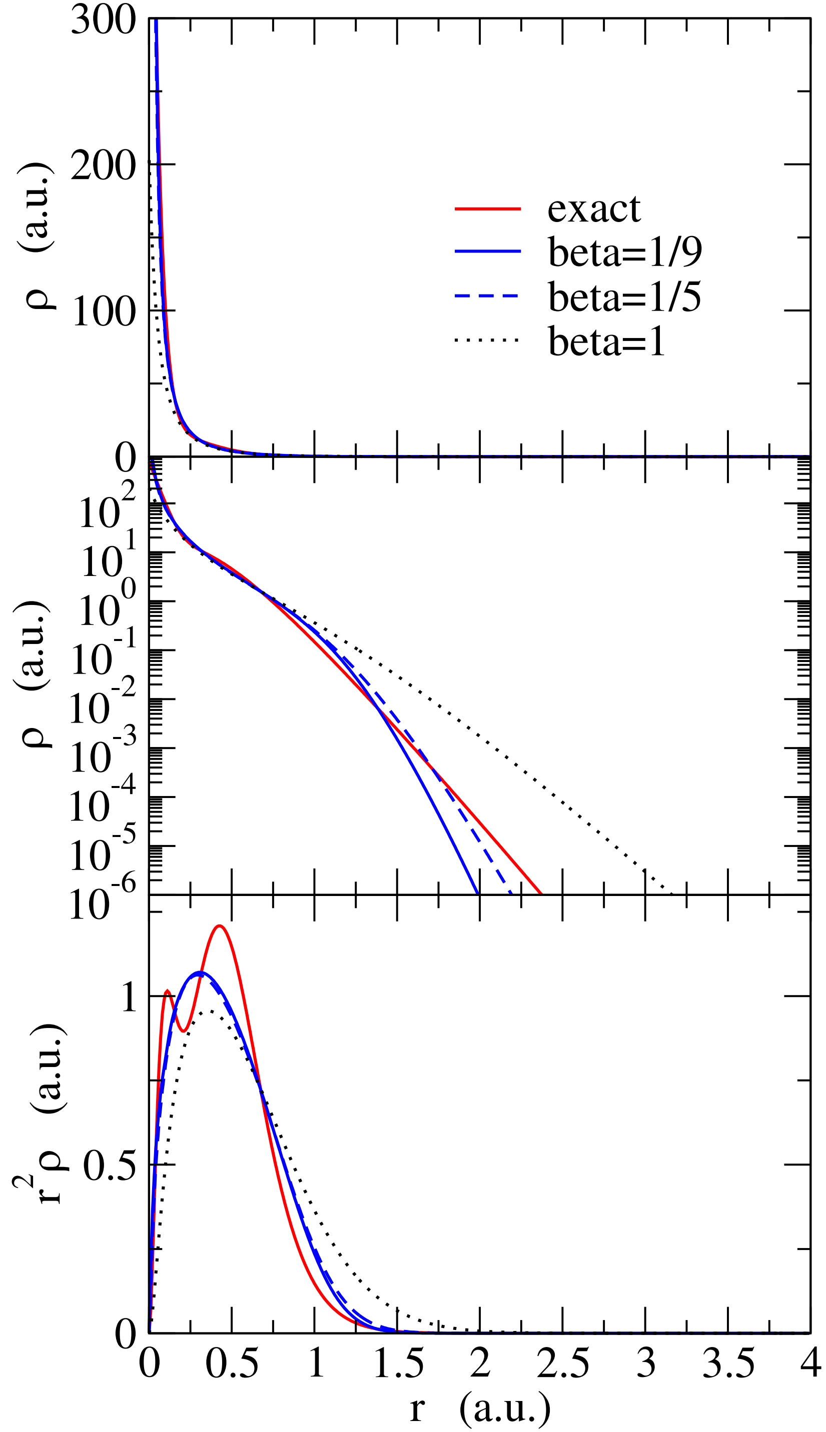
(b) Coulomb systems

$$V(r) = -\frac{10e^2}{r}$$

10 electrons

e(1S) = -50.0 (Ha), (2P) = e(2S) = -12.5 (Ha)

	E_{tot} (Ha)	Rms radius (a.u.)
exact	-200.0	0.27
OF-DFT (β = 1/9)	-208.6	0.30
OF-DFT (β = 1/5)	-196.1	0.318
OF-DFT (β = 1)	-141.49	0.482



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OF-DFT (β = 1/5)	-196.1	0.318
OF-DFT (β = 1)	-141.49	0.482

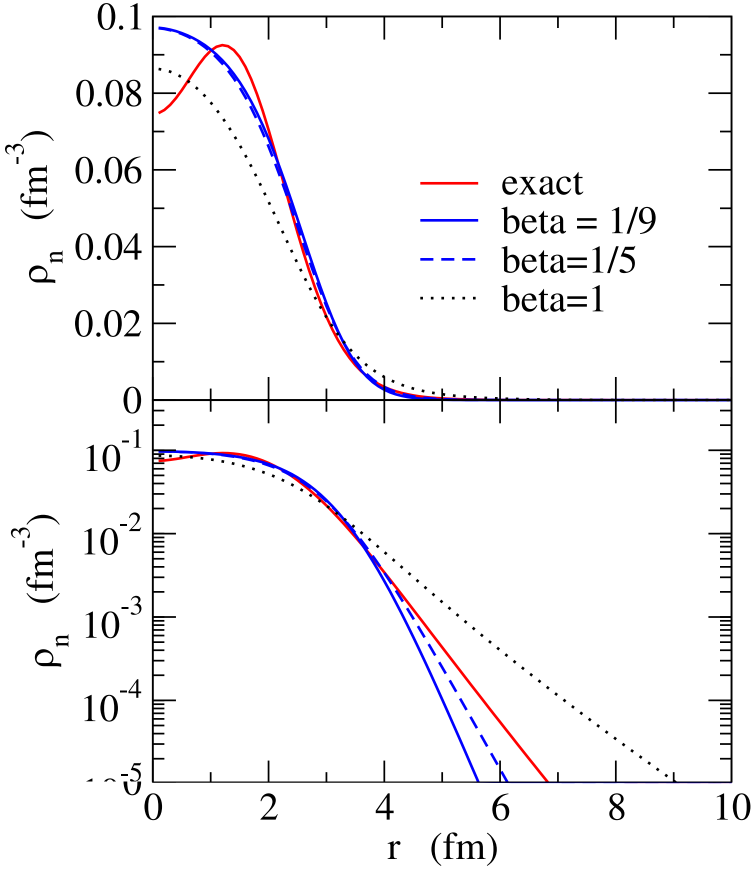
✓ the choice of β=1 is not good

✓ the choice of β=1/5 and 1/9 are both reasonable

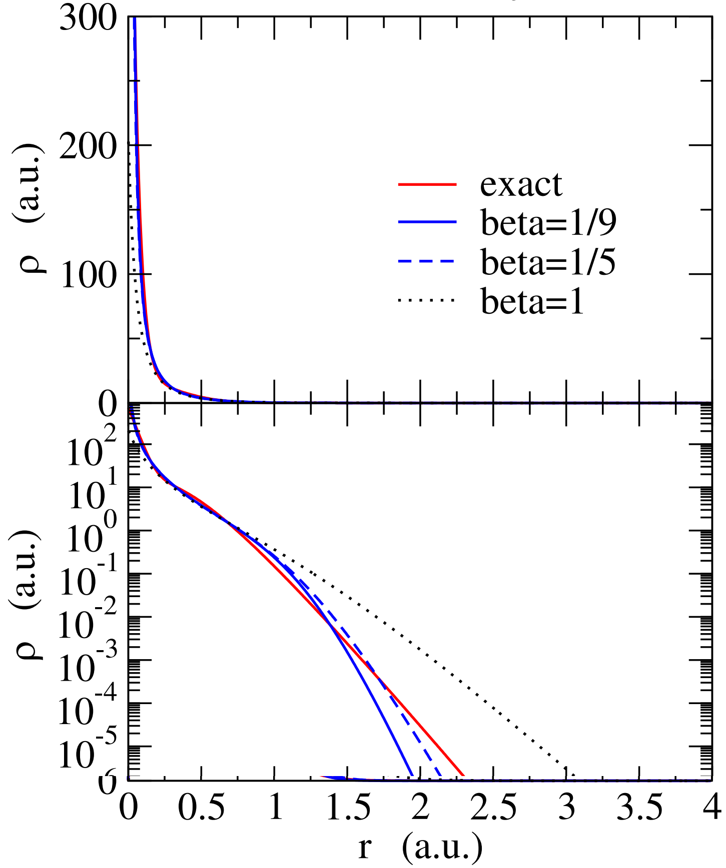
- the dependence on β is mild
  ← the long range int.
- the tail problem appears only at very large *r*

Comparisons between nuclear and electric systems

a nuclear system



an electron system



nuclear systems → a saturation property

(the density at the central part: not large)

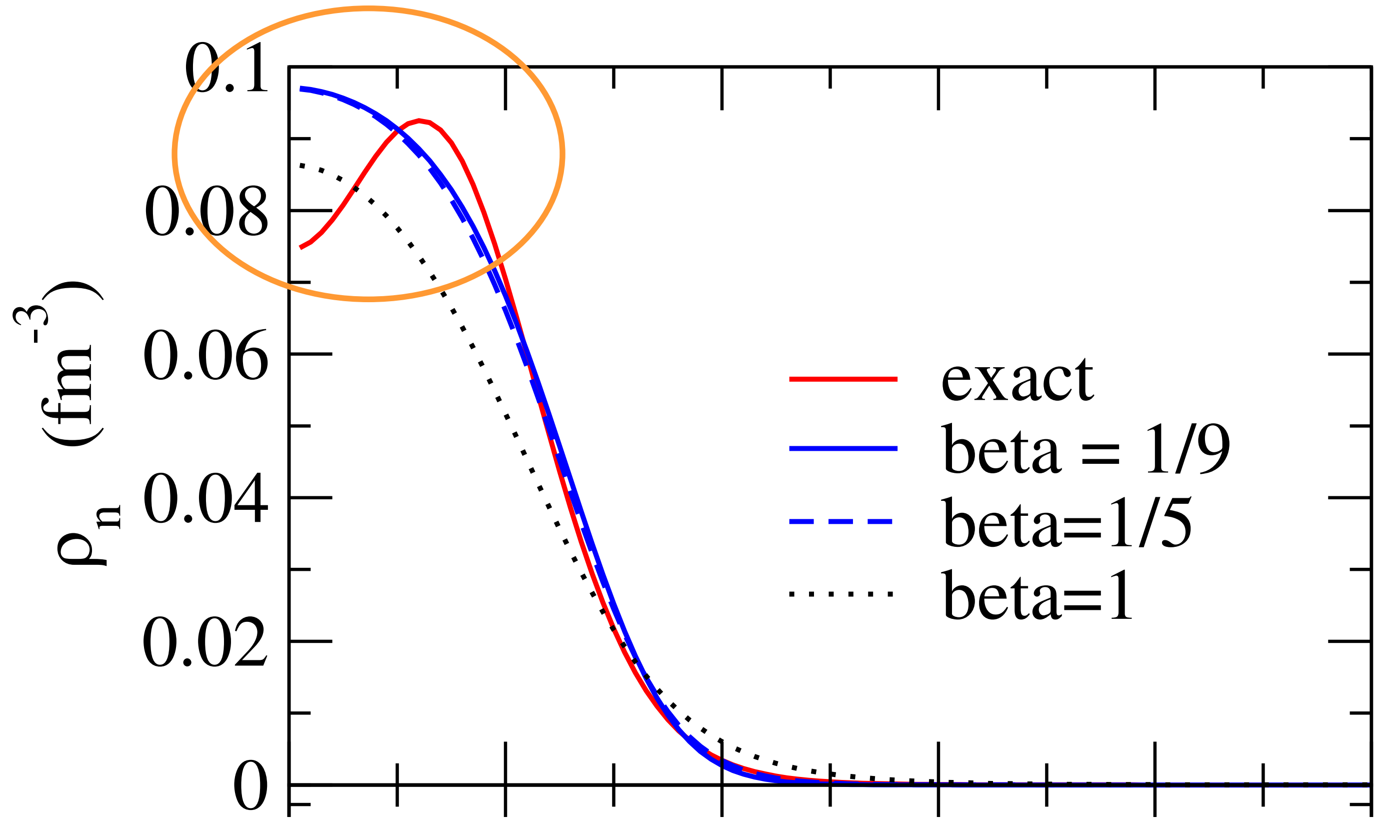
→ the tail problem is more relevant

G. Colo and K. Hagino, PTEP 2023, 103D01 (2023)

Remark 1: shell corrections?

(Extended) Thomas-Fermi: semi-classical approximation

→ basically no shell effect



shell corrections?

OF-DFT + 1 more iteration with KS

cf. O. Bohigas et al., PLB64, 381 (1976).

OF-DFT → convergence: ρ

→ solve KS-eq. only one time with this density

the simplified Skyrme interaction (the t_0 and t_3 terms only)

$$v_{NN}(\boldsymbol{r},\boldsymbol{r}') = \left[t_0 + \frac{t_3}{6}\rho\left(\frac{\boldsymbol{r}+\boldsymbol{r}'}{2}\right)^{\alpha}\right]\delta(\boldsymbol{r}-\boldsymbol{r}')$$

$$\to E = \int d\boldsymbol{r}\,\left[\frac{\hbar^2}{2m}\tau(\boldsymbol{r}) + \frac{3}{8}t_0\rho(\boldsymbol{r})^2 + \frac{t_3}{16}\rho(\boldsymbol{r})^{\alpha+2}\right]$$

(Z=N, no Coulomb)

parameters: Agrawal, Shlomo, Sanzhur, PRC67 (2003) 034314

shell corrections?

OF-DFT + 1 more iteration with KS

cf. O. Bohigas et al., PLB64, 381 (1976).

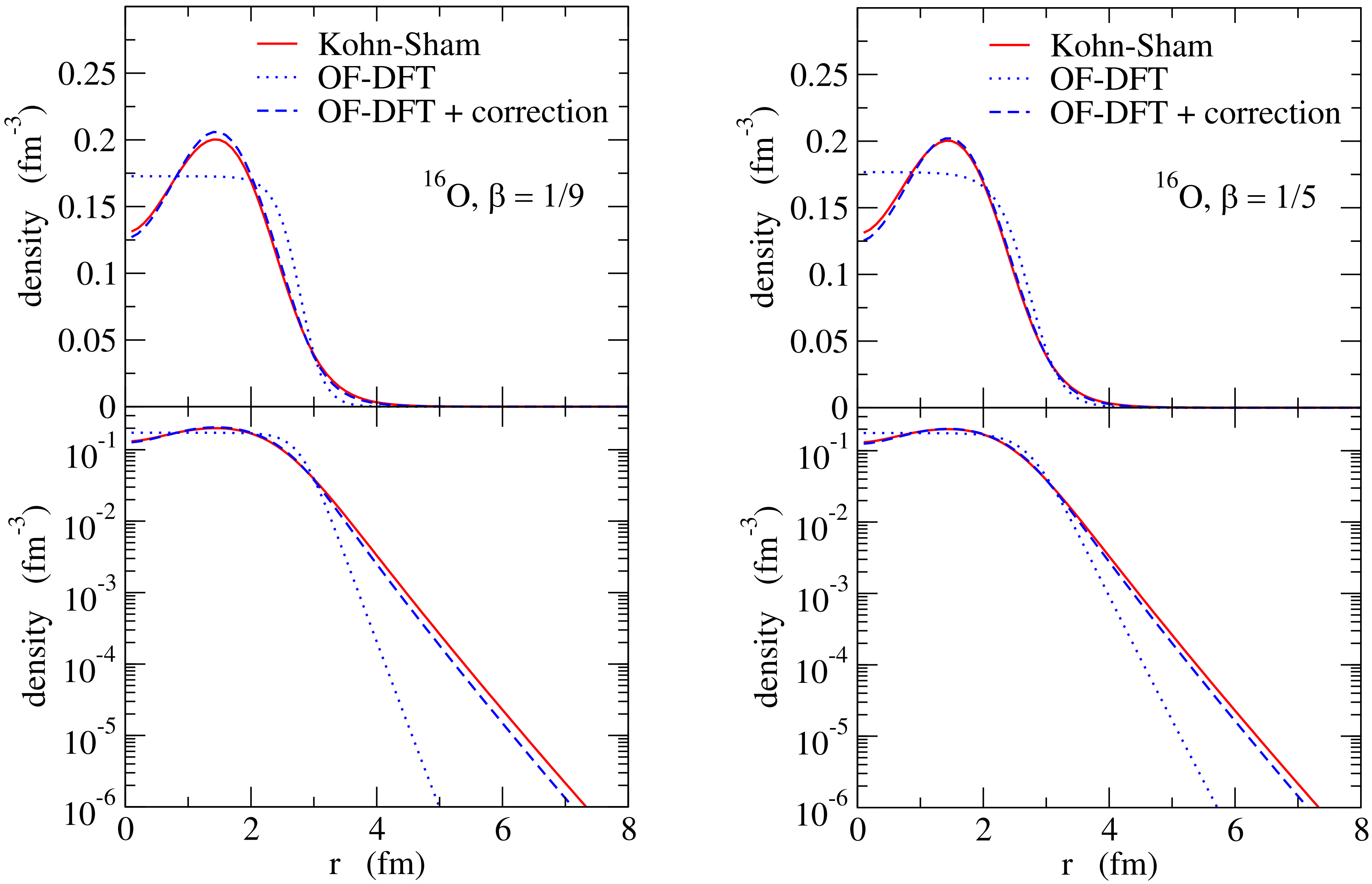
the simplified Skyrme interaction (the t_0 and t_3 terms only)

$$E = \int d\boldsymbol{r} \left[\frac{\hbar^2}{2m} \tau(\boldsymbol{r}) + \frac{3}{8} t_0 \rho(\boldsymbol{r})^2 + \frac{t_3}{16} \rho(\boldsymbol{r})^{\alpha+2} \right]$$

^{16}O	E_{tot} (MeV)	Rms radius (fm)
exact	-187.6	2.364
OF-DFT (β = 1/9)	-201.2	2.253
OF-DFT (β = 1/5)	-180.4	2.296
OF-DFT+corr. (β = 1/9)	-186.6	2.317
OF-DFT+corr. (β = 1/5)	-187.2	2.339

β = 1/9 and 1/5 lead to similar results after the correction.

shell corrections?

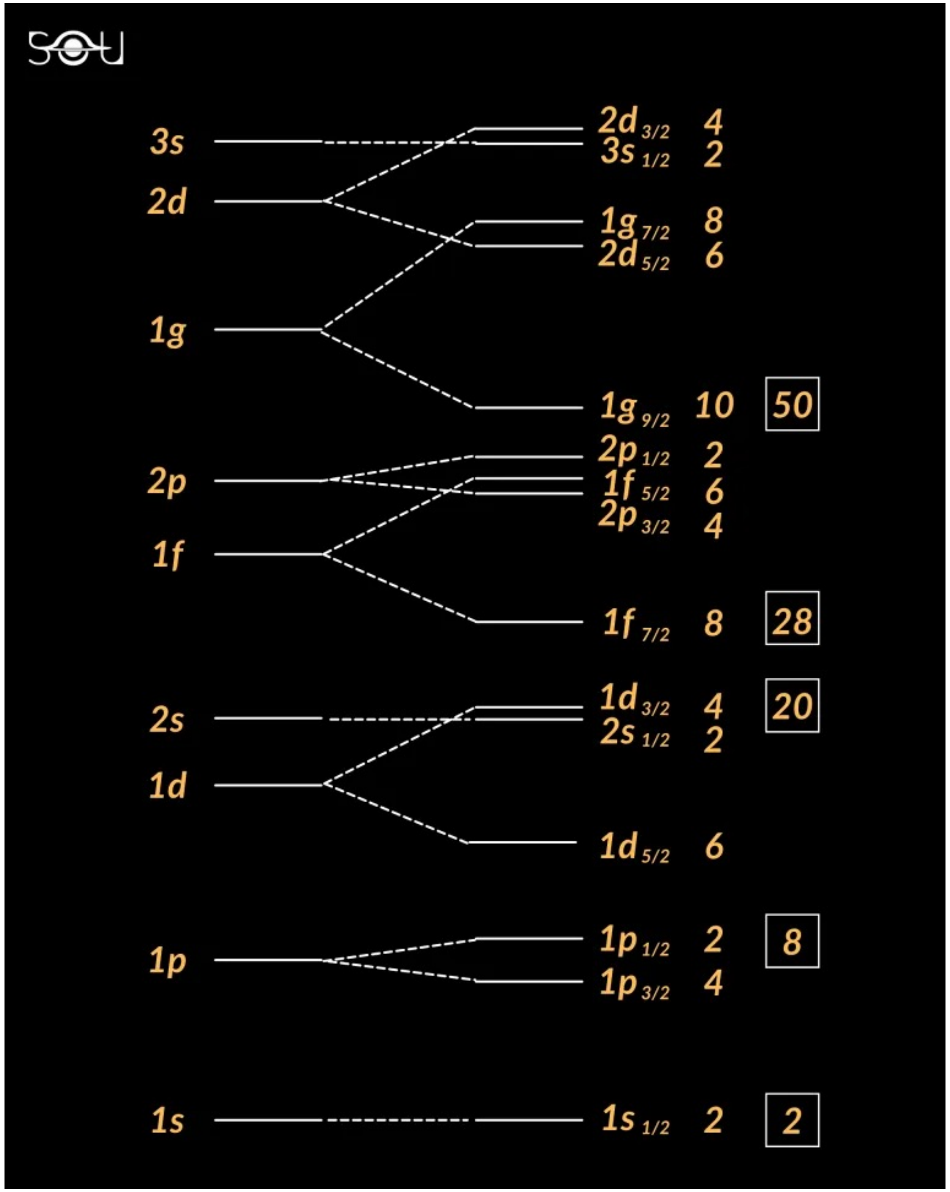


✓ weak dependence on β

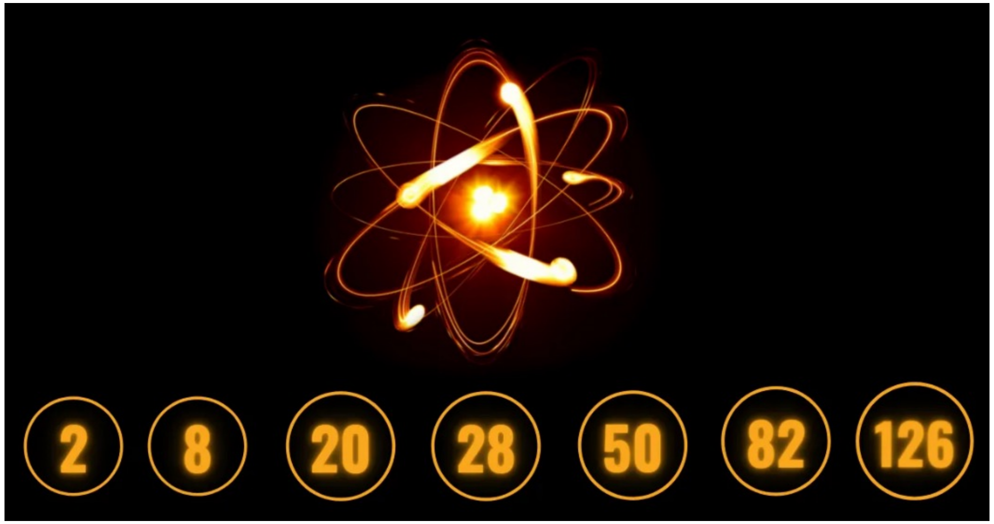
G. Colo and K. Hagino, PTEP 2023, 103D01 (2023)

Remark 2: a spin-orbit potential

an *ls* interaction: an important ingredient of nuclear magic numbers



$$V(r) + V_{ls}(r)\boldsymbol{l} \cdot \boldsymbol{s}$$



https://www.secretsofuniverse.in/magic-numbers-in-physics/

Remark 2: a spin-orbit potential

OF-DFT with spin-orbit

$$\epsilon_{ls} = -\frac{3}{4}W_0\rho\boldsymbol{\nabla}\cdot\boldsymbol{J} \to -\frac{2m}{\hbar^2}\left(\frac{3}{4}W_0\right)^2\rho(\boldsymbol{\nabla}\rho)^2$$

B. Grammaticos and A. Voros, Ann. of Phys. 129, 153 (1980).
A. Bulgac et al., PRC97, 044313 (2018).

◆ A test with a simplified Skyrme functional

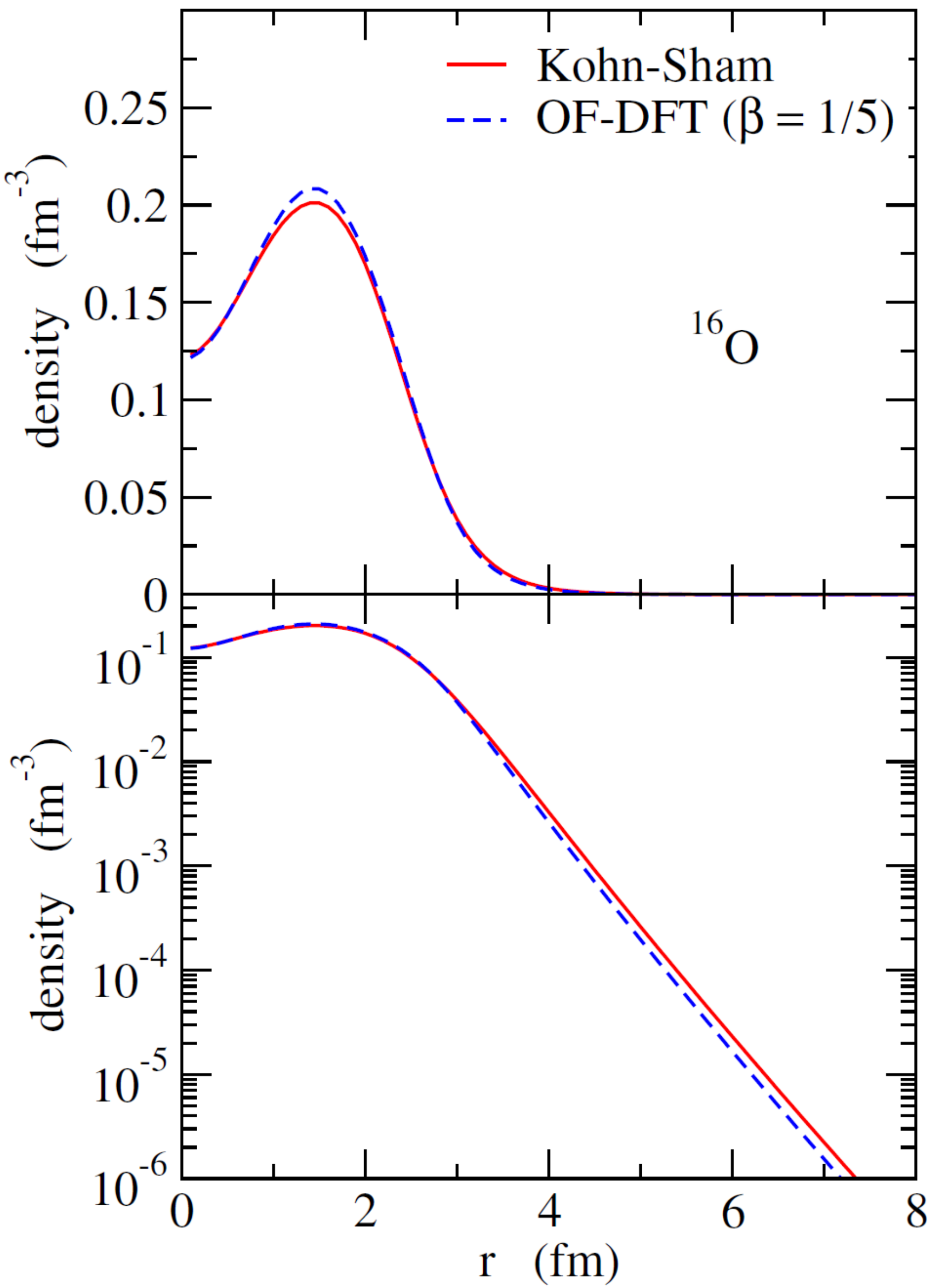
a standard value: W_0 = 120-130 MeV fm^5 → no convergence

a test with W_0 = 50 MeV fm^5

^{16}O	E_{tot} (MeV)	Rms radius (fm)
exact (KS)	-187.99	2.362
OF-DFT (β = 1/9)	no convergence	no convergence
OF-DFT (β = 1/5)	-186.37	2.262

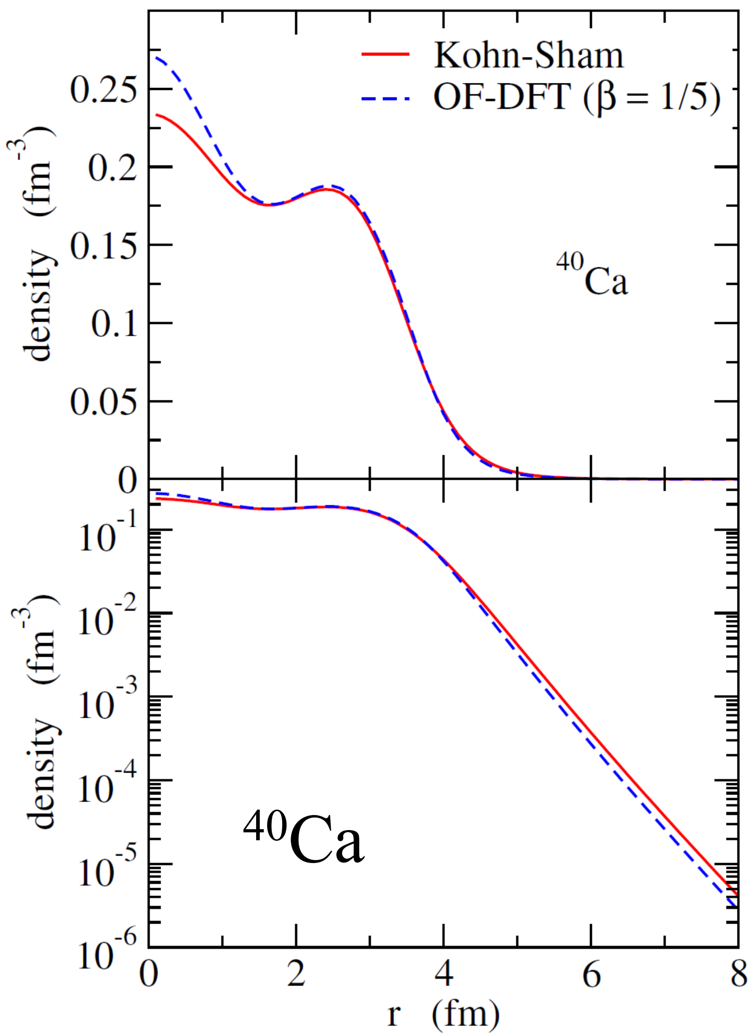
* a simple OF-DFT (without KS correction)

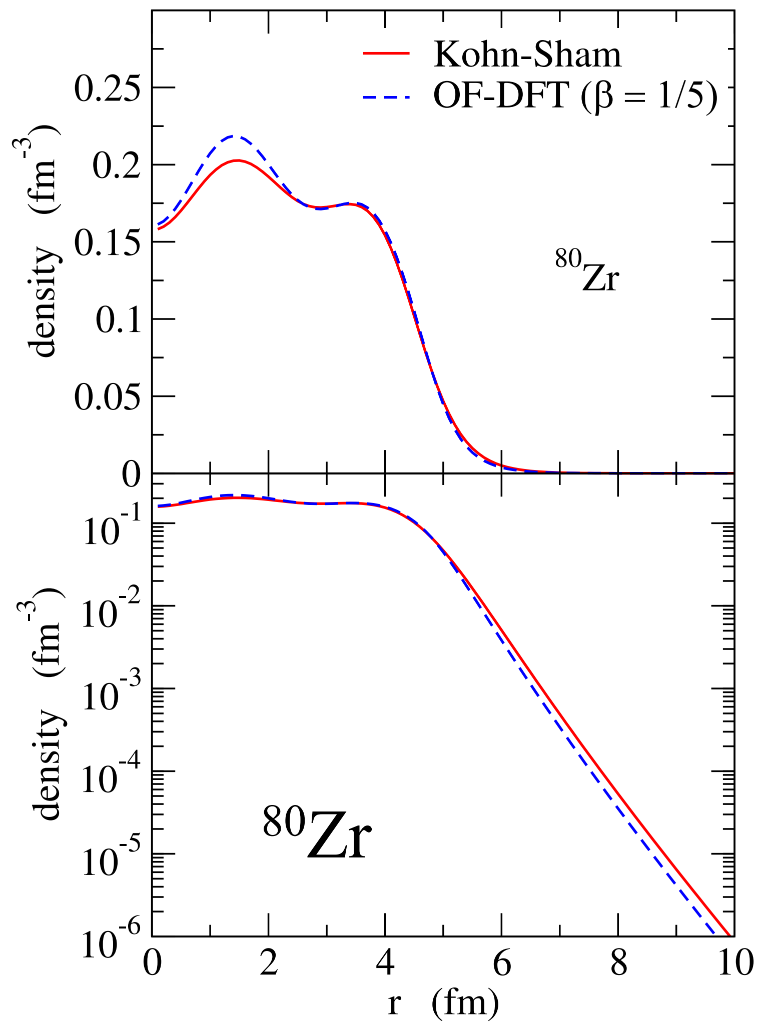
simplified Skyrme with ls (W_0=50 MeV fm^5)



- the structure
- the tail

well reproduced





$E_{\mathrm{KS}} = -510.54$ MeV
$E_{\mathrm{OF\text{-}DFT}} = -515.37$ MeV

$E_{\mathrm{KS}} = -1063.43$ MeV
$E_{\mathrm{OF\text{-}DFT}} = -1085.67$ MeV

the spin-orbit interaction seems to restore shell effects to some extent

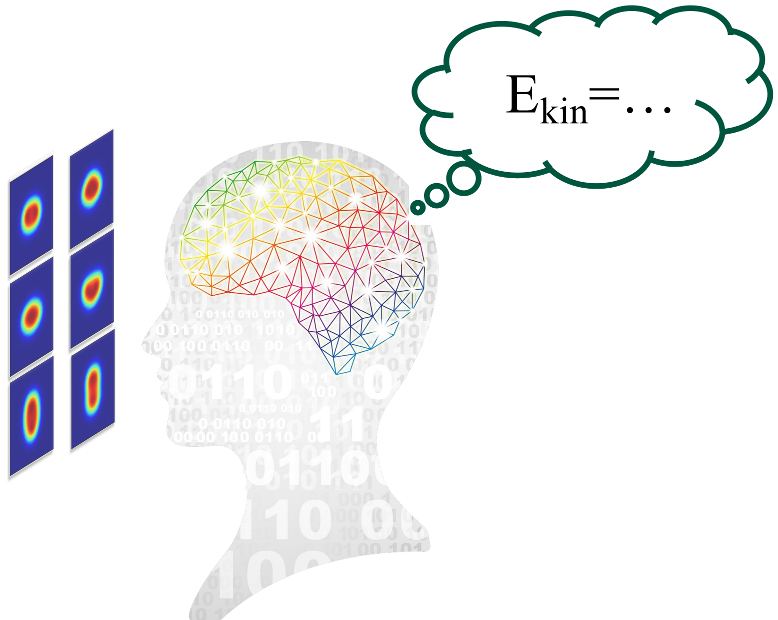
K. Hagino and G. Colo, in preparation

Applications of machine learning to OF-DFT

OF-DFT: $E_{\mathrm{phenom}} \sim E[\rho]$

$$\tau_{\mathrm{TF}}(\boldsymbol{r}) = \alpha\rho^{5/3} + \frac{\beta}{4}\frac{(\boldsymbol{\nabla}\rho)^2}{\rho}$$

Can AI tell us E by looking at ρ?



1. "Nuclear energy density functionals from machine learning"
   X.H. Wu, Z.X. Ren, and P.W. Zhao, PRC105, L031303 (2022).

2. "Analysis of a Skyrme energy density functional with deep learning"
   N. Hizawa, K. Hagino, and K. Yoshida, PRC108, 034311 (2023).

Applications of machine learning to OF-DFT

1. "Nuclear energy density functionals from machine learning"
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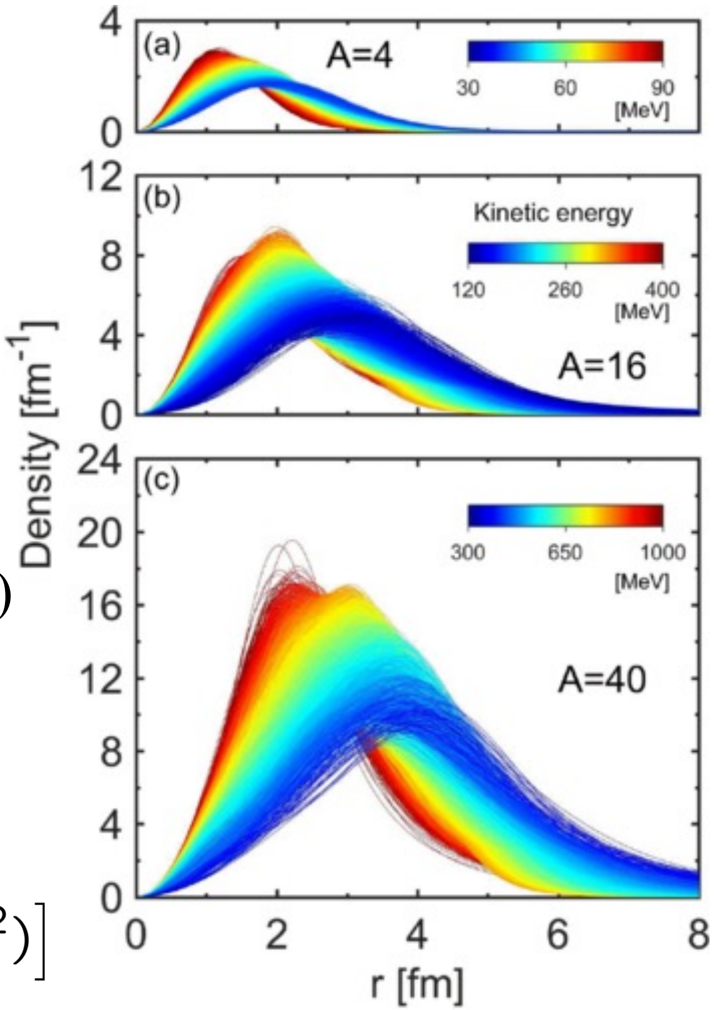
Kohn-Sham eq. with a single-particle random potential

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{\mathrm{rand}}(r)\right)\varphi_i(\boldsymbol{r}) = \epsilon_i\varphi_i(\boldsymbol{r})$$

✓ systems: ^{4}He, ^{16}O, ^{40}Ca without Coulomb

✓ 30,000 (= 3 x 10,000) training sets
  → $E_{\mathrm{kin}}[\rho_i]$ (see the right figure)



➡ machine learning (Kernel Ridge Regression)

$$E_{\mathrm{kin}}[\rho] = \sum_{i=1}^{30,000} w_i K(\rho_i, \rho)$$

$$K(\rho_i, \rho) = \exp\left[-||\rho_i(\boldsymbol{r}) - \rho(\boldsymbol{r})||^2/(2A_i A\sigma^2)\right]$$

Applications of machine learning to OF-DFT

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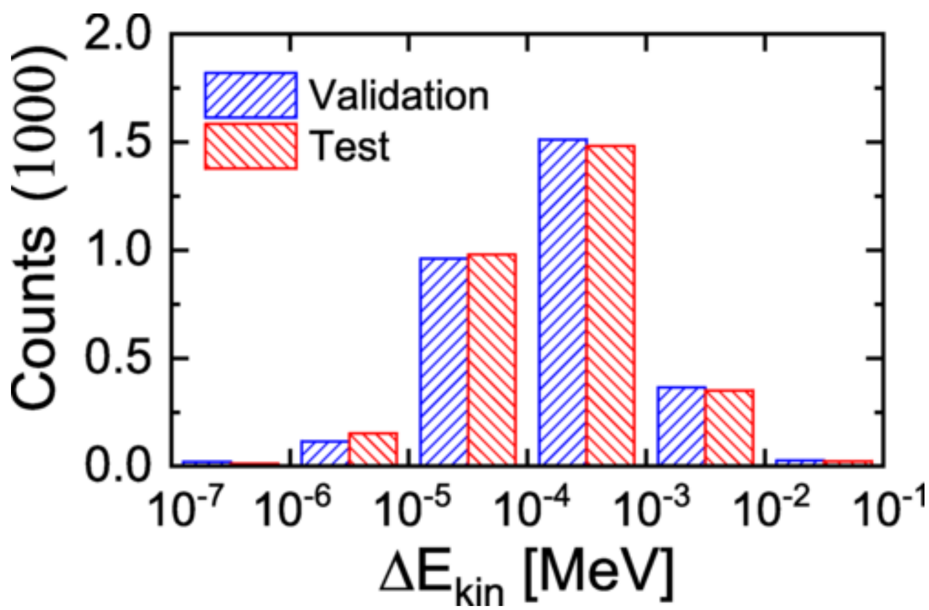
$$E_{\rm kin}[\rho] = \sum_{i=1}^{30,000} w_i K(\rho_i, \rho) \qquad K(\rho_i,\rho) = \exp\left[-||\rho_i(\boldsymbol{r}) - \rho(\boldsymbol{r})||^2/(2A_iA\sigma^2)\right]$$

a loss function to determine the hyper parameters

$$L(\boldsymbol{w}) = \sum_{i=1}^{m} (E_{\rm kin}^{\rm ML}[\rho_i] - E_{\rm kin}[\rho_i])^2 + \lambda ||\boldsymbol{w}||^2$$

σ, λ → minimization with
3,000 (=3x1,000) validation sets

✓ test sets: 3,000 (=3x1,000)



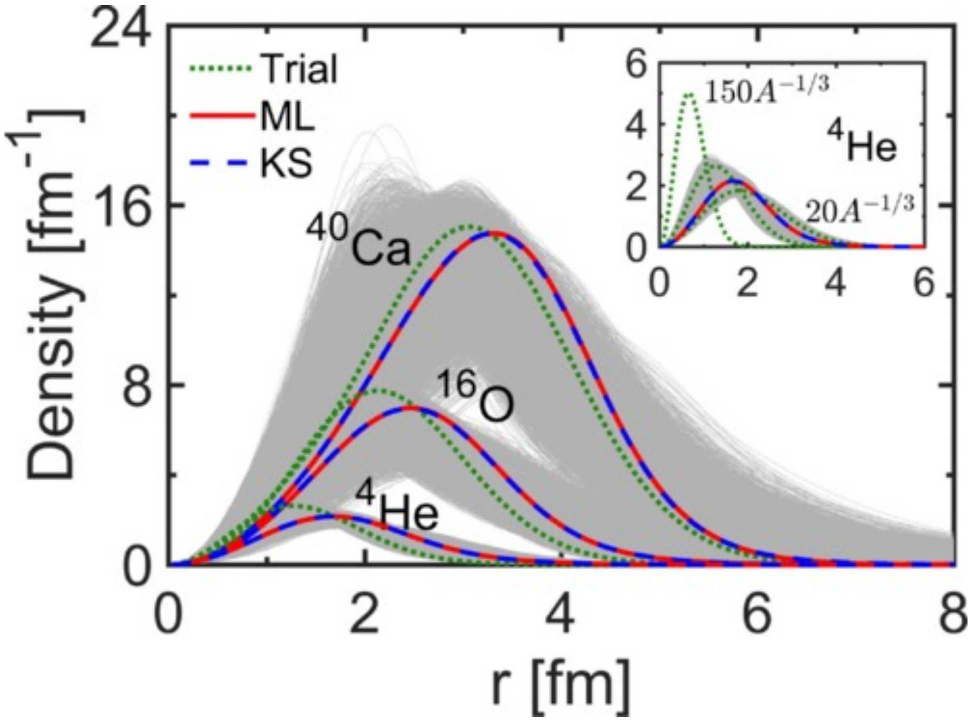
Applications of machine learning to OF-DFT

Test with $E[\rho] = E_{kin}^{ML}[\rho] + E_{int}[\rho]$

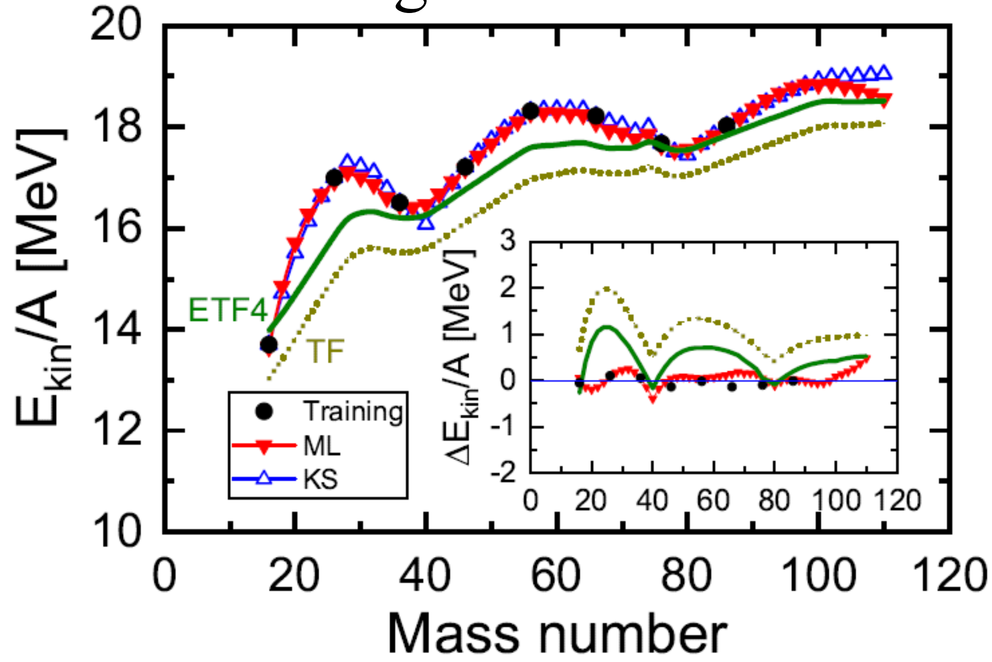
→ Skyrme functional (ρ-terms only)

$$\mathcal{E}_{\rm int} = \frac{3}{8}t_0\rho(\boldsymbol{r})^2 + \frac{t_3}{16}\rho(\boldsymbol{r})^{\alpha+2} + \frac{1}{64}(9t_1 - 5t_2 - 4t_2x_2)(\boldsymbol{\nabla}\rho(\boldsymbol{r}))^2$$

$$\rho_{n+1} = \rho_n - \epsilon\frac{\delta E_{\rm tot}[\rho]}{\delta\rho}$$



training with more nuclei



Applications of machine learning to OF-DFT

2. “Analysis of a Skyrme energy density functional with deep learning”
   N. Hizawa, K. Hagino, and K. Yoshida, PRC108, 034311 (2023).

Towards a mapping from a full Skyrme EDF to OF-DFT

$$
\begin{aligned}
E_{\mathrm{Sk}} &= E[\tau, \rho, \boldsymbol{\nabla}\rho, \boldsymbol{\nabla}^2\rho, \boldsymbol{J}] \\
E_{\mathrm{pair}} &= E[\rho_{\mathrm{pair}}]
\end{aligned}
$$

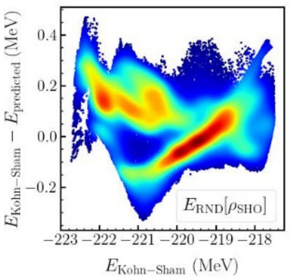
One needs to construct: $E_{\mathrm{SkHFB-OFDFT}} = E[\rho]$

Deep Learning?

Skyrme Kohn-Sham with random external potentials

training

$$E = E_{\mathrm{sk}} + E_{\mathrm{ext}}(i) \rightarrow \{\rho_i, E_i,\} \rightarrow E[\rho]$$



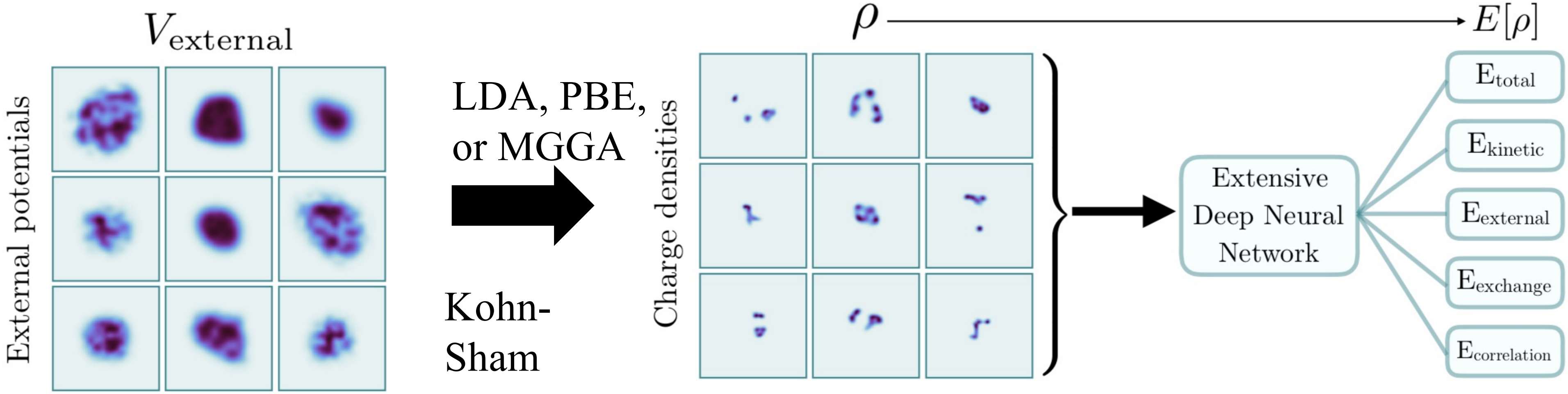
N. Hizawa, K. Hagino, and K. Yoshida,
PRC108, 034311 (2023) Editor’s suggestion.

Applications of machine learning to OF-DFT

N. Hizawa, K. Hagino, and K. Yoshida, PRC108, 034311 (2023).

A similar work for multi-electron systems:

K. Ryczko, D.A. Strubbe, and I. Tamblyn, PRA100, 022512 (2019).



→ application to a nuclear system (Hizawa, Hagino, Yoshida)

$$E_{\rm int} = E_{\rm Sk}[\tau, \rho, \boldsymbol{J}] + E[\rho_{\rm pair}]$$

red: nuclear systems

Applications of machine learning to OF-DFT

N. Hizawa, K. Hagino, and K. Yoshida, PRC108, 034311 (2023).

Skyrme EDF + random external potentials

- ^{24}Mg with SLy4 + DDDI (BCS)
- axial symmetry, no Coulomb
- Kohn-Sham with 2D mesh

$\rightarrow \rho_{ij} = \rho(r_i, z_j)$ i: 1-10, j: 1-20 $\rightarrow$ 200 mesh points

- external potentials
  - ✓ an axial harmonic oscillator
  - ✓ a spatially random potential + smearing

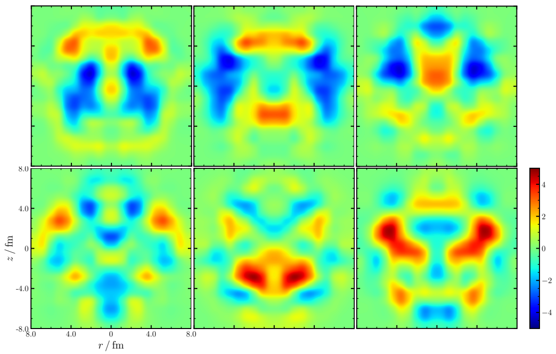
⇨ $V_k^{(\mathrm{ext})} \longrightarrow \{\rho^{(k)}, E_k\}$

$k = 1 - 250{,}000$ { 90% for training data; 10% for test data }

Applications of machine learning to OF-DFT

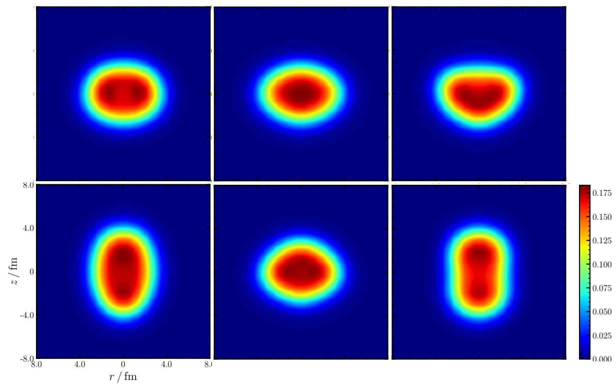
N. Hizawa, K. Hagino, and K. Yoshida, PRC108, 034311 (2023).

external potentials



KS

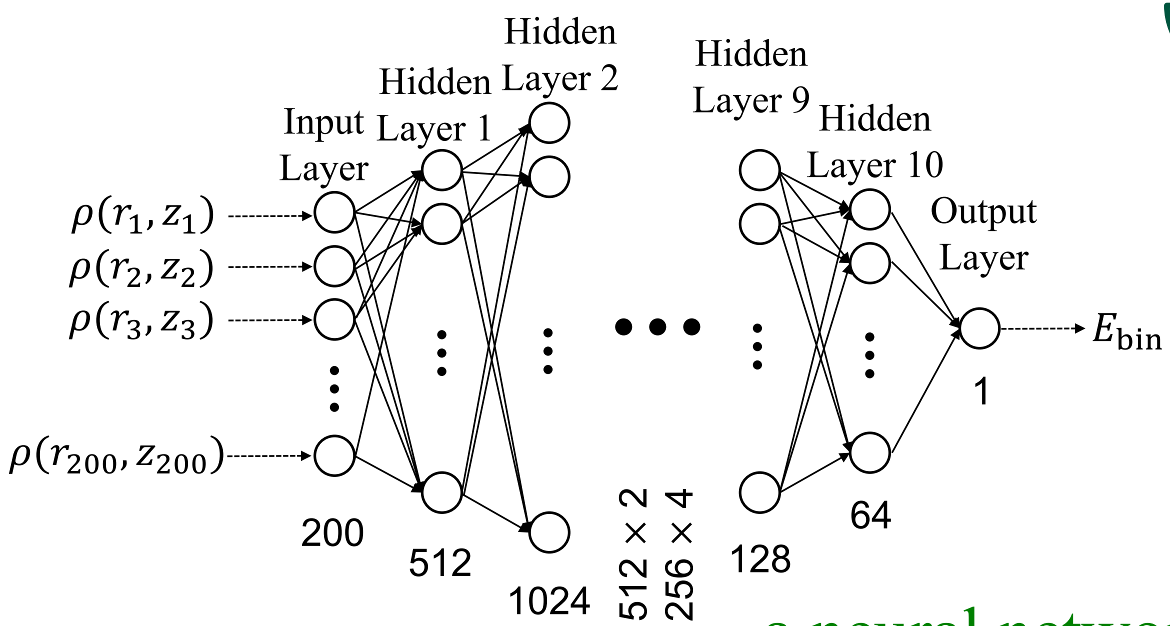
densities



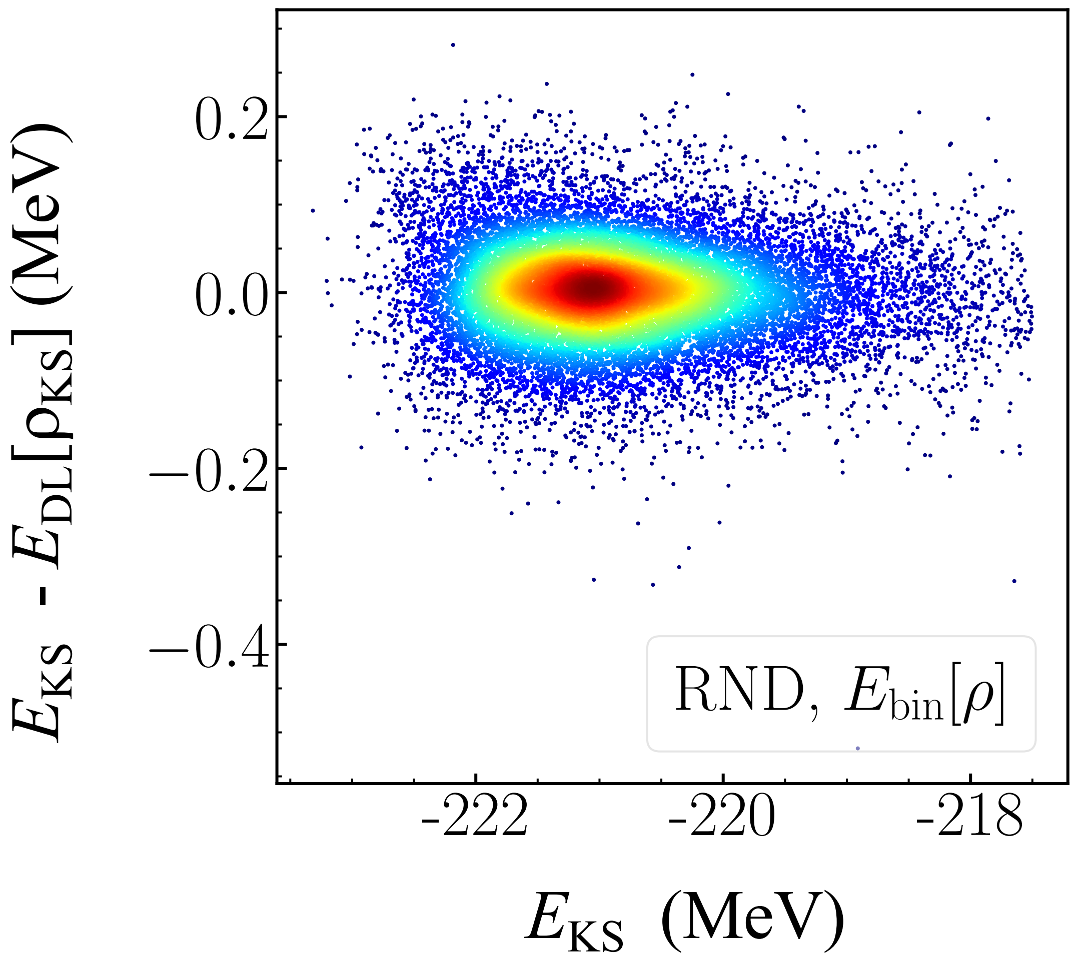
\+

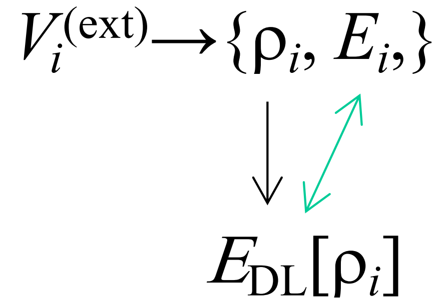
$$E_{\mathrm{kin}}[\tau]$$
$$E_{\mathrm{int}}[\rho, \tau, \boldsymbol{J}]$$
$$E_{\mathrm{pair}}[\rho, \tilde{\rho}]$$
$$E_{\mathrm{external}}[\rho]$$
$$E_{\mathrm{bind}}[\rho, \tau, \boldsymbol{J}, \tilde{\rho}]$$

deep learning



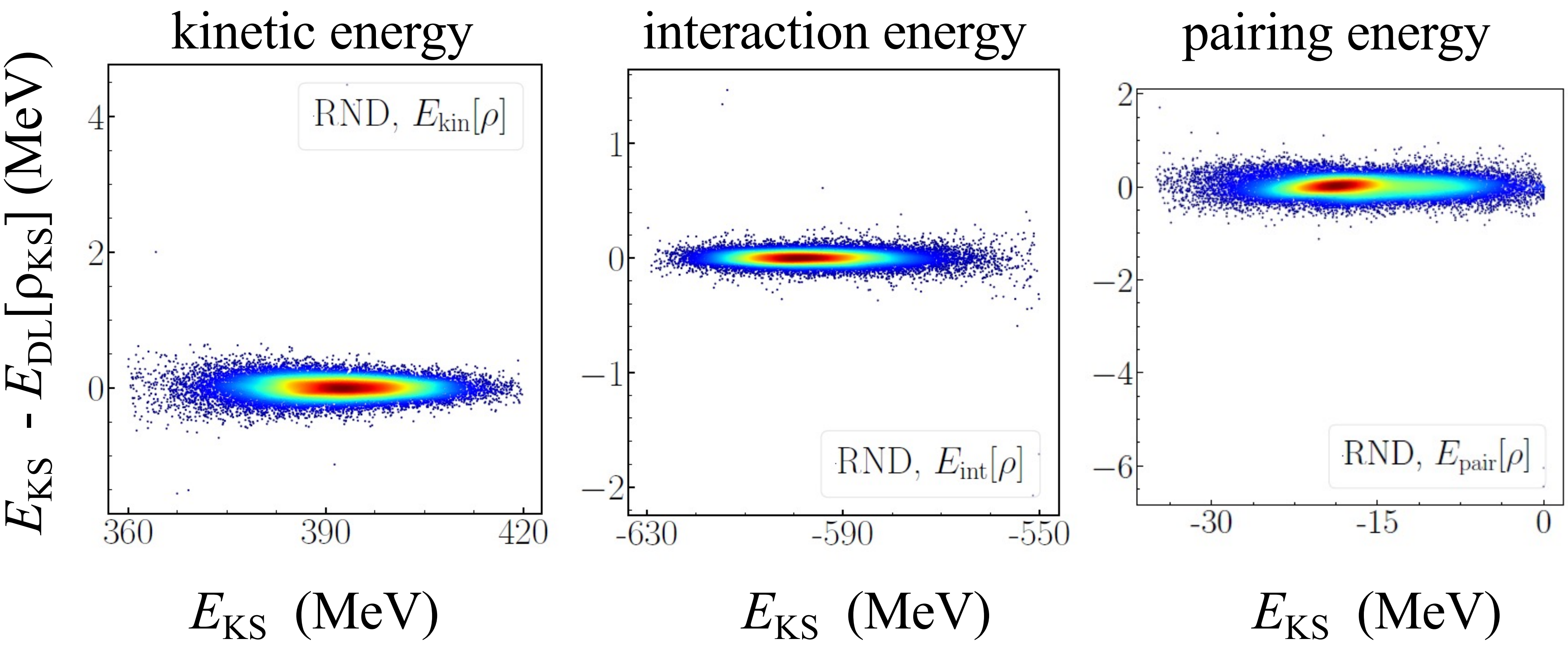
a neural network with fully connected layers performance for the test data (the total binding energy)





$E_{DL}[\rho]$ which reproduced the original E_{KS} within 0.04 MeV

N. Hizawa, K. Hagino, and K. Yoshida,
PRC108, 034311 (2023) Editor's suggestion.



MAE = 0.11 MeV MAE = 0.043 MeV MAE = 0.16 MeV

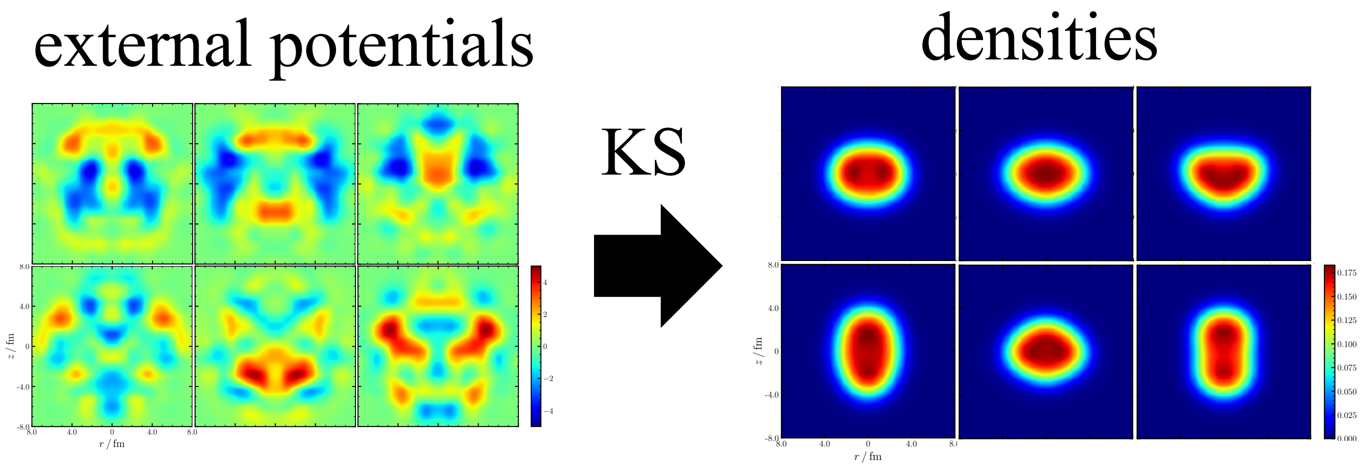
HO external potentials:

MAE = 0.0165 MeV MAE = 0.0105 MeV MAE = 0.0233 MeV

(note) MAE for E_{tot} = 0.0433 MeV (RND), 0.0051 MeV (SHO)

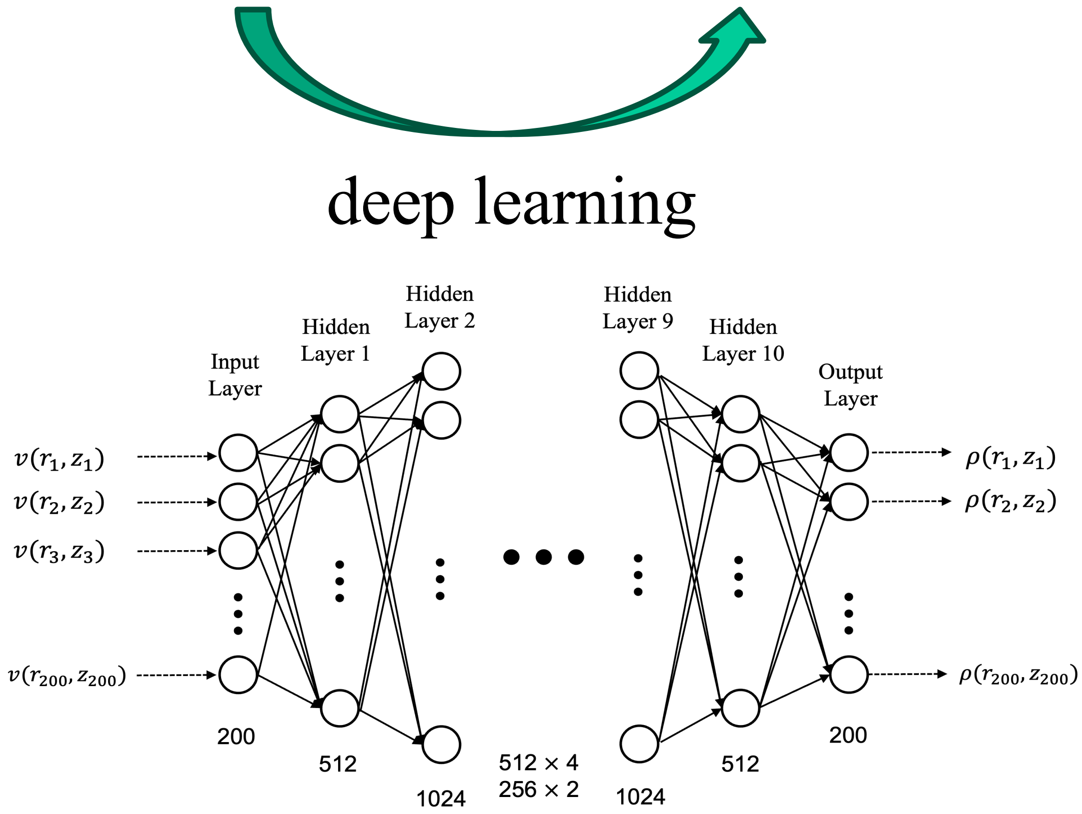
* MEA = Mean Absolute Error

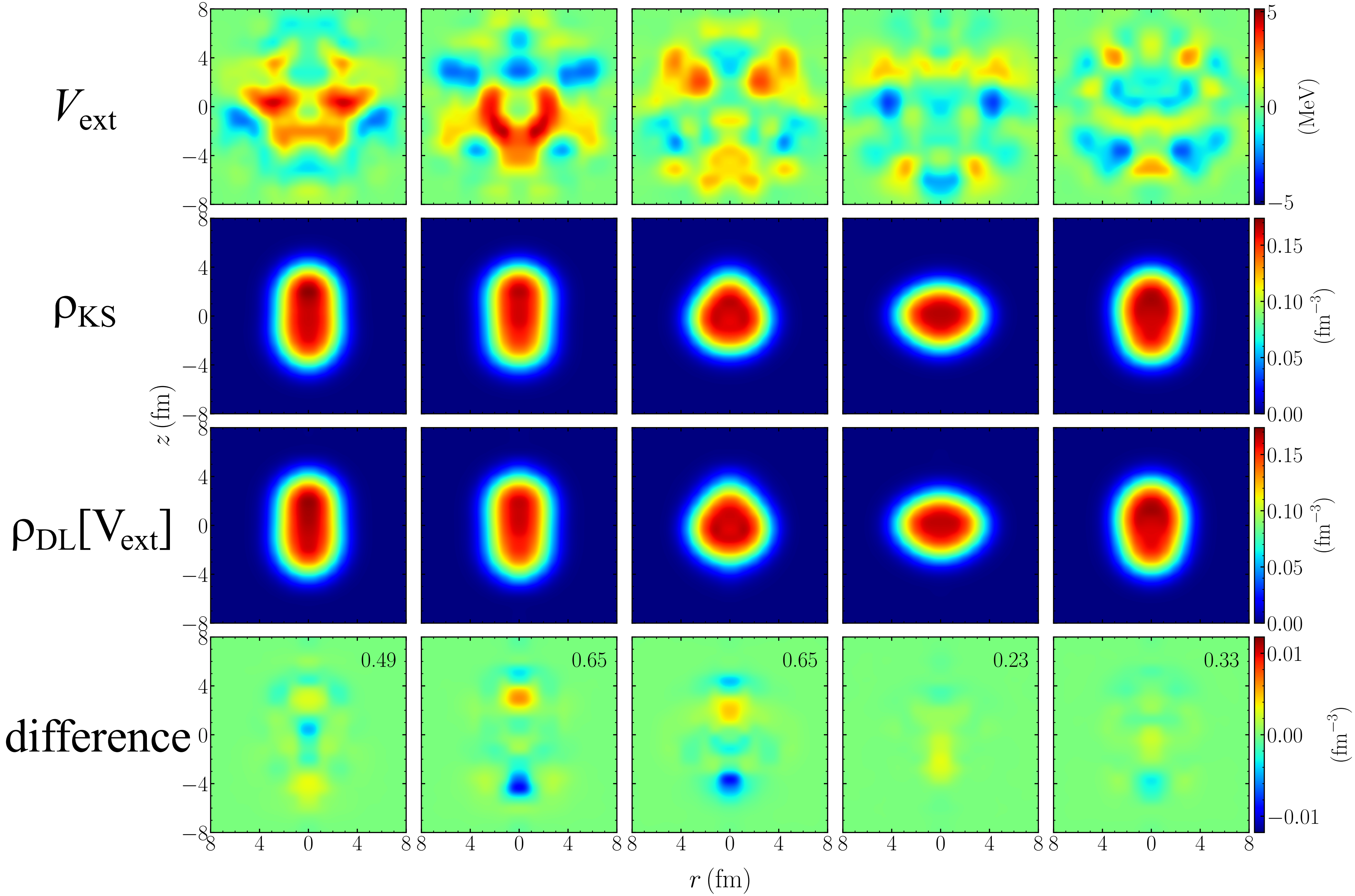
from external potential to ρ



$+$

$$E_{\text{kin}}[\tau]$$
$$E_{\text{int}}[\rho, \tau, \boldsymbol{J}]$$
$$E_{\text{pair}}[\rho, \tilde{\rho}]$$
$$E_{\text{external}}[\rho]$$
$$E_{\text{bind}}[\rho, \tau, \boldsymbol{J}, \tilde{\rho}]$$





V_{ext}
ρ_{KS}
$\rho_{DL}[V_{ext}]$
difference
z (fm)
r (fm)
(MeV)
(fm^{-3})
0.49
0.65
0.65
0.23
0.33

Summary 1: conventional OF-DFT

- OF-DFT: reasonable approximation both for Coul. and Nucl. systems
- OF-DFT: simpler than KS.   cf. an application to ^{1800}Sn
- OF-DFT + Extended Thomas-Fermi
  - ✓ reasonably good, but may have a problem in ρ (in the tail region)
  - ✓ a prescription: to modify the coefficients in ETF
- OF-DFT + 1 KS iteration
  - ✓ good both for E_{gs} and ρ
  - ✓ weak dependence on the coefficients in ETF
- Spin-orbit interaction
  - ✓ seems to restore (a part of) shell effects

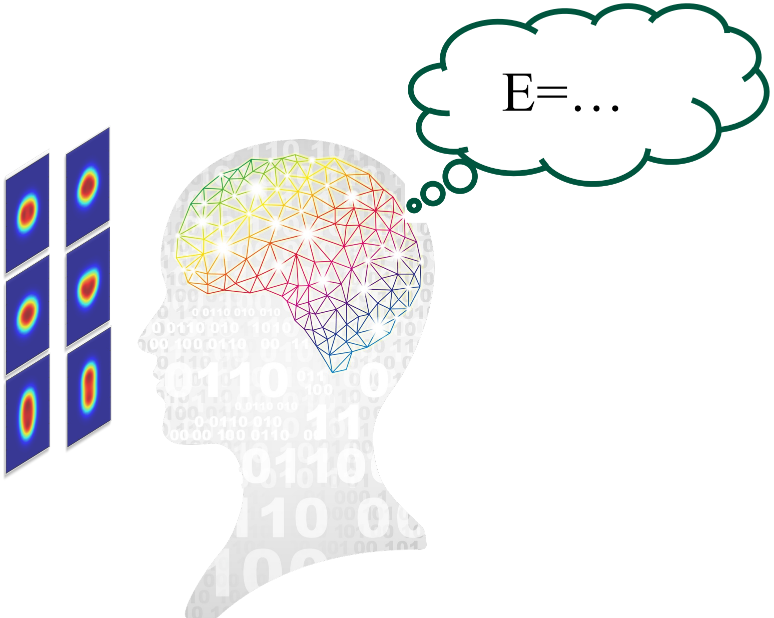
Future challenges

- ◆ full Skyrme functional
- ◆ deformation property

Summary 2: Machine/Deep learning for OF-DFT

- Machine Learning for E_{kin}
  - ✓ an accurate and a global (hopefully) functional
- Deep Learning for Skyrme functional
  - ✓ a mapping from $E_{\mathrm{sk}}[\rho,\tau,J,\rho_{\mathrm{pair}}]$ to $E_{\mathrm{OF\text{-}DFT}}[\rho]$
  - ✓ $\{\rho_i, E_i,\}$ with random external fields
  - ✓ for ^{24}Mg with SLy4 → successful within 0.04 MeV

a promising tool

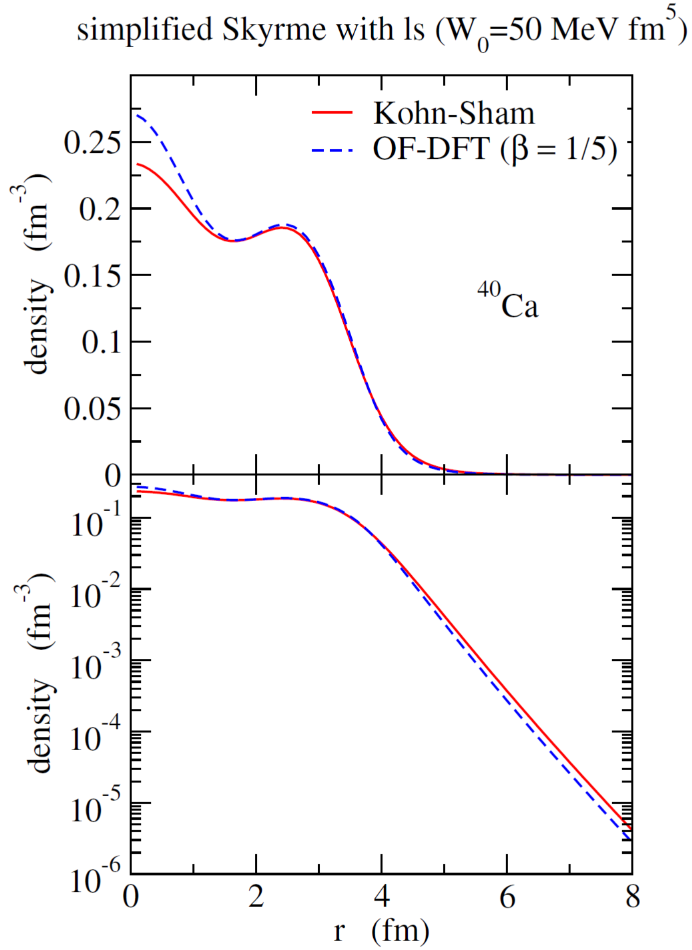


Future challenges

◆ a global functional

◆ deformation property (fission barrier,….)

^{40}Ca	E_{tot} (MeV)	Rms radius (fm)
exact (KS)	-510.54	3.098
OF-DFT (β = 1/9)	no convergence	no convergence
OF-DFT (β = 1/5)	-515.37	3.029



^{80}Zr	E_{tot} (MeV)	Rms radius (fm)
exact (KS)	-1063.43	3.845
OF-DFT (β = 1/9)	no convergence	no convergence
OF-DFT (β = 1/5)	-1085.67	3.800