1. A short comment on GCM
2. Orbital-Free DFT

K. Hagino (Kyoto University)

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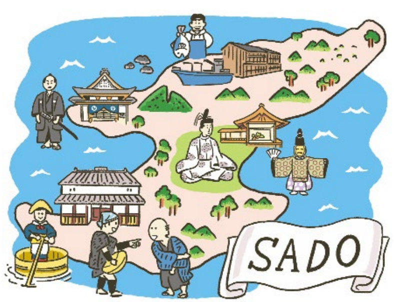
3. Deep-learning for OF-DFT
4. Summary



The 6th workshop on many-body correlations in microscopic nuclear models, Sado, September 28-30, 2023

A short comment on GCM

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M. Matsumoto (Tohoku University, D2)
Y. Tanimura (Soongsil University, Seoul)

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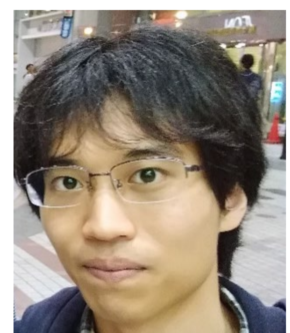


M. Matsumoto, Y. Tanimura, K.H., arXiv: 2308.13233

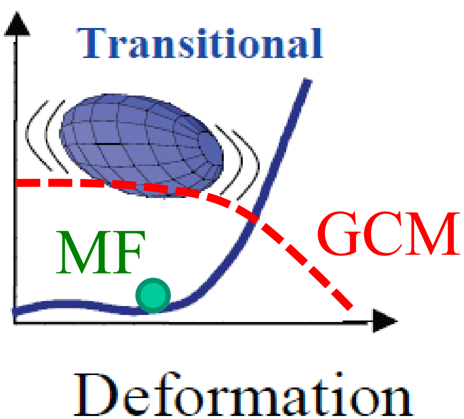
A short comment on GCM

An ansatz of the Generator Coordinate Method (GCM)

$$|\Psi\rangle = \int dQ\, f(Q)|\Phi_Q\rangle$$

$$\delta\langle\Phi_Q|H - \lambda\hat{Q}|\Phi_Q\rangle = 0$$

a SD for the local g.s.



determined variationally
($\rightarrow$ Hill-Wheeler equation)

"beyond mean-field" (BMF) method

We question: to what extend does this ansatz hold?

M. Matsumoto, Y. Tanimura, K.H., arXiv: 2308.13233

The Optimized GCM (OptGCM)

M. Matsumoto, Y. Tanimura, K.H., arXiv: 2308.13233

the conventional GCM:

$$|\Psi\rangle = \int dQ\, f(Q)|\Phi_Q\rangle$$

variational　　pre-fixed (CHF/CHFB)

usually: local g.s. at Q

the OptGCM:

$$|\Psi\rangle = \int dQ\, f(Q)|\Phi_Q\rangle$$

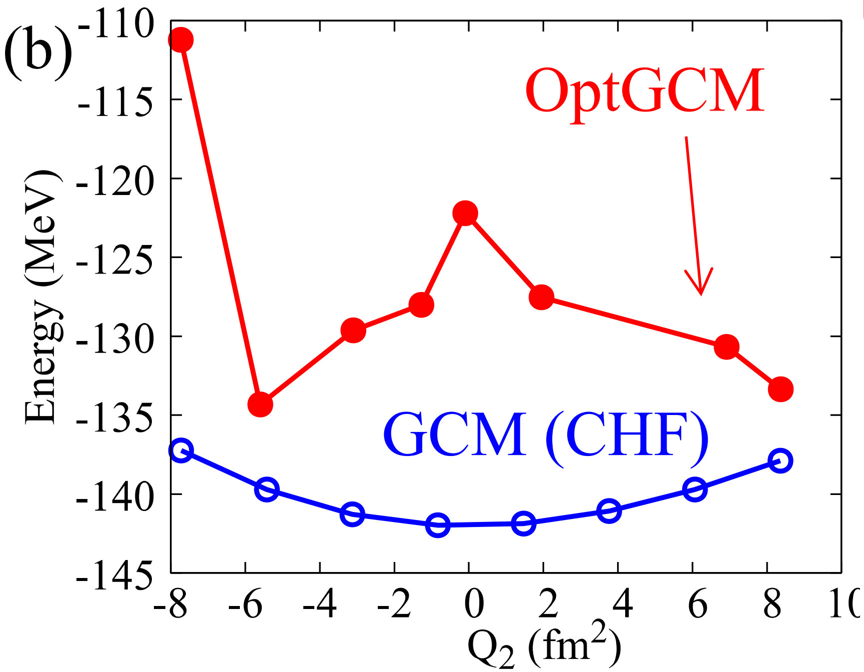
variational　　variational

The Optimized GCM (OptGCM)

M. Matsumoto, Y. Tanimura, K.H., arXiv: 2308.13233

results for ^{16}O with SIII

$\langle \Phi_a | H | \Phi_a \rangle$



E_{HF} = -142.024 MeV
E_{GCM} = -142.407 MeV
E_{OptGCM} = -143.109 MeV

a superposition of local g.s.
→ not optimum

$E_{\mathrm{g.s.}}$: decreases by including excited state configuraitons

↑

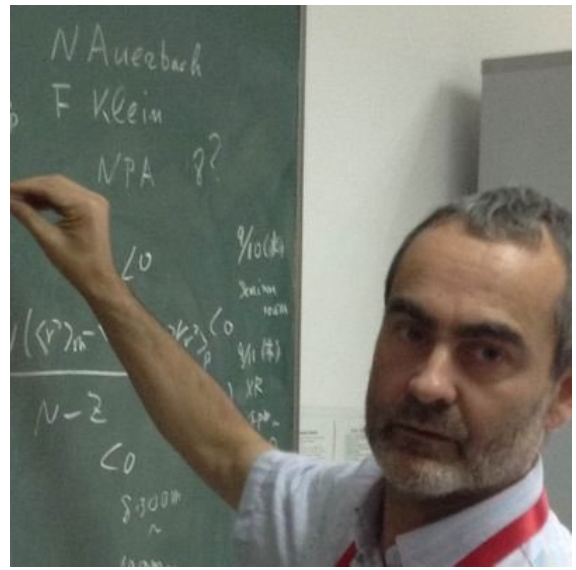
even though $\langle \Phi_a | H | \Phi_a \rangle > \langle \Phi_a^{(0)} | H | \Phi_a^{(0)} \rangle$

$|\langle \Phi_a | H | \Phi_b \rangle| > |\langle \Phi_a^{(0)} | H | \Phi_b^{(0)} \rangle|$

* also for N_{ab}

Orbital Free DFT

K. Hagino (Kyoto University)
Gianluca Colo (U. of Milano/YITP)



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YITP YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

Gianluca Colo: 2022.12 – 2023.2 at YITP as a visiting professor

G. Colo and K. Hagino,
PTEP in press. arXiv: 2308.00357

Density Functional Theory

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

Kohn-Sham scheme (“orbital-based” DFT)

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

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

A simpler approach: orbital-free DFT

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

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

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

the extended Thomas-Fermi approximation

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

$$\alpha = \frac{3}{5}(3\pi^2)^{2/3}, \quad \beta = \frac{1}{9}$$

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

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

electron systems: β → a free parameter

popular choices: β = 1/9, 1/5, 1

Nuclear systems:

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

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

- 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?

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)

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

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

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

neutrons only, with N=8

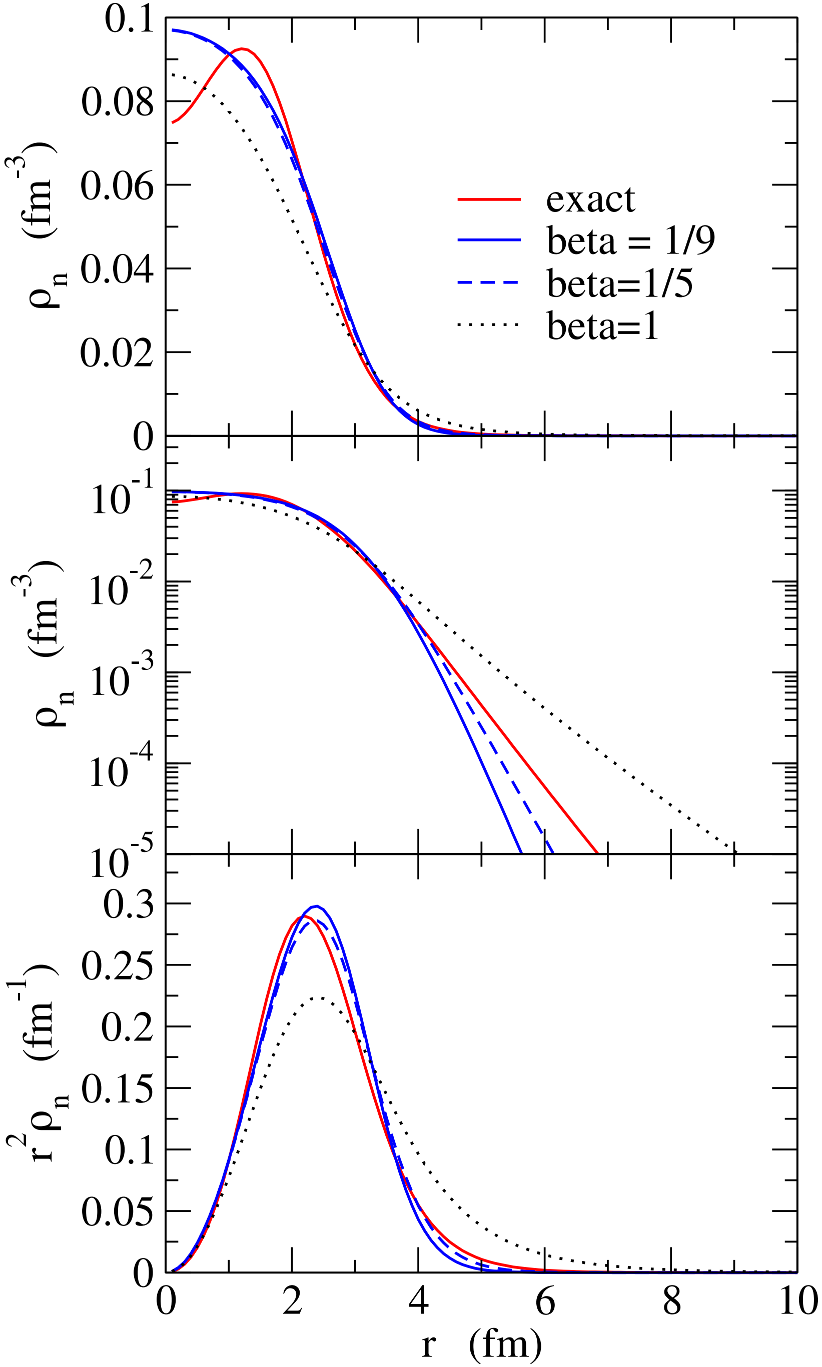
e($1s_{1/2}$) = -32.6 MeV, e($1p_{3/2}$) = e($1p_{1/2}$) = -16.8 MeV

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

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

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

$$\rightarrow E = \int d\boldsymbol{r}\left(\frac{\hbar^2}{2m}\tau[\rho_{\mathrm{OF-DFT}}(\boldsymbol{r})] + V(\boldsymbol{r})\rho_{\mathrm{OF-DFFT}}(\boldsymbol{r})\right)$$



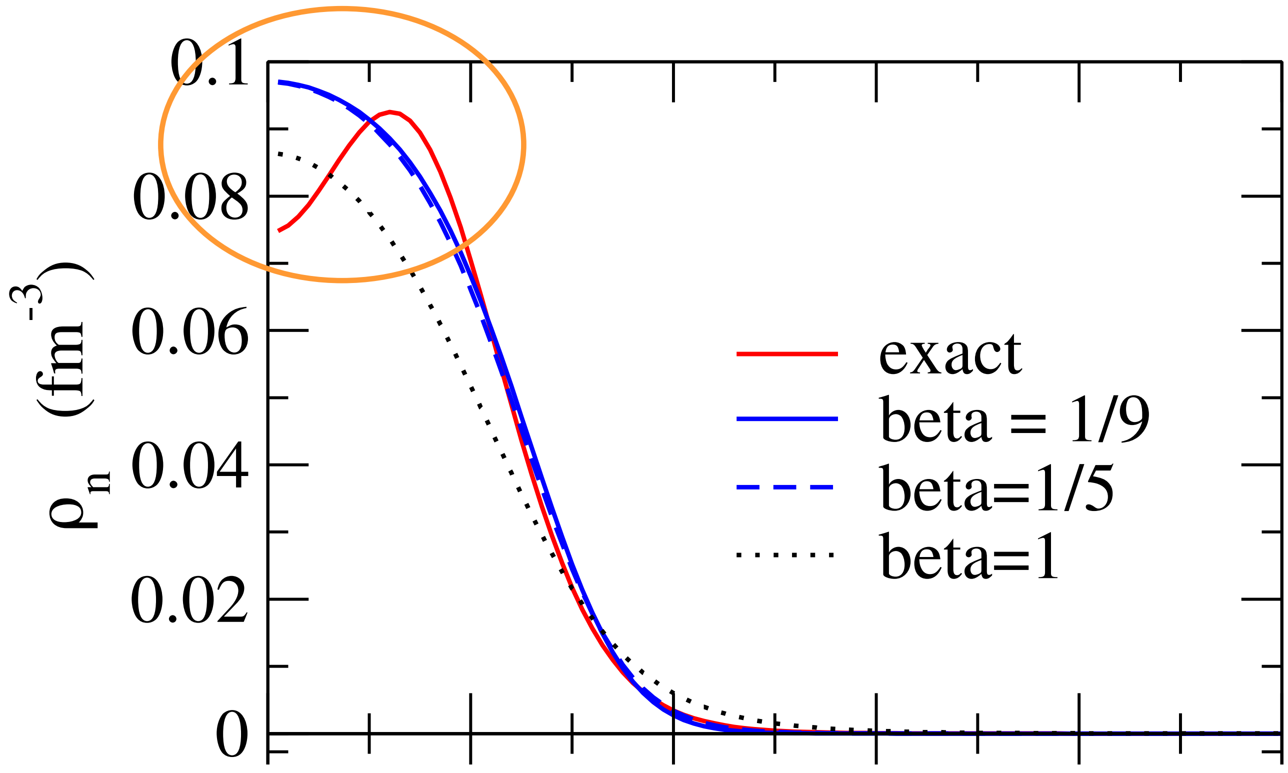
	E_{tot} (MeV)	Rms radius (fm)
exact	-142.27	2.575
$\beta = 1/9$	-140.85	2.500
$\beta = 1/5$	-135.19	2.562
$\beta = 1$	-96.31	3.12

- ✓ 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

$r \rightarrow \beta$=1/5 is slightly better 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).

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)

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

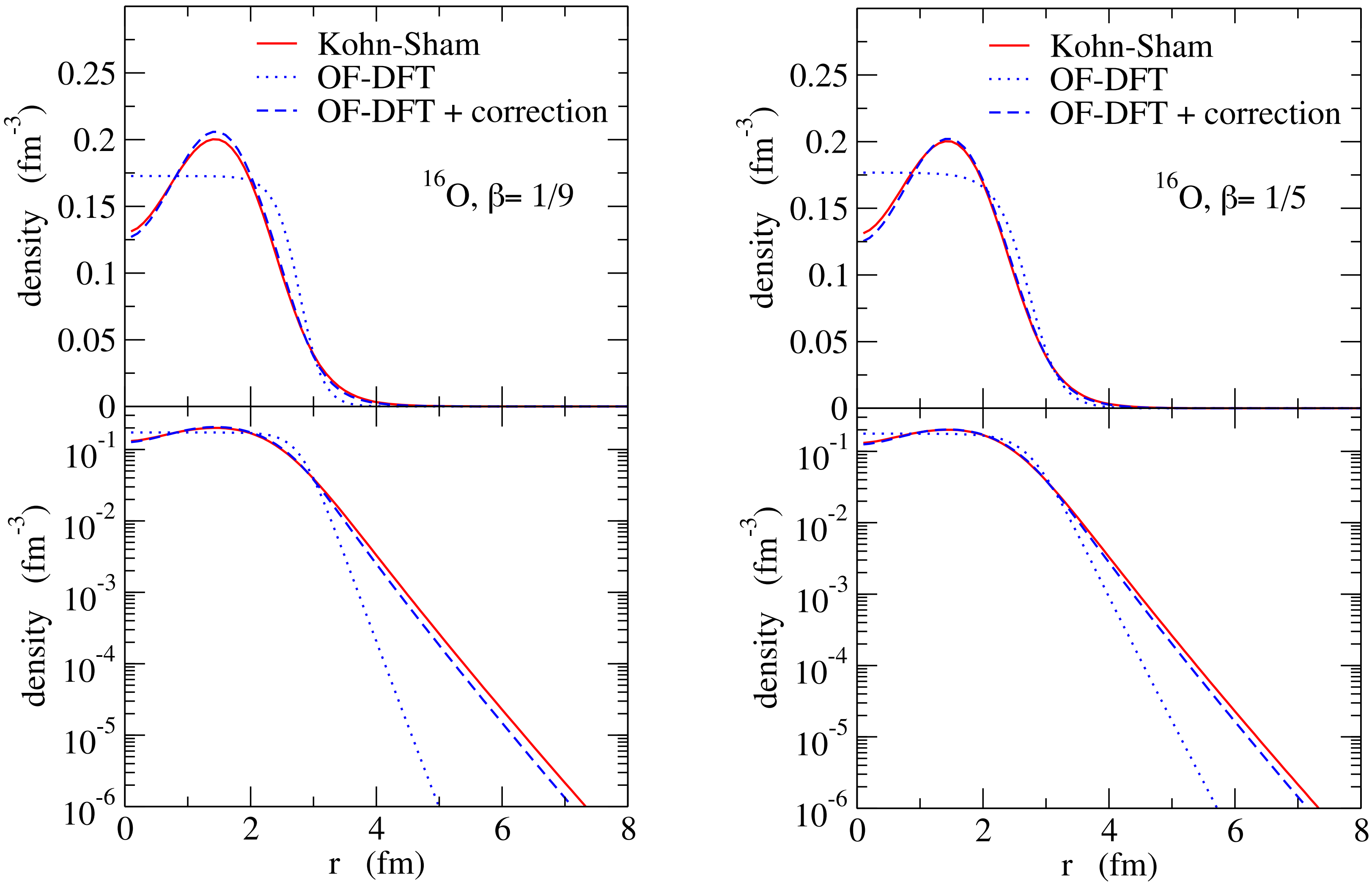
^{16}O	E_{tot} (MeV)	Rms radius (fm)
exact	-187.6	2.364
OF-DFT (β = 1/9)	-201.2	2.253
OF-DFT (β = 1/5)	-180.4	2.296
OF-DFT+corr. (β = 1/9)	-186.6	2.317
OF-DFT+corr. (β = 1/5)	-187.2	2.339

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

[shell corrections?](#)

OF-DFT + 1 more iteration with KS

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



Deep Learning for OF-DFT

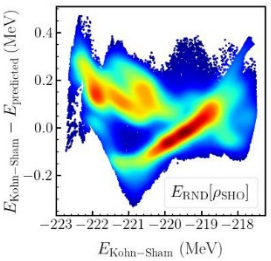
Towards a mapping from a full Skyrme EDF to OF-DFT

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

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

Deep Learning?

$$\{\rho_i, E_i,\} \rightarrow E[\rho]$$



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

Deep Learning for OF-DFT

Skyrme EDF + a random external potential

✓ an axial HO
✓ a spatially random potential + smearing

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

$$k = 1 - 250{,}000$$

$$\left\{ \begin{array}{l} \text{90\% for training data} \\ \text{10\% for test data} \end{array} \right.$$

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

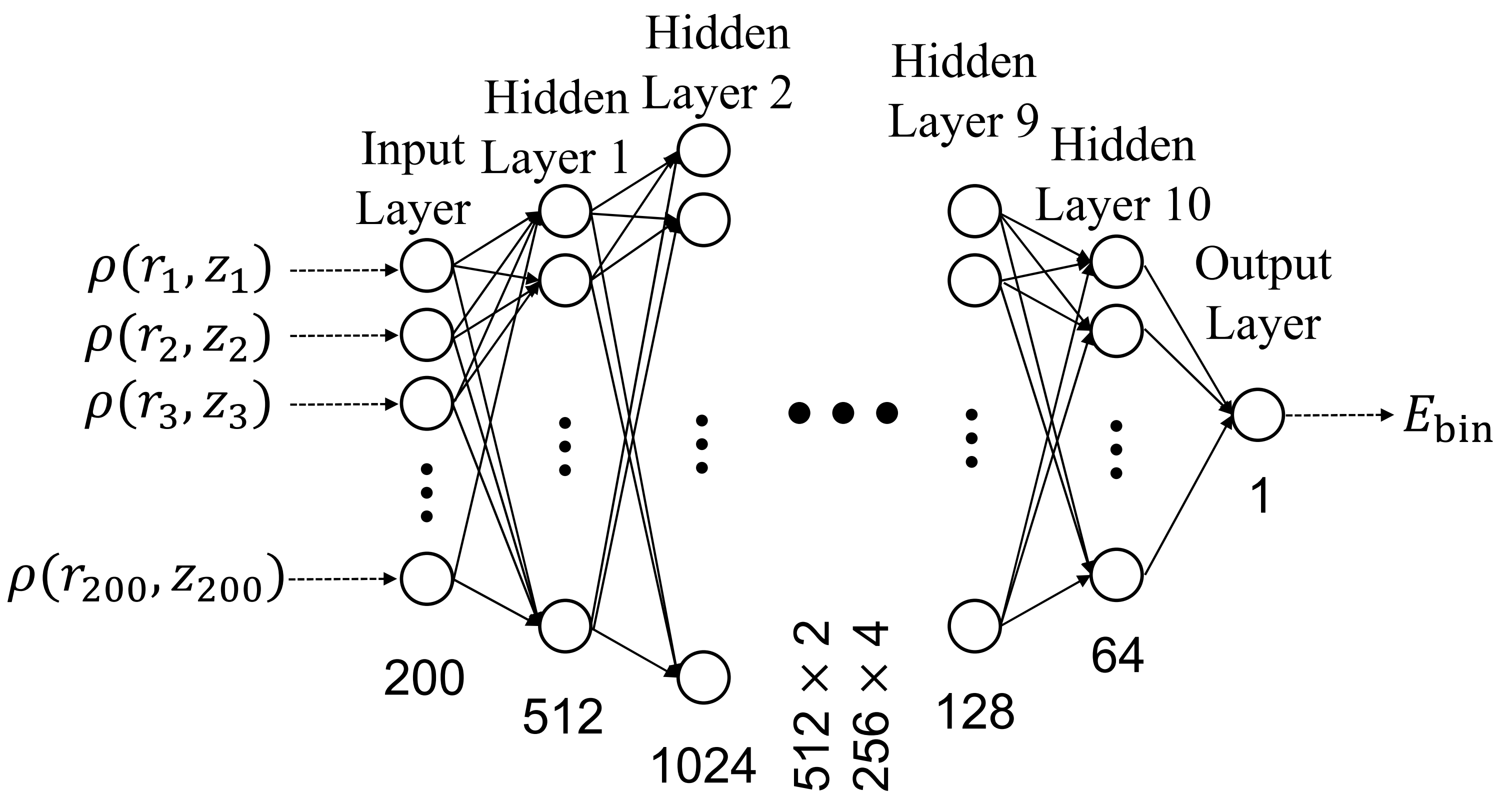
$$\rightarrow \rho_{ij} = \rho(r_i, z_j)$$

i: 1-10, j: 1-20 → 200 mesh points

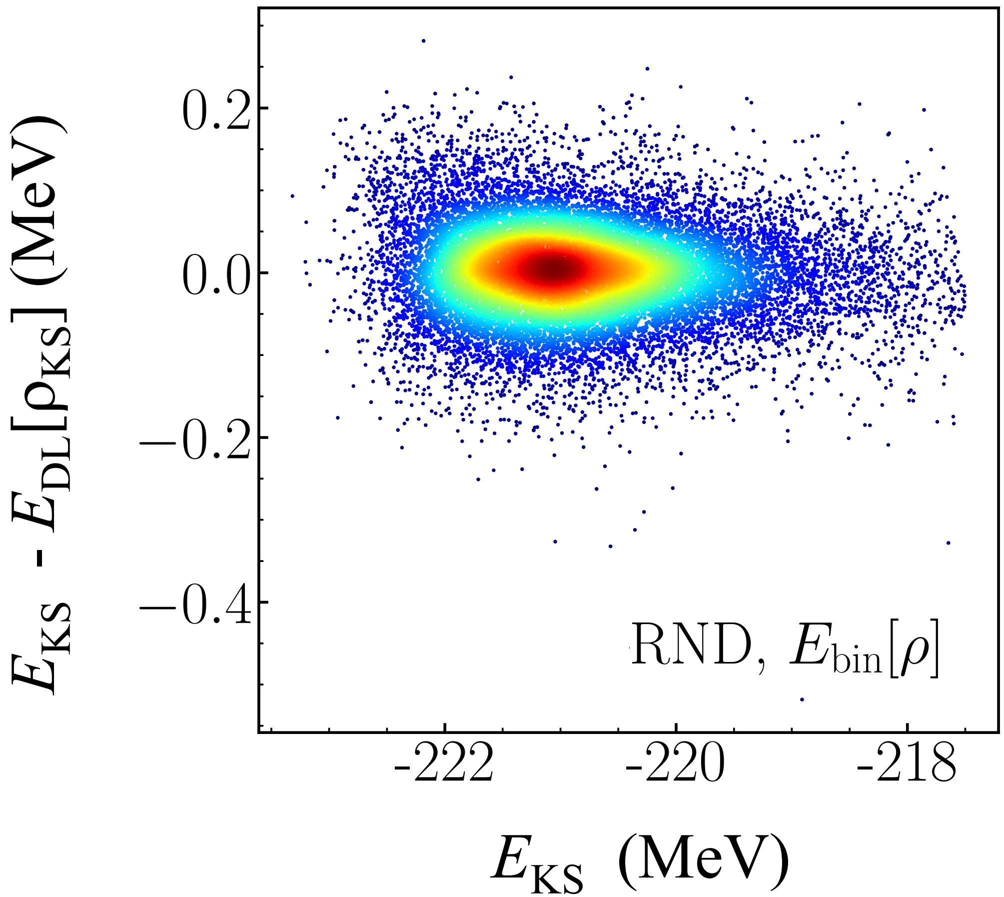
- Skyrme + a random external potential

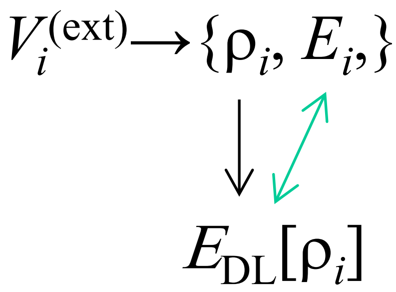
$$V_k^{(\mathrm{ext})} \longrightarrow \rho_{ij}^{(k)},\ E_k \qquad k = 1 - 250{,}000,\ (\mathrm{i,j}) = 1\text{-}200$$

$$\begin{cases} \text{90\% for training data} \\ \text{10\% for test data} \end{cases}$$



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





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

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

Summary

- GCM: a linear superposition of local ground states → not sufficient
  OptGCM: variationally determines both $f(Q)$ and SD

- OF-DFT + Extended Thomas-Fermi→ fast computation cf. ^{1700}Sn
  - ✓ 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

- Deep Learning for OF-DFT
  - ✓ a mapping from $E_{sk}[\rho,\tau,J,\rho_{pair}]$ to $E_{OF\text{-}DFT}[\rho]$
  - ✓ $\{\rho_i, E_i,\}$ with random external fields
  - ✓ for ^{24}Mg with SLy4 → successful within 0.04 MeV

a global $E_{OF\text{-}DFT}[\rho]$? → a future challenge