A first step in the nuclear inverse Kohn-Sham problem: from densities to potentials

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Density Functional Theory

- A successful approach in facing the problem of many interacting fermions is based on **Density Functional Theory** (DFT)

- **Hohenberg – Kohn theorems**

→ The **basic variable** for describing **ground state** properties is not the full many-body g.s. wave function $|\Psi\rangle$, but the much simpler **density** $\rho(\boldsymbol{r})$

$$\rho(\boldsymbol{r}) = \langle\Psi|\hat{\rho}(\boldsymbol{r})|\Psi\rangle$$

$$E[\rho] = \langle\Psi|\hat{H}|\Psi\rangle$$

→ The energy is a **functional** of the density $E[\rho]$ and the exact g.s. density ρ_{gs} minimizes *E*

$$E_{gs} = \min_{\rho(\boldsymbol{r})} E[\rho(\boldsymbol{r})] = E[\rho = \rho_{gs}]$$

- The **exact** energy functional is **not known** → approximated or phenomenological functionals

R. G. Parr and W. Yang, Density-functional theory of atoms and molecules

Nuclear Energy Density Functionals (EDF)

- A successful strategy in nuclear physics is based on building **phenomenological EDF** $E[\rho]$
- They depend on different types of **density** (number, spin, isoscalar/isovector…)
- They include ≈10 free parameters **fitted** to experimental data
- Examples: Skyrme (local) and Gogny (finite range) interactions

- **Limitations** → **no** clear way for **systematic improvement** of the EDF

N. Schunck, Energy Density Functional Methods for Atomic Nuclei

Exploring a different strategy

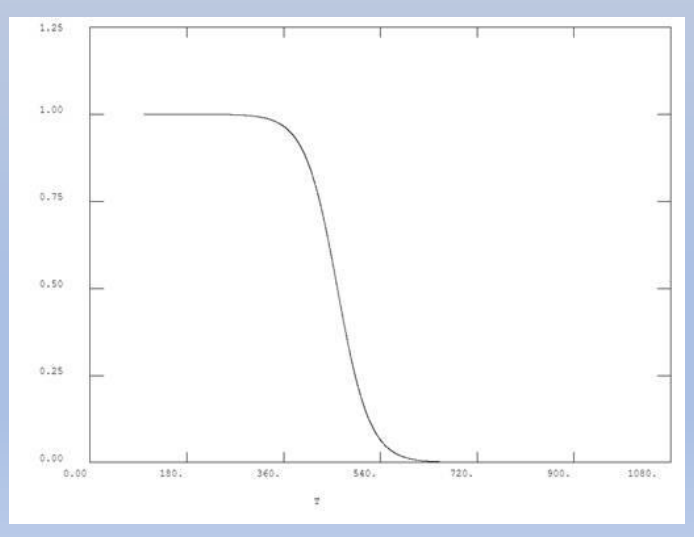
Hohenberg-Kohn theorems establish a **biunivocal** correspondence between the ground state **density** $\boldsymbol{\rho(r)}$ and effective single-particle **potential** $\boldsymbol{U(r)}$

Direct problem

Given an expression for the **energy** $E[\rho]$,
determine the ground state **density** $\rho(\boldsymbol{r})$

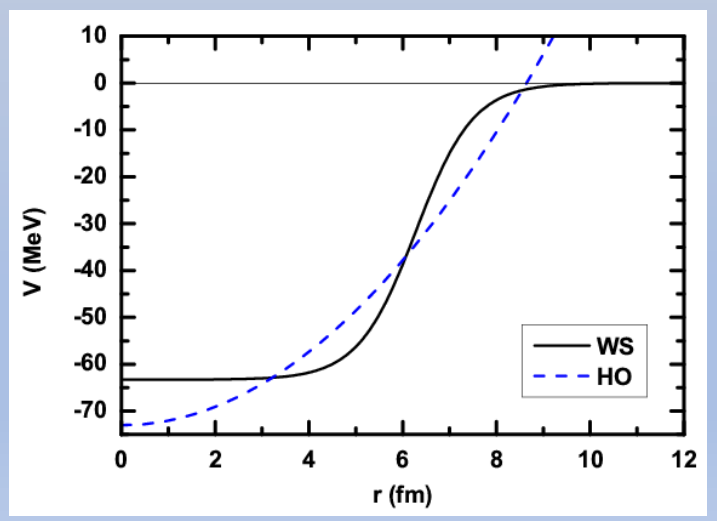
Inverse problem

Given the ground state **density** $\boldsymbol{\tilde{\rho}(r)}$,
determine the **potential** $U[\rho]$



Inverse

Direct



Kohn – Sham method

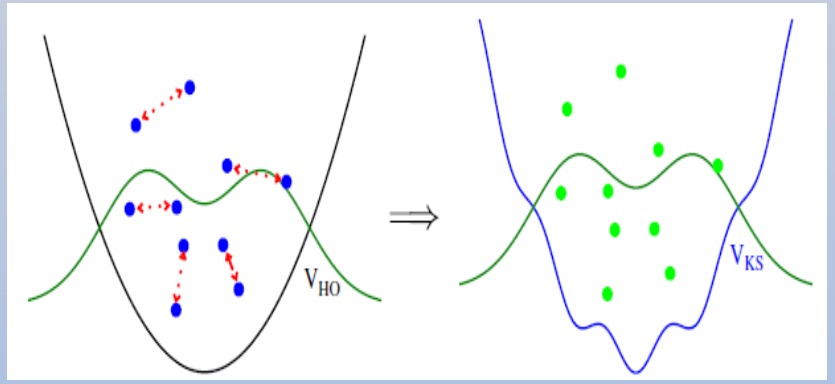
- K.-S. hypothesis: for every interacting system, ∃ a system of **independent** particles with the **same** g.s. **density** as the interacting one

- The problem can be restated in terms of **single-particle orbitals** $\{\phi_j(\boldsymbol{r})\}$ $\quad E_s[\rho] = T_s[\rho] + F[\rho]$

- The variational eq. $\frac{\delta E}{\delta \phi_j^*} = 0$ yields self-consistent Schrödinger eqs.

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{\delta F[\rho]}{\delta \rho}\right]\phi_j(\boldsymbol{r}) = \epsilon_j \phi_j(\boldsymbol{r})$$

$$\rho(\boldsymbol{r}) = \sum_j \left|\phi_j(\boldsymbol{r})\right|^2$$



- $U[\rho] \equiv \frac{\delta F[\rho]}{\delta \rho}$ is the **effective Kohn-Sham potential**

$$T_s[\phi_j] = \sum_j \int d\boldsymbol{r}\, \phi_j^*(\boldsymbol{r}) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \phi_j(\boldsymbol{r})$$

- The potential is unique given the g.s. density (and viceversa)

Assumptions

- We employ **proton and neutron densities** only. The KS potential is a function of only the **spatial coordinates:** $U[\rho] = U(\boldsymbol{r})$.
- Assume **spherical symmetry** for simplicity → study **doubly magic** nuclei
- The method gives the **KS potential** $U[\rho] = \frac{\delta F[\rho]}{\delta \rho}$.

Outline of the calculations

- We have applied **two methods** (**vLB** and **CV**) to the solution of inverse Kohn-Sham (IKS) problem
- We have tested on **Hartree-Fock** and **experimental densities** for ^{40}Ca and ^{208}Pb

G. Accorto et al., arxiv: 1908.03068 (2019)

Constrained Variational (CV) method

Minimize the kinetic **energy functional** $T_s[\phi_j(\boldsymbol{r})]$ where the orbitals $\phi_j(\boldsymbol{r})$ are subject to:

1. **Orthonormality** constraints $\quad G_{ij}[\phi_j(\boldsymbol{r})] \equiv \int d\boldsymbol{r}\, \phi_i^*(\boldsymbol{r})\phi_j(\boldsymbol{r}) = \delta_{ij}$
2. **Density** constraint $\quad \rho(\boldsymbol{r}) = \tilde{\rho}(\boldsymbol{r}) \;\; \forall \boldsymbol{r}$

- $\tilde{\rho}(\boldsymbol{r})$***: input density***
- $\rho(\boldsymbol{r})$***: theoretical density***
  $\rho(\boldsymbol{r}) = \sum_j |\phi_j(\boldsymbol{r})|^2$

Introduce **Lagrange multipliers** ϵ_{ij} and $U(\boldsymbol{r})$**.** The problem is equivalent to the free minimization of the **objective functional** $J[\{\phi_j\}]$:

$$J[\phi_j(\boldsymbol{r})] \equiv T_s[\phi_j(\boldsymbol{r})] + \int d\boldsymbol{r}\, \rho(\boldsymbol{r})\, U(\boldsymbol{r}) - \sum \epsilon_{ij} G_{ij}[\phi_j(\boldsymbol{r})]$$

$$\frac{\delta J\,[\{\phi_j\}]}{\delta \phi_k(\boldsymbol{r})} = 0$$

- *$U(\boldsymbol{r})$ has the meaning of* ***single particle potential***

D. S. Jensen and A. Wasserman, International Journal of Quantum Chemistry 118, e25425 (2018)

Constrained Variational (CV) method

- **Spherically symmetric** systems → one dimensional problem in *r*, **radial** wave functions $u_j(r)$
- The constrained minimization of $T_s[u_j(r)]$ is carried out **numerically** using the **IPOPT** library → $u_j(r)$
- Convergence criteria → relative tolerance on constraints; tolerance on the value of the objective function
- $\delta J/\delta\phi_k = 0$ → **linear** eqs in the multipliers $\boldsymbol{U(r)}$ $\forall r$ and $\boldsymbol{\epsilon_{ij}}$
- **No assumption** on form of the potential is needed. The **only input** is the density $\tilde{\rho}(\boldsymbol{r})$

Target density $\tilde{\rho}(\boldsymbol{r})$

↓

Eigenfunctions $u_j(r)$

↓

Multipliers $U(r)$ and ϵ_{ij}

Van Leeuwen - Baerends (vLB) method

Reduced radial wave-function

KS equation in spherical symmetry: $$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2mr^2}+U(r)\right]u_i(r)=\varepsilon_i u_i(r)$$

Theoretical density (KS ansatz): $$\rho(r)=\frac{1}{4\pi r^2}\sum_{i=0}^{N_{orb}} n_i u_i^2(r)$$

Manipulating these expressions we can write

$$U(r)=\frac{1}{4\pi r^2\rho(r)}\sum_{i=0}^{N_{orb}}\left[n_i u_i(r)\left(\frac{\hbar^2}{2m}\frac{d^2}{dr^2}-U_l\right)u_i+\varepsilon_i n_i u_i^2\right]$$

And then, defining the **iterative procedure**

$$U^{(k+1)}(r)=\frac{1}{4\pi r^2\tilde{\rho}(r)}\sum_{i=0}^{N_{orb}}\left[n_i u_i^{(k)}(r)\left(\frac{\hbar^2}{2m}\frac{d^2}{dr^2}-U_l\right)u_i^{(k)}+\varepsilon_i n_i (u_i^{(k)})^2\right]=\frac{\rho^{(k)}(r)}{\tilde{\rho}(r)}U^{(k)}(r)$$

R. van Leeuwen and E. J. Baerends, Phys. Rev. A 49, 2421 (1994)

Van Leeuwen - Baerends (vLB) method

We used a slightly different equation for the inverse algorithm, obtained by a manipultation on the previous one[†]:

$$U^{(k+1)}(r) = U^{(k)}(r) + \gamma \frac{\rho^{(k)}(r) - \tilde{\rho}(r)}{\tilde{\rho}(r)}$$

- Correct behaviour for the nuclear case (**negative** potentials)
- There is not dependence of the algorithm on a **shift** of the potential

The iterative procedure requires a convergence condition to **stop**. We chose

$$\max_r \left| U^{(k+1)}(r) - U^{(k)}(r) \right| < \alpha$$

with $\alpha \leq 5\,\mathrm{keV}$.

D. S. Jensen and A. Wasserman, International Journal of Quantum Chemistry 118, e25425 (2018)

Van Leeuwen - Baerends (vLB) method

Iterative scheme:

Inverse problem:

$$U^{(k+1)}(r) = U^{(k)}(r) + \gamma \frac{\rho^{(k)}(r) - \tilde{\rho}(r)}{\tilde{\rho}(r)}$$

Direct problem:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + U(r) \right] u_i(r) = \varepsilon_i u_i(r)$$

(starting WS+C)
POTENTIAL

EIGENFUNCTIONS

$$\rho(r) = \frac{1}{4\pi r^2} \sum_{i=0}^{N_{orb}} n_i u_i^2(r)$$

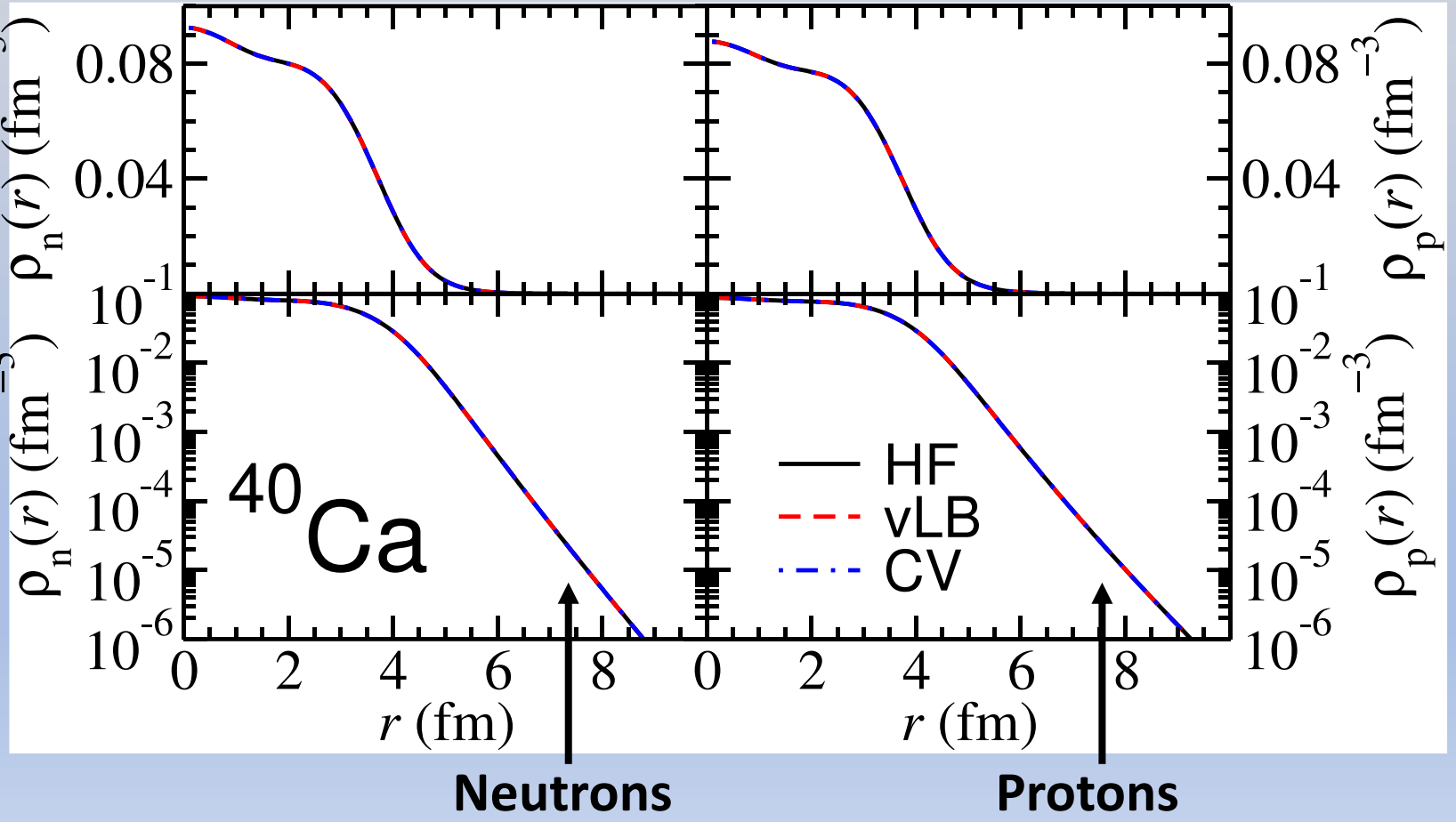
THEORETICAL DENSITY

The algorithm is strong enough to be **independent** from the starting potential

Hartree-Fock densities

- Test the inversion methods on **Hartree-Fock densities** for ^{208}**Pb** and ^{40}**Ca** obtained from **SkX** interactions.
- **Skyrme** interactions → very mild non-localities ($\frac{m^*}{m} \approx 1$)

$\boldsymbol{m^*}$: effective mass



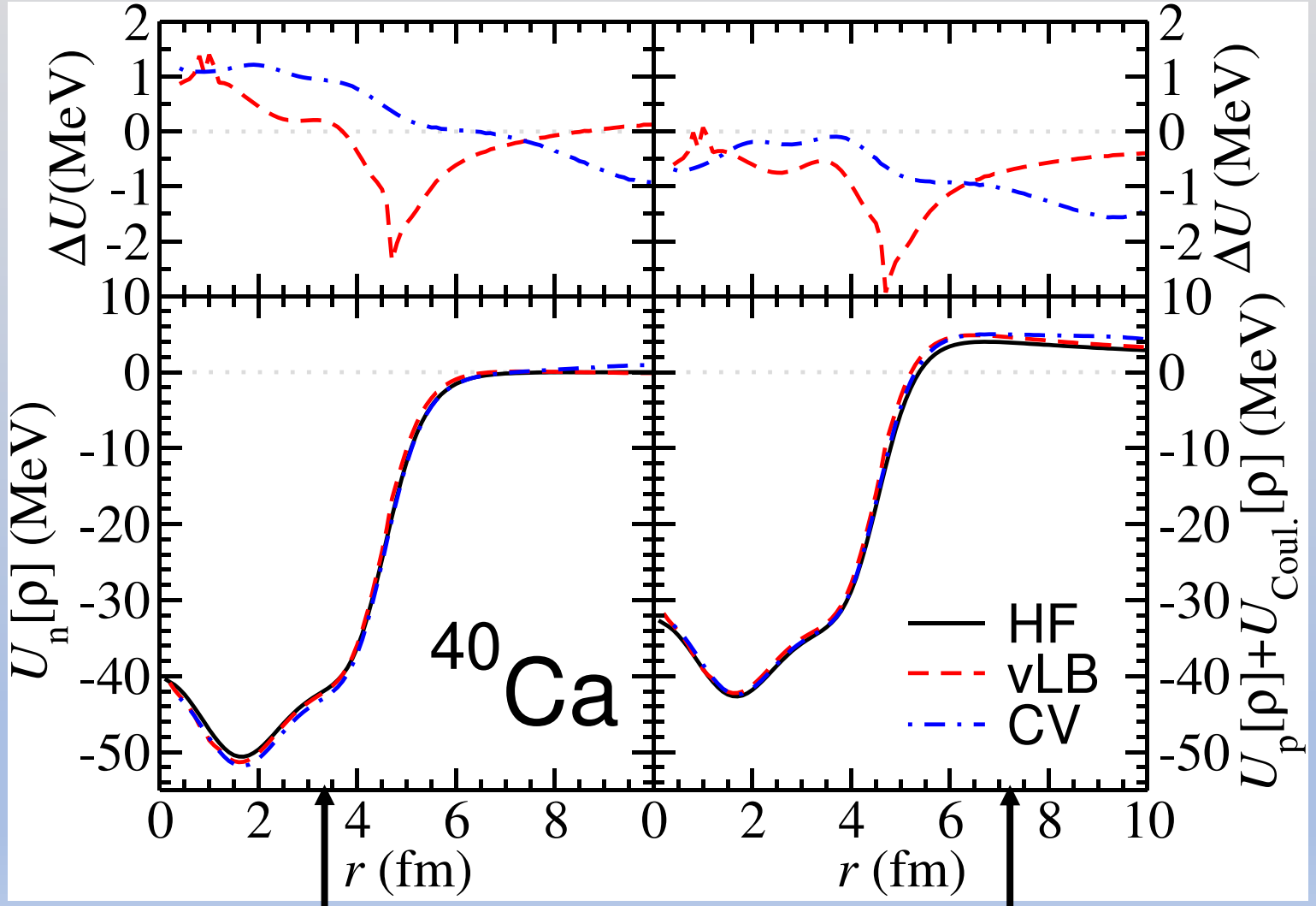
*Target **densities** (neutrons and protons) from **HF**, **vLB** and **CV** calculations for ^{40}**Ca** as a function of the radial coordinate*

Upper panel: linear scale
Lower panel: logarithmic scale

$$\rho(r) = \frac{1}{4\pi r^2} \sum_{i=1}^{N_{orb}} n_i u_i^2(r)$$

n_i: *occupation number*
u_i: *radial wave function*

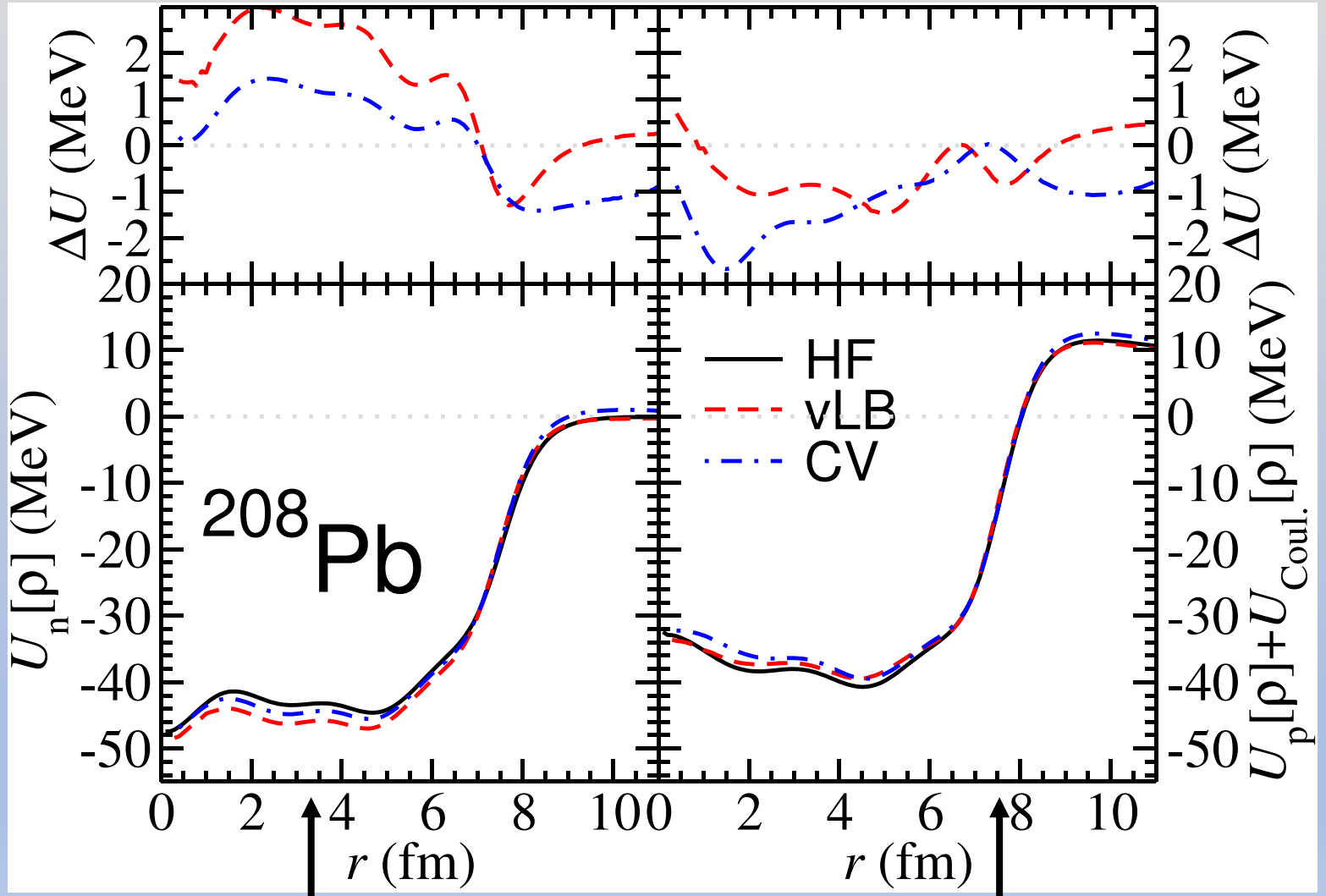
^{40}Ca potential from HF density



*Lower panel: **vLB** and **CV** potentials from ^{40}Ca density corresponding to SkX **HF** potential.*

Upper panel: differences $U_{vLB} - U_{HF}$ and $U_{CV} - U_{HF}$

^{208}Pb potential from HF density



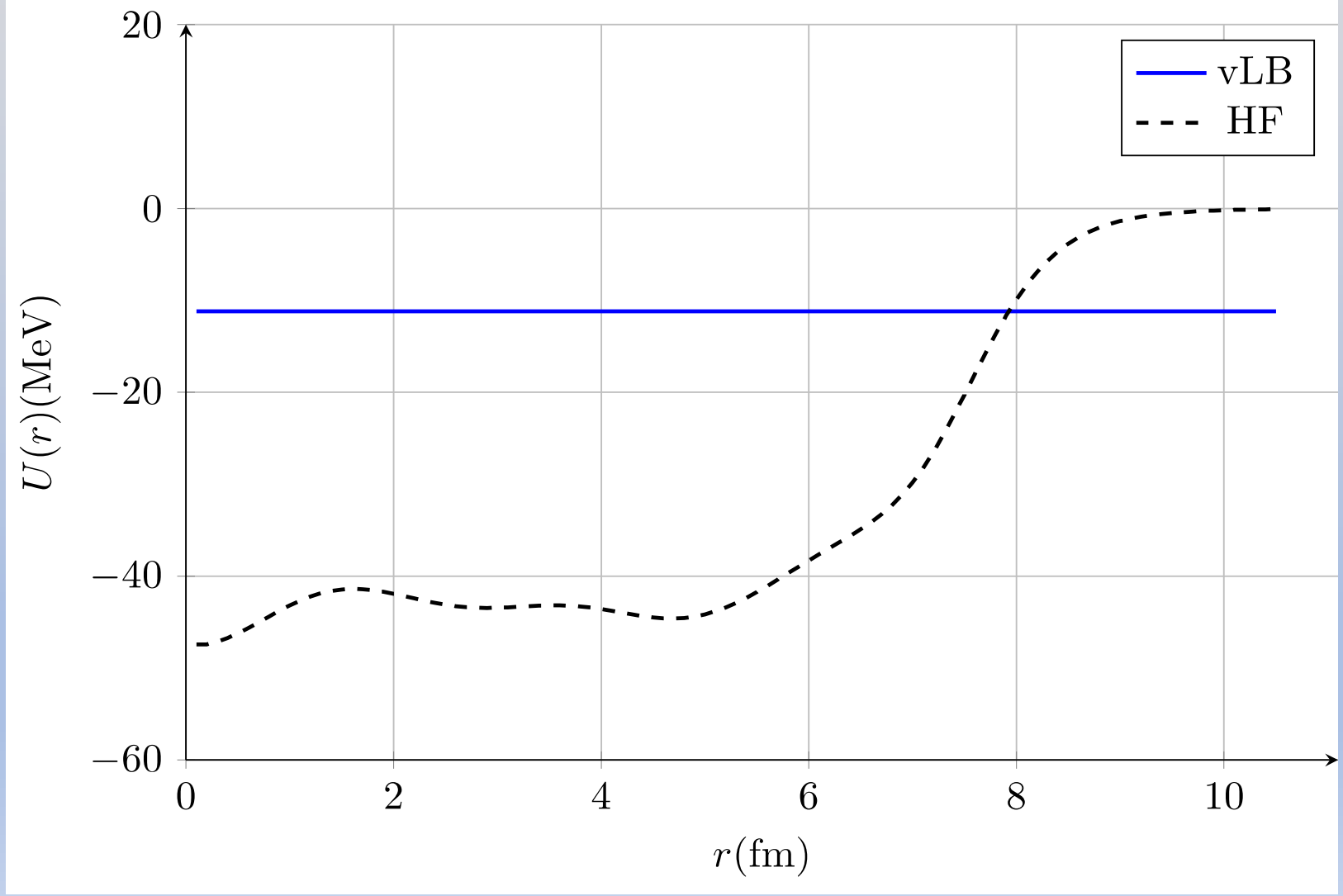
*Lower panel: **vLB** and **CV** potentials from ^{208}Pb density corresponding to SkX **HF** potential.*

Upper panel: differences $U_{vLB} - U_{HF}$ and $U_{CV} - U_{HF}$

Van Leeuwen - Baerends (vLB) method

Evolution of the vLB potential from a constant potential

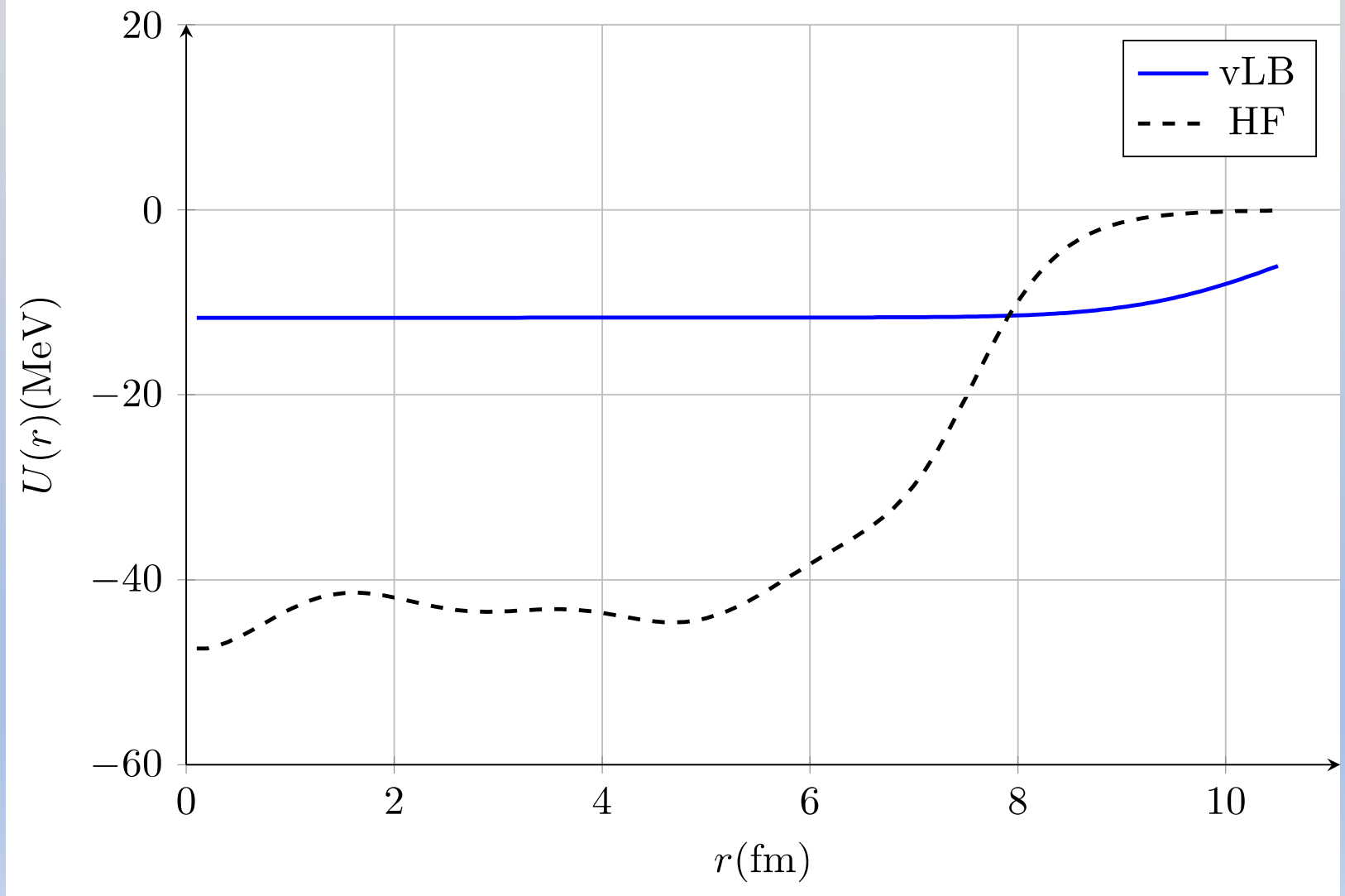
Iteration: 0



Van Leeuwen - Baerends (vLB) method

Evolution of the vLB potential from a constant potential

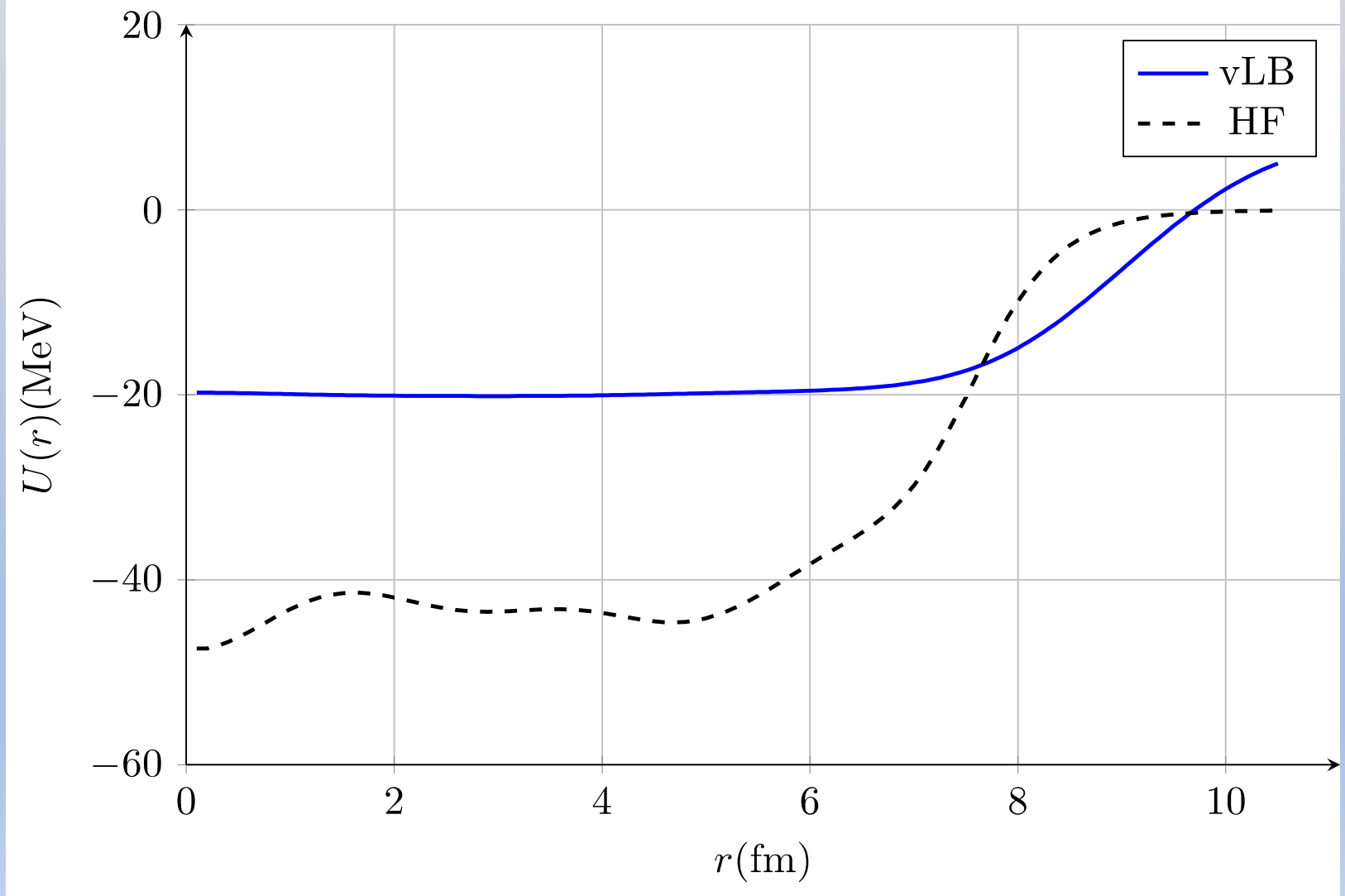
Iteration: 5



Van Leeuwen - Baerends (vLB) method

Evolution of the vLB potential from a constant potential

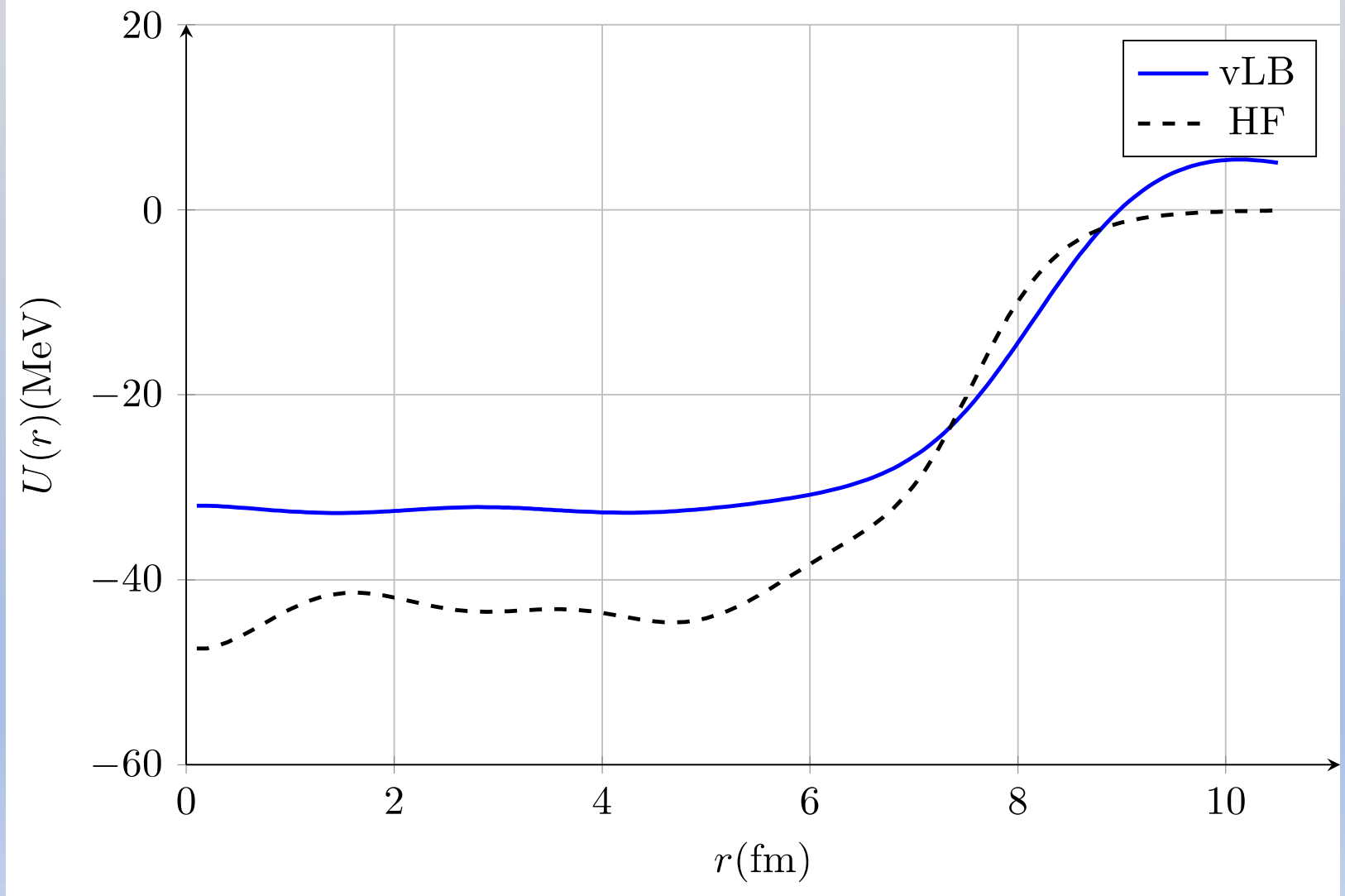
Iteration: 100



Van Leeuwen - Baerends (vLB) method

Evolution of the vLB potential from a constant potential

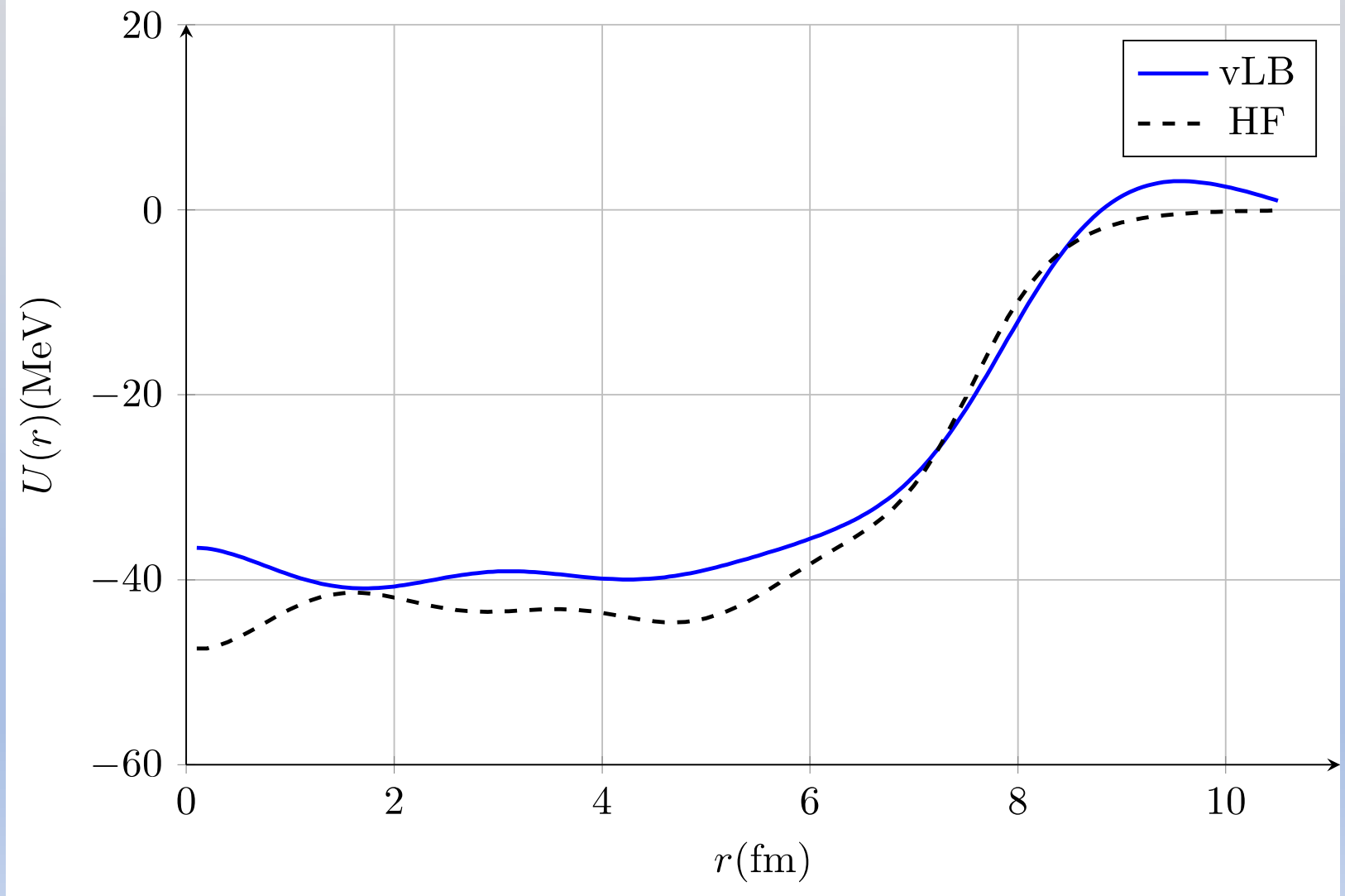
Iteration: 300



Van Leeuwen - Baerends (vLB) method

Evolution of the vLB potential from a constant potential

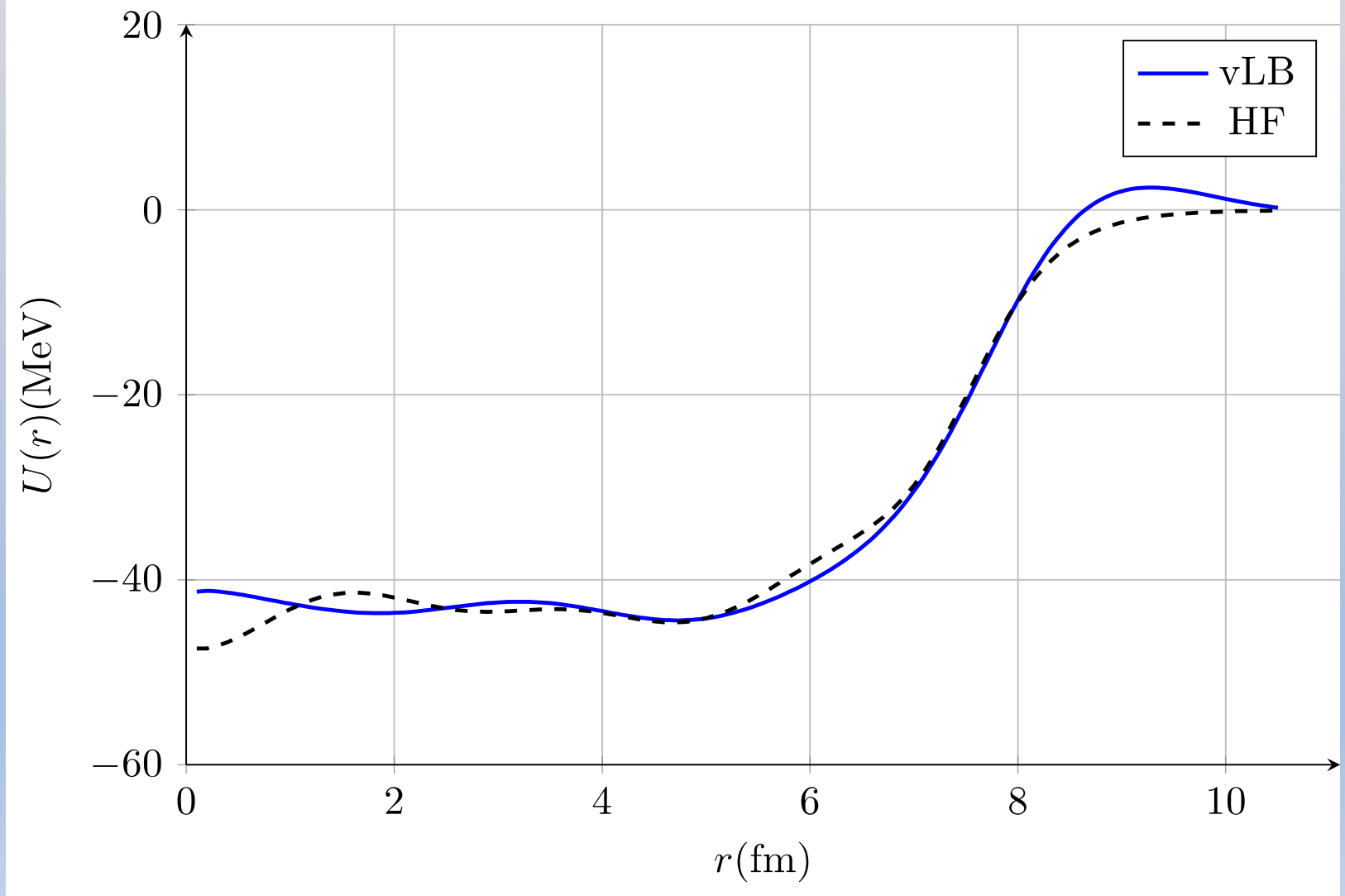
Iteration: 500



Van Leeuwen - Baerends (vLB) method

Evolution of the vLB potential from a constant potential

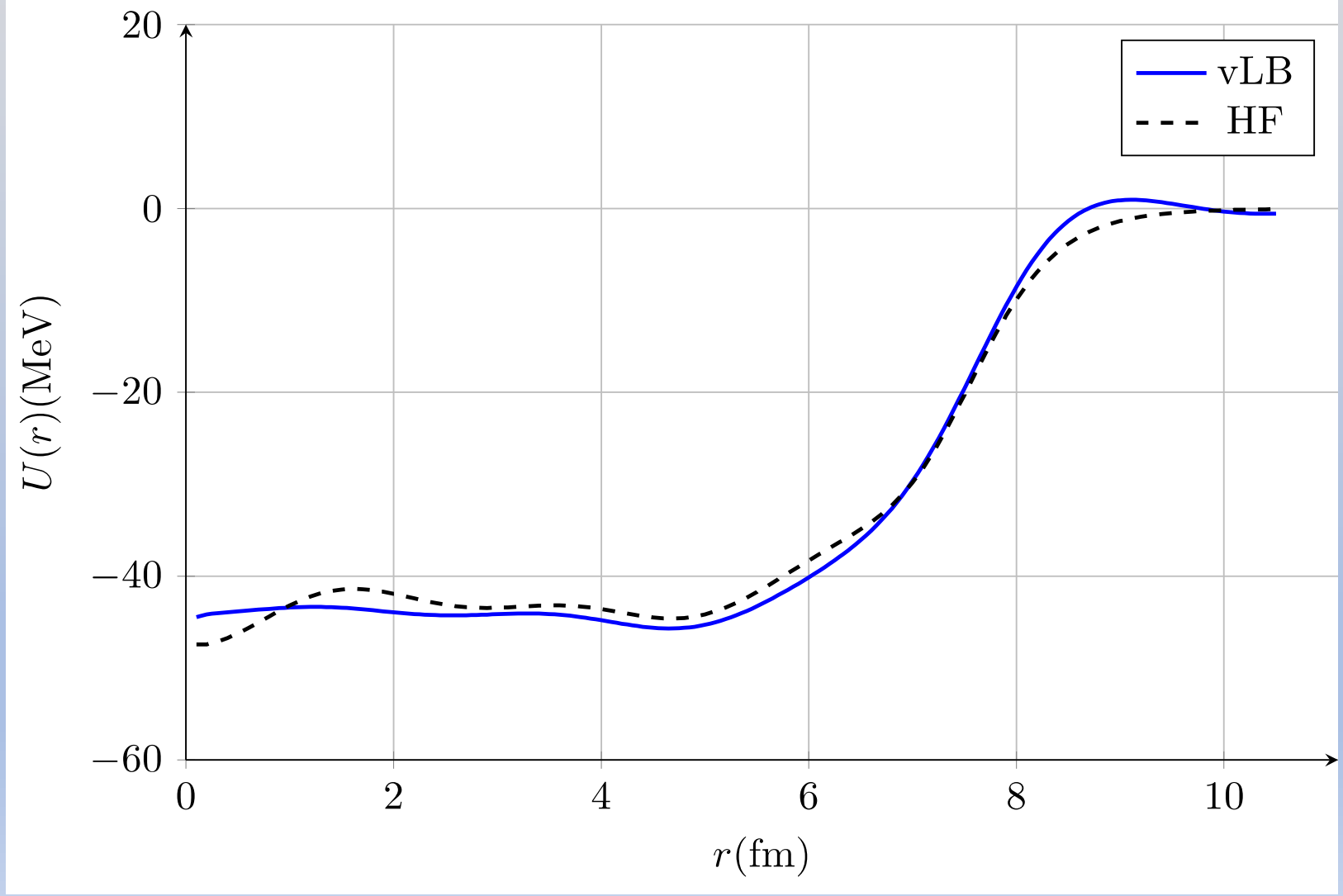
Iteration: 800



Van Leeuwen - Baerends (vLB) method

Evolution of the vLB potential from a constant potential

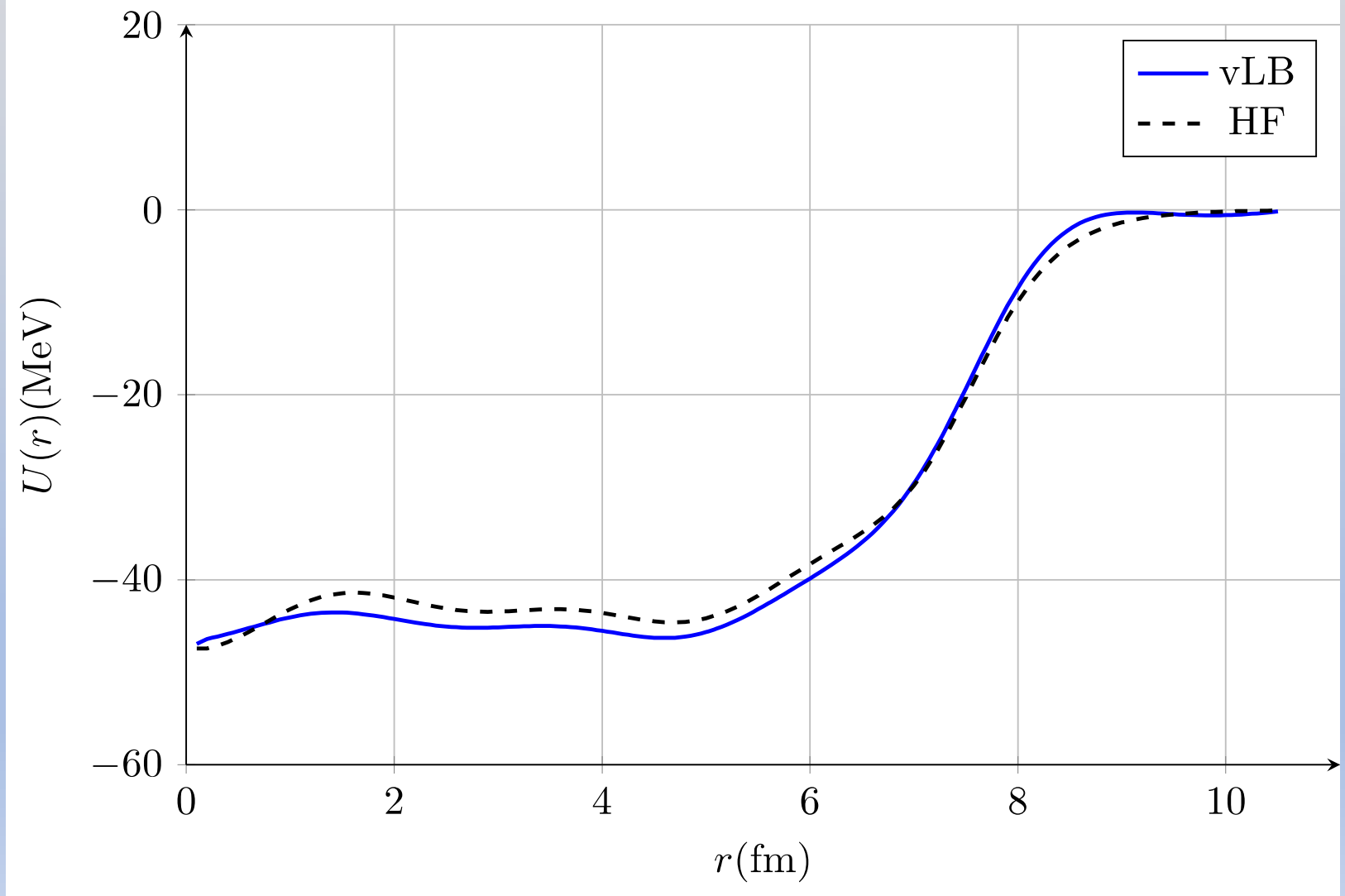
Iteration: 1100



Van Leeuwen - Baerends (vLB) method

Evolution of the vLB potential from a constant potential

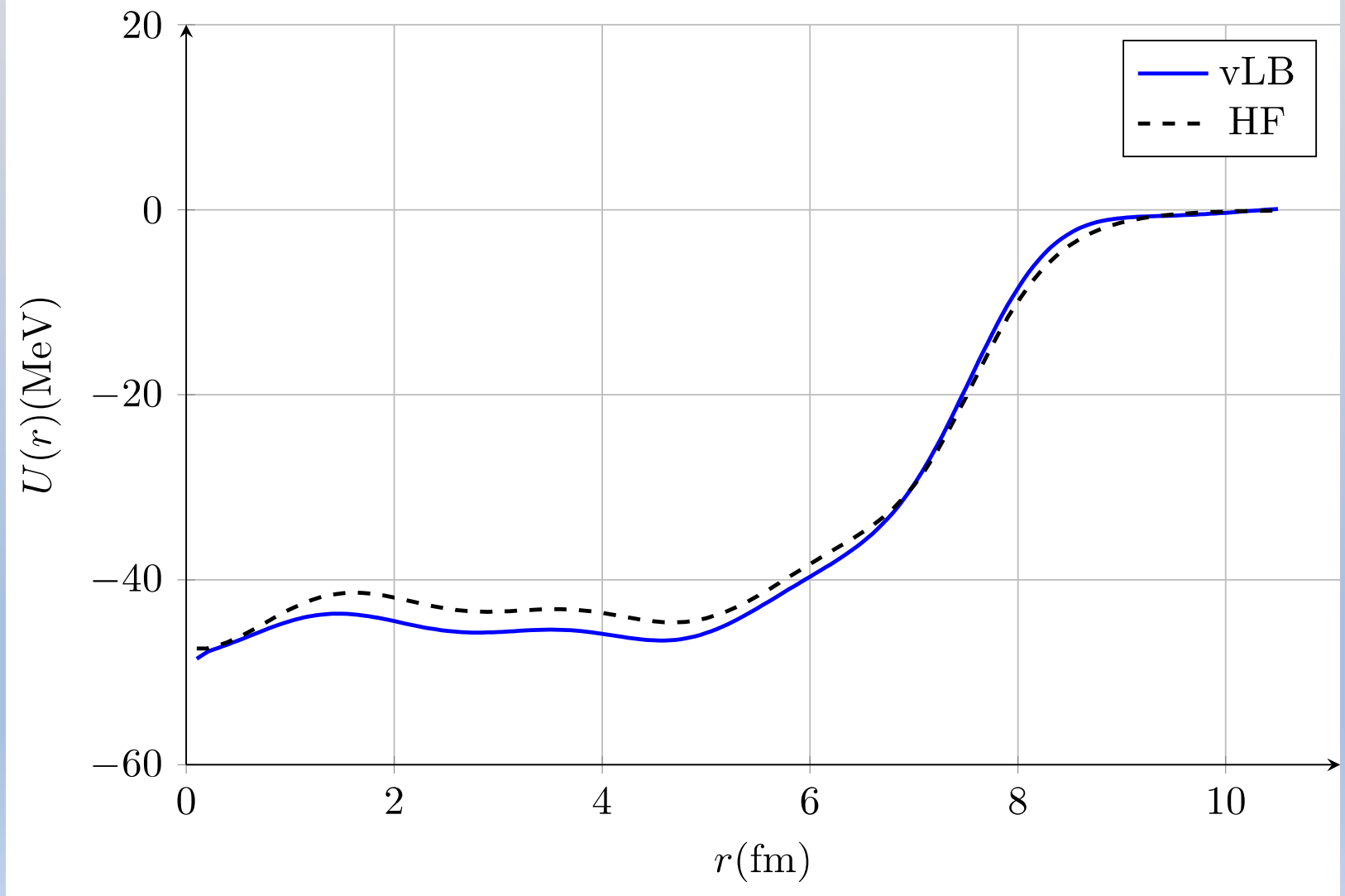
Iteration: 1500



Van Leeuwen - Baerends (vLB) method

Evolution of the vLB potential from a constant potential

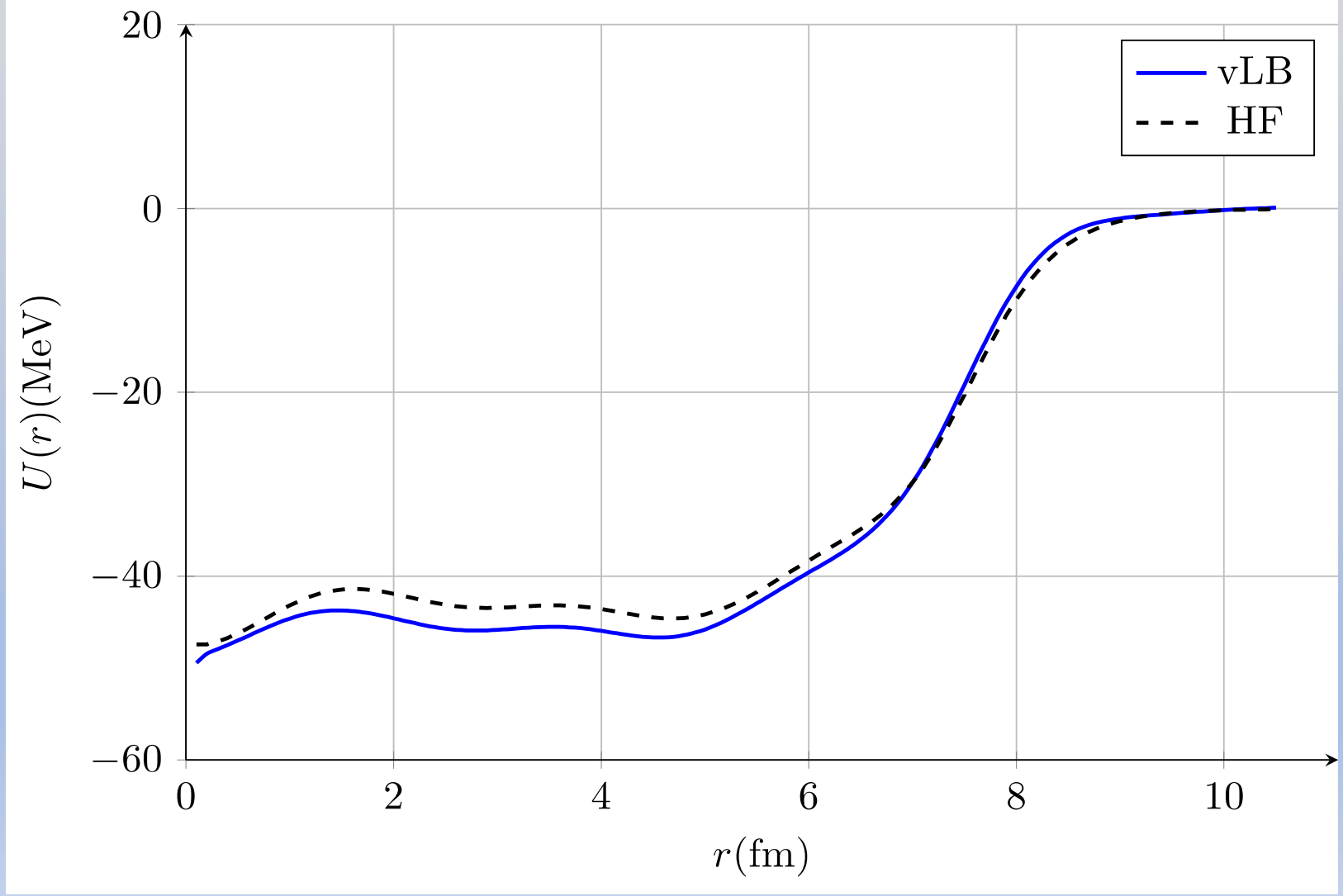
Iteration: 2000



Van Leeuwen - Baerends (vLB) method

Evolution of the vLB potential from a constant potential

Iteration: 2500



Experimental densities

Apply the inversion methods to **experimental densities** parametrized as Sum of Gaussians (**SOG**)

- **Proton density** (^{208}Pb, ^{40}Ca) → deconvolution of experimental charge density
- **Neutron density** (^{208}Pb) → data from proton scattering

$$\rho_{charge}(r) = \sum_i A_i^{charge} \left(e^{-\left(\frac{r-R_i}{\gamma}\right)^2} + e^{-\left(\frac{r+R_i}{\gamma}\right)^2} \right)$$

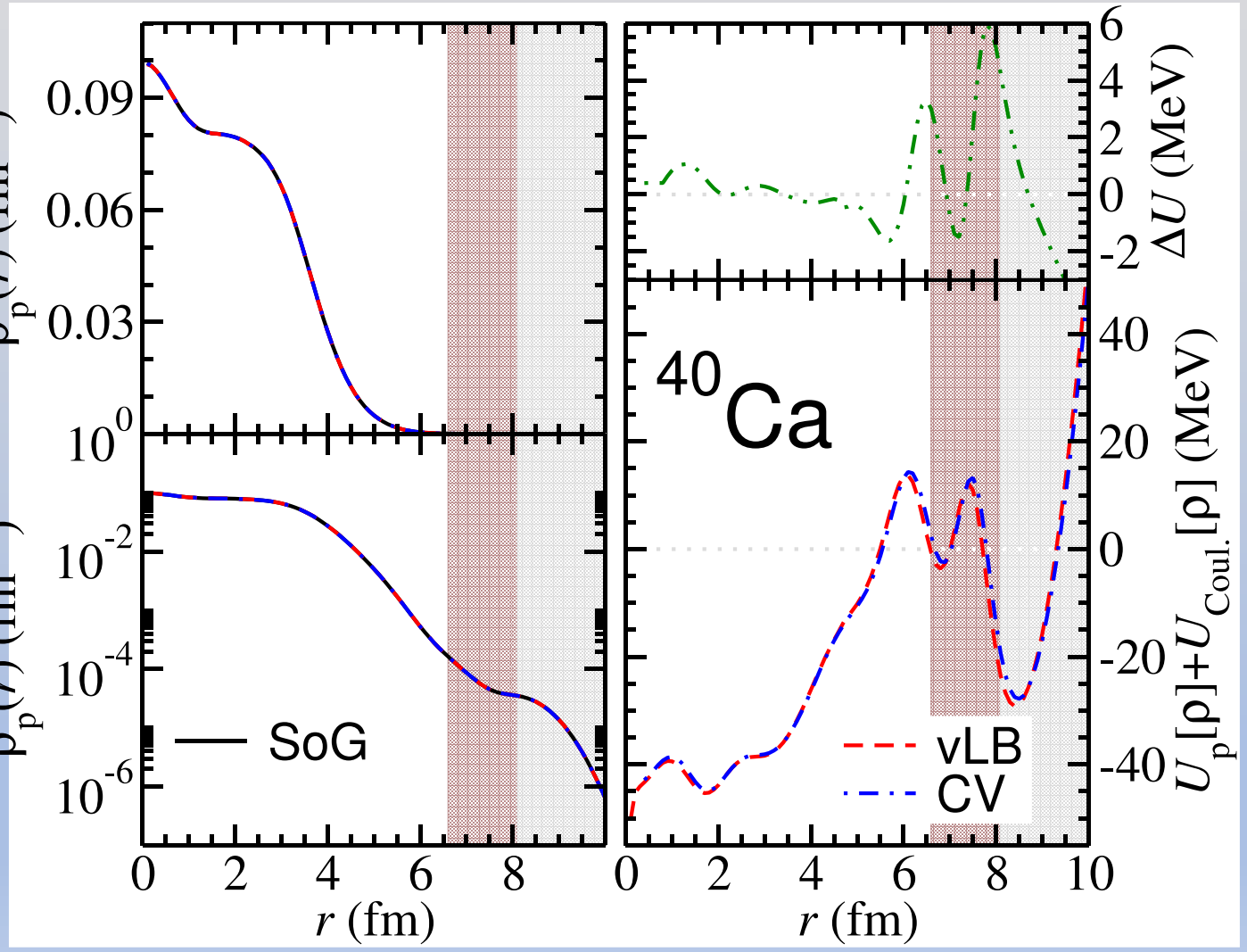
$$\rho_{charge}(\boldsymbol{r}) = \int d\boldsymbol{r}' f(\boldsymbol{r}') \rho_p(\boldsymbol{r} - \boldsymbol{r}')$$

R_i: center of i-th Gaussian
f: proton form factor

PROS	CONS
Model independent parametrization	The Gaussian behaviour is **not realistic** in the **tail** of the distribution
The nuclear surface density is well reproduced	

J. Zenihiro et al., Phys. Rev. C 82, 044611 (2010)
H. D. Vries, C. D. Jager, and C. D. Vries, Atomic Data and Nuclear Data Tables 36, 495 (1987)

^{40}Ca potential from SOG density

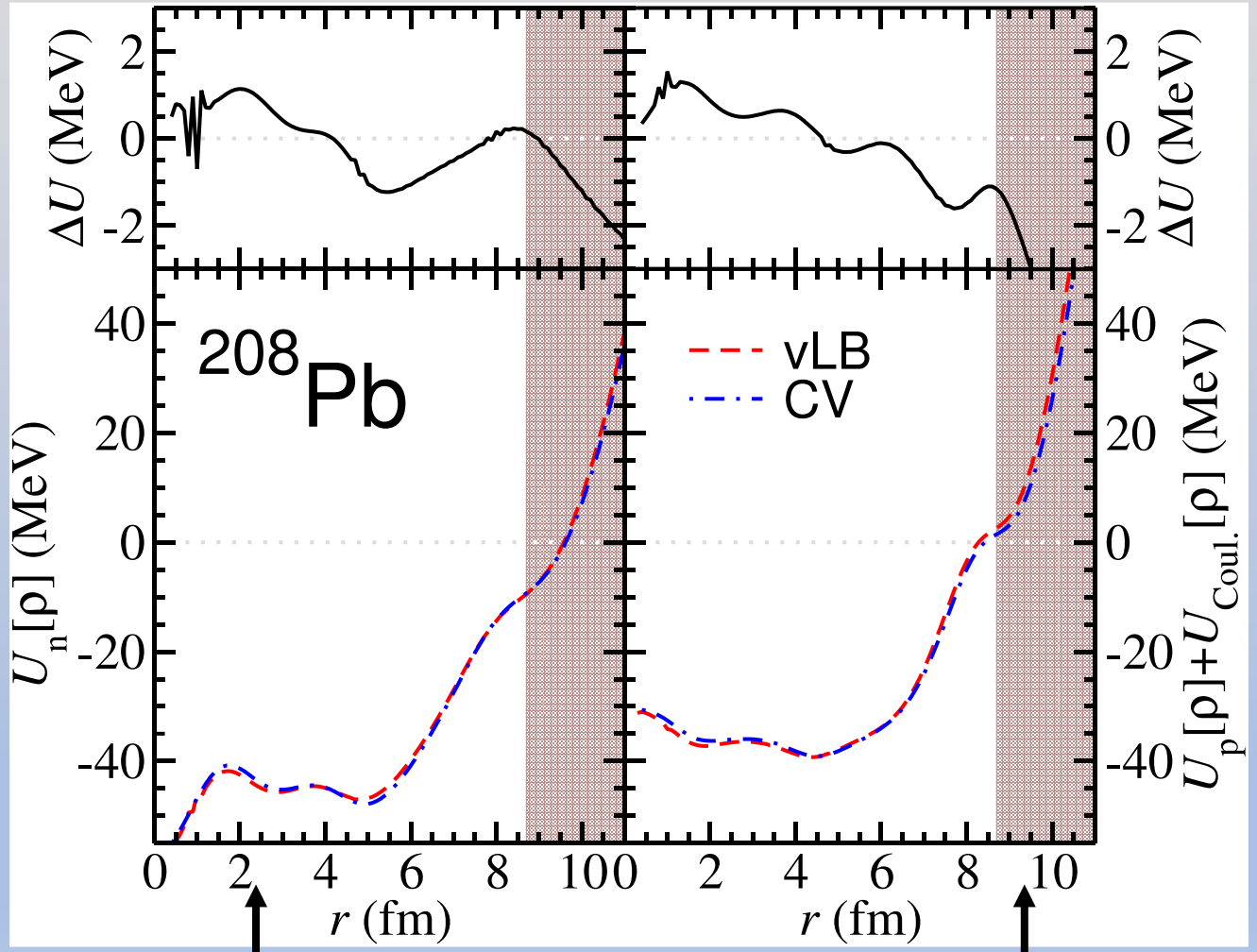


Left: ***SoG***, ***vLB*** *and* ***CV*** ***proton*** *densities for ^{40}Ca in linear (top) and logarithmic scale (bottom)*

Right: ***vLB*** *and* ***CV*** *potentials from ^{40}Ca proton SOG density (lower panel); difference* $U_{CV} - U_{vLB}$ *(upper panel)*

Shadowed: regions corresponding to r larger than the radius of the outermost (second outermost) Gaussian

^{208}Pb potential from SOG density



*Lower panel: **vLB** and **CV** potentials from SOG densities for ^{208}Pb.*

Upper panel: differences $U_{vLB} - U_{CV}$

Shadowed: regions corresponding to r larger than the radius of the outermost Gaussian

Neutrons

Protons

Conclusions and further developments

- We have used **two** different methods (CV and vLB) for the solution of the **Inverse Kohn-Sham** (IKS) problem in magic nuclei

→ Using a known neutron or proton **density** $\tilde{\rho}(r)$ as the **only input**, the **effective** single-particle **potential** $U(r)$ has been calculated

→ The two methods are in **good agreement** with each other and have been benchmarked with HF potentials

- This is a **first step**. Possible further steps are:

→ Use systematically ab initio densities as input

→ Find a way to introduce spin and gradient terms

Credits

A first step in the nuclear inverse Kohn-Sham problem: from densities to potentials

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(Dated: August 8, 2019)

G. Accorto, P. Brandolini, F. Marino, A. Porro, A. Scalesi, G. Colò, X. Roca-Maza and E. Vigezzi, arxiv: 1908.03068 (2019)