Description of nucleus-nucleus interaction using the Skyrme energy density functional

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Motivation

To describe the ground state characteristics of the nucleus, it is necessary to adhere to the strategy of matching these characteristics to experimental data. The characteristics are

- Binding energy
- Charge radii
- Nucleon distribution densities
- Single-particle spectra

However, we can’t talk about the description of interaction between nuclei. In work [1], using the Giessen EDF, authors succeeded in description of sub-burrier fusion. Therefore, this work is devoted to obtain fusion barriers using the Skyrme EDF.

[1] N. V. Antonenko ,G. G. Adamian, V. V. Sargsyan, H. Lenske,
Eur. Phys. J. A 58, 211 (2022)

Nucleus-nucleus interaction potential

The nucleus-nucleus interaction potential is represented as the sum

$$V(R) = V_C(R) + V_N(R) + V_r(R)$$

The double-folding procedure $$V_N(R) = \int d\boldsymbol{r_1} d\boldsymbol{r_2}\, \rho_1(\boldsymbol{r_1})\rho_2(\boldsymbol{R}-\boldsymbol{r_2})\mathcal{F}(\boldsymbol{r_1}-\boldsymbol{r_2})$$

$\rho_i(\boldsymbol{r_i})$ – density distribution of i nucleus

$\mathcal{F}(\boldsymbol{r_1}-\boldsymbol{r_2})$ – Nucleon-Nucleon force, chosen in Migdal type:

$$\mathcal{F}(\boldsymbol{r_2}-\boldsymbol{r_1}) = C_0\left[\left(F_{in}\frac{\rho_1(\boldsymbol{r_1})+\rho_2(\boldsymbol{R}-\boldsymbol{r_1})}{\rho_0} + F_{ex}\left(1-\frac{\rho_1(\boldsymbol{r_1})+\rho_2(\boldsymbol{R}-\boldsymbol{r_1})}{\rho_0}\right)\right)\delta(\boldsymbol{r_2}-\boldsymbol{r_1})\right]$$

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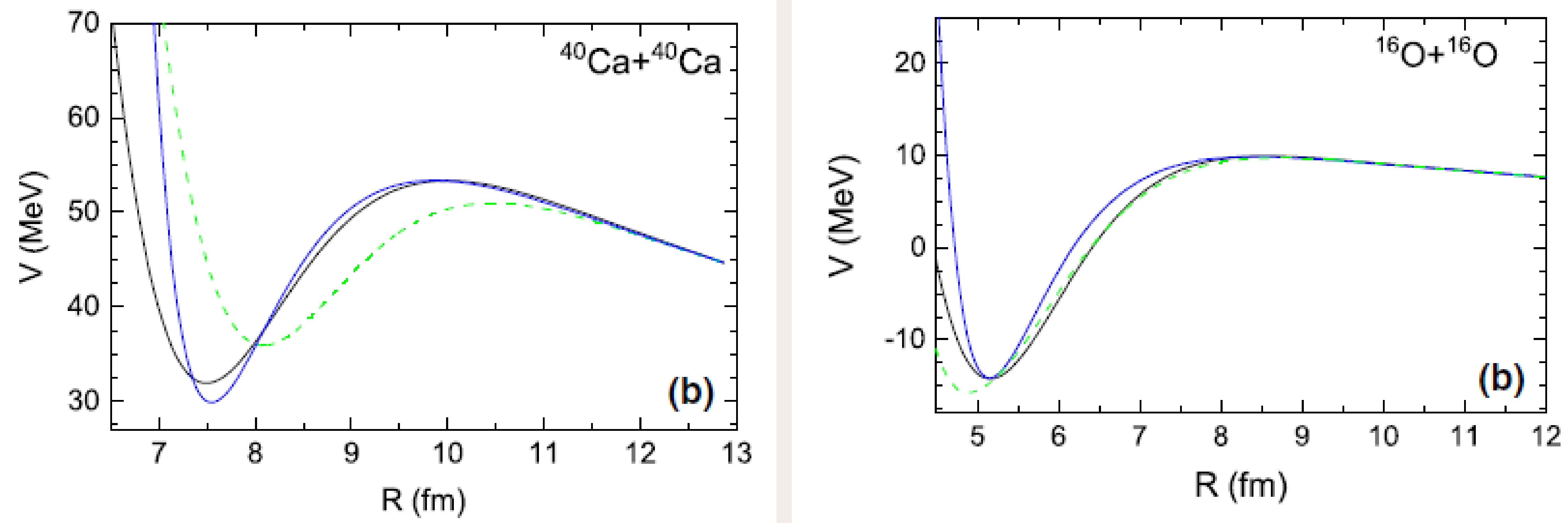
Nucleus-nucleus interaction potential



Comparison of nucleus-nucleus interaction potentials calculated with self-consistent (solid lines) and phenomenological (dashed lines) nucleon densities for the reactions ^{40}Ca+^{40}Ca and ^{16}O+^{16}O. The results of calculation with the parametrization of the nuclear part of the potential are shown by blue lines.

N. V. Antonenko ,G. G. Adamian, V. V. Sargsyan, H. Lenske,
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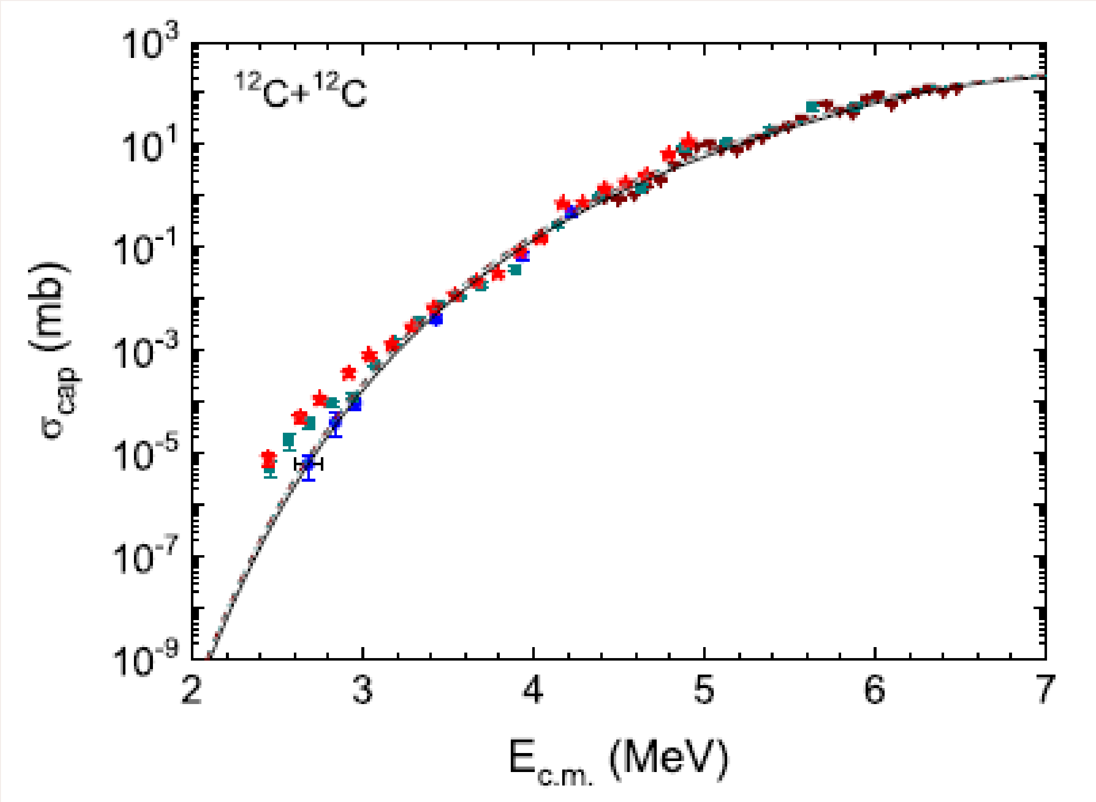
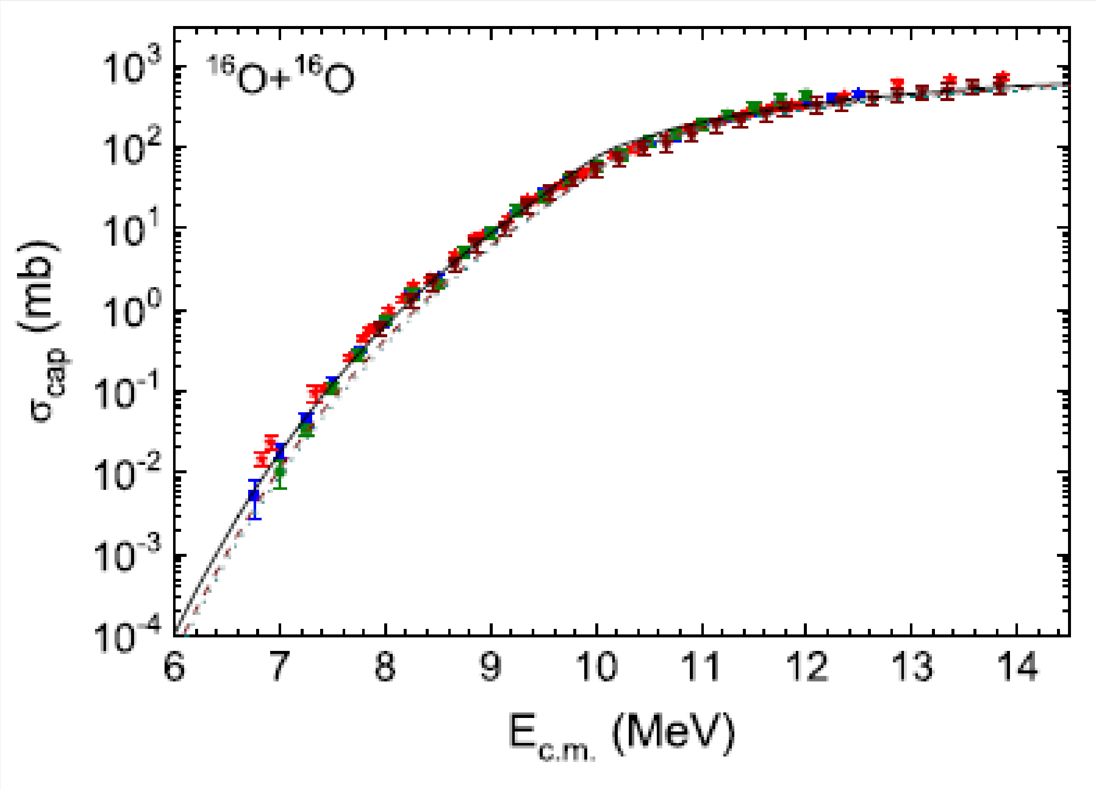
The fusion excitation functions





The fusion excitation functions calculated with phenomenologically adjusted (solid lines), self-consistent (dashed line), and parameterized (dotted line) potentials for the $^{12}C+^{12}C$ and $^{16}O+^{16}O$ reactions.

N. V. Antonenko ,G. G. Adamian, V. V. Sargsyan, H. Lenske,
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Skyrme force

The Skyrme-like effective interactions is represented as

$$V(\boldsymbol{r}_1, \boldsymbol{r}_2) = t_0(1 + x_0 P_\sigma)\delta(\boldsymbol{r})$$ Central term

$$+\frac{1}{2}t_1(1 + x_1 P_\sigma)\left[\boldsymbol{k}'^2\delta(\boldsymbol{r}) + \delta(\boldsymbol{r})\boldsymbol{k}^2\right]$$

$$+t_2(1 + x_2 P_\sigma)\,\boldsymbol{k}'\delta(\boldsymbol{r})\boldsymbol{k}$$ Non-local terms

$$+\frac{1}{6}t_3(1 + x_3 P_\sigma)[\rho(\boldsymbol{R})]^\alpha\delta(\boldsymbol{r})$$ Density-dependent term

$$+iW_0\boldsymbol{\sigma}[\boldsymbol{k}' \times \delta(\boldsymbol{r})\boldsymbol{k}]$$ Spin-orbit term

$\boldsymbol{\sigma}$ –the Pauli matrices, P_σ – spin-exchange operator, $\boldsymbol{k}'$, $\boldsymbol{k}$– relative wave vectors and

$t_0, t_1, t_2, t_3, x_0, x_1, x_2, x_3, W_0, \alpha$ – parameters of Skyrme EDF

D. Vautherin and D.M. Brink, Phys. Rev. C 5, 626 (1972)

Skyrme Energy Density Functional

$$E_0 = \langle \phi | (T+V) | \phi \rangle = \int \mathcal{H}(\boldsymbol{r}) d\boldsymbol{r}$$ Expectation value of the energy

$$\rho_q(\boldsymbol{r}) = \sum_{i,\sigma} |\phi_i(\boldsymbol{r},\sigma,q)|^2$$

$$\tau_q(\boldsymbol{r}) = \sum_{i,\sigma} |\nabla\phi_i(\boldsymbol{r},\sigma,q)|^2$$

$$\boldsymbol{J}_q(\boldsymbol{r}) = (-i) \sum_{i,\sigma,\sigma'} \phi_i^* [\nabla\phi_i(\boldsymbol{r},\sigma',q) \times \langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle]$$

$$\begin{aligned}
\mathcal{H}(\boldsymbol{r}) &= \frac{1}{4} t_0 \left[(2+x_0)\rho^2 - (2x_0+1)\left(\rho_n^2 + \rho_p^2\right)\right] \\
&+ \frac{1}{24} t_3 \rho^\alpha \left[(2+x_3)\rho^2 - (2x_3+1)\left(\rho_n^2 + \rho_p^2\right)\right] \\
&+ \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\tau\rho + \frac{1}{8}[t_2(2x_2+1) - t_1(2x_1+1)]\left(\tau_n\rho_n + \tau_p\rho_p\right) \\
&+ \frac{1}{32}[3t_1(2+x_1) - t_2(2+x_2)](\nabla\rho)^2 - \frac{1}{32}[3t_1(2x_1+1) + t_2(2x_2+1)]\left[(\nabla\rho_n)^2 + \left(\nabla\rho_p\right)^2\right] \\
&+ \frac{1}{2} W_0 \left[\boldsymbol{J}\nabla\rho + \boldsymbol{J}_n\nabla\rho_n + \boldsymbol{J}_p\nabla\rho_p\right] - \frac{1}{16}(t_1x_1 + t_2x_2)\boldsymbol{J}^2 + \frac{1}{16}(t_1 - t_2)\left[\boldsymbol{J}_n^2 + \boldsymbol{J}_p^2\right]
\end{aligned}$$

E. Chabanat, P. Bonche, P. Haensel, J. Meyer, R. Schaeffer, Nuclear Phys. A 635 (1998) 231

Hartree-Fock equations

$$\left[-\vec{\nabla}^2 \frac{\hbar^2}{2m_q^*(\vec{r})} + U_q(\vec{r}) + \vec{W}_q(\vec{r}) \cdot (-i)\left(\vec{\nabla} \times \vec{\sigma}\right)\right] \phi_i = e_i \phi_i$$

$$\frac{\hbar^2}{2m_q^*(\vec{r})} = \frac{\hbar^2}{2m} + \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\rho + \frac{1}{8}[t_2(2x_2+1) - t_1(2x_1+1)]\rho_q$$

Effective mass

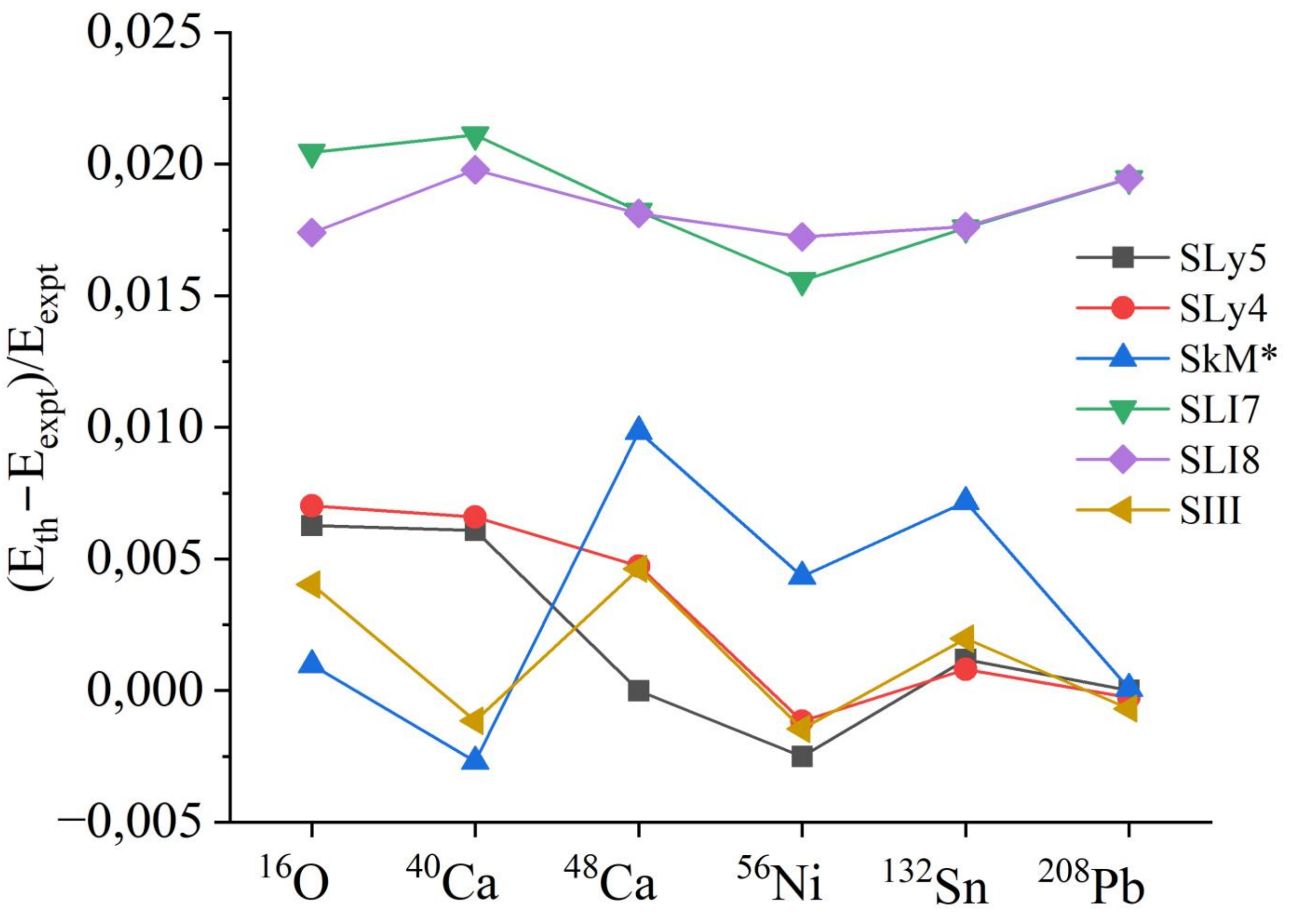
$$\begin{aligned} U_q(\vec{r}) = {} & \frac{1}{2} t_0\left[(2+x_0)\rho - (2x_0+1)\rho_q\right] \\ & + \frac{1}{24} t_3 \left[(\alpha+2)(2+x_3)\rho^{\alpha+1} - (2x_3+1)\left(2\rho^\alpha \rho_q + \alpha \rho^{\alpha-1}\left(\rho_n^2 + \rho_p^2\right)\right)\right] \\ & - \frac{1}{16}[3t_1(2+x_1) - t_2(2+x_2)]\nabla^2\rho + \frac{1}{16}[3t_1(2x_1+1) + t_2(2x_2+1)]\nabla^2\rho_q \\ & + \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\tau + \frac{1}{8}[t_2(2x_2+1) - t_1(2x_1+1)]\tau_q \\ & - \frac{1}{2} W_0\left(\nabla \cdot \boldsymbol{J} + \nabla \cdot \boldsymbol{J}_q\right) \end{aligned}$$

Nuclear central potential

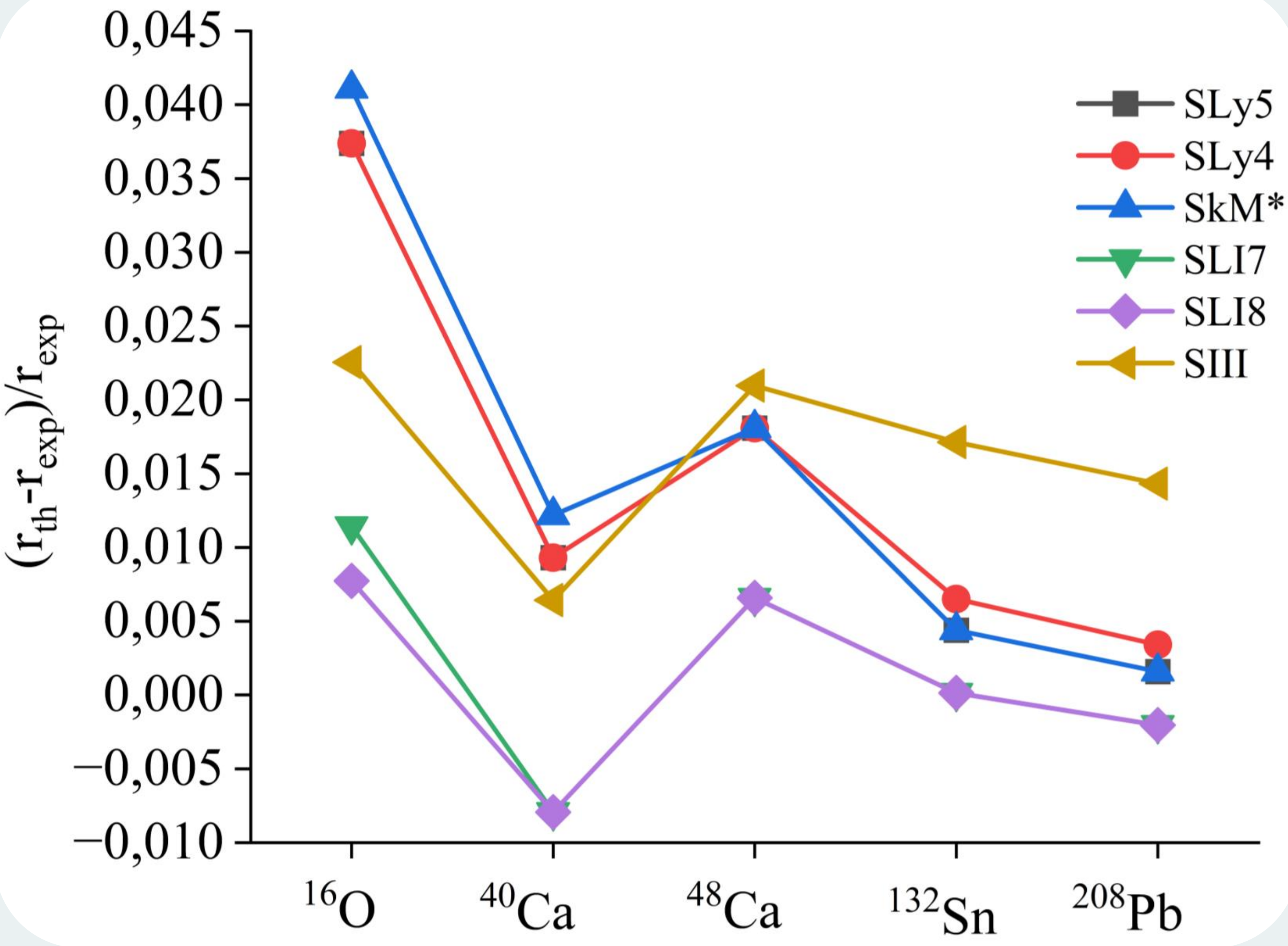
$$\vec{W}_q(\vec{r}) = \frac{1}{2} W_0\left(\nabla\rho + \nabla\rho_q\right) + \frac{1}{8}(t_1 - t_2)\boldsymbol{J}_q - \frac{1}{8}(t_1 x_1 + t_2 x_2)\boldsymbol{J}$$

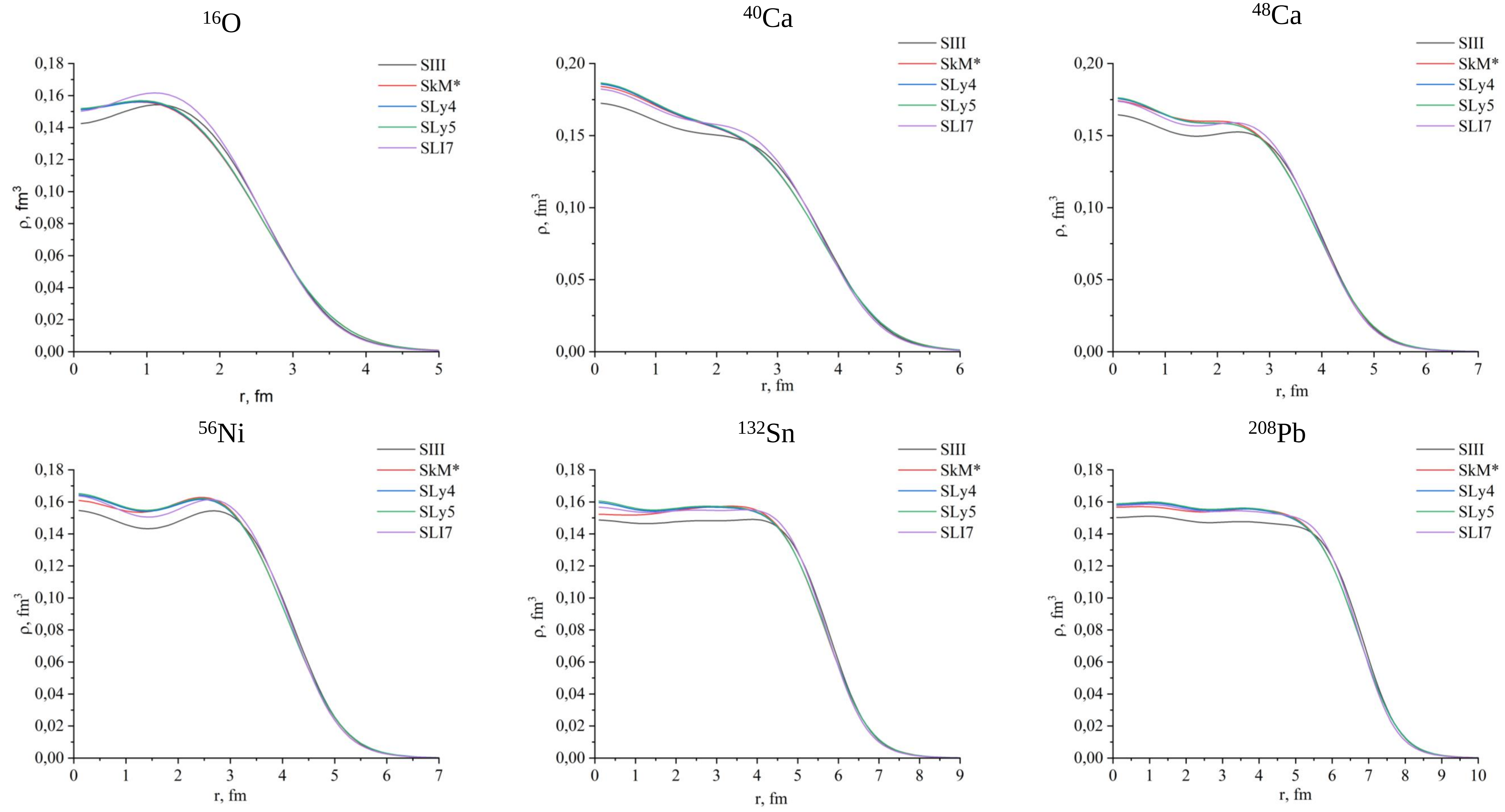
Single-particle spin-orbital potential

Binding energies



Charge radii





^{16}O
^{40}Ca
^{48}Ca
^{56}Ni
^{132}Sn
^{208}Pb
SIII
SkM*
SLy4
SLy5
SLI7
ρ, fm3
r, fm

Skyrme-Landau-Migdal force

$$\mathcal{F} = N_0 \sum_l \left[F_l + F_l'(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j) + G_l(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) + G_l'(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)\right] P_l\left(\frac{\boldsymbol{k_1 k_2}}{k_F^2}\right) \qquad N_0 = \frac{\pi^2 \hbar^2}{2 k_F m^*}$$

where F_l, F_l', G_l, G_l' - Landau-Migdal parameters; P_l - Legendre polynomials; $\boldsymbol{\sigma}$ – spin, $\boldsymbol{\tau}$ – isospin

A.B. Migdal, Theory of Finite Fermi Systems and Applications to Atomic Nuclei (Wiley, New York, 1967)

The most significant part of decomposition is zero harmonics. Thus in coordinate space Landau-Migdal interaction is given in following form

$$\mathcal{F}(\boldsymbol{r}_1, \boldsymbol{r}_2) = N_0\left[F_0 + G_0(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) + (F_0' + G_0')(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)\right]\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)$$

Severyukhin A. P. Rol phonon-phononnogo vzaimodejstviya v strukture nejtronno-izbytochnyh yader. [The role of phonon-phonon interaction in the structure of neutron-rich nuclei Dokt. Diss.]. Dubna, 2025. 263 p.

Skyrme-Landau-Migdal force

To calculate the Landau-Migdal parameters we need to calculate second variational derivative:

$$\frac{\delta^2\mathcal{H}(\boldsymbol{r})}{\delta\rho_1\delta\rho_2} = \sum_{\sigma,\tau,\sigma',\tau'} \frac{\left(1+(-1)^{\sigma-\sigma'}\boldsymbol{\sigma_1\sigma_2}\right)}{4}\frac{\left(1+(-1)^{\tau-\tau'}\boldsymbol{\tau_1\tau_2}\right)}{4}\frac{\delta^2\mathcal{H}(\boldsymbol{r})}{\delta\rho_{\sigma\tau}\delta\rho_{\sigma'\tau'}}$$

$$F_0 = N_0^{-1}\left\{\frac{3}{4}t_0 + \frac{1}{16}\rho^\alpha(\alpha+1)(\alpha+2) + \frac{1}{8}k_F^2[3t_1+(5+4x_2)t_2]\right\}$$

$$F_0' = -N_0^{-1}\left\{\frac{1}{4}t_0(1+2x_0) + \frac{1}{24}t_3\rho^\alpha(1+2x_3) + \frac{1}{8}k_F^2[t_1(1+2x_1)-t_2(1+2x_2)]\right\}$$

$$G_0 = N_0^{-1}\left\{\frac{1}{4}t_0(1-2x_0) + \frac{1}{24}t_3\rho^\alpha(1-2x_3) + \frac{1}{8}k_F^2[t_1(1-2x_1)-t_2(1+2x_2)]\right\}$$

$$G_0' = N_0^{-1}\left[\frac{1}{4}t_0 + \frac{1}{24}t_3\rho^\alpha + \frac{1}{8}k_F^2(t_1-t_2)\right]$$

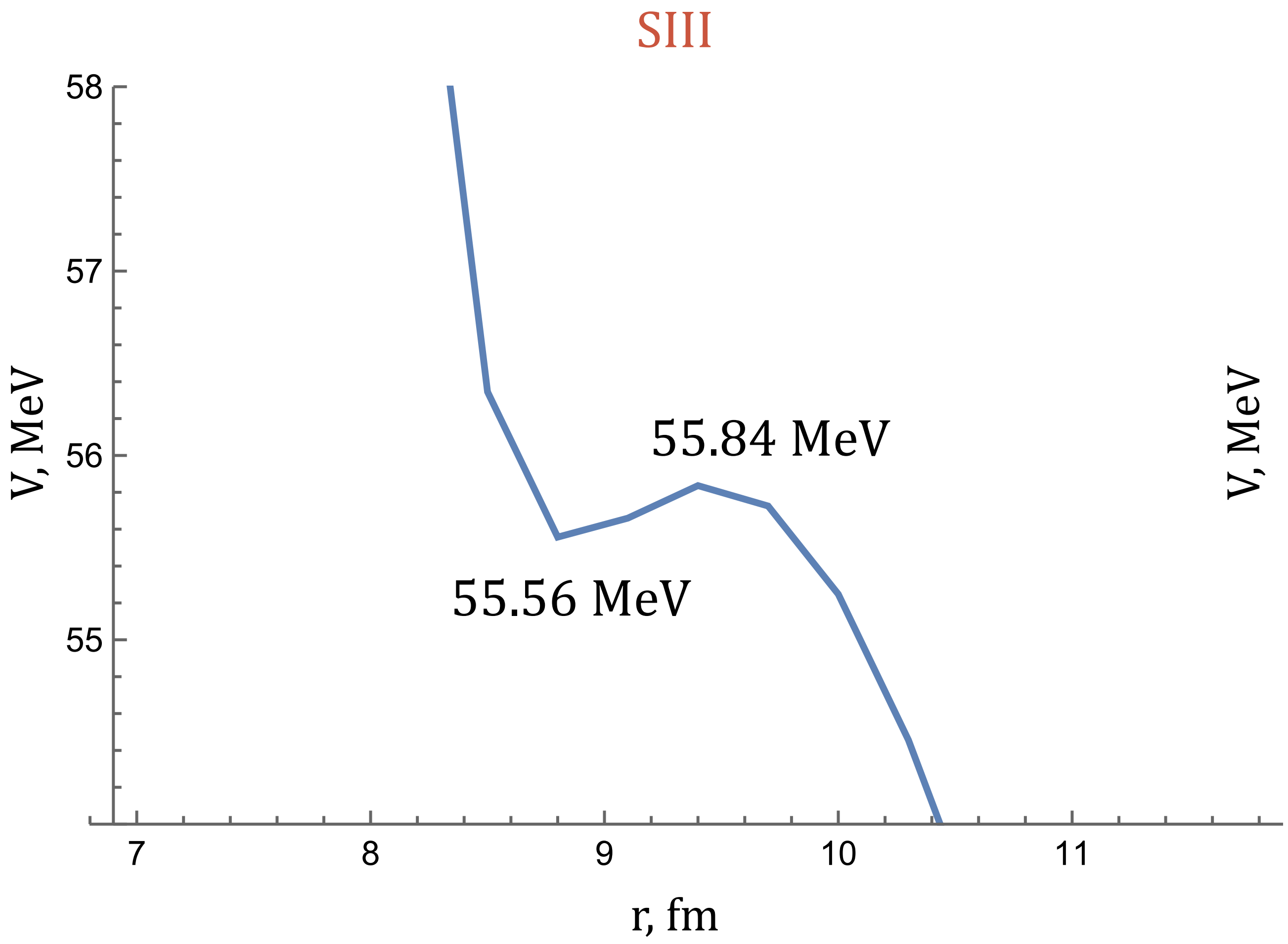
N. Van Giai, H. Sagawa, Phys. Lett. B106 (1981) 379

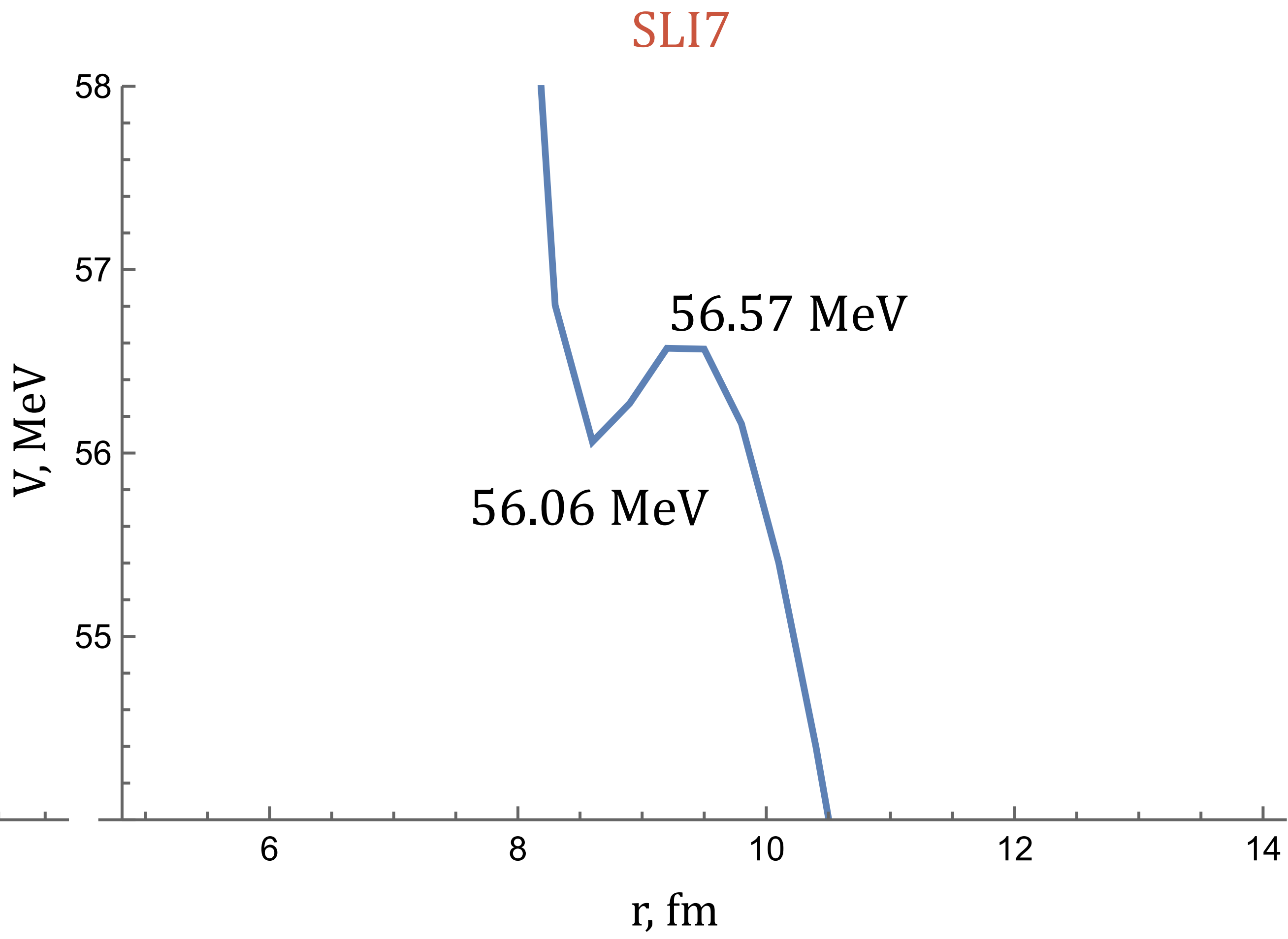
G.F. Bertsch and S.F. Tsai, Phys. Rep. 18C, 126 (1975)

Nucleus-nucleus interaction potential with Skyrme EDF

$r_{phen} = 10.58\ fm\ , V_{phen} = 50.46$ MeV

$^{48}Ca+^{48}Ca$

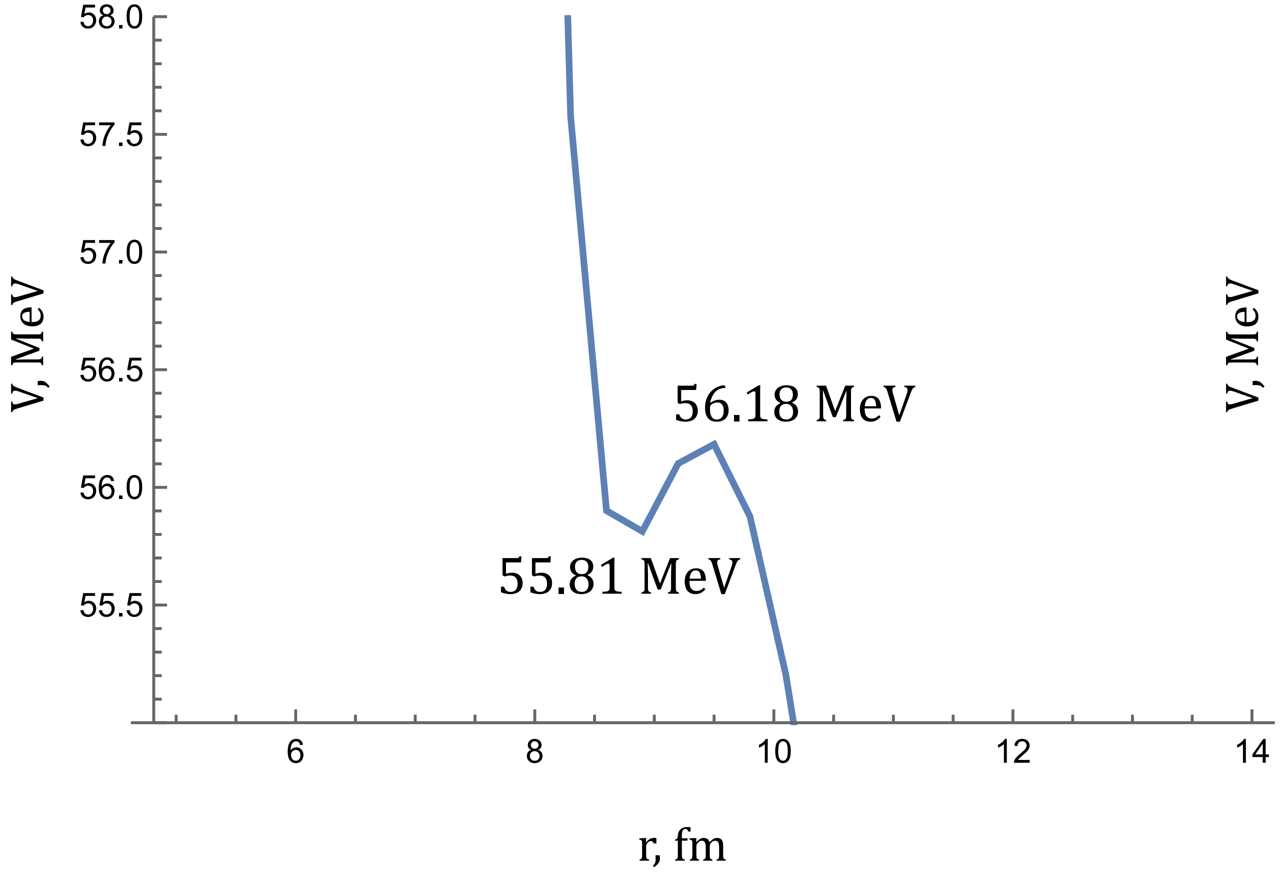




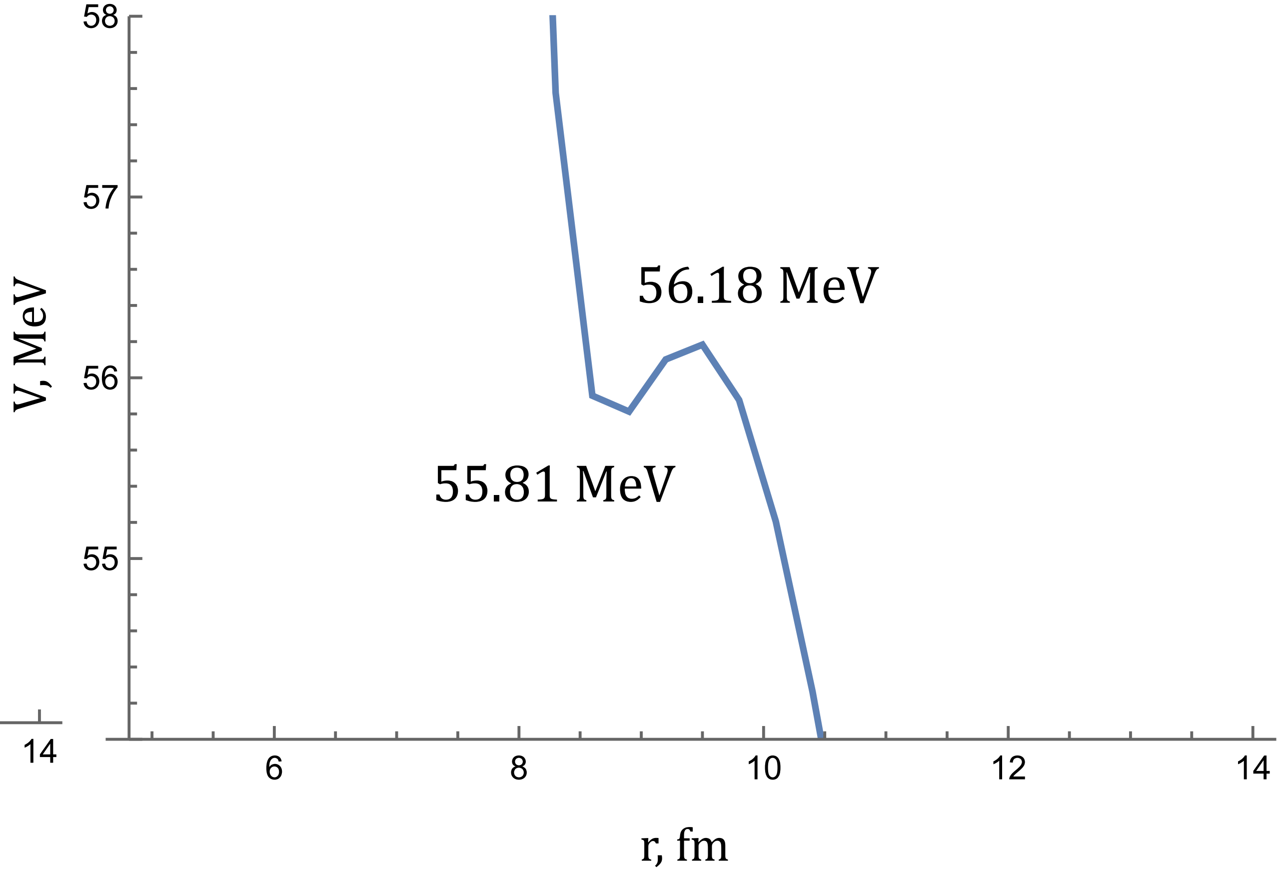
$r_{phen} = 10.58\ fm$, $V_{phen} = 50.46$ MeV

$^{48}Ca + ^{48}Ca$

SLI8



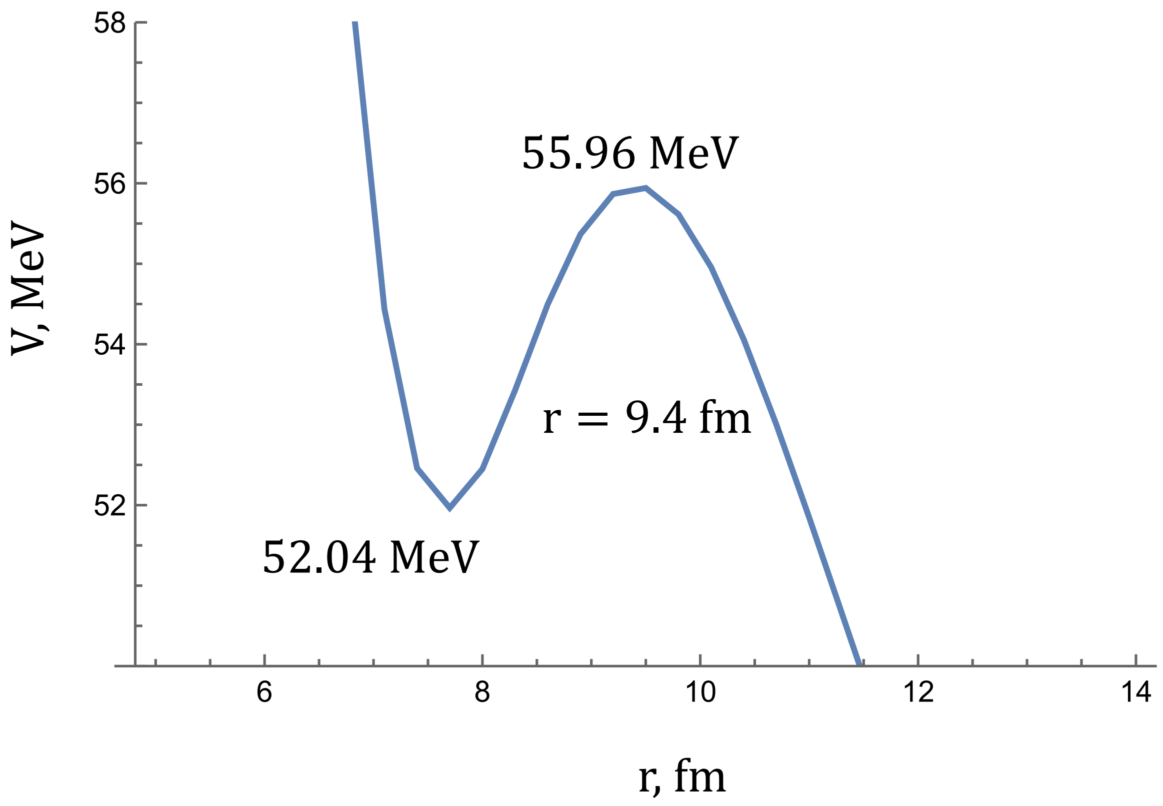
SLI9



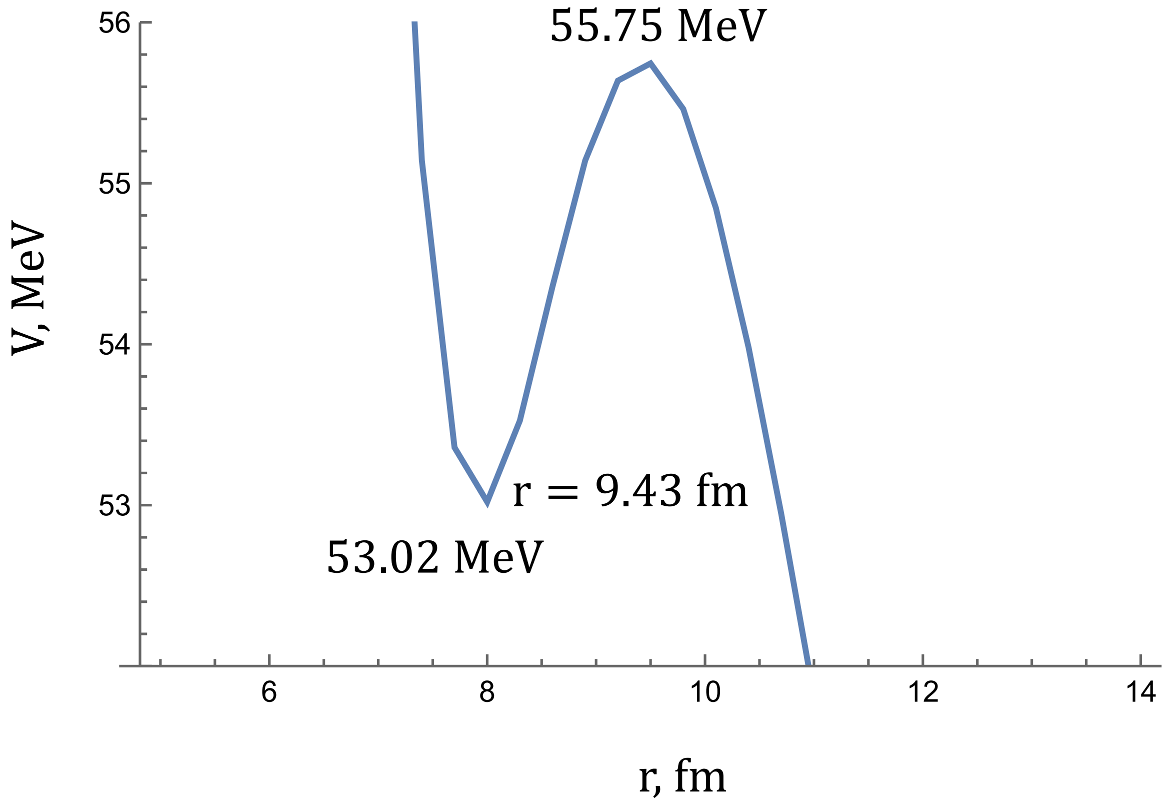
$r_{phen} = 10.58\ fm\ , V_{phen} = 50.46$ MeV

$^{48}Ca+^{48}Ca$

SLy4



SkM*



As we can see, the original Skyrme parameterizations give overestimated barrier values, compared to the Giessen EDF. But we can try to reduce it

Velocity term scaling

The first step in the construction of an effective interaction is to fix the saturation point of the symmetric infinite nuclear matter. Four quantities must be adjusted: the density at this point, the corresponding energy per nucleon, incompressibility modulus and isoscalar effective mass.

For a zero-range Skyrme force, the density functional gives the following energy per nucleon for symmetric matter:

$$\frac{E}{A}(\rho) = \frac{3\hbar^2}{10m}\left(\frac{3\pi^2}{2}\right)^{2/3}\rho^{2/3} + \frac{3}{8}t_0\rho + \frac{3}{80}\theta_s\left(\frac{3\pi^2}{2}\right)^{2/3}\rho^{5/3} + \frac{1}{16}t_3\rho^{\alpha+1}$$

where $\theta_s = [3t_1 + (5+4x_2)t_2]$ and defines effective mass on nucleons

Such construction also presents in Landau-Migdal parameter F_0

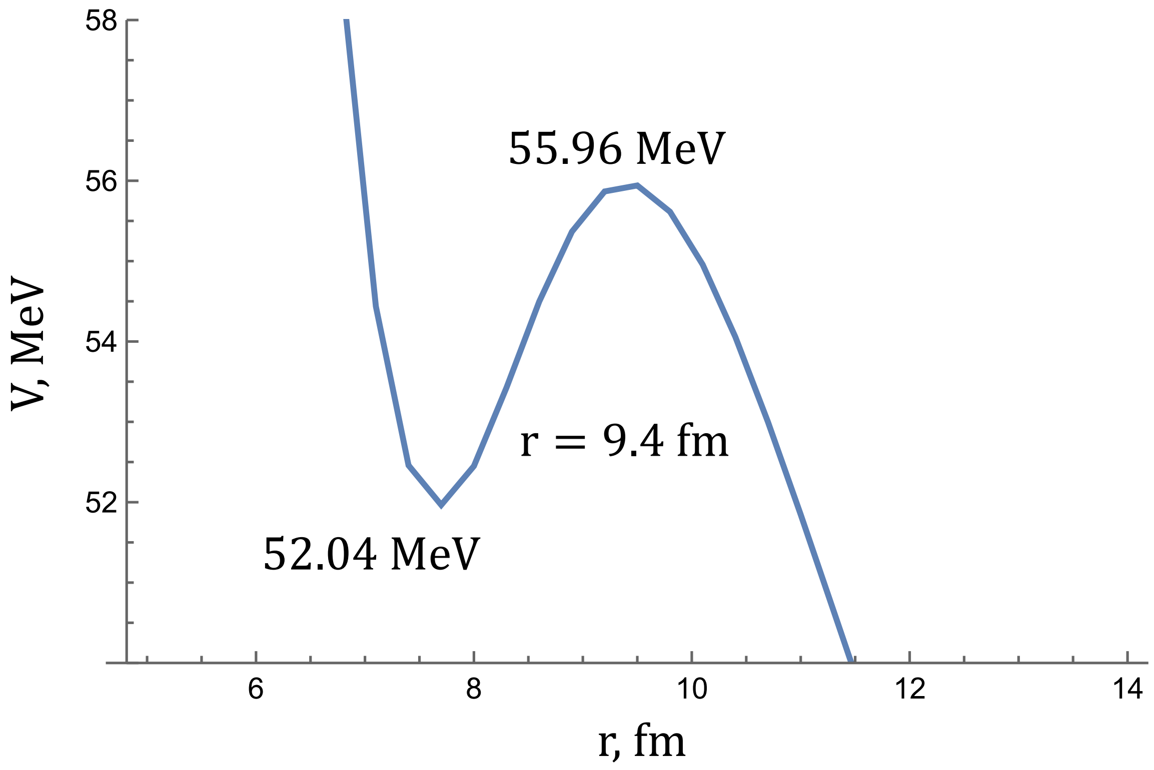
$$F_0 = N_0^{-1}\left\{\frac{3}{4}t_0 + \frac{1}{16}\rho^{\alpha}(\alpha+1)(\alpha+2) + \frac{1}{8}k_F^2[3t_1 + (5+4x_2)t_2]\right\}$$

This term comes from gradient terms (velocity), which we will change, finding the dependence how increasing of F_0 change the barrier

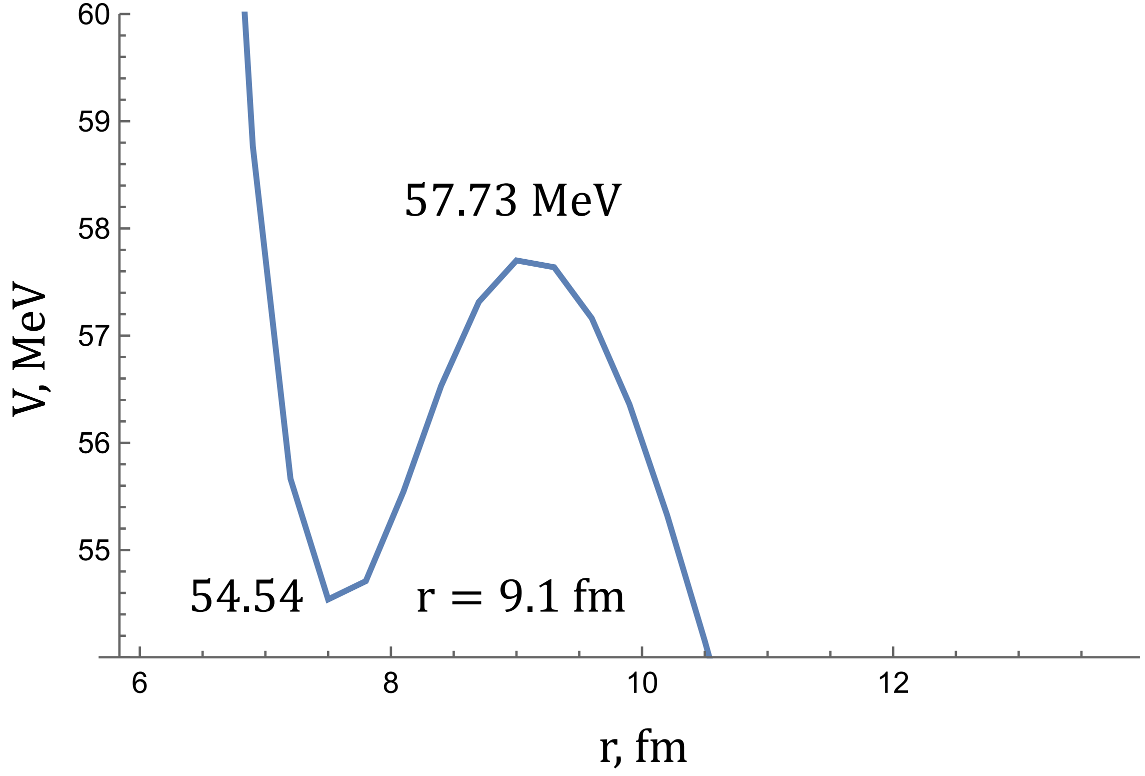
$r_{phen} = 10.58\ fm\ , V_{phen} = 50.46$ MeV

SLy4 ^{48}Ca+ ^{48}Ca

$\theta_s = 906$ MeV·fm^5, (original)

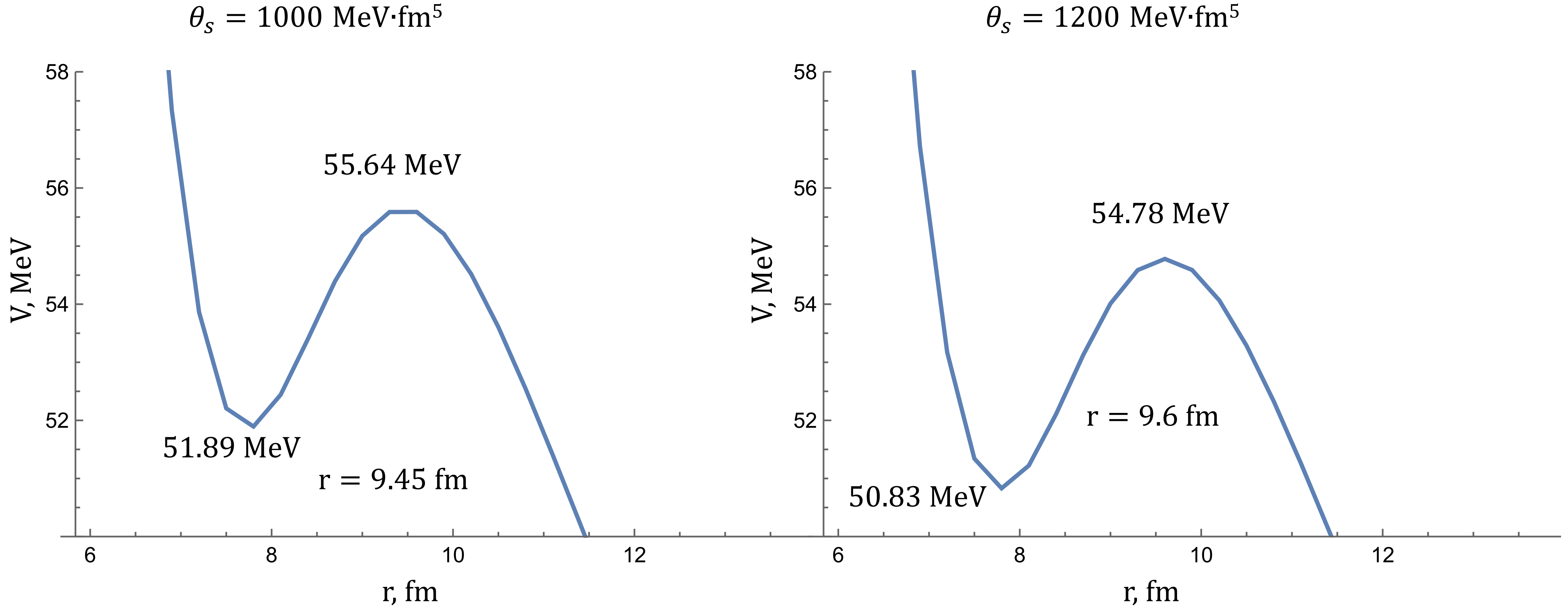


$\theta_s = 600$ MeV·fm^5



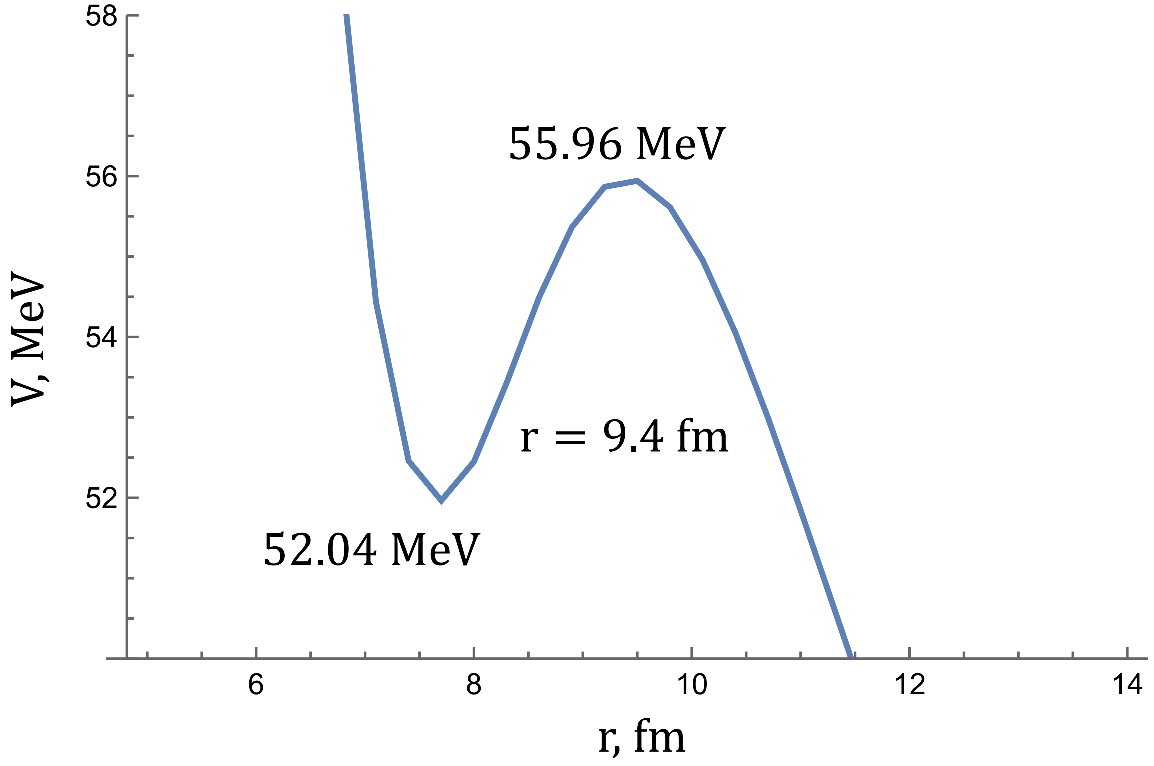
$r_{phen} = 10.58\ fm$, $V_{phen} = 50.46$ MeV

$^{48}Ca + ^{48}Ca$

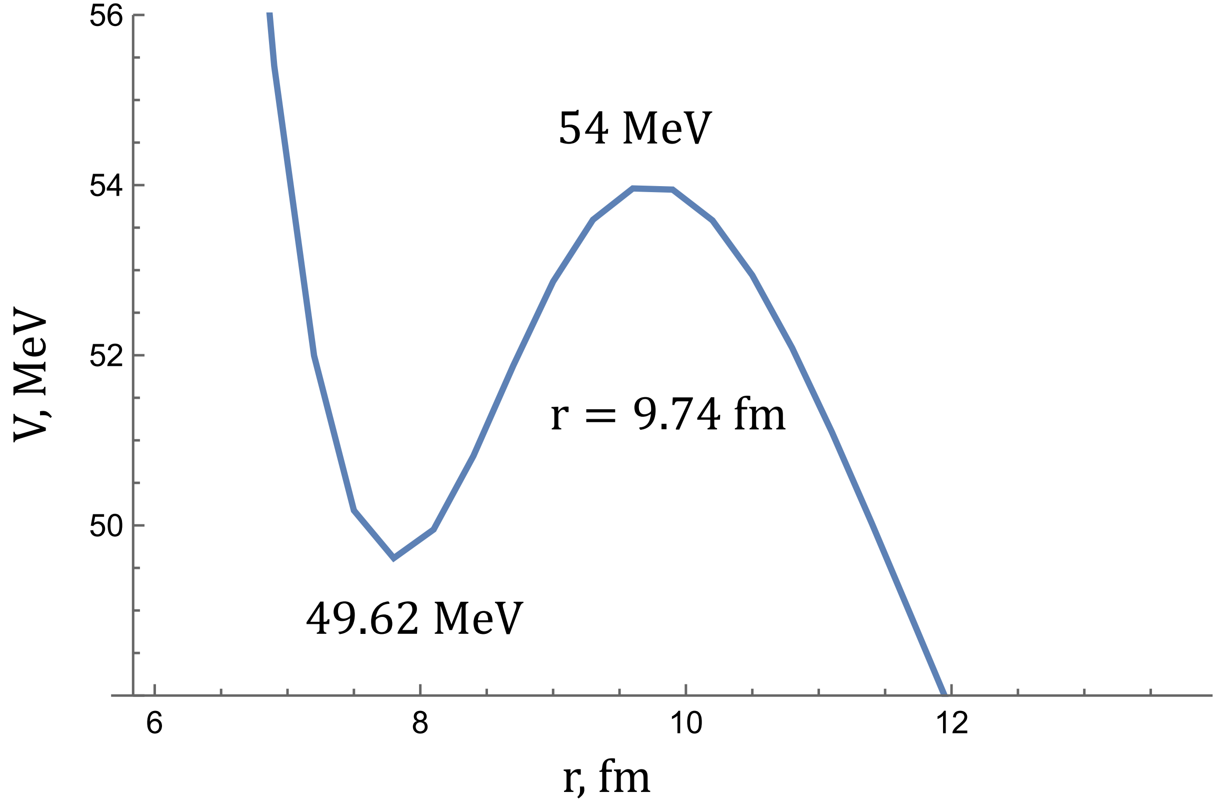


$r_{phen} = 10.58\ fm\ , V_{phen} = 50.46$ MeV $\ {}^{48}Ca + {}^{48}Ca$

$\theta_s = 906$ MeV·fm^5, (original)



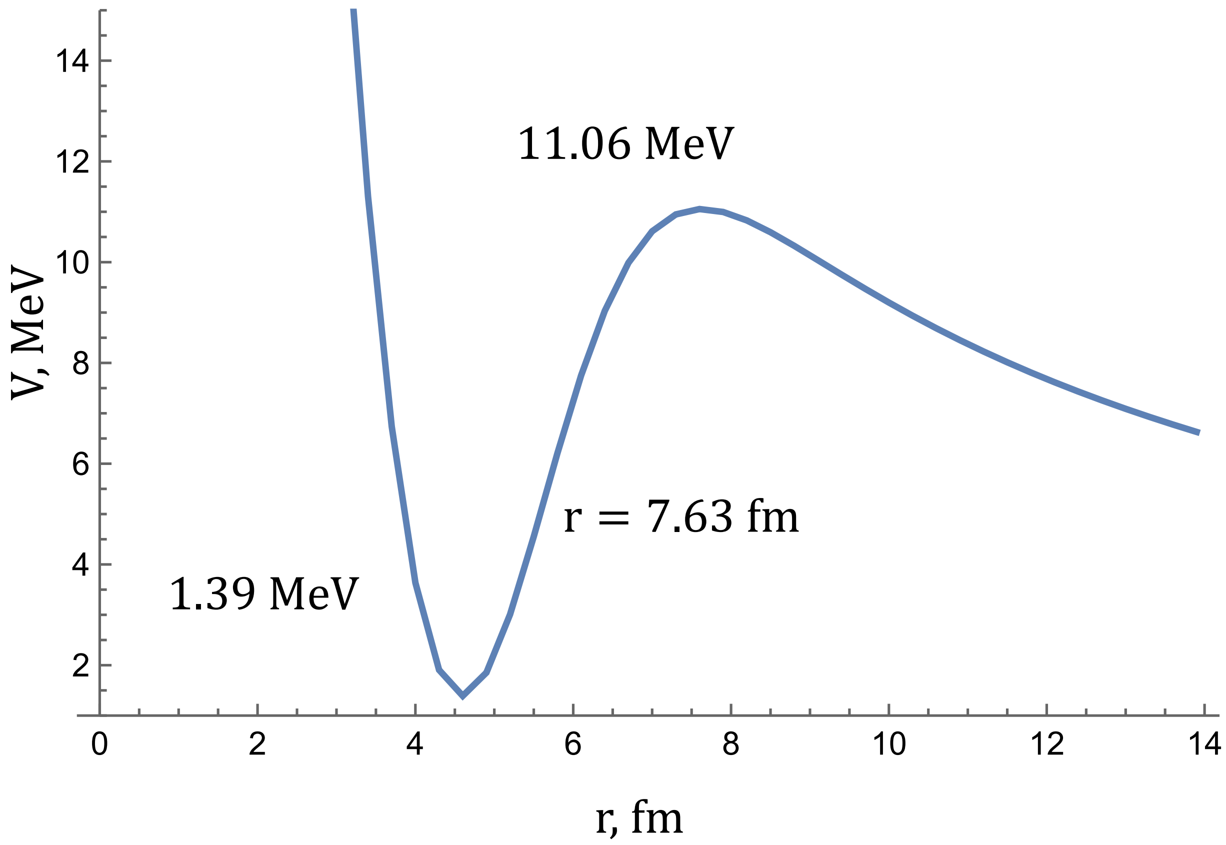
$\theta_s = 1400$ MeV·fm^5



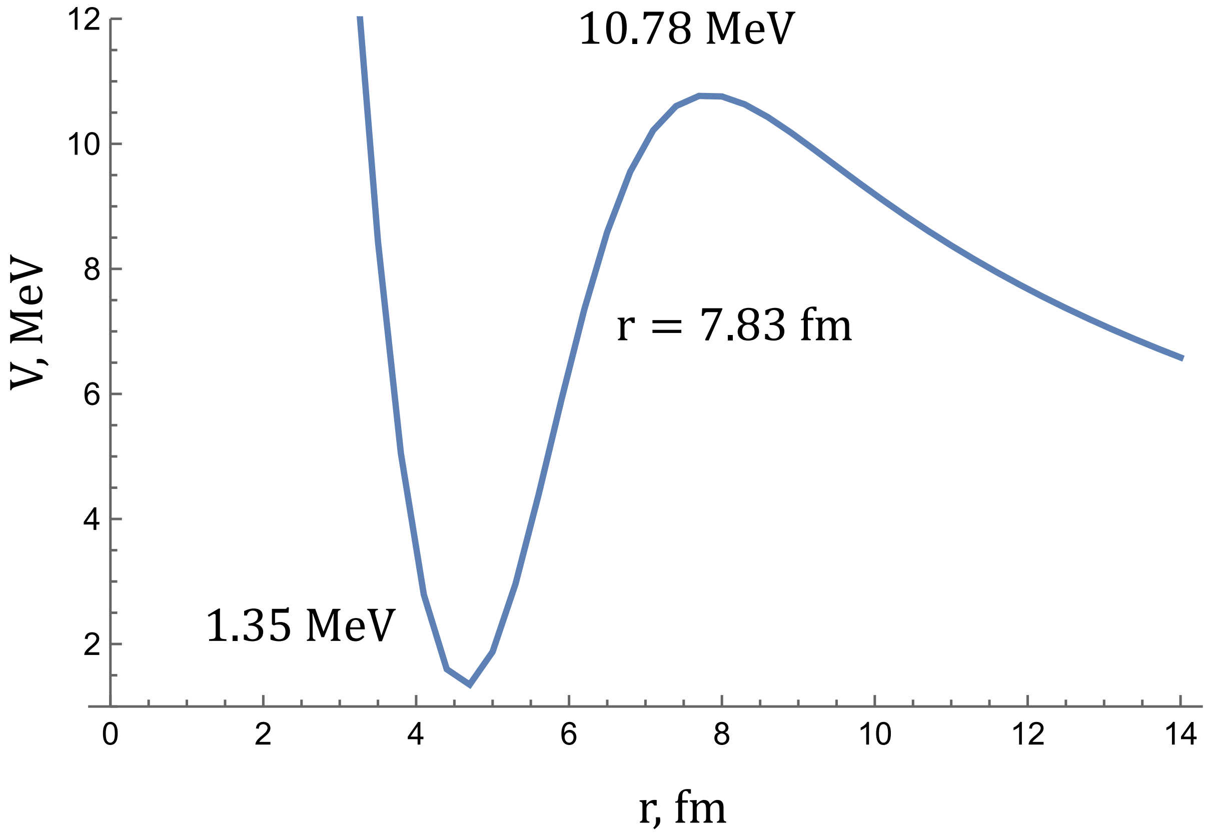
$^{16}O + ^{16}O$

$r_{phen} = 8.69\ fm\ , V_{phen} = 9.75$ MeV

$\theta_s = 906$ MeV·fm^5



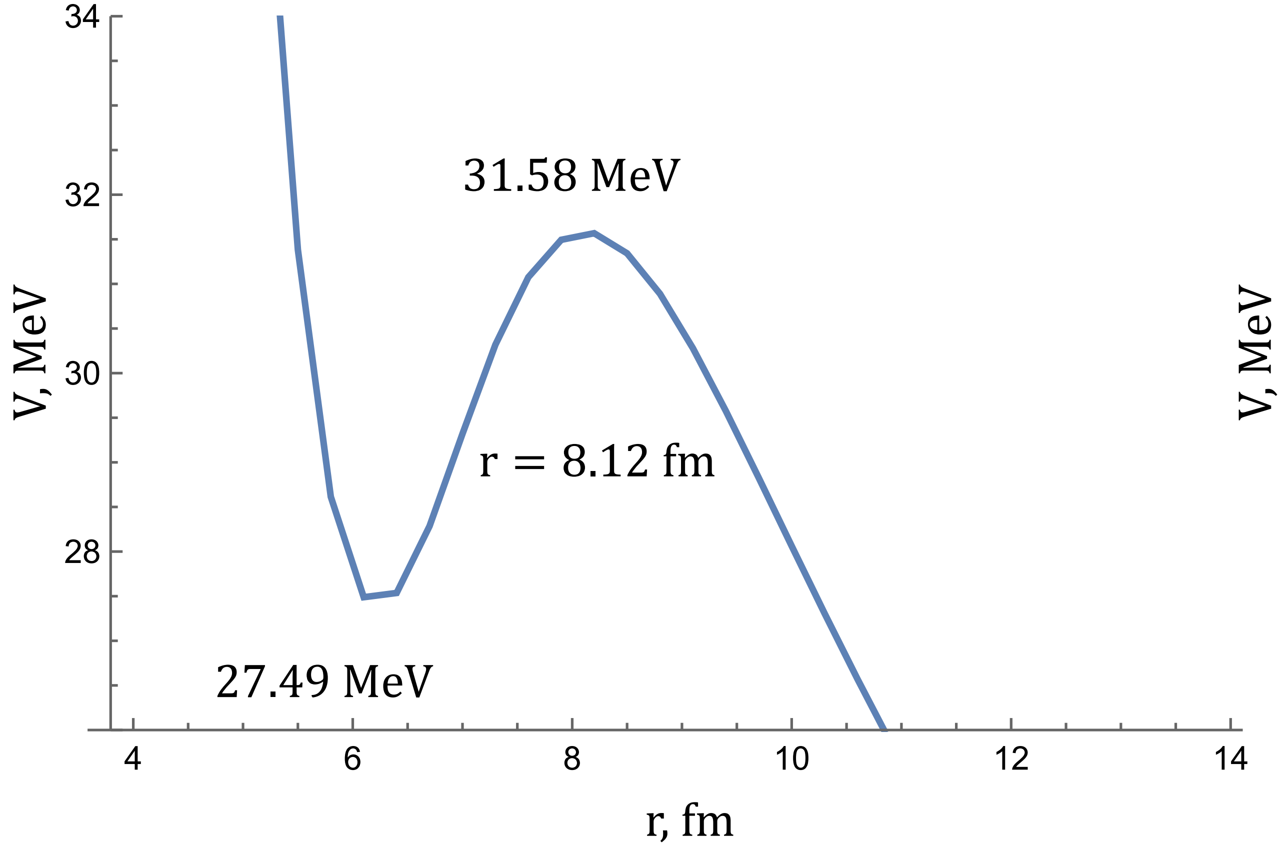
$\theta_s = 1400$ MeV·fm^5



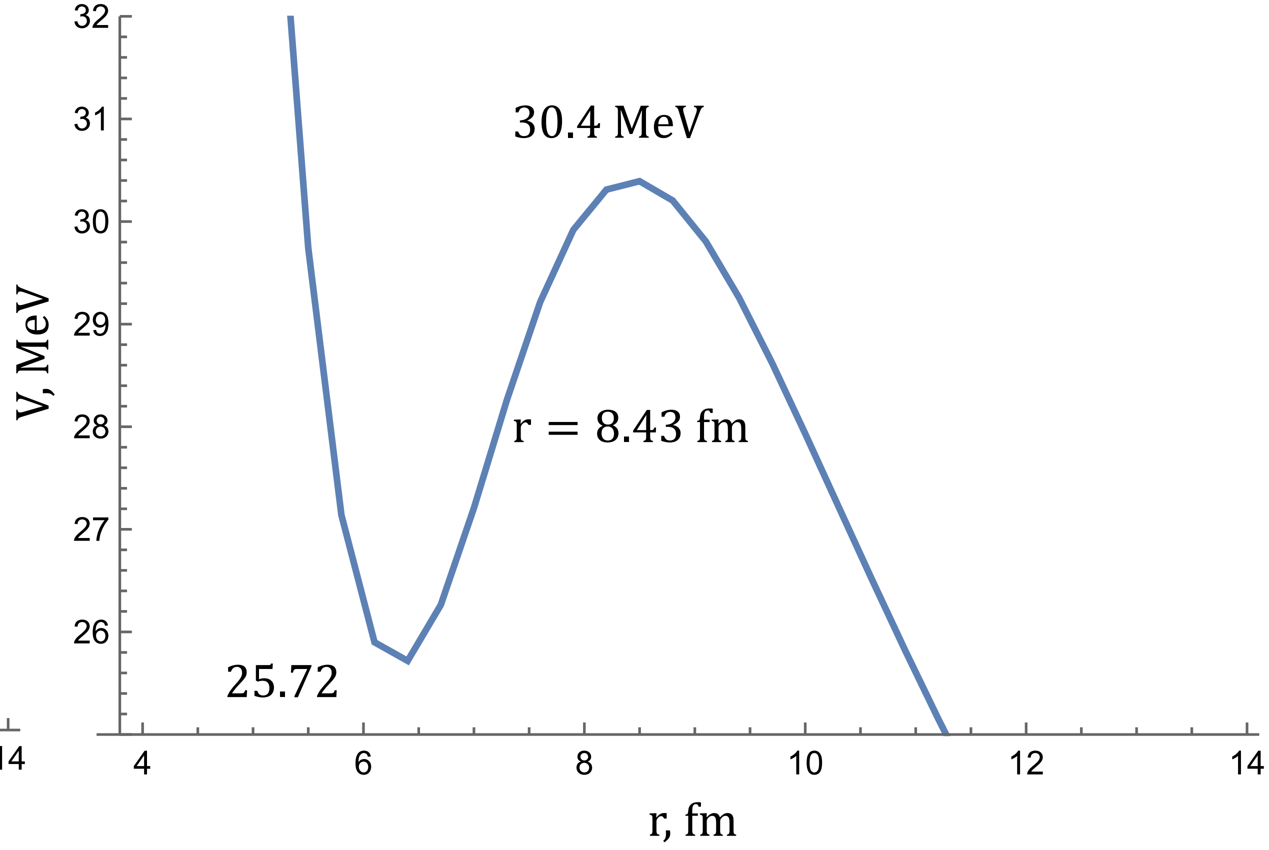
$r_{phen} = 9.08\ fm\ , V_{phen} = 28.64$ MeV

$^{28}Si + ^{28}Si$

$\theta_s = 906$ MeV·fm^5



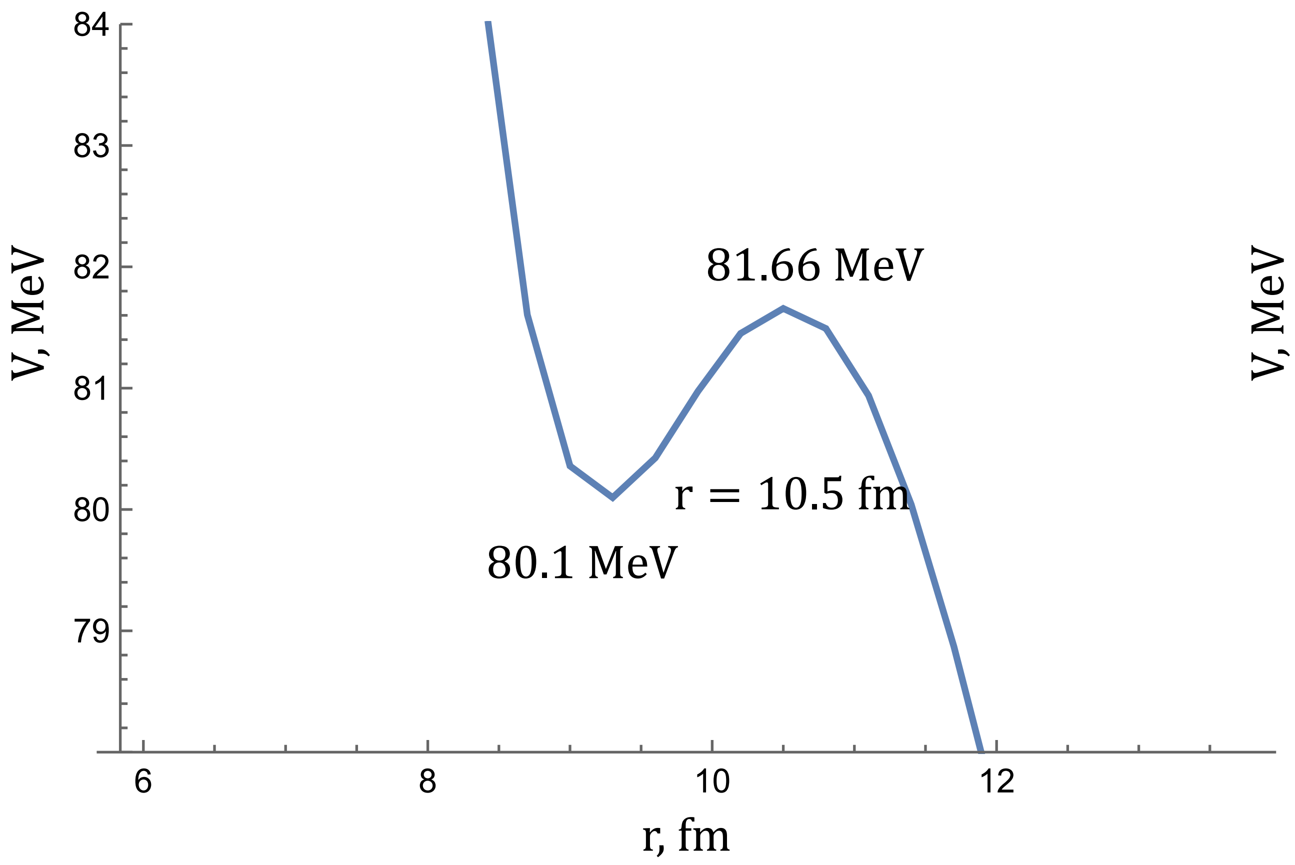
$\theta_s = 1400$ MeV·fm^5



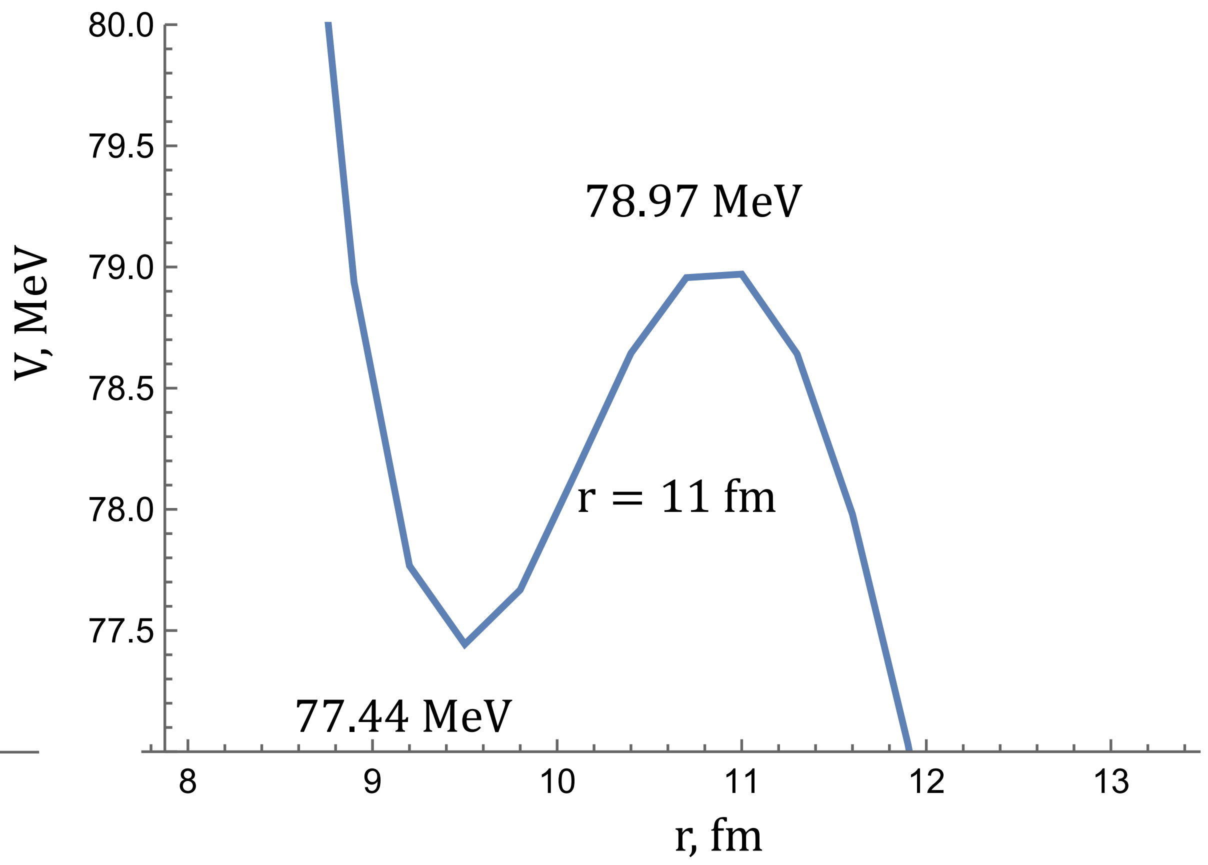
$^{16}O+^{208}Pb$

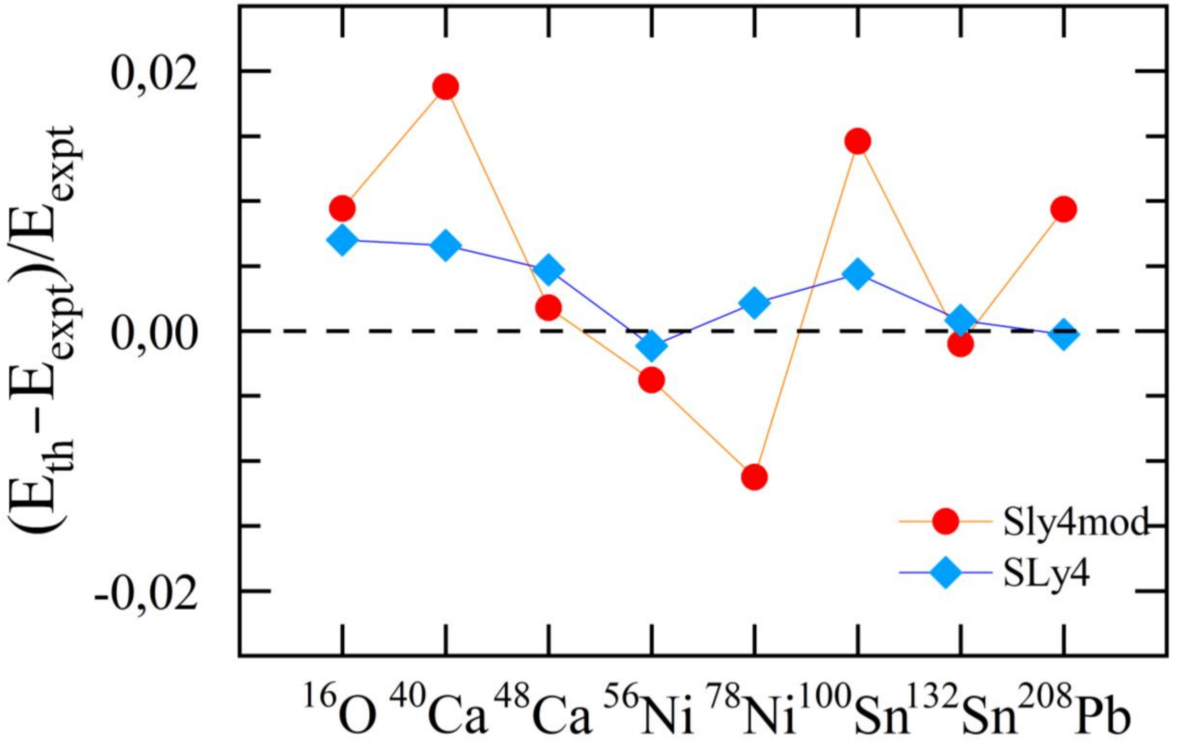
$V_{phen} = 71.5$ MeV

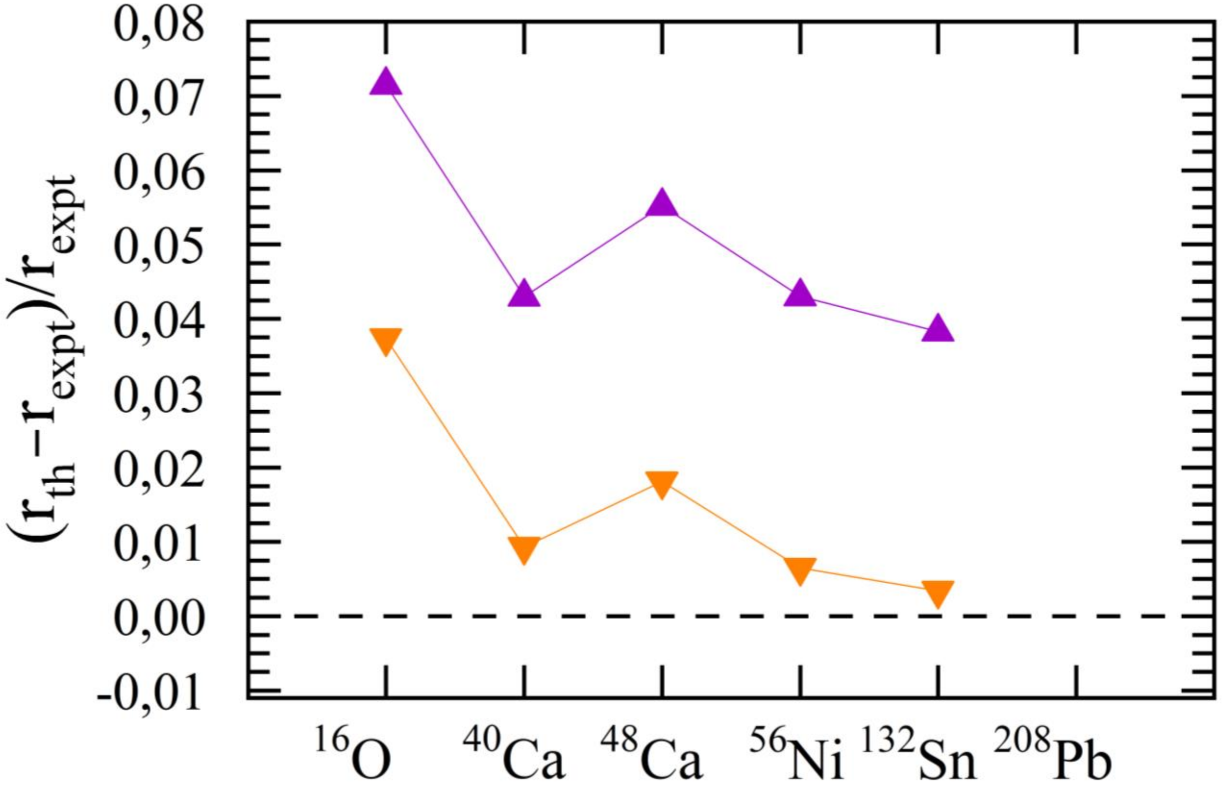
$\theta_s = 906$ MeV·fm^5



$\theta_s = 1400$ MeV·fm^5




0,02
0,00
-0,02
$(E_{th}-E_{expt})/E_{expt}$
Sly4mod
SLy4
^{16}O ^{40}Ca ^{48}Ca ^{56}Ni ^{78}Ni ^{100}Sn ^{132}Sn ^{208}Pb


0,08
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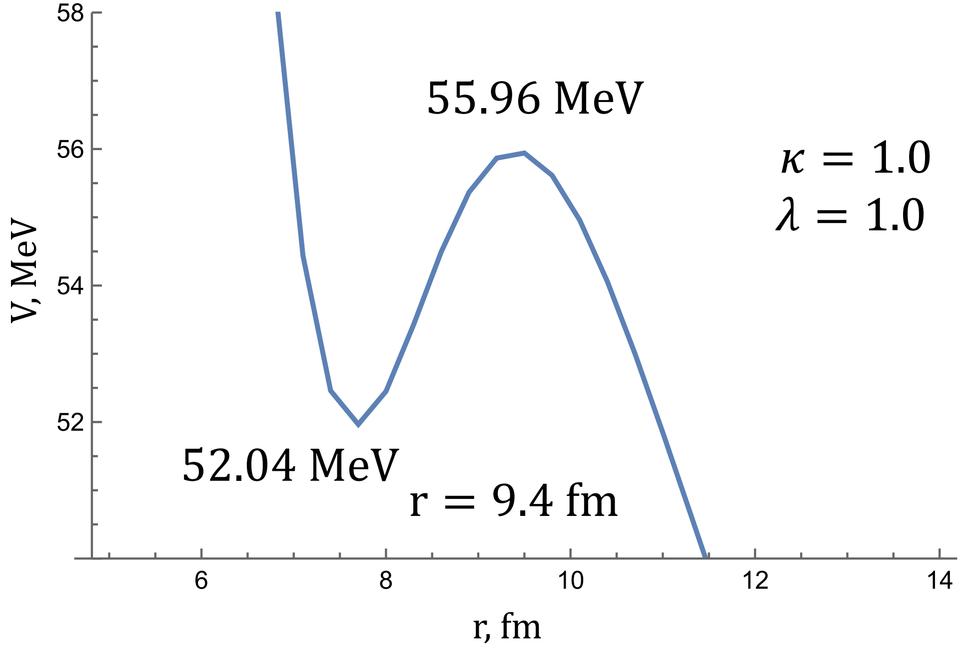
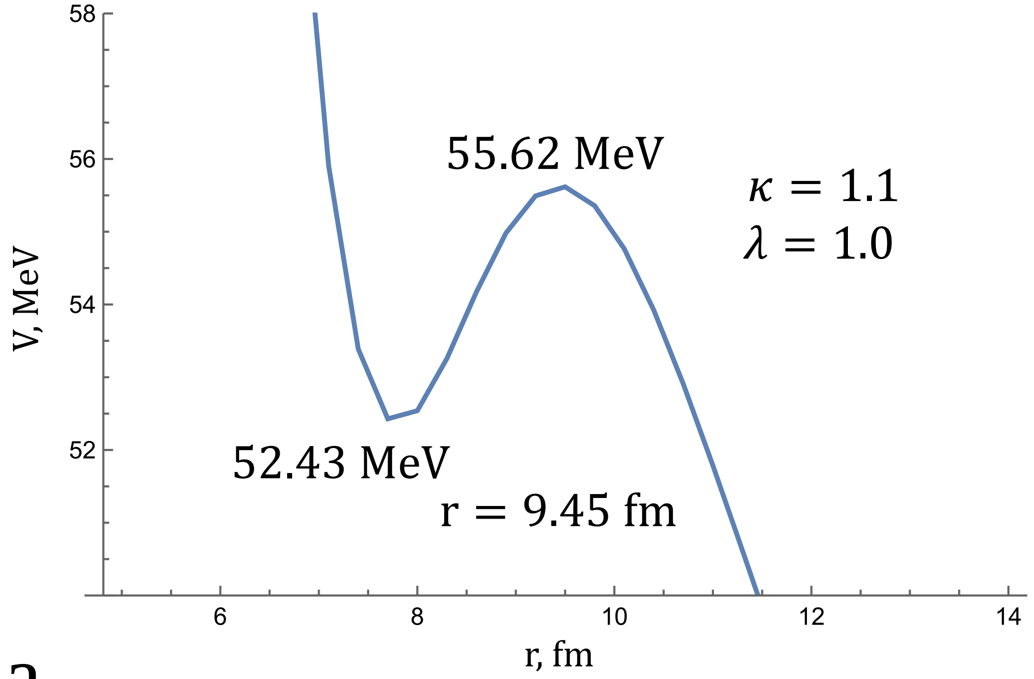
$(r_{th}-r_{expt})/r_{expt}$
^{16}O ^{40}Ca ^{48}Ca ^{56}Ni ^{132}Sn ^{208}Pb

How we could see, increasing the θ_s reduces the Coulomb barrier. Since then we can bring coefficients κ, λ in nuclear central potential to see different affect from gradient terms

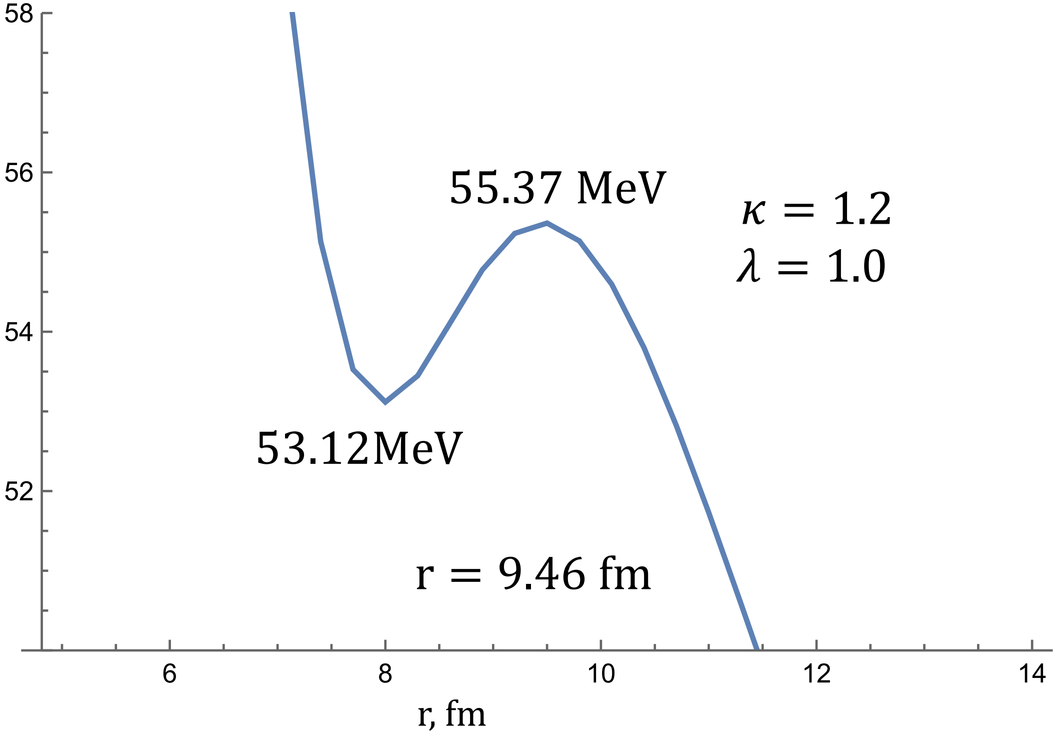
$$
\begin{aligned}
U_q(\vec{r}) \; &= \frac{1}{2} t_0\left[(2+x_0)\rho-(2x_0+1)\rho_q\right] \\
&+\frac{1}{24} t_3\left[(\alpha+2)(2+x_3)\rho^{\alpha+1}-(2x_3+1)\left(2\rho^{\alpha}\rho_q+\alpha\rho^{\alpha-1}\left(\rho_n^2+\rho_p^2\right)\right)\right] \\
&-\frac{1}{16}\kappa[3t_1(2+x_1)-t_2(2+x_2)]\nabla^2\rho+\frac{1}{16}\lambda[3t_1(2x_1+1)+t_2(2x_2+1)]\nabla^2\rho_q \\
&+\frac{1}{8}[t_1(2+x_1)+t_2(2+x_2)]\tau+\frac{1}{8}[t_2(2x_2+1)-t_1(2x_1+1)]\tau_q \\
&-\frac{1}{2} W_0\left(\nabla\cdot\boldsymbol{J}+\nabla\cdot\boldsymbol{J}_q\right)
\end{aligned}
$$

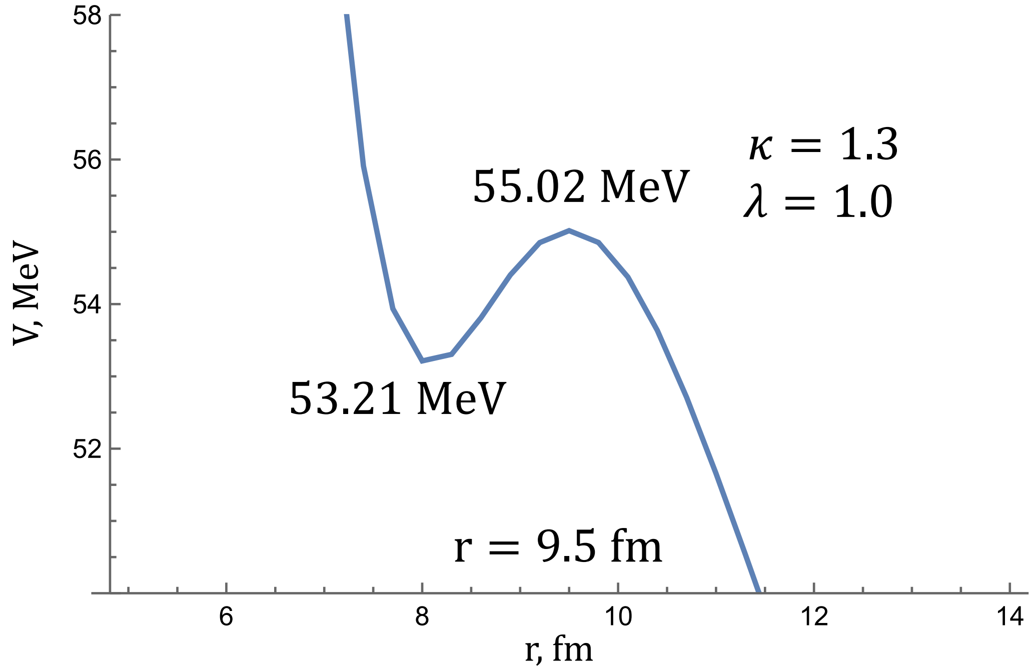




SLy4

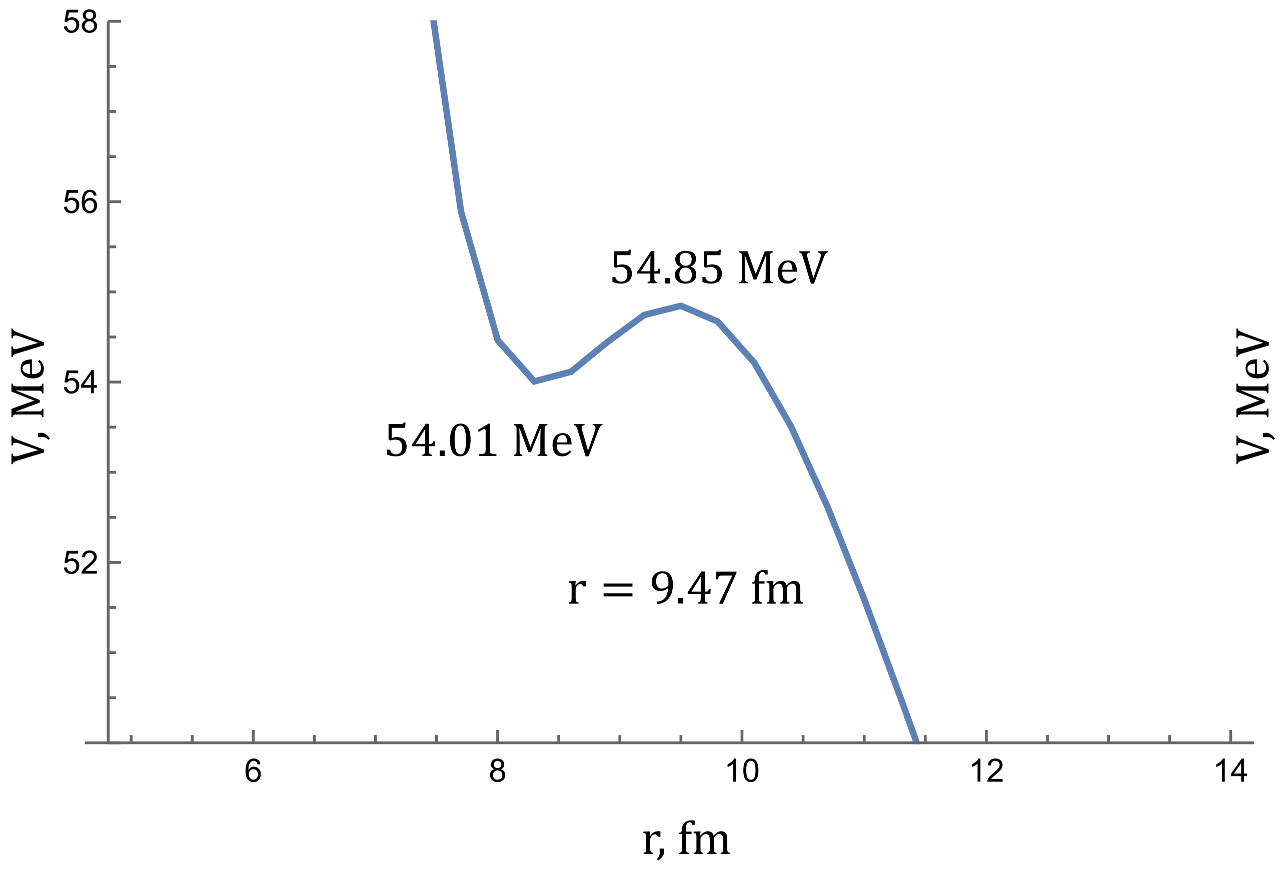
$^{48}Ca + ^{48}Ca$



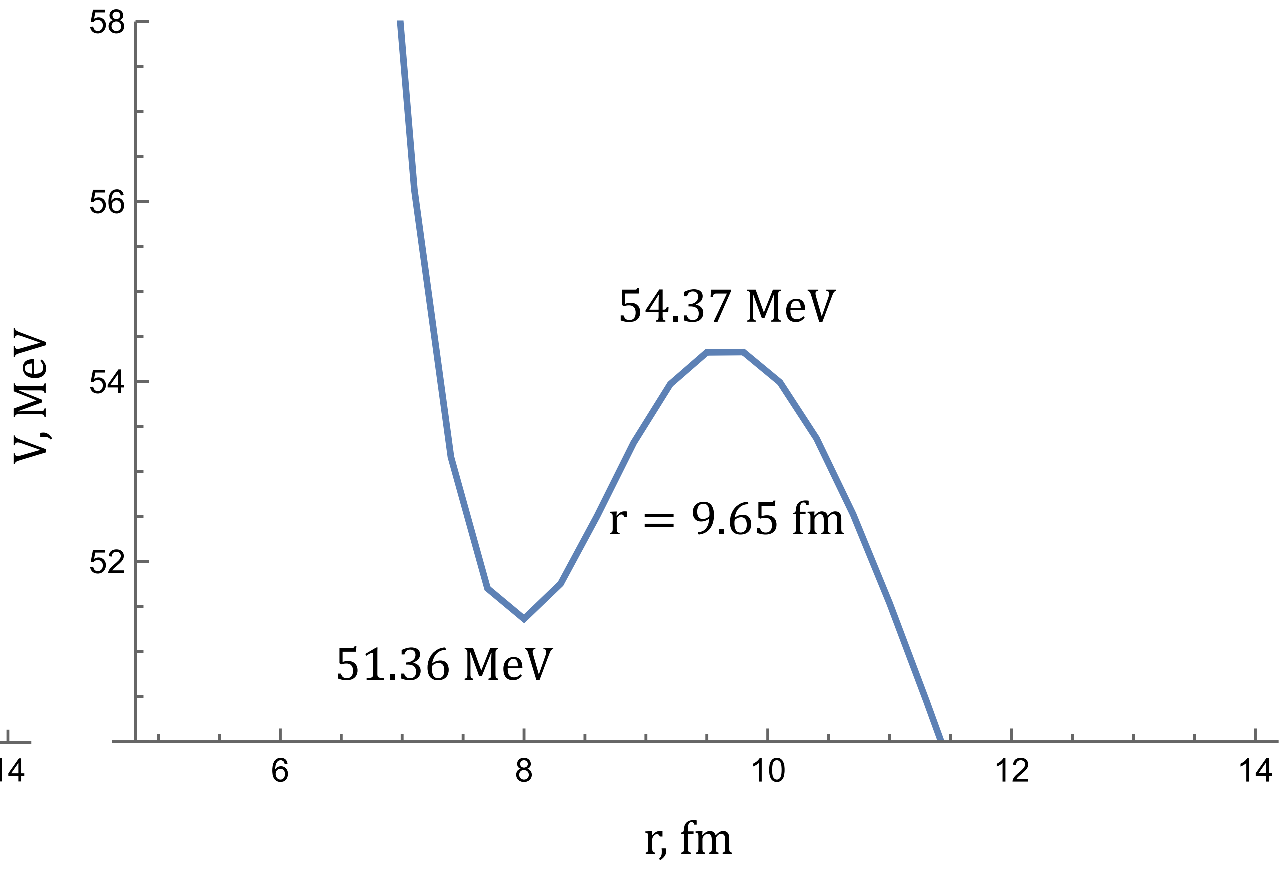


$r_{phen} = 10.58\ fm,\ V_{phen} = 50.46$ MeV

^{48}Ca+ ^{48}Ca



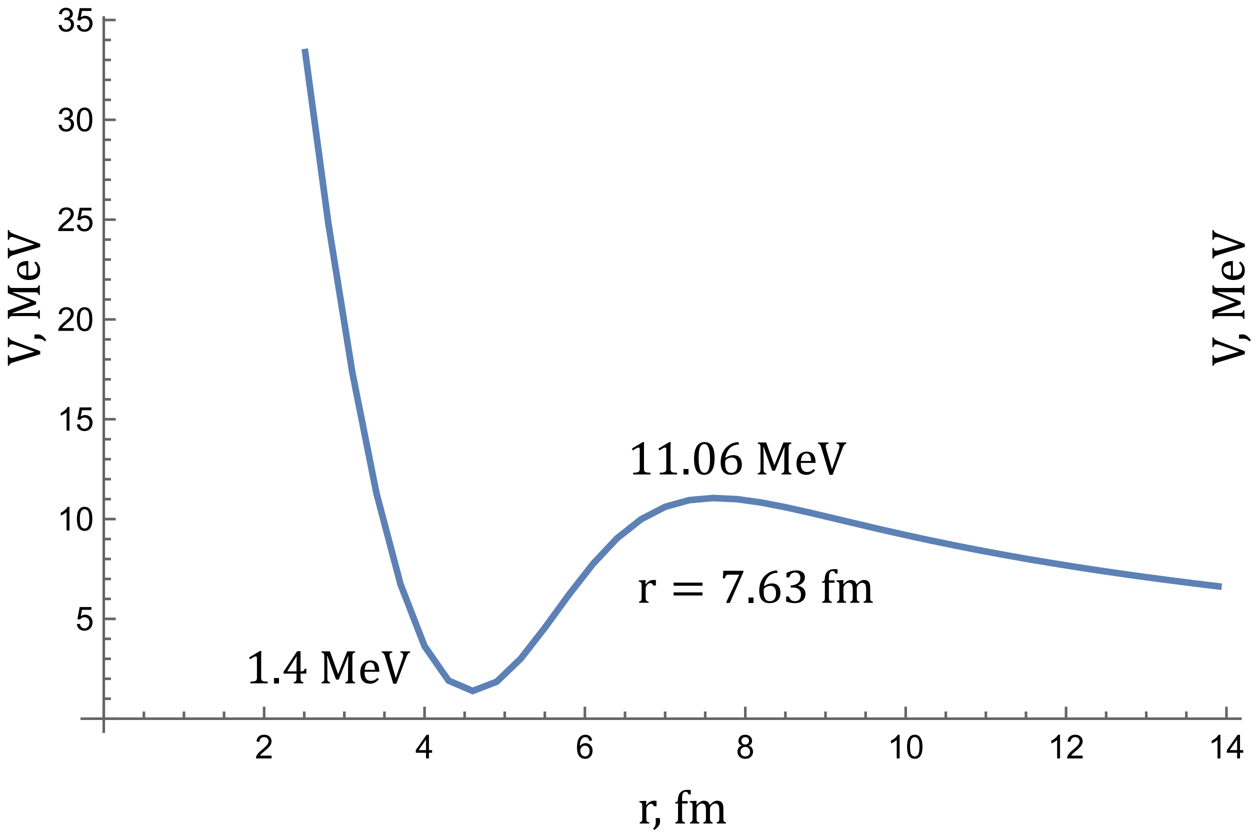
$\kappa = 1.44, \lambda = 1.0$



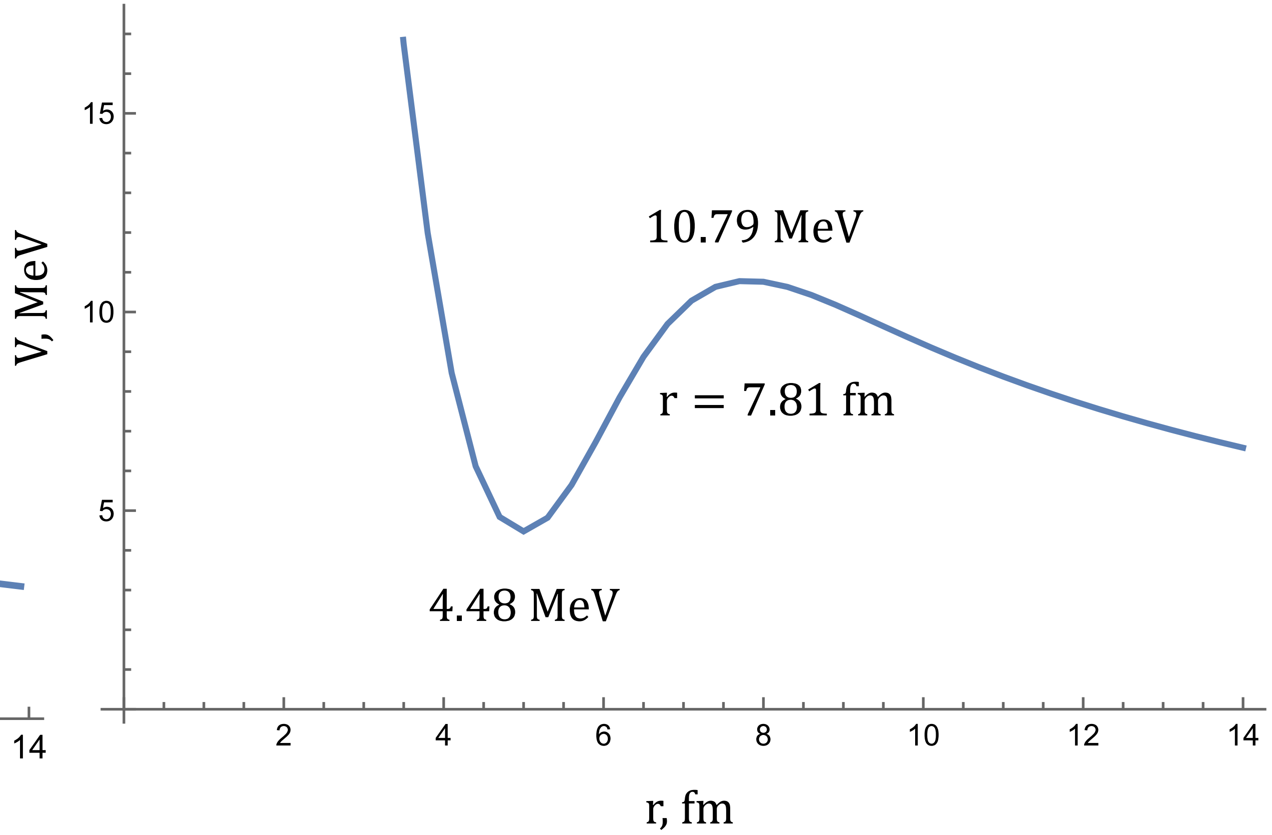
$\kappa = 1.44, \lambda = 0.8$

$^{16}O + ^{16}O$

$r_{phen} = 8.69\ fm\ , V_{phen} = 9.75$ MeV



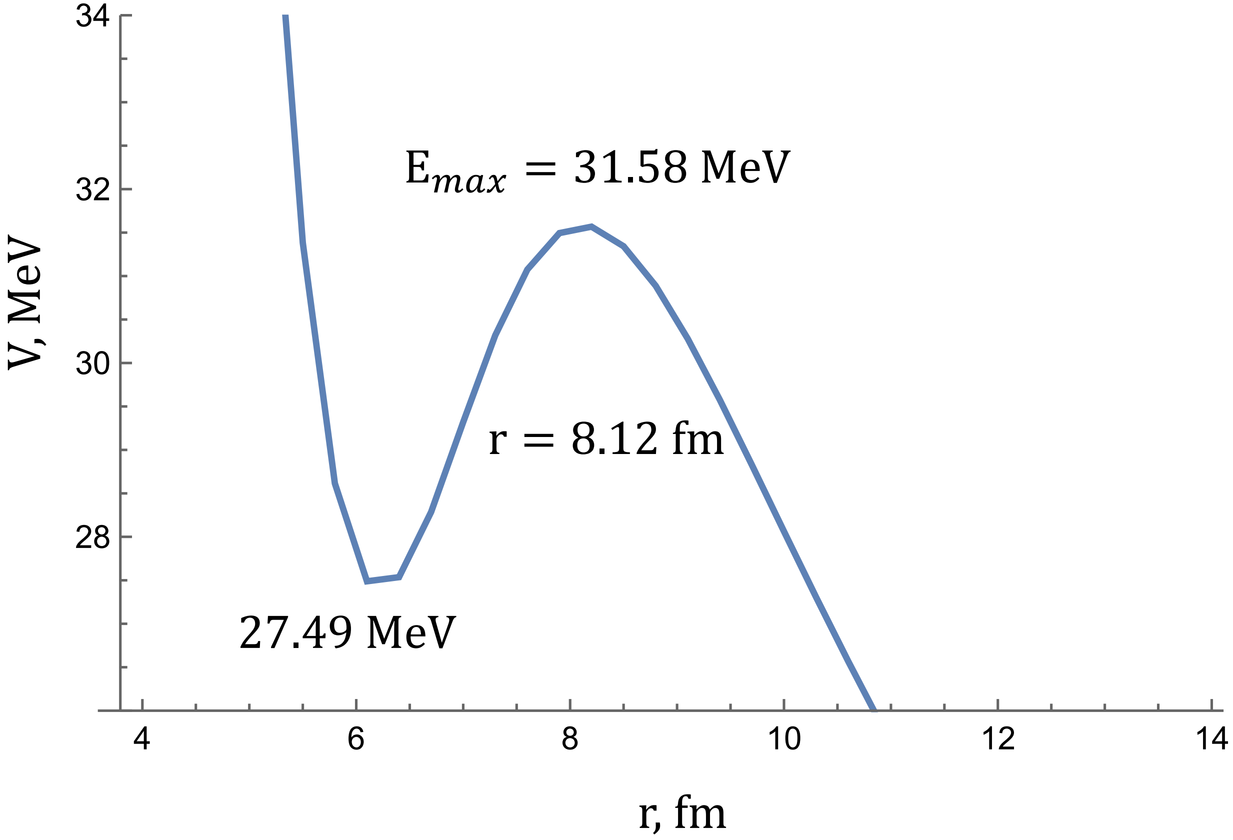
$\kappa = 1.0, \lambda = 1.0$



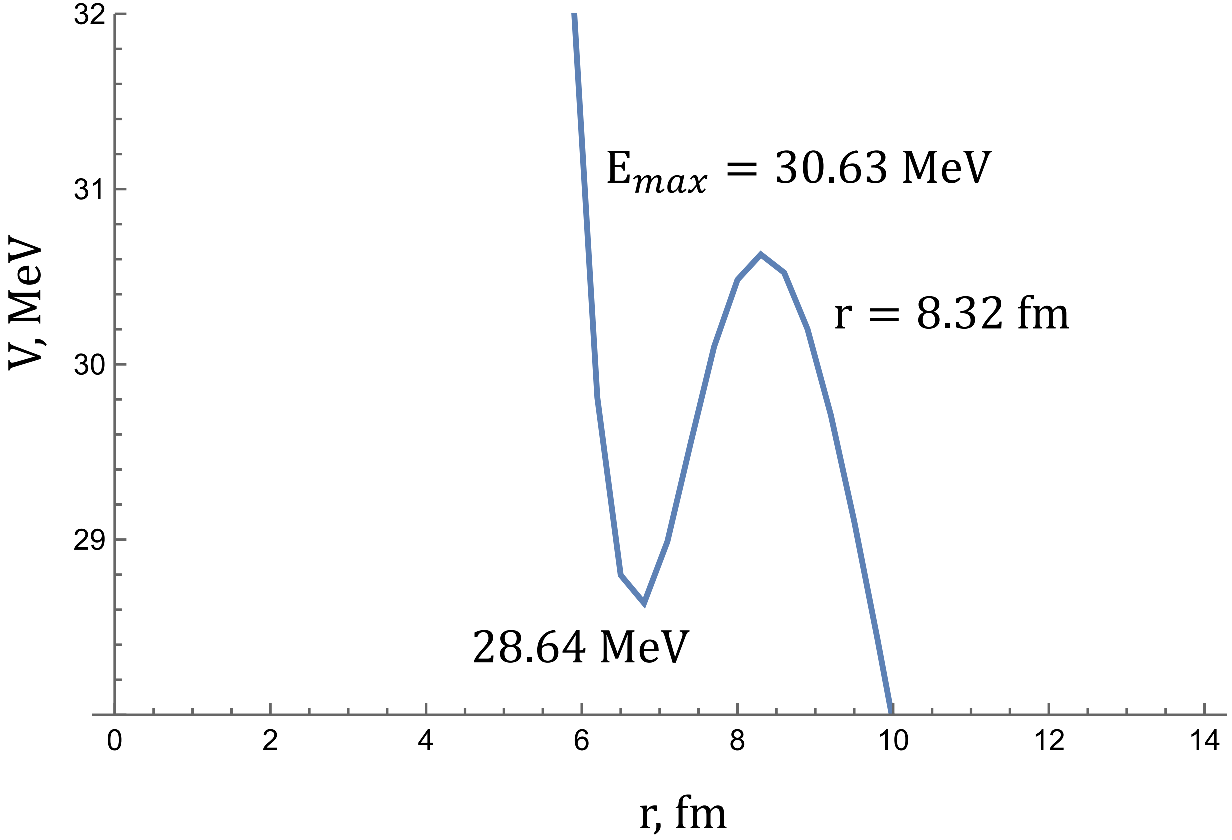
$\kappa = 1.42, \lambda = 1.0$

$^{28}Si + ^{28}Si$

$r_{phen} = 9.08\ fm\ ,V_{phen} = 28.64$ MeV



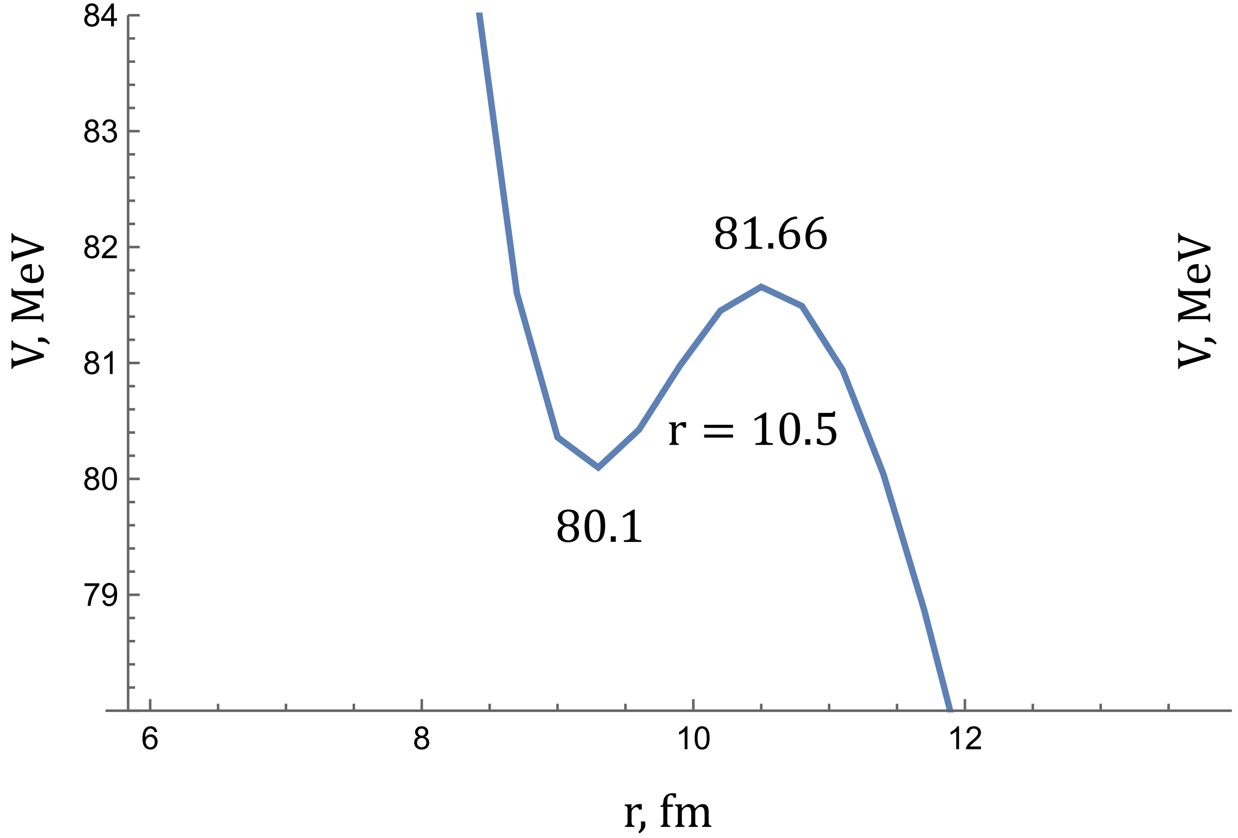
$\kappa = 1.0, \lambda = 1.0$



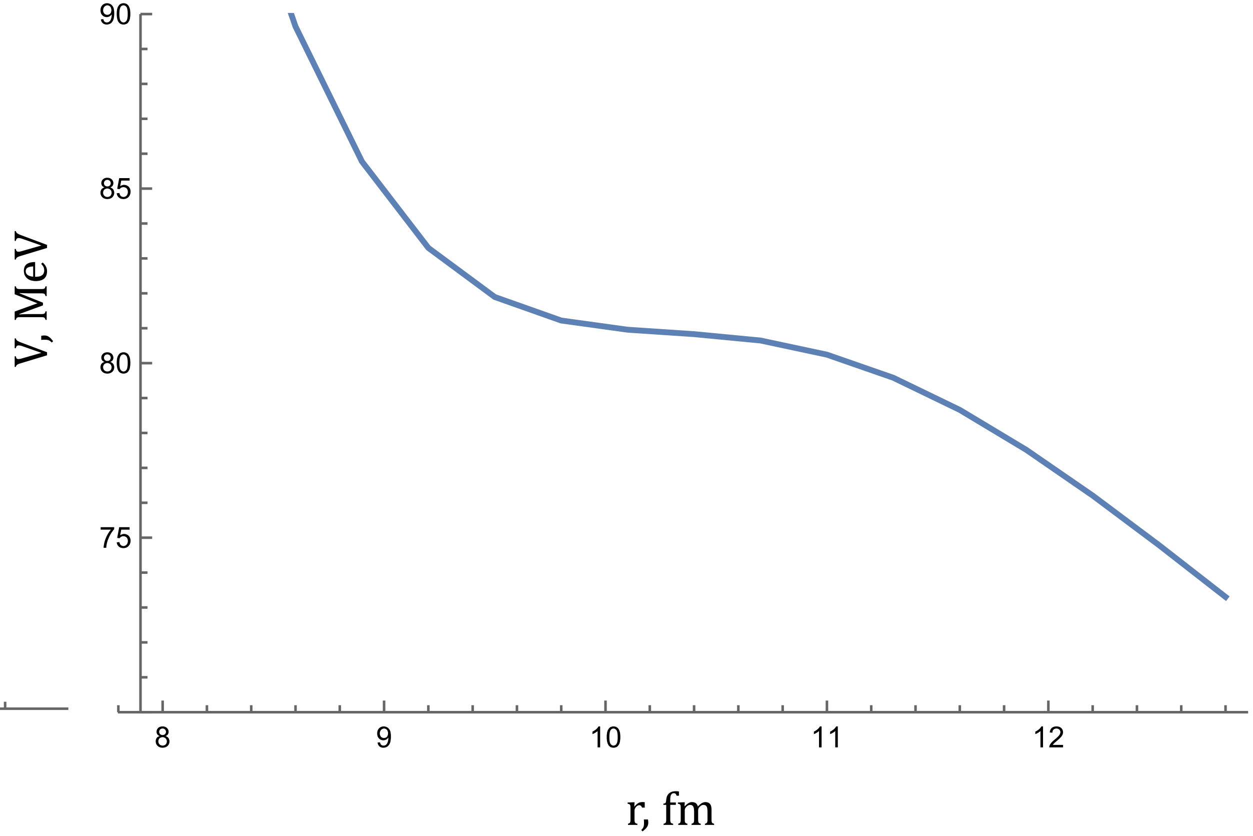
$\kappa = 1.42, \lambda = 1.0$

$^{16}O + ^{208}Pb$

$V_{phen} = 71.5$ MeV



$\kappa = 1.0, \lambda = 1.0$



$\kappa = 1.42, \lambda = 1.0$

Conclusion

The nucleon density distributions of spherical nuclei are calculated within the self-consistent HF approach based on the energy density functional. For the reactions with light nuclei, the nucleus–nucleus interaction potentials are calculated in the double-folding form with these nucleon densities. The Landau–Migdal parameters was applied for calculating the nucleus–nucleus interaction potentials in the double folding form

The characteristics of the Coulomb barriers obtained with original Skyrme EDF parametrizations aren't in good agreement with those required to describe the sub-barrier complete fusion according to work[1]. Since then, we found the way of improving the Skyrme EDF to minimize the Coulomb barrier

[1]V.V. Sargsyan, G.G. Adamian, N.V. Antonenko, H. Lenske, Phys.Lett. B **824**, 136792 (2022)