Thomas-Fermi
and
Extended Thomas-Fermi approaches

Vitali Yurievich DENISOV

Institute for Nuclear Research, Kiev, Ukraine

Taras Shevchenko National University of Kyiv

PLAN

1. **Introduction**
2. **Thomas-Fermi approach**
3. **Extended Thomas-Fermi approach**
4. **Application**
   - Modern energy-density potential
   - Density distributions in nuclei
   - Energy of the nuclei
   - Nucleus-nucleus potential
5. **Conclusions**

There are microscopic and macroscopic approaches for consideration of many-fermion systems.

Microscopic approaches are

⇒ based on microscopical models related to Schrödinger equation, Hartree-Fock or Hartree-Fock-BCS approaches and etc.;

⇒ connected with cumbersome numerical calculations;

⇒ complex in visualization and interpretation.

Macroscopic approaches are

⇒ based on classical or semiclassical models

⇒ connected with simple numerical calculations;

⇒ easy in visualization and interpretation.

2. Thomas-Fermi approach

Thomas, L. H. (1927). "The calculation of atomic fields". Proc. Cambridge Phil. Soc. 23 (5): 542-548.

Fermi, Enrico (1927). "Un Metodo Statistico per la Determinazione di alcune Priopriet dell'Atomo". Rend. Accad. Naz. Lincei 6: 602-607.

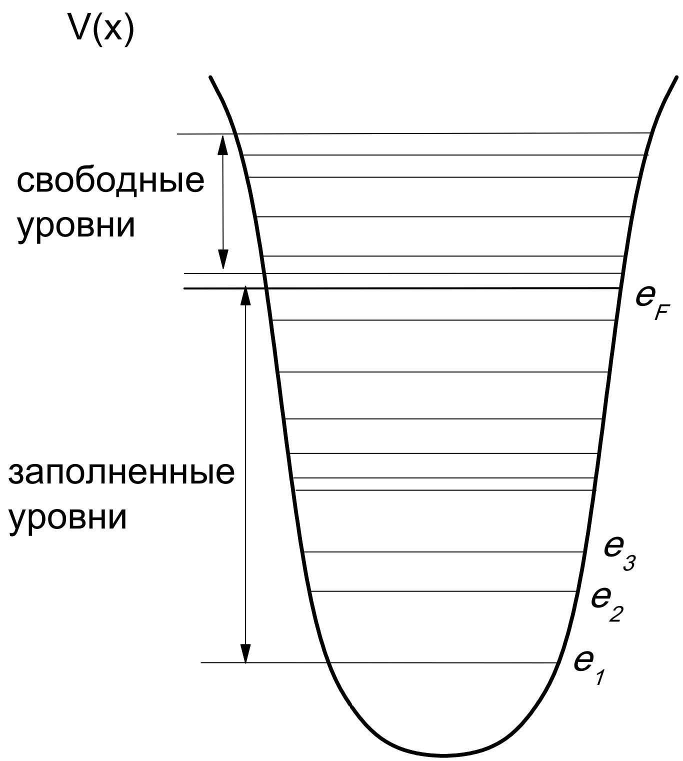
Thomas-Fermi is statistical approach for fermions based on next points:

⇒ All lowest levels including the Fermi level are occupied by particles until the Fermi level.

⇒ Two particles with spin 1/2 are occupied each level.

⇒ The corresponding partition function is $\Theta(E_F - E_i)$, where E_i is the energy of single-particle level in the system, E_F is the Fermi level,

$$\Theta(E_F - E_i) = \begin{cases} 1 \text{ if } E_F \geq E_i, \\ 0 \text{ if } E_F < E_i. \end{cases} \tag{1}$$



The energy of the fermion system is

$$E = \sum_i E_i \Theta(E_F - E_i) = \sum_i E_i n(E_i), \tag{2}$$

where $n(E_i) = \Theta(E_F - E_i)$ is the partition function.

Each quantum state fill the cell of phase space according to the Heisenberg uncertainty principle

$$\delta x \delta p = 2\pi\hbar. \tag{3}$$

Therefore the number of state related to the cell of phase space is

$$\frac{\delta x \delta p}{2\pi\hbar}. \tag{4}$$

If we take into account the spin of fermion 1/2 and therefore two fermions can occupy the same level, than

$$2\frac{\delta x \delta p}{2\pi\hbar}. \tag{5}$$

The density of particles in the volume is

$$\rho = \frac{\text{number of states}}{\delta x \delta y \delta z} = 2 \times \text{the sum on all momentums} \frac{\delta p_x \delta p_y \delta p_z}{(2\pi\hbar)^3} \tag{6}$$

or in integral form

$$\rho = 2 \times \int \frac{d^3p}{(2\pi\hbar)^3} n(p). \tag{7}$$

Here $n(p) = \Theta(p_F - p)$ is the partition function, $E_F = \frac{p_F^2}{2m}$ is the Fermi momentum, $E = \frac{p^2}{2m}$

and m is the fermion mass. We get

$$\rho = 2 \times \int d\Omega \int dp \frac{p^2}{(2\pi\hbar)^3} \Theta(p_F - p) = 2 \times \int d\Omega \frac{p_F^3}{3(2\pi\hbar)^3} = 2 \times 4\pi \frac{p_F^3}{3(2\pi\hbar)^3} = \frac{p_F^3}{3\pi^2\hbar^3}. \quad (8)$$

The energy density of the fermion system is

$$\mathcal{E} = 2 \times \int \frac{d^3p}{(2\pi\hbar)^3} n(p) \frac{p^2}{2m} = 2 \times \int d\Omega \frac{p_F^5}{10m(2\pi\hbar)^3} = \frac{p_F^5}{10\pi^2\hbar^3 m}. \quad (9)$$

Using $p_F = \left(3\pi^2\hbar^3\rho\right)^{1/3}$ we can easy find relation between energy density and the density of particles

$$\mathcal{E} = \frac{(3\pi^2\hbar^3\rho)^{5/3}}{10\pi^2\hbar^3} = \frac{3^{5/3}\pi^{4/3}}{5} \frac{\hbar^2}{2m} \rho^{5/3}. \quad (10)$$

This is well-known Thomas-Fermi relation between the energy density and the density of particles. This expression has been applied in various branches of physics as solid state, atomic and nuclear physics.

3. Extended Thomas-Fermi approach

We try to improve the Thomas-Fermi approach. The improvement will relates to the inhomogeneity of the potential in the space.

We consider single-particle Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V, \tag{11}$$

where V is the single-particle potential, which can be, as example, the self-consistent Hartree-Fock potential. The Schödinger equation is

$$\hat{H}\varphi_i = E_i\varphi_i, \tag{12}$$

where $\varphi_i = \varphi_i(\vec{r})$ is the wave function, E_i is the energy of state i.

The density matrix is

$$\rho(\vec{r}, \vec{r}', E_F) = \sum_{i=1}^{\infty} \varphi_i(\vec{r})\Theta(E_F - \hat{H})\varphi_i^*(\vec{r}'). \tag{13}$$

Note, that $\Theta(E_F - \hat{H})\varphi_i^*(\vec{r}') = \Theta(E_F - E_i)\varphi_i^*(\vec{r}')$, therefore

$$\rho(\vec{r}, \vec{r}', E_F) = \sum_{i=1}^{\infty} \varphi_i(\vec{r})\Theta(E_F - E_i)\varphi_i^*(\vec{r}'). \tag{14}$$

Our goal to get expression for

$$\rho(\vec{r}, \vec{r}', E_F) = \sum_{i=1}^{\infty} \varphi_i(\vec{r}) \Theta(E_F - \hat{H}) \varphi_i^*(\vec{r}').$$

with the classical hamiltonian

$$H(\vec{q}, \vec{p}) = \frac{\vec{p}^2}{2m} + V(\vec{q}), \tag{15}$$

i.e. without operator $\hat{H}$.

The Laplace and inverse Laplace transformations are, respectively,

$$F(s) = \mathcal{L}\{f(E)\} = \int_0^{\infty} dE\ e^{-sE} f(E), \tag{16}$$

$$f(E) = \mathcal{L}^{-1}\{F(s)\} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds\ e^{sE} F(s). \tag{17}$$

Useful examples are

$$\Theta(E_F - E_i) = \mathcal{L}^{-1}\{\frac{e^{-\beta E_i}}{\beta}\} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta\ e^{\beta E_F}\ \frac{e^{-\beta E_i}}{\beta}, \tag{18}$$

$$\delta(E_F - E_i) = \mathcal{L}^{-1}\{e^{-\beta E_i}\} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta\ e^{\beta E_F}\ e^{-\beta E_i}. \tag{19}$$

$$\Theta(E_F - E_i) = \mathcal{L}^{-1}\{\frac{e^{-\beta E_i}}{\beta}\} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta\ e^{\beta E_F}\ \frac{e^{-\beta E_i}}{\beta}. \quad (20)$$

Taking into account

$$\Theta(E_F - E_i) = \mathcal{L}^{-1}\{\frac{e^{-\beta E_i}}{\beta}\} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta\ e^{\beta E_F}\ \frac{e^{-\beta E_i}}{\beta}. \quad (21)$$

and spin of fermions 1/2 we present the density matrix into form

$$\rho(\vec{r}, \vec{r}', E_F) = 2\sum_{i=1}^{\infty} \varphi_i(\vec{r})\Theta(E_F - \hat{H})\varphi_i^*(\vec{r}') = 2\sum_{i=1}^{\infty} \varphi_i(\vec{r})\mathcal{L}^{-1}\{\frac{e^{-\beta \hat{H}}}{\beta}\}\varphi_i^*(\vec{r}')$$
$$= 2\mathcal{L}^{-1}\{\frac{C^{\beta}(\vec{r}, \vec{r}')}{\beta}\}, \quad (22)$$

where

$$C^{\beta}(\vec{r}, \vec{r}') = \sum_{i=1}^{\infty} \varphi_i(\vec{r}) e^{-\beta \hat{H}} \varphi_i^*(\vec{r}'). \quad (23)$$

Let A is a single-particle operator. The Wigner transform of a single-particle operator A_W is defined as

$$A_W \equiv A(\vec{q},\vec{p}) = \int d^3s\; e^{-i(\vec{p}\vec{s})/\hbar} < \vec{q} + \vec{s}/2|A|\vec{q} - \vec{s}/2 > . \tag{24}$$

The inverse Wigner transform is

$$< \vec{r}|A|\vec{r}' >= \frac{1}{(2\pi\hbar)^3} \int d^3p\; e^{i\vec{p}(\vec{r}-\vec{r}')/\hbar}\; A((\vec{r}+\vec{r}')/2,\vec{p}). \tag{25}$$

Note that the Wigner transform of the Hamiltonian operator is

$$H_W = H(\vec{q},\vec{p}) = \frac{\vec{p}^2}{2m} + V. \tag{26}$$

So the Wigner transform of the Hamiltonian has classical form.

Example:

$$\begin{aligned}\hat{H}^2 = (\hat{T}+\hat{V})^2 = \left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\left(\frac{-\hbar^2}{2m}\nabla^2 + V\right) = \hat{T}^2 + \hat{T}\hat{V} + \hat{V}\hat{T} + \hat{V}^2 \\ = \hat{T}^2 + \hat{V}\hat{T} + \hat{V}^2 + \hat{T}\hat{V} = \hat{T}^2 + 2\hat{V}\hat{T} + \hat{V}^2 + \frac{-\hbar^2}{2m}(2\nabla\hat{V}\nabla + \nabla^2\hat{V}).\end{aligned} \tag{27}$$

Here $\hat{V}$ is the potential energy, which is the function of coordinate only. Similar:

$$\hat{H}^2{}_W = (\hat{T}_W + \hat{V}_W)^2 - \frac{1}{2}\frac{\hbar^2}{2m}\Delta V_W = H^2(\vec{q},\vec{p}) - \frac{1}{2}\frac{\hbar^2}{2m}\Delta V_W. \tag{28}$$

The Wigner transform of function $C^\beta(\vec{r},\vec{r}') = \sum_{i=1}^{\infty} \varphi_i(\vec{r}) e^{-\beta\hat{H}} \varphi_i^*(\vec{r}')$ is

$$C^\beta(\vec{q},\vec{p}) = \left(e^{-\beta\hat{H}}\right)_W = \sum_{i=0}^{\infty} \frac{1}{n!} \left((-\beta\hat{H})^n\right)_W . \tag{29}$$

Using the formula

$$(AB)_W = A(\vec{q},\vec{p}) e^{\frac{i\hbar}{2}(\overleftarrow{\nabla}_q \overrightarrow{\nabla}_p - \overleftarrow{\nabla}_p \overrightarrow{\nabla}_q)} B(\vec{q},\vec{p}) \tag{30}$$

we get

$$C^\beta(\vec{q},\vec{p}) = \left(e^{-\beta\hat{H}}\right)_W = \sum_{i=0}^{\infty} \frac{1}{n!} \left((-\beta\hat{H})^n\right)_W \tag{31}$$

$$\approx \exp\left[-\beta\left(\frac{p^2}{2m} + V(q)\right)\right] \left[1 + \frac{\hbar^2\beta^2}{8m}\left(-\nabla^2 V + \frac{\beta}{3}(\nabla V)^2 + \frac{\beta}{3m}(\vec{p}\nabla)^2 V\right) + \mathcal{O}(\hbar^4)\right].$$

The Wigner transform $f(\vec{q},\vec{p})$ of the semiclassical density matrix

$$\begin{aligned} f(\vec{q},\vec{p},E_F) &= \int d^3s\, e^{-i(\vec{p}\vec{s})/\hbar}\, \rho(\vec{q}+\vec{s}/2, \vec{q}-\vec{s}/2, E_F) \\ &= 2\int d^3s\, e^{-i(\vec{p}\vec{s})/\hbar}\, \mathcal{L}^{-1}\{\frac{C^\beta(\vec{q}+\vec{s}/2, \vec{q}-\vec{s}/2)}{\beta}\} = 2\mathcal{L}^{-1}\{\frac{C^\beta(\vec{q},\vec{p})}{\beta}\} \\ &= 2\Theta(E_F - \frac{p^2}{2m} - V(q)) + 2\frac{\hbar^2}{8m}\Big[-\nabla^2 V\, \delta'(E_F - \frac{p^2}{2m} - V(q)) \\ &+ \frac{1}{3}\left((\nabla V)^2 + \frac{(\vec{p}\nabla)^2 V}{m}\right)\delta''(E_F - \frac{p^2}{2m} - V(q))\Big] + \mathcal{O}(\hbar^4). \end{aligned} \tag{32}$$

The Thomas-Fermi part of Wigner semiclassical density matrix

$$f_{\rm TF}(\vec{q},\vec{p},E_F) = 2\Theta(E_F - \frac{p^2}{2m} - V(q)). \tag{33}$$

The Thomas-Fermi density

$$\begin{aligned}\rho_{\rm TF}(\vec{r}) &= \frac{1}{(2\pi\hbar)^3}\int d^3p\ f_{\rm TF}(\vec{r},\vec{p},E_F) = 2\frac{1}{(2\pi\hbar)^3}\int d^3p\ \Theta(E_F - \frac{p^2}{2m} - V(q)) \\ &= \frac{1}{4\pi^3\hbar^3}\int d\Omega\int_0^\infty dp\ p^2\ \Theta(E_F - \frac{p^2}{2m} - V(q)) = \frac{1}{\pi^2\hbar^3}\int_0^{[2m(E_F-V(q))]^{1/2}} dp\ p^2 \\ &= \frac{1}{3\pi^2\hbar^3}[2m(E_F - V(q))]^{3/2} = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}[E_F - V(q)]^{3/2} = \frac{p_F^3}{3\pi^2\hbar^3},\end{aligned} \tag{34}$$

where $p_F = [2m(E_F - V(q))]^{1/2}$.

The kinetic energy density is defined as

$$\tau = \frac{\hbar^2}{2m}\nabla_r\nabla_{r'}\rho(\vec{r},\vec{r}',E_F)|_{\vec{r}'=\vec{r}} = \sum_i \frac{\hbar^2}{2m}\nabla_r\varphi_i(\vec{r})\nabla_{r'}\varphi_i(\vec{r}'). \tag{35}$$

Similar way we get

$$\begin{aligned}\tau_{\rm TF}(\vec{r}) &= \frac{1}{(2\pi\hbar)^3}\int d^3p\ \frac{p^2}{2m}\ f_{\rm TF}(\vec{r},\vec{p},E_F) = \frac{1}{2m\pi^2\hbar^3}\int_0^{[2m(E_F-V(q))]^{1/2}} dp\ p^4 \\ &= \frac{1}{5\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}[E_F - V(q)]^{5/2} = \frac{p_F^5}{10\pi^2 m\hbar^3}.\end{aligned} \tag{36}$$

The Wigner transform $f(\vec{q},\vec{p})$ of the semiclassical density matrix

$$f(\vec{q},\vec{p},E_F) = 2\Theta(E_F - \frac{p^2}{2m} - V(q)) + 2\frac{\hbar^2}{8m}\Big[-\nabla^2 V\ \delta'(E_F - \frac{p^2}{2m} - V(q)) + \frac{1}{3}\left((\nabla V)^2 + \frac{(\vec{p}\nabla)^2 V}{m}\right)\delta''(E_F - \frac{p^2}{2m} - V(q))\Big] + \mathcal{O}(\hbar^4). \tag{37}$$

Let's consider contribution

$$\rho_{21} = \frac{1}{(2\pi\hbar)^3}\int d^3p\ \left[2\frac{\hbar^2}{8m}(-1)\nabla^2 V\ \delta'(E_F - \frac{p^2}{2m} - V(q))\right] = \frac{-\nabla^2 V}{32m\pi^3\hbar}\int d^3p\ \ \delta'(E_F - \frac{p^2}{2m} - V(q)) \tag{38}$$

Taking into account that

$$\delta'(E_F - \frac{p^2}{2m} - V(q)) = \frac{d\delta(E_F - \frac{p^2}{2m} - V(q))}{dE} = -\frac{d\delta(E_F - \frac{p^2}{2m} - V(q))}{d(p^2/(2m))} = -2m\frac{d\delta(E_F - \frac{p^2}{2m} - V(q))}{d(p^2)} = -2m\frac{d\delta(E_F - \frac{p^2}{2m} - V(q))}{dp}\frac{1}{\frac{dp^2}{dp}} = \frac{-m}{p}\ \frac{d\delta(E_F - \frac{p^2}{2m} - V(q))}{dp} \tag{39}$$

we get

$$\rho_{21} = \frac{-\nabla^2 V}{32m\pi^3\hbar}\int d^3p\ \ \frac{-m}{p}\ \frac{d\delta(E_F - \frac{p^2}{2m} - V(q))}{dp}$$

$$= \frac{\Delta V}{32\pi^3\hbar}\int d\Omega \int dp\, p^2\, \frac{1}{p}\, \frac{d\delta(E_F - \frac{p^2}{2m} - V(q))}{dp} = \frac{\Delta V}{8\pi^2\hbar}\int dp\, p\, \frac{d\delta(E_F - \frac{p^2}{2m} - V(q))}{dp}. \quad (40)$$

Taking integral by parts we get

$$\rho_{21} = -\frac{\Delta V}{8\pi^2\hbar}\int dp\, \frac{dp}{dp}\, \delta(E_F - \frac{p^2}{2m} - V(q))$$
$$= -\frac{\pi\Delta V}{8\pi^2\hbar}\int dp\, \delta\left(\left(\sqrt{E_F - V(q)} - \frac{p}{\sqrt{2m}}\right)\left(\sqrt{E_F - V(q)} + \frac{p}{\sqrt{2m}}\right)\right)$$
$$= -\frac{\Delta V}{8\pi^2\hbar}\, \frac{\sqrt{2m}}{2\sqrt{E_F - V(q)}} = -\frac{1}{16\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2} \frac{\Delta V}{\sqrt{E_F - V(q)}} \quad (41)$$

Similar

$$\rho_{22} = \frac{1}{(2\pi\hbar)^3}\int d^3p\, \left[2\frac{\hbar^2}{8m}\frac{1}{3}(\nabla V)^2 \delta''(E_F - \frac{p^2}{2m} - V(q))\right]$$
$$= \frac{(\nabla V)^2}{96m\hbar}\int d^3p\, \delta''(E_F - \frac{p^2}{2m} - V(q)) = \frac{\pi(\nabla V)^2}{24m\hbar}\int dp\, p^2\, \delta''(E_F - \frac{p^2}{2m} - V(q))$$
$$= \frac{-1}{96\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2} \frac{(\nabla V)^2}{(E_F - V(q))^{3/2}}. \quad (42)$$

The last term is

$$\rho_{23} = \frac{1}{(2\pi\hbar)^3} \int d^3p \ \left[2\frac{\hbar^2}{8m} \frac{(\vec{p}\nabla)^2 V}{3m} \delta''(E_F - \frac{p^2}{2m} - V(q)) \right]$$
$$= \frac{1}{96\pi^3 \hbar m^2} \int d^3p \ \sum_{i,j} p_i \nabla_i p_j \nabla_j V \delta''(E_F - \frac{p^2}{2m} - V(q)). \tag{43}$$

We use expansion on the basis of covariant and contravariant orts

$$\vec{p} = \left(\frac{4\pi}{3}\right)^{1/2} p \ \sum_i \vec{e^i} \ Y_{1i}(\Omega) = \left(\frac{4\pi}{3}\right)^{1/2} p \ \sum_i \vec{e_i} \ Y^*_{1i}(\Omega) \tag{44}$$

and obtain

$$\rho_{23} = \frac{1}{72\pi^2 \hbar m^2} \int d\Omega \int dp \ p^2 \sum_{i,j} Y_{1i}(\Omega) \vec{e^i} \nabla_i Y^*_{1j}(\Omega) \vec{e_j} \nabla_j V p^2 \delta''(E_F - \frac{p^2}{2m} - V(q))$$
$$= \frac{1}{72\pi^2 \hbar m^2} \int dp \ p^4 \sum_{i,j} \vec{e^i} \nabla_i \vec{e_j} \nabla_j \delta_{ij} V \delta''(E_F - \frac{p^2}{2m} - V(q))$$
$$= \frac{1}{72\pi^2 \hbar m^2} \int dp \ p^4 \sum_i (\nabla_i)^2 V \delta''(E_F - \frac{p^2}{2m} - V(q))$$
$$= \frac{\Delta V}{72\pi^2 \hbar m^2} \int dp \ p^4 \delta''(E_F - \frac{p^2}{2m} - V(q))$$
$$= \frac{\Delta V}{72\pi^2 \hbar m^2} \frac{3m^2\sqrt{2m}}{2(E_F - V(q))^{1/2}} = \frac{1}{48\pi^2} \left(\frac{2m}{\hbar^2}\right)^{1/2} \frac{\Delta V}{(E_F - V(q))^{1/2}}. \tag{45}$$

As the result we get the semiclassical density matrix in the form

$$\rho(\vec{r}) = \frac{1}{(2\pi\hbar)^3}\int d^3p\, f(\vec{r},\vec{p},E_F) = \left[\frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(E_F - V(\vec{r}))^{3/2} - \frac{1}{24\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\left(\frac{\Delta V}{(E_F - V(\vec{r}))^{1/2}} + \frac{(\nabla V)^2}{4\,(E_F - V(\vec{r}))^{3/2}}\right) + \ldots\right]. \tag{46}$$

Note that semiclassical density diverges at the classical turning point $E_F = V(\vec{r})$.

The kinetic energy

$$\tau(\vec{r}_1,\vec{r}_2) = \frac{\hbar^2}{2m}\vec{\nabla}_{r_1}\vec{\nabla}_{r_2}\rho(\vec{r}_1,\vec{r}_2,E_F) = \sum_i \frac{\hbar^2}{2m}\vec{\nabla}_{r_1}\varphi_i(\vec{r}_1)\vec{\nabla}_{r_2}\varphi_i(\vec{r}_2) \tag{47}$$

can be rewritten as

$$\tau = \sum_i \left[\frac{1}{4}\vec{\nabla}_r^2 - \vec{\nabla}_s^2\right]\rho(\vec{r}-\vec{s}/2,\vec{r}+\vec{s}/2,E_F), \tag{48}$$

where $\vec{r} = (\vec{r}_1 + \vec{r}_2)/2$ and $\vec{s} = (\vec{r}_1 - \vec{r}_2)/2$. The Wigner transform of this equation is

$$\begin{aligned}\tau_W = \tau(\vec{r},\vec{p}) &= \frac{1}{4}\vec{\nabla}_r^2\rho_W(\vec{r},\vec{p}) + \frac{p^2}{\hbar^2}\rho_W(\vec{r},\vec{p}) \\ &= \frac{1}{4}\vec{\nabla}_r^2 f(\vec{r},\vec{p}) + \frac{p^2}{\hbar^2}f(\vec{r},\vec{p})\end{aligned} \tag{49}$$

Substituting semiclassical expression for distribution function $f(\vec{r},\vec{p})$, which takes into account all terms with $\hbar^2$ (see Eq. (34)), and performing the inverse Wigner we get the kinetic energy density

$$\tau(\vec{r}) = \tau(\vec{r},\vec{r}')|_{\vec{r}')=\vec{r}} = \frac{1}{(2\pi\hbar)^3}\int d^3p\left[\frac{1}{4}\vec{\nabla}_r^2 f(\vec{r},\vec{p}) + \frac{p^2}{\hbar^2}\vec{\nabla}_r^2 f(\vec{r},\vec{p})\right]$$

$$= \left[\frac{1}{5\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(E_F - V(\vec{r}))^{5/2}\right.$$

$$\left. -\frac{1}{8\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\left(\frac{5}{3}(\Delta V)\left(E_F - V(\vec{r})\right)^{1/2} - \frac{3}{4}\,\frac{(\nabla V)^2}{\left(E_F - V(\vec{r})\right)^{1/2}}\right) + ...\right]. \tag{50}$$

So there are series

$$\rho(\vec{r}) = \rho_{\mathrm{TF}} + \rho_2 + ... \tag{51}$$

$$\tau_{\mathrm{ETF}} = \tau_{\mathrm{TF}} + \tau_2(\rho) + ... \tag{52}$$

It is useful to obtain relation between the kinetic energy density and the local fermion density, i. e.

$$\tau_{\mathrm{ETF}}(\rho) = \tau_{\mathrm{TF}}(\rho) + \tau_2(\rho) + ... \tag{53}$$

Similar expression exist for Thomas-Fermi approach

$$\tau_{\mathrm{TF}}(\rho) = \frac{3^{5/3}\pi^{4/3}}{5}\frac{\hbar^2}{2m}\rho^{5/3} = \frac{1}{5\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(E_F - V(\mathbf{r}))^{5/2}\,. \tag{54}$$

The correction is (D.A. Kirzhnits (1967))

$$\tau_2 = \frac{\hbar^2}{2m}\left[\frac{(\nabla\rho)^2}{36\rho} + \frac{\Delta\rho}{3}\right]. \tag{55}$$

Application

- Modern energy-density potential
- Density distributions in nuclei
- Energy of the nuclei
- Nucleus-nucleus potential

Modern energy-density potential

The energy density functional

$$\mathcal{E}[\rho_p(\vec{r}), \rho_n(\vec{r})] = \frac{\hbar^2}{2m}[\tau_p(\vec{r}) + \tau_n(\vec{r})] + \mathcal{V}(\vec{r}),$$

where m is the nucleon mass. The expressions for proton τ_p and neutron τ_n kinetic energy density functionals are taken into account $\hbar^2$ corrections. The potential energy density functional splits into Skyrme and Coulomb (direct and exchange) parts

$$\mathcal{V}(\vec{r}) = \mathcal{V}_{\text{Skyrme}}(\vec{r}) + \mathcal{V}_{\text{Coul}}(\vec{r}).$$

The expressions for proton τ_p and neutron τ_n kinetic energy density functional taken into account $\hbar^2$ corrections are

$$\tau_{p(n)}(\vec{r}) = \frac{3}{5}(3\pi^2)^{2/3}\rho_{p(n)}^{5/3} + \frac{1}{36}\frac{(\nabla\rho_{p(n)})^2}{\rho_{p(n)}} + \frac{1}{3}\Delta\rho_{p(n)} - \frac{1}{12}\rho_{p(n)}\left(\frac{\nabla f_{p(n)}}{f_{p(n)}}\right)^2$$
$$+\frac{1}{6}\frac{\nabla\rho_{p(n)}\nabla f_{p(n)} + \rho_{p(n)}\Delta f_{p(n)}}{f_{p(n)}} + \frac{\rho_{p(n)}}{2}\left(\frac{2m}{\hbar^2}\,\frac{W_0}{2}\,\frac{2\nabla\rho_{p(n)} + \nabla\rho_{n(p)}}{f_{p(n)}}\right)^2,$$

where

$$f_{p(n)}(\vec{r}) = 1 + \frac{2m}{\hbar^2}\left(\frac{3t_1 + 5t_2}{16} + \frac{t_2x_2}{4}\right)\rho_{p(n)}(\vec{r}).$$

The Skyrme energy density functional is

$$\mathcal{V}_{\text{Skyrme}}\vec{r} = \frac{t_0}{2}[(1+\frac{1}{2}x_0)\rho^2 - (x_0+\frac{1}{2})(\rho_p^2+\rho_n^2)] + \frac{1}{12}t_3\rho^\alpha[(1+\frac{1}{2}x_3)\rho^2 - (x_3+\frac{1}{2})(\rho_p^2+\rho_n^2)]$$
$$+\frac{1}{4}[t_1(1+\frac{1}{2}x_1)+t_2(1+\frac{1}{2}x_2)]\tau\rho + \frac{1}{4}[t_2(x_2+\frac{1}{2})-t_1(x_1+\frac{1}{2})](\tau_p\rho_p+\tau_n\rho_n)$$
$$+\frac{1}{16}[3t_1(1+\frac{1}{2}x_1)-t_2(1+\frac{1}{2}x_2)](\nabla\rho)^2 - \frac{1}{16}[3t_1(x_1+\frac{1}{2})+t_2(x_2+\frac{1}{2})]((\nabla\rho_n)^2+(\nabla\rho_p)^2)$$
$$-\frac{W_0^2}{4}\frac{2m}{\hbar^2}[\frac{\rho_p}{f_p}(2\nabla\rho_p+\nabla\rho_n)^2+\frac{\rho_n}{f_n}(2\nabla\rho_n+\nabla\rho_p)^2].$$

t_0, t_1, t_2, x_0, x_1, x_2, α and W_0 - parameters of the Skyrme forces, the last term is the spin-orbit interaction obtained in $\hbar^2$ approximation.

The Coulomb energy density functional is the sum of direct and exchange terms

$$\mathcal{V}_{\text{Coul}}(\vec{r}) = \frac{e^2}{2}\rho_p(\vec{r})\int \frac{\rho_p(\vec{r}\prime)}{|\vec{r}-\vec{r}\prime|}d\vec{r}\prime - \frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}(\rho_p(\mathbf{r}))^{4/3}.$$

Density distributions in nuclei

There are two method:

$\Rightarrow$ variational method based on trial functions:

Examples: $\rho_{p(n)} = \frac{\rho_{0,p(n)}}{1+exp\frac{r-R_{p(n)}}{d_{p(n)}}}$

This is simple method.

$\Rightarrow$ direct variational method:

$$\delta\left[\int d^3r\mathcal{E}(\rho) - \lambda \text{ condition}]\right] = 0 \qquad (56)$$

We get complex integro-differential equation(s), which can be solved. Conditions can be related to particle conservation $\int d^3r\rho(\vec{r}) - N = 0$ and etc.

Semi-Microscopic Potential (SMP) between heavy nuclei. Frozen density potenti

The interaction energy between spherical and axial-symmetric nuclei in the frozen density approximation is

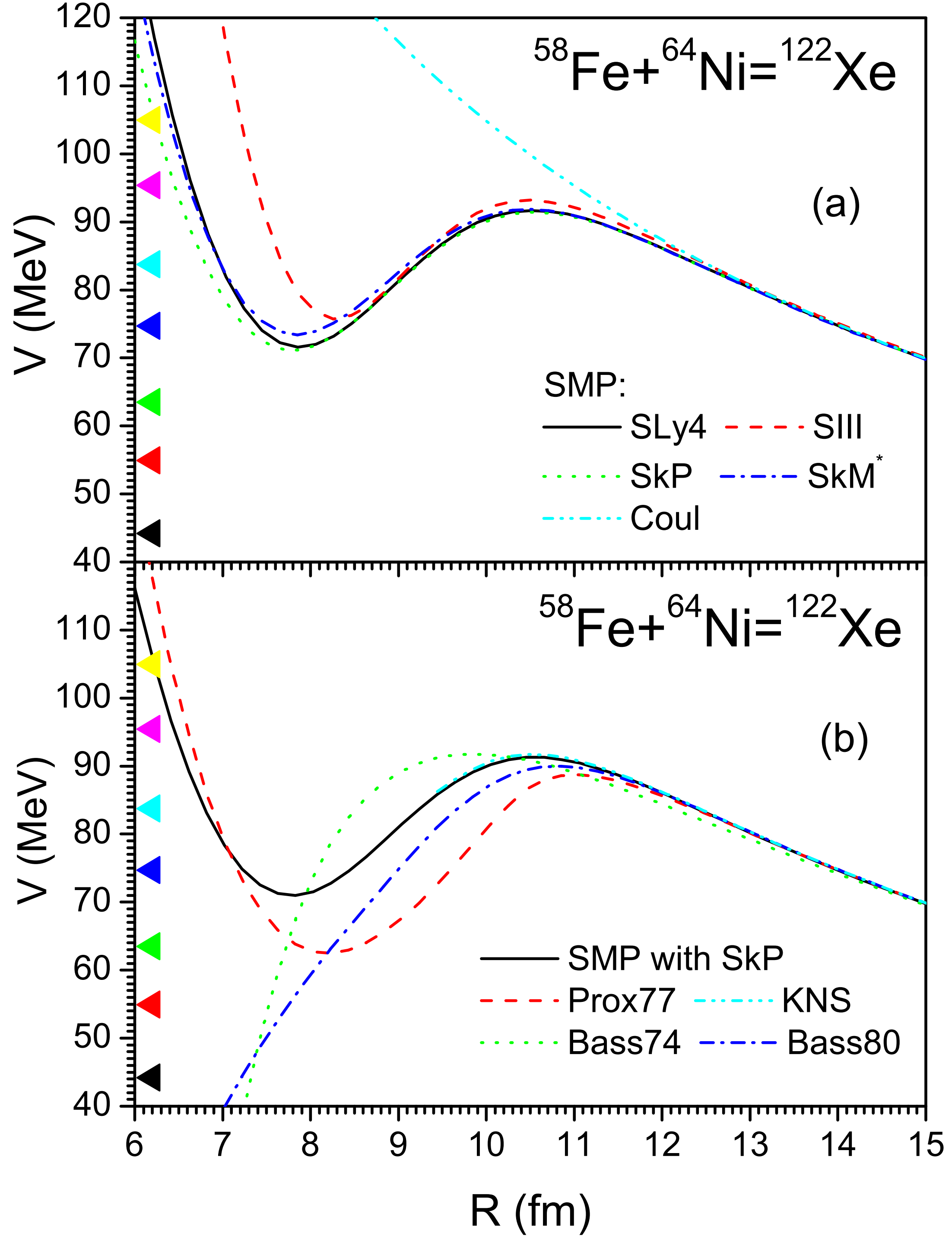
$$V(R,\vartheta) = E_{12}(R,\vartheta) - E_1 - E_2,$$

R is the distance between mass centers of colliding nuclei,

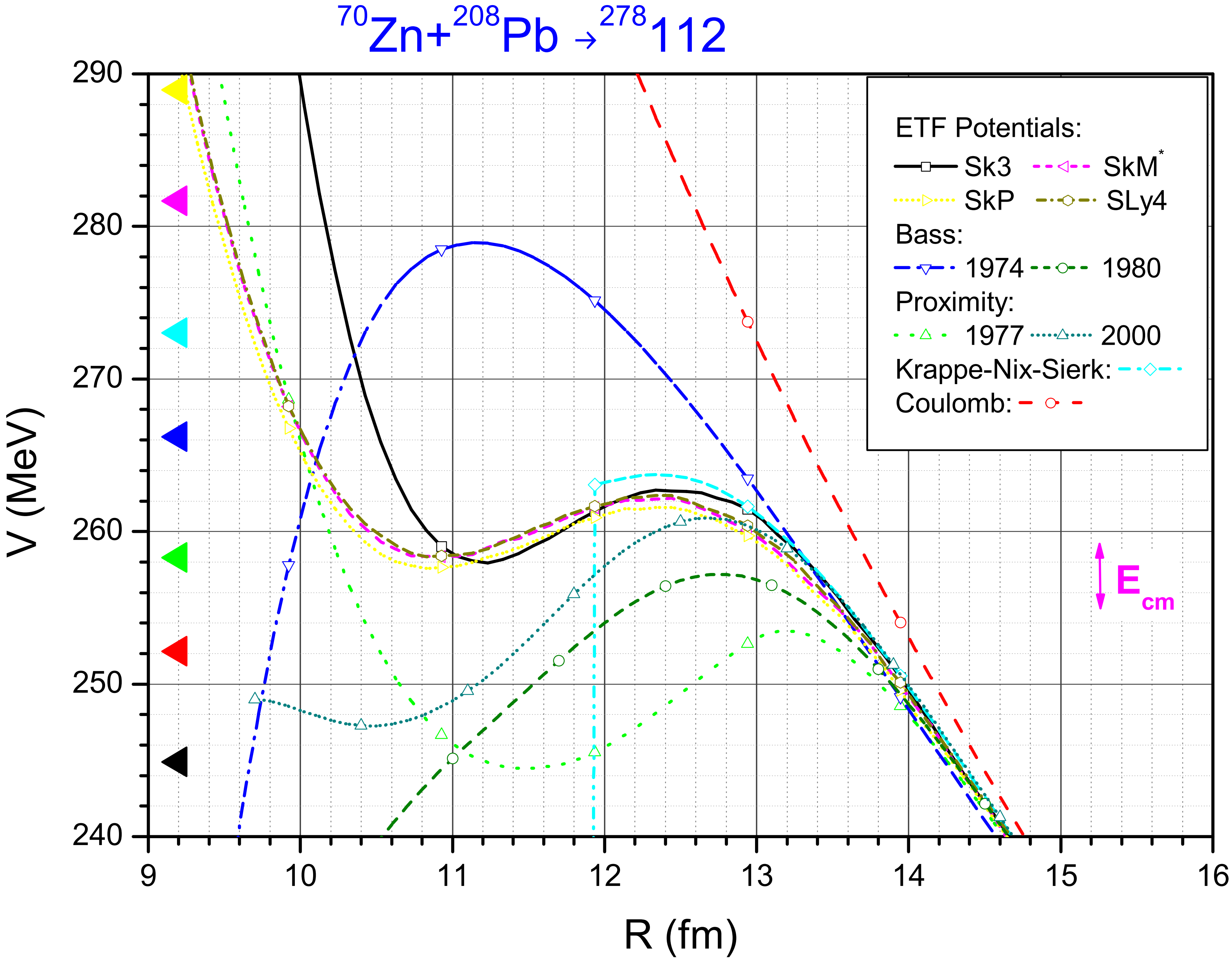
ϑ is the angle between the axial-symmetry axis of deformed nuclei and the line connected the mass centers of nuclei, binding energies are

$$E_{12}(R,\vartheta) = \int d^3r\ \mathcal{E}[\rho_{1p}(\vec{r}) + \rho_{2p}(R,\vartheta,\vec{r}), \rho_{1n}(\vec{r}) + \rho_{2n}(R,\vartheta,\vec{r})],$$

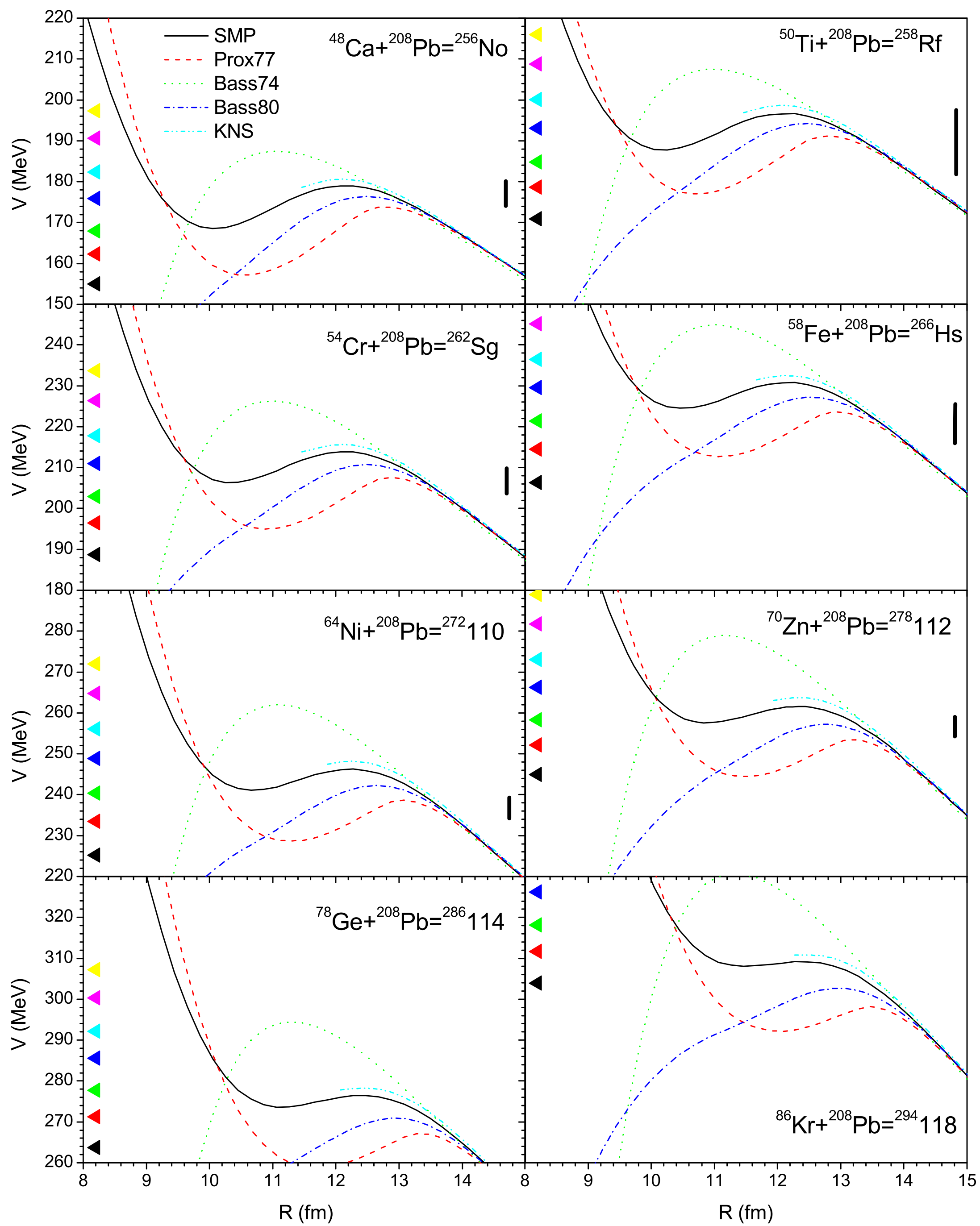
$$E_1 = \int d^3r\ \mathcal{E}[\rho_{1p}(\vec{r}), \rho_{1n}(\vec{r})], \quad E_2 = \int d^3r\ \mathcal{E}[\rho_{2p}(\vec{r}), \rho_{2n}(\vec{r})].$$



$^{58}Fe+^{64}Ni=^{122}Xe$
(a)
SMP:
SLy4
SIII
SkP
SkM*
Coul
$^{58}Fe+^{64}Ni=^{122}Xe$
(b)
SMP with SkP
Prox77
KNS
Bass74
Bass80
V (MeV)
R (fm)



$^{70}Zn+^{208}Pb \rightarrow ^{278}112$
ETF Potentials:
Sk3
SkM*
SkP
SLy4
Bass:
1974
1980
Proximity:
1977
2000
Krappe-Nix-Sierk:
Coulomb:
E_{cm}
V (MeV)
R (fm)
290
280
270
260
250
240
9
10
11
12
13
14
15
16


SMP
Prox77
Bass74
Bass80
KNS
$^{48}Ca+^{208}Pb=^{256}No$
$^{50}Ti+^{208}Pb=^{258}Rf$
$^{54}Cr+^{208}Pb=^{262}Sg$
$^{58}Fe+^{208}Pb=^{266}Hs$
$^{64}Ni+^{208}Pb=^{272}110$
$^{70}Zn+^{208}Pb=^{278}112$
$^{78}Ge+^{208}Pb=^{286}114$
$^{86}Kr+^{208}Pb=^{294}118$
V (MeV)
R (fm)

Thanks for your attention!