COULOMB INTERACTION IN HORSE FORMALISM

V. A. Kulikov
A. M. Shirokov, U. M. Yanikov

2024

Outline

1. HORSE formalism
2. HORSE and Coulomb interaction
3. Expansion coefficients for the wave function
4. Results for the scattering phase

HORSE formalism

Radial Schrödinger equation $$H^l u_l(k,r) = E u_l(k,r)$$

w.f. expansion $$u_l(k,r) = \sum_{n=0}^{\infty} a_{nl}(k)\varphi_{nl}(r)$$

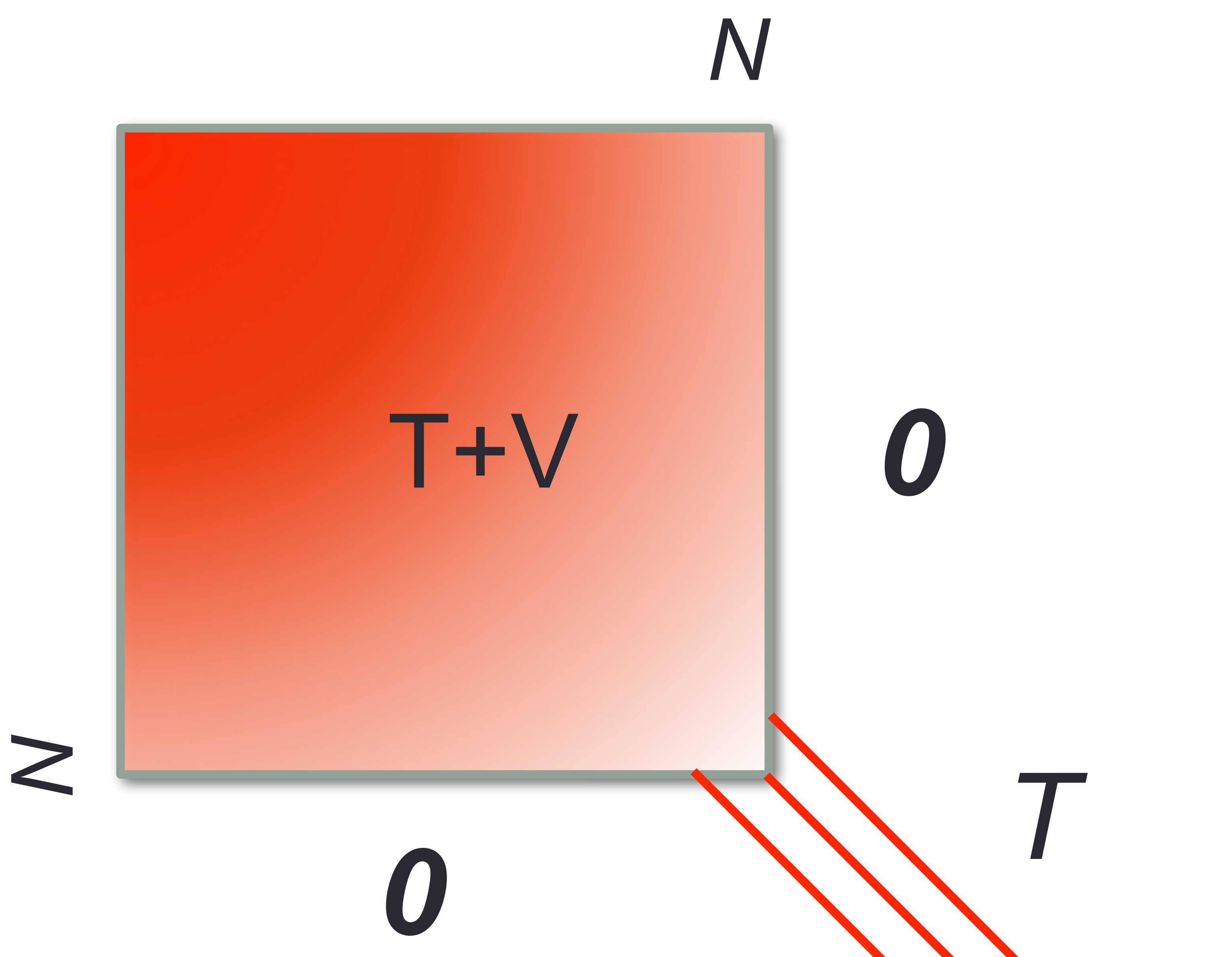
$\varphi_{nl}(r)$ – oscillator function

$$\sum_{n'=0}^{\infty} (H^l_{nn'} - \delta_{nn'}E)a_{n'l}(k) = 0 \qquad \text{n=0,1,…}$$

$$H^l_{nn'} = \langle \varphi_{nl}(r) \,|\, H^l \,|\, \varphi_{n'l}(r) \rangle$$

HORSE formalism

Hamiltonian structure:



Hamiltonian matrix elements:

$$H^l_{nn'} = T^l_{nn'} + V^l_{nn'}$$

Non-zero kinetic energy m. e.

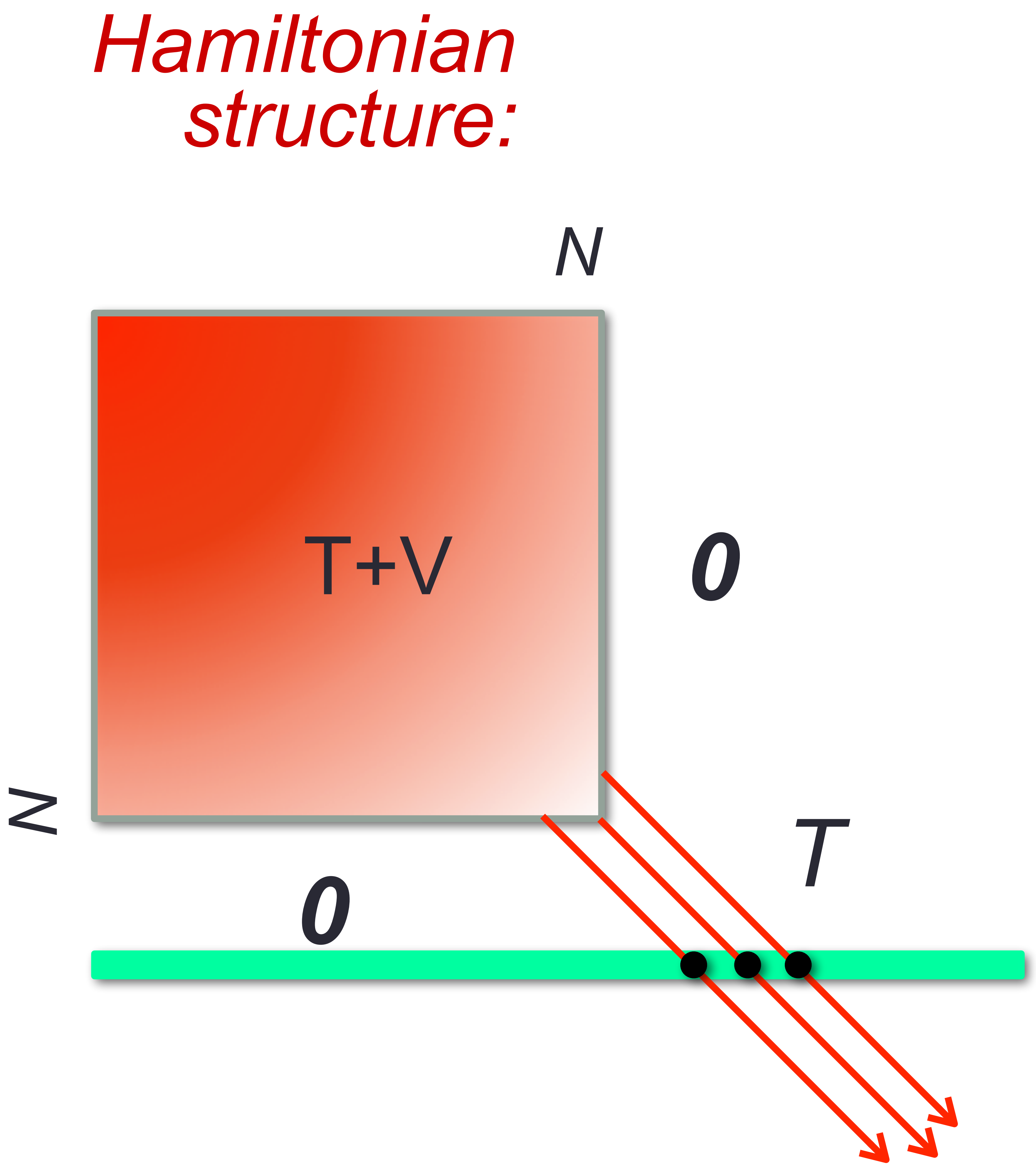
$$T^l_{nn} = \frac{\hbar\omega}{2}\left(2n + l + \frac{3}{2}\right)$$

$$T^l_{n+1,n} = T^l_{n,n+1} = -\frac{\hbar\omega}{2}\sqrt{(n+1)\left(n + l + \frac{3}{2}\right)}$$

Truncated potential energy matrix

$$V^l_{nn'} = \begin{cases} V^l_{nn'} & \text{if} \quad n \le N \quad \text{and} \quad n' \le N \\ 0 & \text{if} \quad n > N \quad \text{or} \quad n' > N \end{cases}$$

HORSE formalism



Hamiltonian matrix elements:

$$H^l_{nn'} = T^l_{nn'} + V^l_{nn'}$$

Potential m. e. decrease with nn'

Kinetic energy m. e. increase with nn'

$N, \hbar\omega$ — basis parameters

$$\sum_{n'}^{\infty} (H^l_{nn'} - \delta_{nn'}E)a_{n'l}(k) = 0$$

HORSE formalism

When *n*, *n'* > *N* $\sum_{n'}^{\infty} (H^{l}_{nn'} - \delta_{nn'}E)a_{n'l}(k) = 0$ reduce to

$$T^{l}_{n,n-1}a^{as}_{n-1,l}(k) + (T^{l}_{n,n} - E)a^{as}_{nl}(k) + T^{l}_{n,n+1}a^{as}_{n+1,l}(k) = 0$$

$$a^{as}_{nl}(k) = \cos\delta_l S_{nl}(k) + \sin\delta_l C_{nl}(k)$$

When *n*, *n'* ≤ *N*: E_λ – *eigenvalues*, $\gamma_{\lambda n}$ – *eigenvectors*

$$\mathfrak{G}_{nn'} = -\sum_{\lambda=0}^{N} \frac{\gamma^{*}_{\lambda n}\gamma_{\lambda n'}}{E_\lambda - E} \qquad \tan\delta_l = -\frac{S_{Nl}(k) - \mathfrak{G}_{NN}S_{N+1,l}(k)}{C_{Nl}(k) - \mathfrak{G}_{NN}C_{N+1,l}(k)}$$

HORSE formalism

Coulomb interaction

$$V = V^{Nucl} + V^{Coul}$$

$$V^{Coul}(r) = \frac{Z_1 Z_2 e^2}{r}$$

$$u_l(k, r) \sim \cos\delta_l(k) F_l(\eta, kr) + \sin\delta_l(k) G_l(\eta, kr), \quad r \to \infty$$

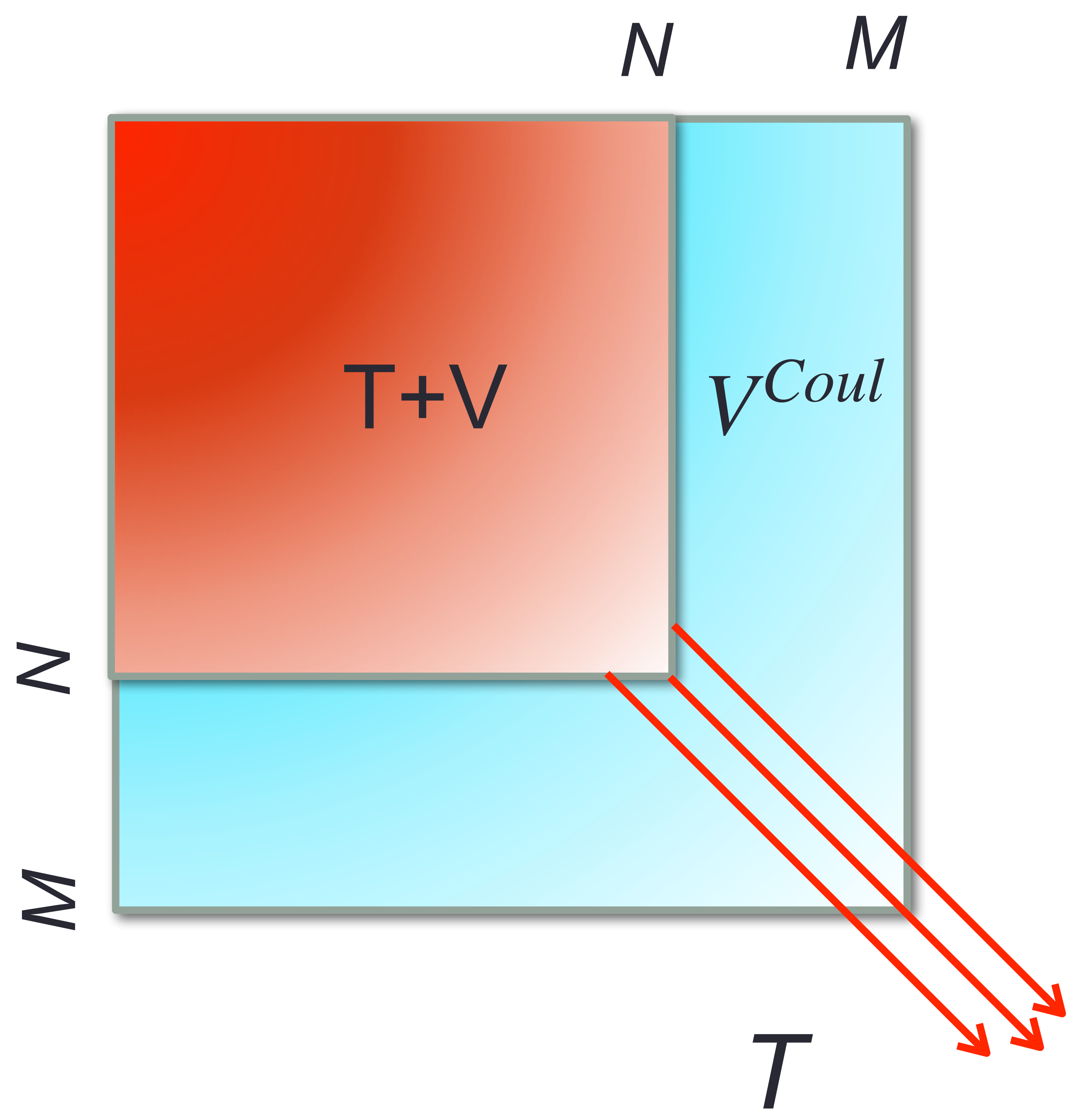
$F_l(\eta, kr)$ — regular Coulomb function

$G_l(\eta, kr)$ — irregular Coulomb function

$\eta = \dfrac{\mu Z_1 Z_2 e^2}{\hbar^2 k}$ — Sommerfeld parameter

HORSE formalism

Coulomb interaction



Hamiltonian matrix elements:

$$H^l_{nn'} = T^l_{nn'} + V^l_{nn'}$$

$$V^l_{nn'} = V^{Nucl}_{nn'} + V^{Coul}_{nn'}$$

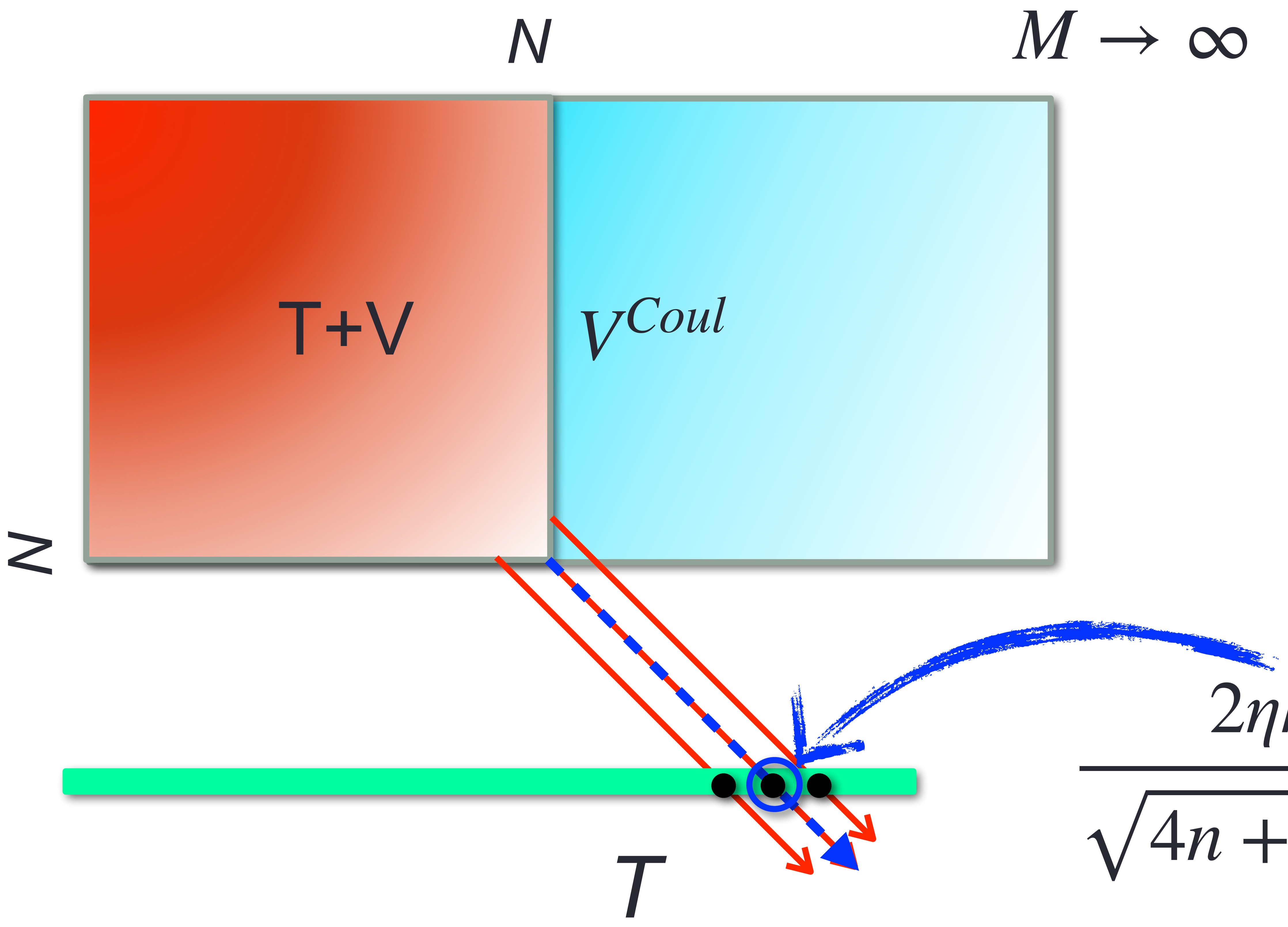
Nuclear potential m. e. decrease with nn’

Kinetic energy m. e. increase with nn’

Coulomb m. e. decrease slowly than nuclear potential m. e.

HORSE formalism

Coulomb interaction method of I. P. Okhrimenko:



$$\frac{2\eta k r_0}{\sqrt{4n+2l+3}}$$

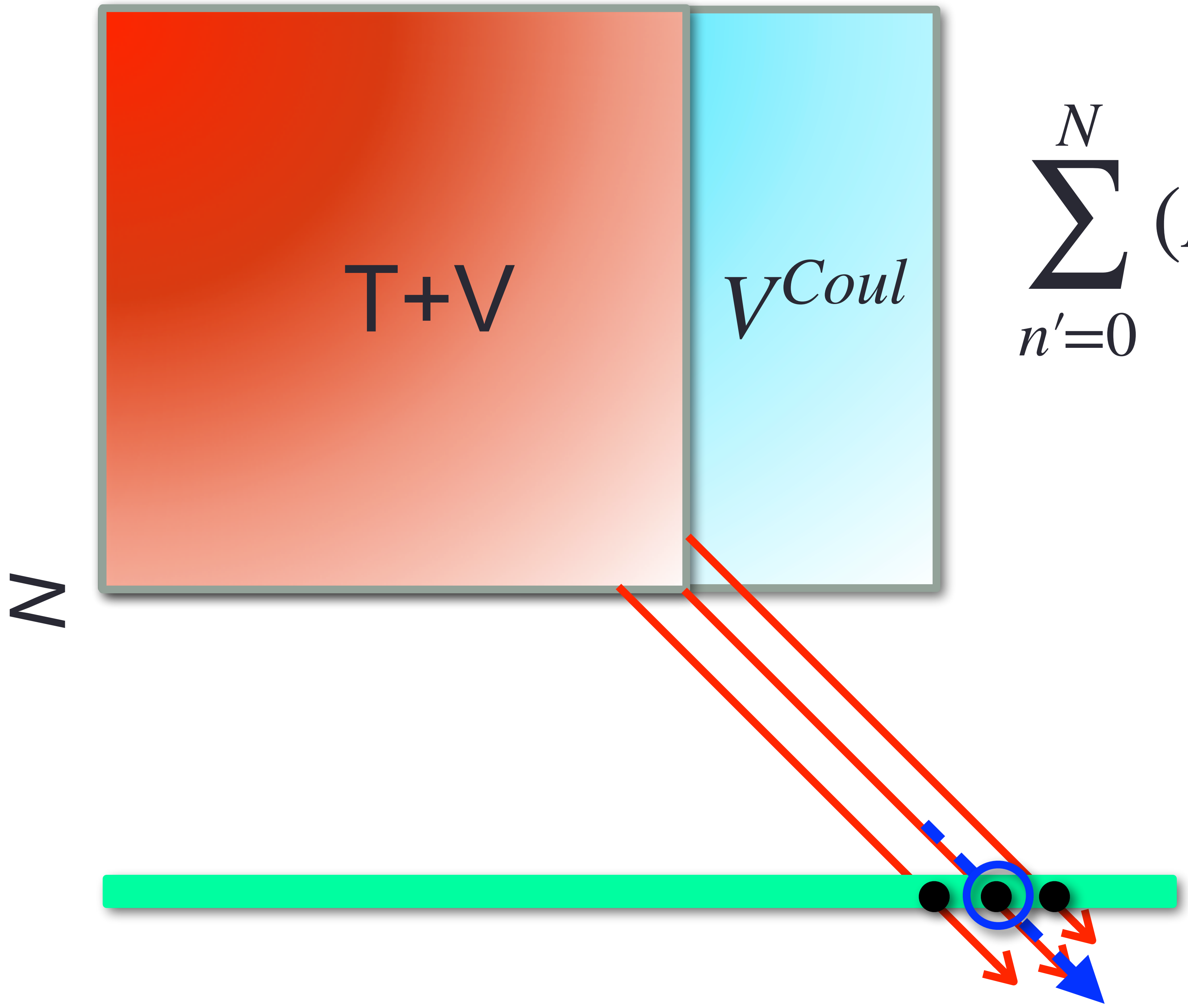
I. P. Okhrimenko, Nucl. Phys. A 424,121 (1984).

HORSE formalism

Coulomb interaction

$$T^l_{n,n-1}a^{as}_{n-1,l}(k) + (T^l_{n,n} - E)a^{as}_{n,l}(k) + T^l_{n,n+1}a^{as}_{n+1,l}(k) + \frac{2\eta k r_0}{\sqrt{4n+2l+3}}a^{as}_{n,l}(k) = 0$$

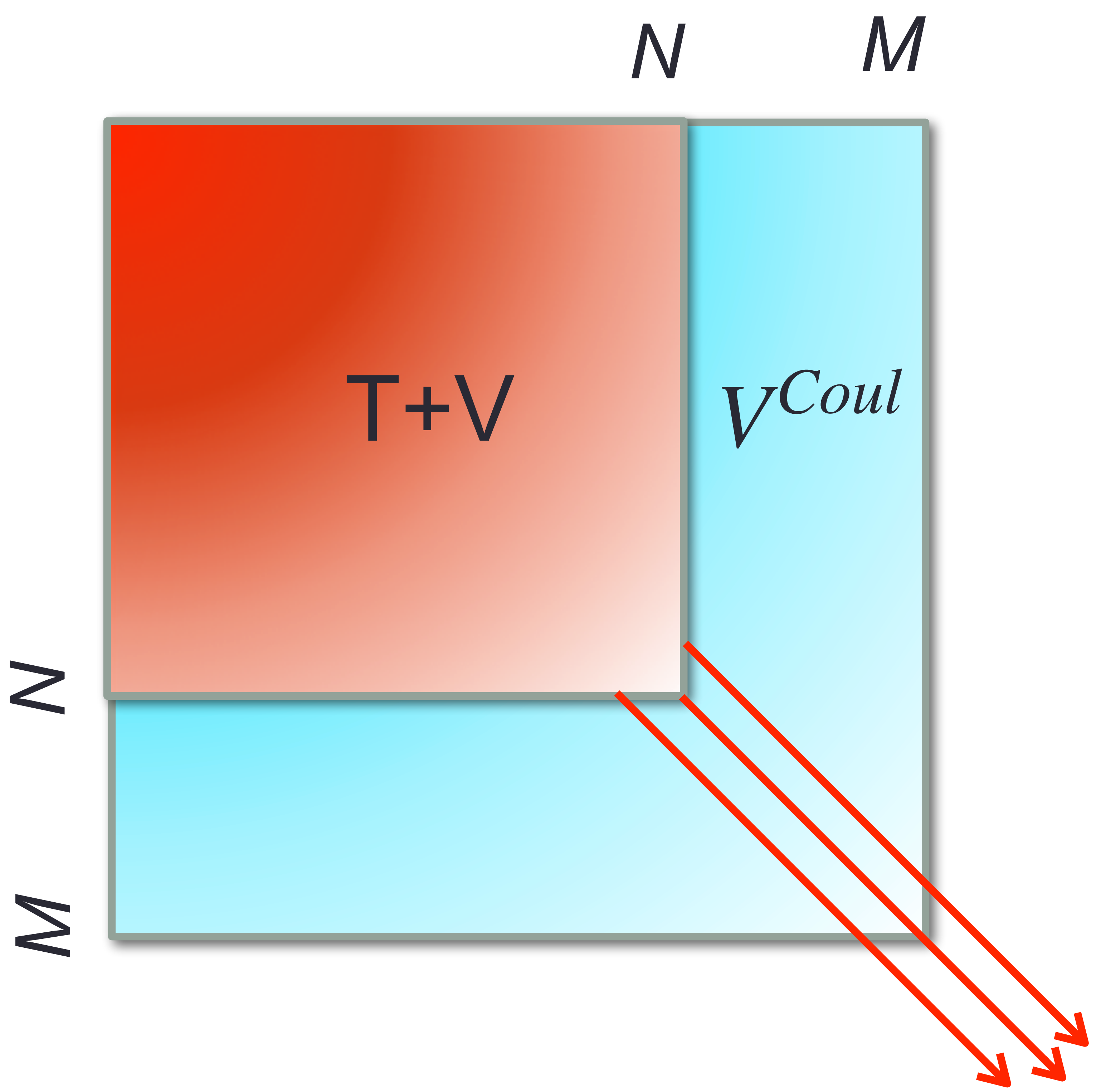
I. P. Okhrimenko, Nucl. Phys. A 424,121 (1984).



$$\sum_{n'=0}^{N}(H^l_{nn'} - \delta_{nn'}E)a_{n'l}(k) + \sum_{n'=N+1}^{\infty} H^l_{nn'}a_{n'l} = 0$$

HORSE formalism

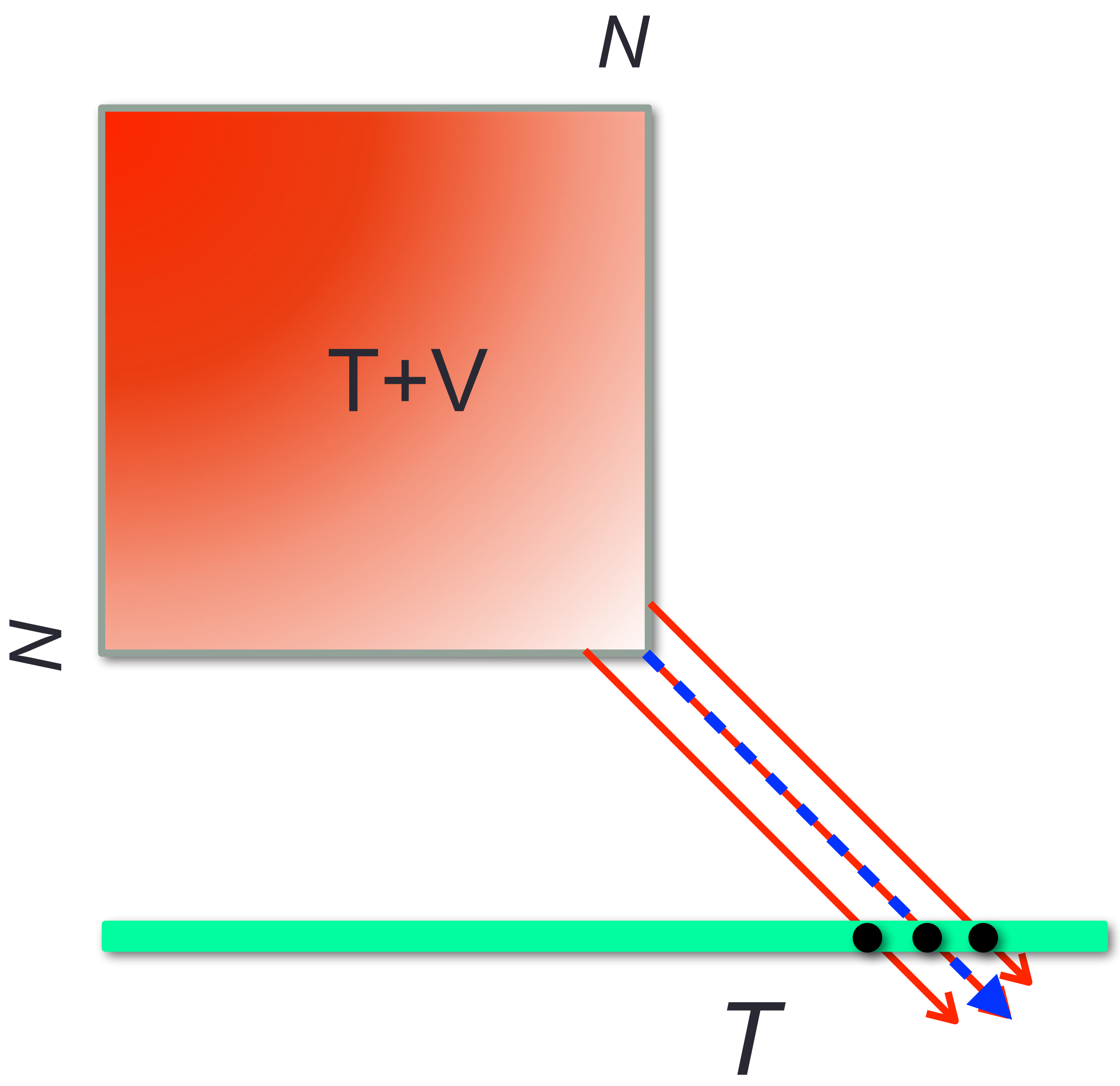
Coulomb interaction



Modified Okhrimenko method: use M>N, but Coulomb matrix is square.

HORSE formalism

Coulomb interaction



Hamiltonian matrix elements:

$$H^l_{nn'} = T^l_{nn'} + V^l_{nn'}$$

$$V^l_{nn'} = V^{Nucl}_{nn'} + V^{Coul}_{nn'}$$

Both components of interaction are cutted with the same N

HORSE formalism

Coulomb interaction

$$u_l(k,r) \sim \cos\delta_l(k) F_l(\eta,kr) + \sin\delta_l(k) G_l(\eta,kr), \qquad r \to \infty$$

$$u_l(k,r) = \sum_{n=0}^{\infty} a_{nl}(k)\varphi_{nl}(r)$$

$$a_{nl}^{as}(k) = \cos\delta_l(k) S_{nl}(k) + \sin\delta_l(k) C_{nl}(k)$$

$$F_l(\eta,kr) = \sum_{n=0}^{\infty} S_{nl}(k)\varphi_{nl}(r)$$

$$\widetilde{G}_l(\eta,kr) = \sum_{n=0}^{\infty} C_{nl}(k)\varphi_{nl}(r) \xrightarrow[r\to\infty]{} G_l(\eta,kr)$$

HORSE formalism

Coulomb interaction

Near to the classical turning point $r_{turn} = r_0\sqrt{4n + 2l + 3}$:

$$\varphi_{nl}(r) \xrightarrow[n\to\infty]{} \sqrt{\frac{2r_0}{\nu}}\delta(r - \nu r_0)$$

$$v = \hbar k/\mu$$

$$S_{nl}(k) = \frac{1}{\sqrt{v}}\int F_l(\eta, kr)\varphi_{nl}(r)dr \xrightarrow[n\to\infty]{} \frac{1}{\sqrt{v}}\sqrt{\frac{2r_0}{\nu}}F_l(\eta, \nu k r_0)$$

$$C_{nl}(k) \xrightarrow[r\to\infty]{} \frac{1}{\sqrt{v}}\int G_l(\eta, kr)\varphi_{nl}(r)dr \xrightarrow[n\to\infty]{} \frac{1}{\sqrt{v}}\sqrt{\frac{2r_0}{\nu}}G_l(\eta, \nu k r_0)$$

HORSE formalism

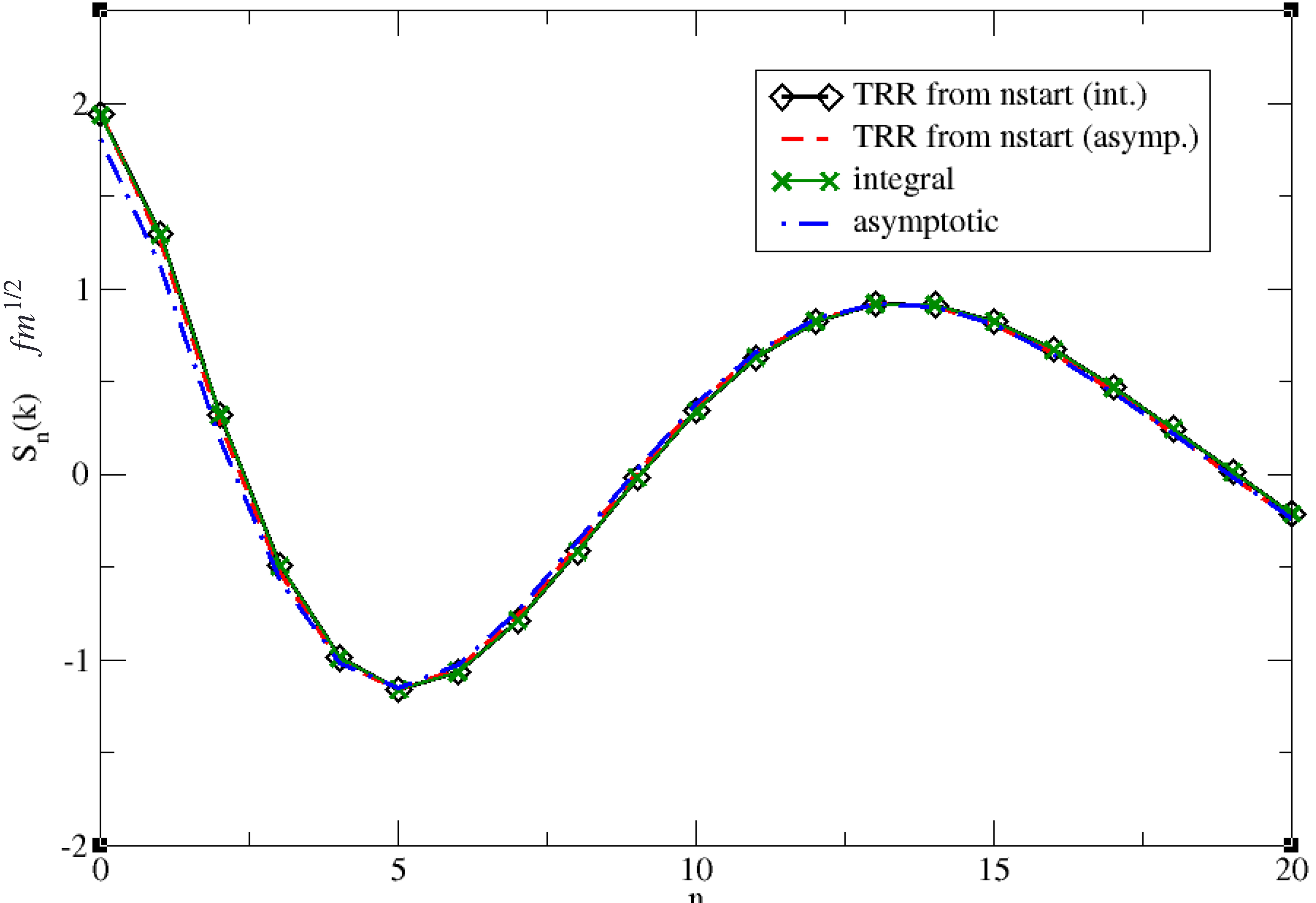
Coulomb interaction

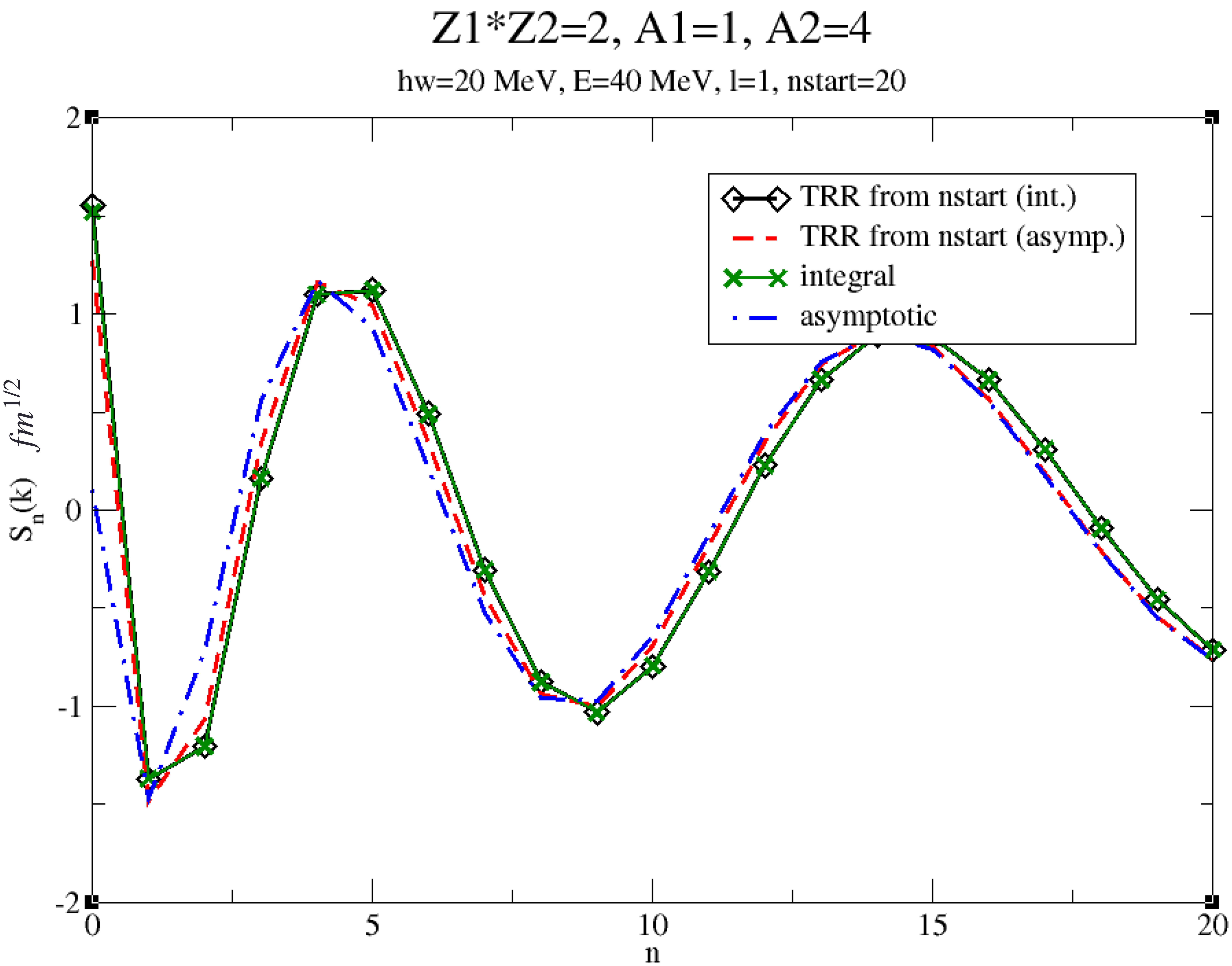
Ways to calculate $S_{nl}(k)$:

- Numerical integration at n $\frac{1}{\sqrt{v}}\int F_l(\eta, kr)\varphi_n^l(r)dr$
- Asymptotic relation $\frac{1}{\sqrt{v}}\sqrt{\frac{2r_0}{\nu}}F_l(\eta, \nu k r_0)$
- Calculation at large n and use the TRR for going down to small n

Z1*Z2=2, A1=1, A2=4

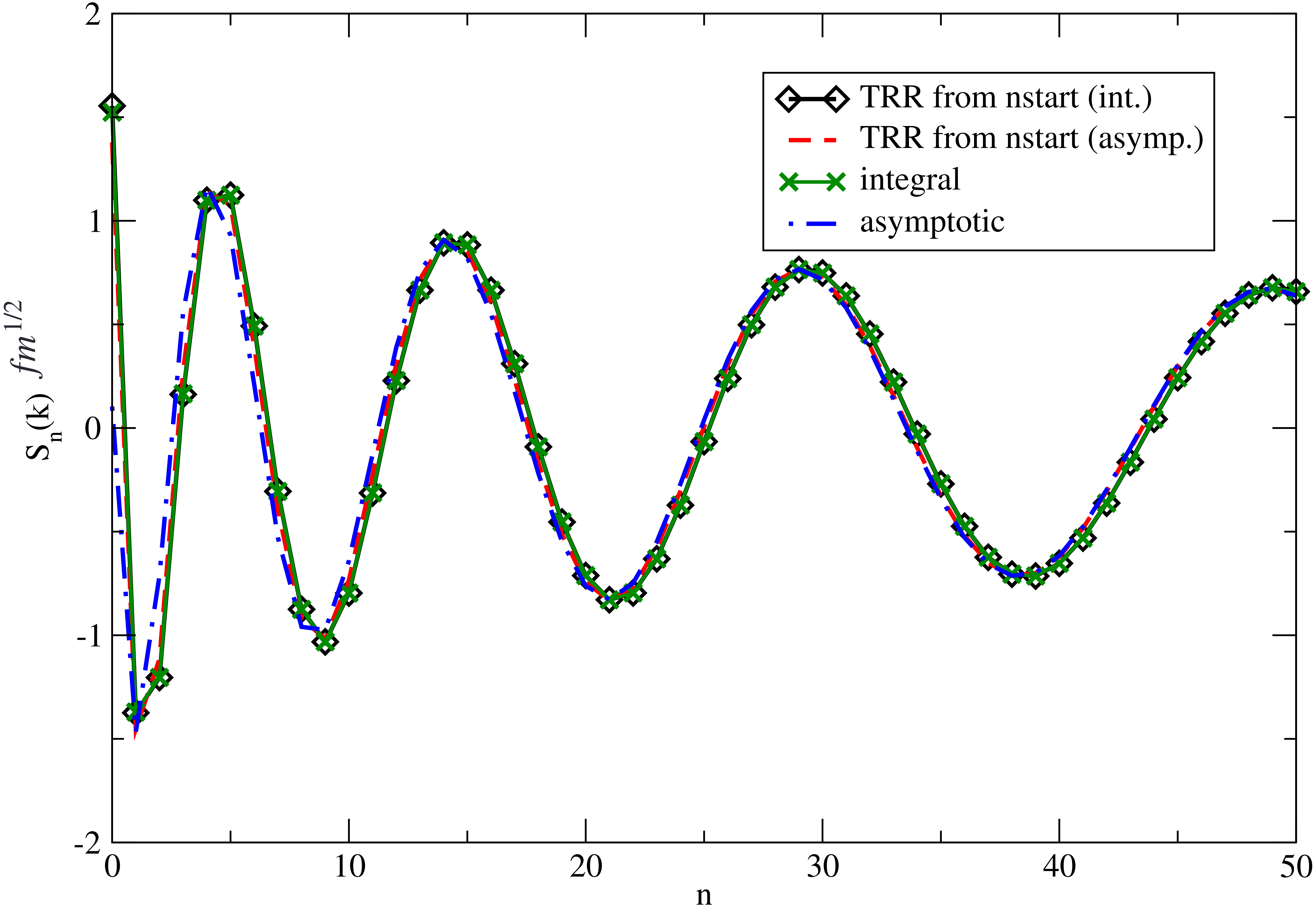
hw=20 MeV, E=15 MeV, l=1, nstart=20

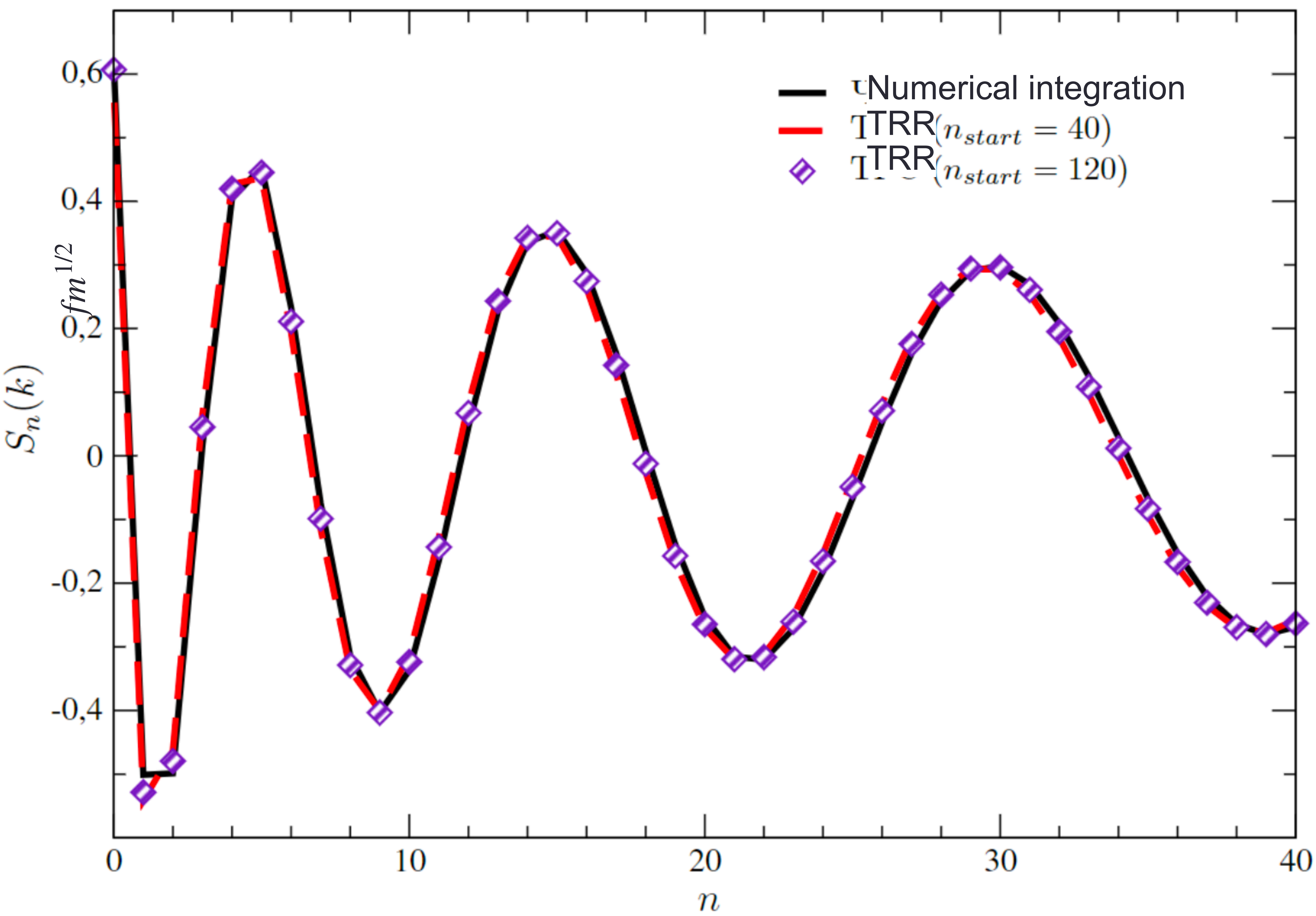



Z1*Z2=2, A1=1, A2=4
hw=20 MeV, E=40 MeV, l=1, nstart=20
TRR from nstart (int.)
TRR from nstart (asymp.)
integral
asymptotic
$S_n(k)$ $fm^{1/2}$
n
2
1
0
-1
-2
0
5
10
15
20

Z1*Z2=2, A1=1, A2=4

hw=20 MeV, E=40 MeV, l=1, nstart=50





Numerical integration
TRR(n_{start} = 40)
TRR(n_{start} = 120)
0,6
0,4
0,2
0
-0,2
-0,4
0
10
20
30
40
n
$S_n(k)$ $fm^{1/2}$

HORSE formalism

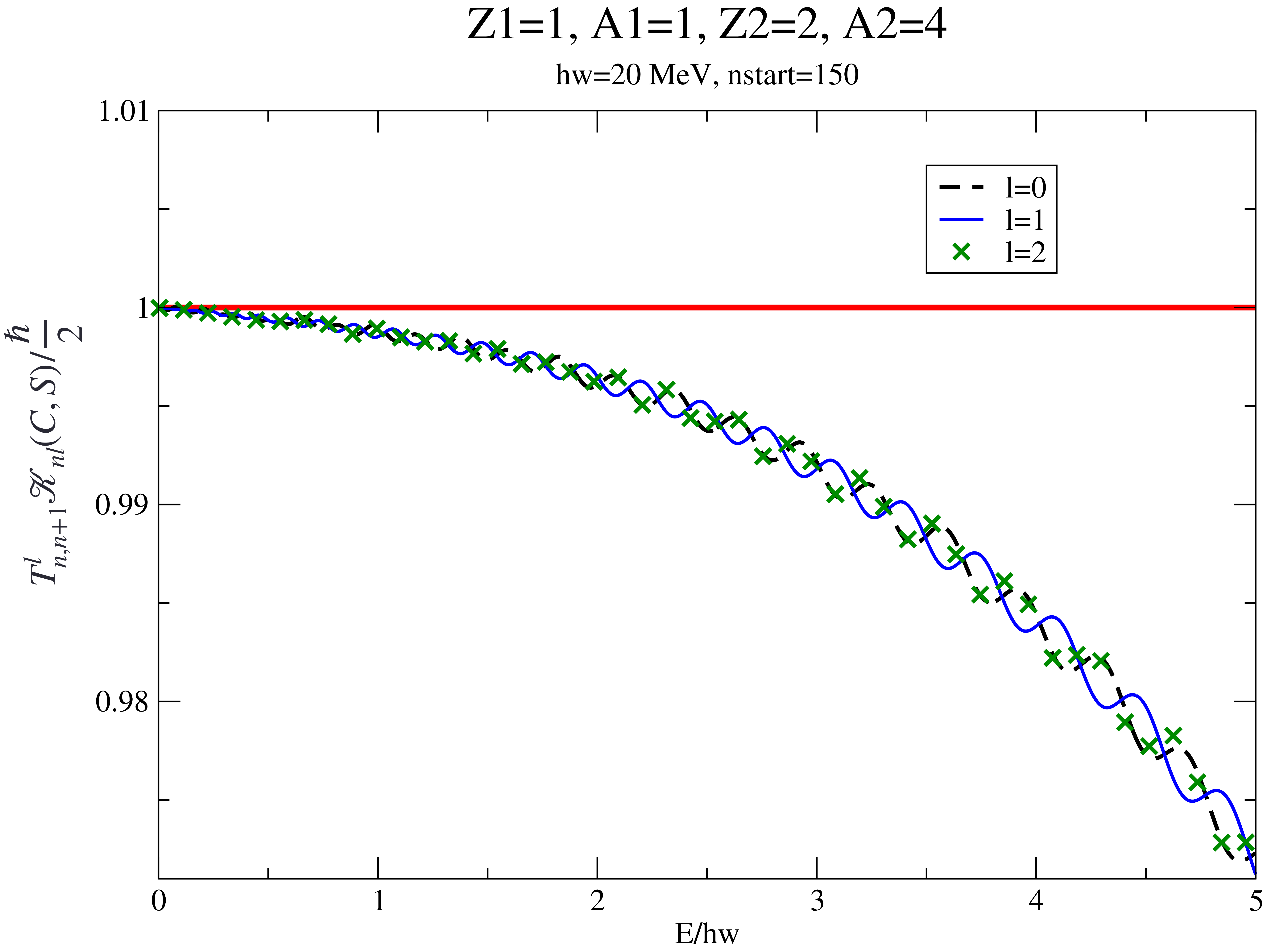
Coulomb interaction

Casorati determinant:

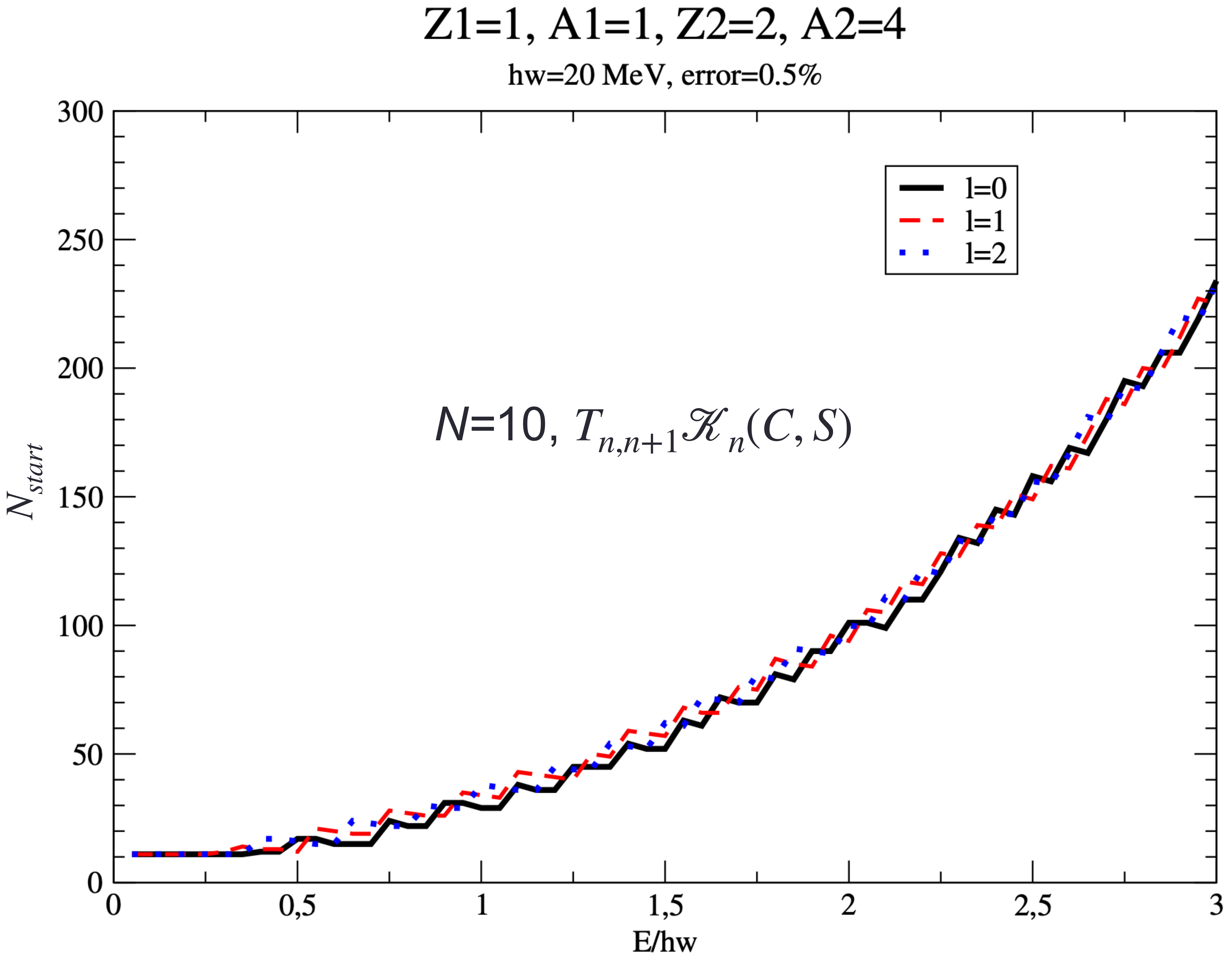
$$\mathscr{K}_{nl}(C,S) = C_{n+1,l}(k)S_{nl}(k) - S_{n+1,l}(k)C_{nl}(k)$$

$$T^{l}_{n,n+1}\mathscr{K}_{nl}(C,S) = \frac{\hbar}{2}$$

This combination doesn't depend on n, we could use it for calculation starting from large n and going down with TRR:



Z1=1, A1=1, Z2=2, A2=4
hw=20 MeV, nstart=150
1.01
1
0.99
0.98
$T^l_{n,n+1}\mathcal{K}_{nl}(C,S)/\frac{\hbar}{2}$
0
1
2
3
4
5
E/hw
l=0
l=1
l=2


Z1=1, A1=1, Z2=2, A2=4
hw=20 MeV, error=0.5%
N=10, $T_{n,n+1}\mathscr{K}_n(C,S)$
l=0
l=1
l=2
N_{start}
E/hw
0
50
100
150
200
250
300
0,5
1
1,5
2
2,5
3

HORSE formalism

Coulomb interaction

$$\tan \delta_l = -\frac{S_{Nl}(k) - \mathfrak{G}_{NN} S_{N+1,l}(k)}{C_{Nl}(k) - \mathfrak{G}_{NN} C_{N+1,l}(k)}$$

Model problem

- Woods–Saxon potential:

$$V^{WS}(r) = \frac{V_0}{1 + \exp\left(\frac{r - R_0}{\alpha_0}\right)} + (\mathbf{l} \cdot \mathbf{s}) \frac{1}{r} \frac{d}{dr} \frac{V_{ls}}{1 + exp\left(\frac{r - R_1}{\alpha_1}\right)}$$

- with Coulomb interaction:

$$V^{Coul}(r) = \frac{Z_1 Z_2 e^2}{r}$$

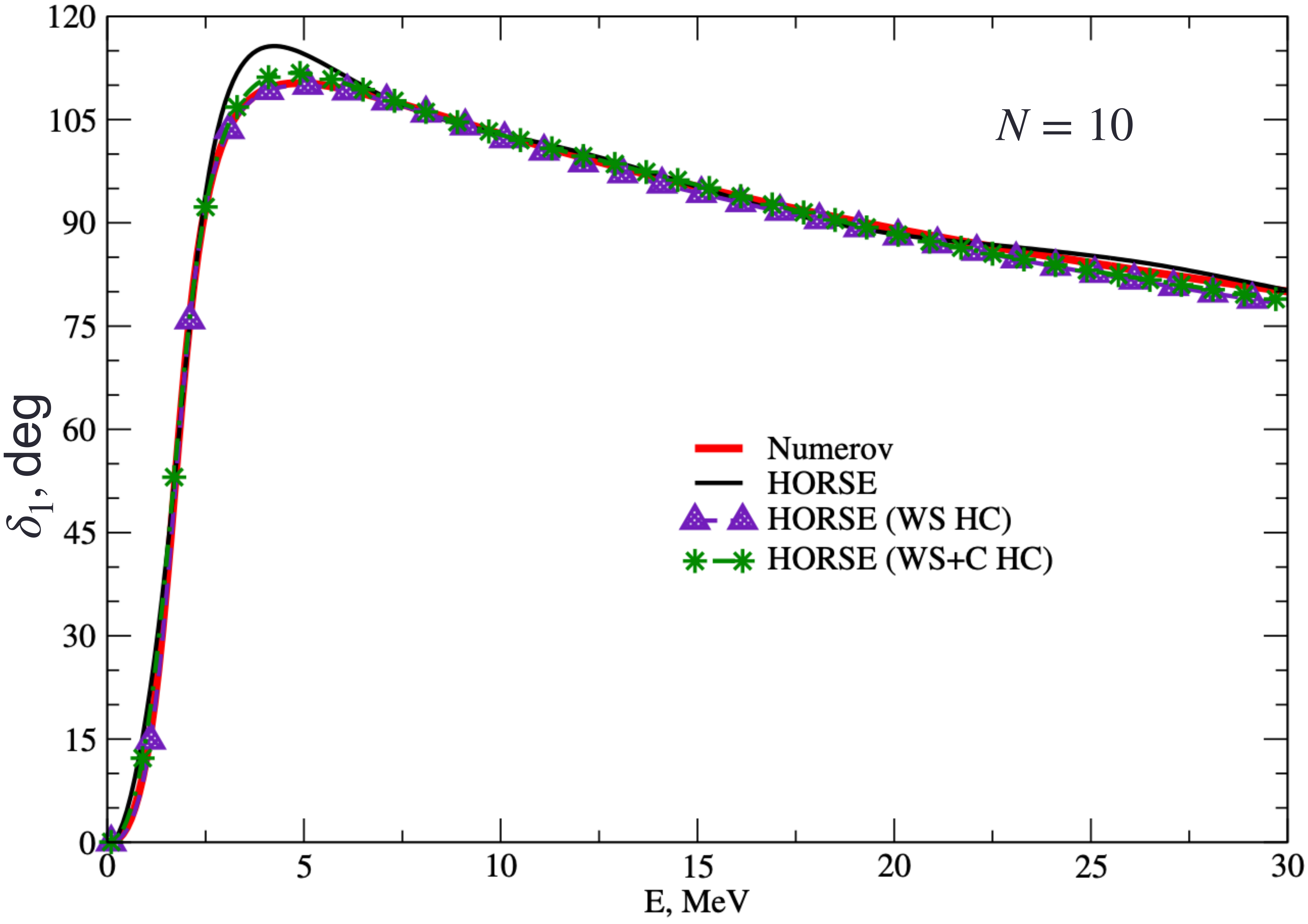
Smoothing of potential energy m. e.

$$\tilde{V}^N_{nm} = \sigma^N_n V^N_{nm} \sigma^N_m$$

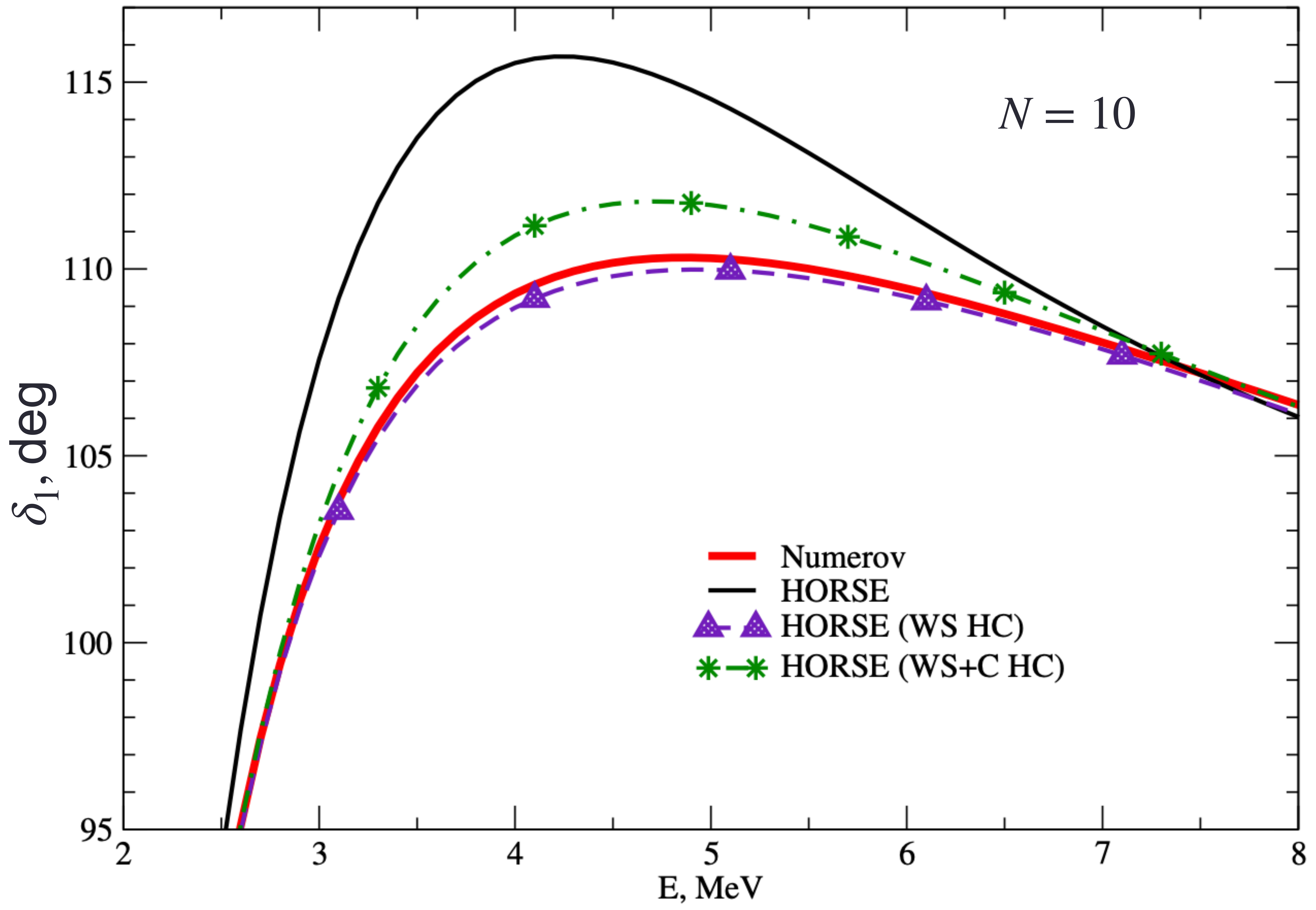
$$\sigma^N_n = \frac{1 - \exp\{-[\alpha(n - N - 1)/(N+1)]^2\}}{1 - \exp\{-\alpha^2\}}$$

$$\alpha = 5$$

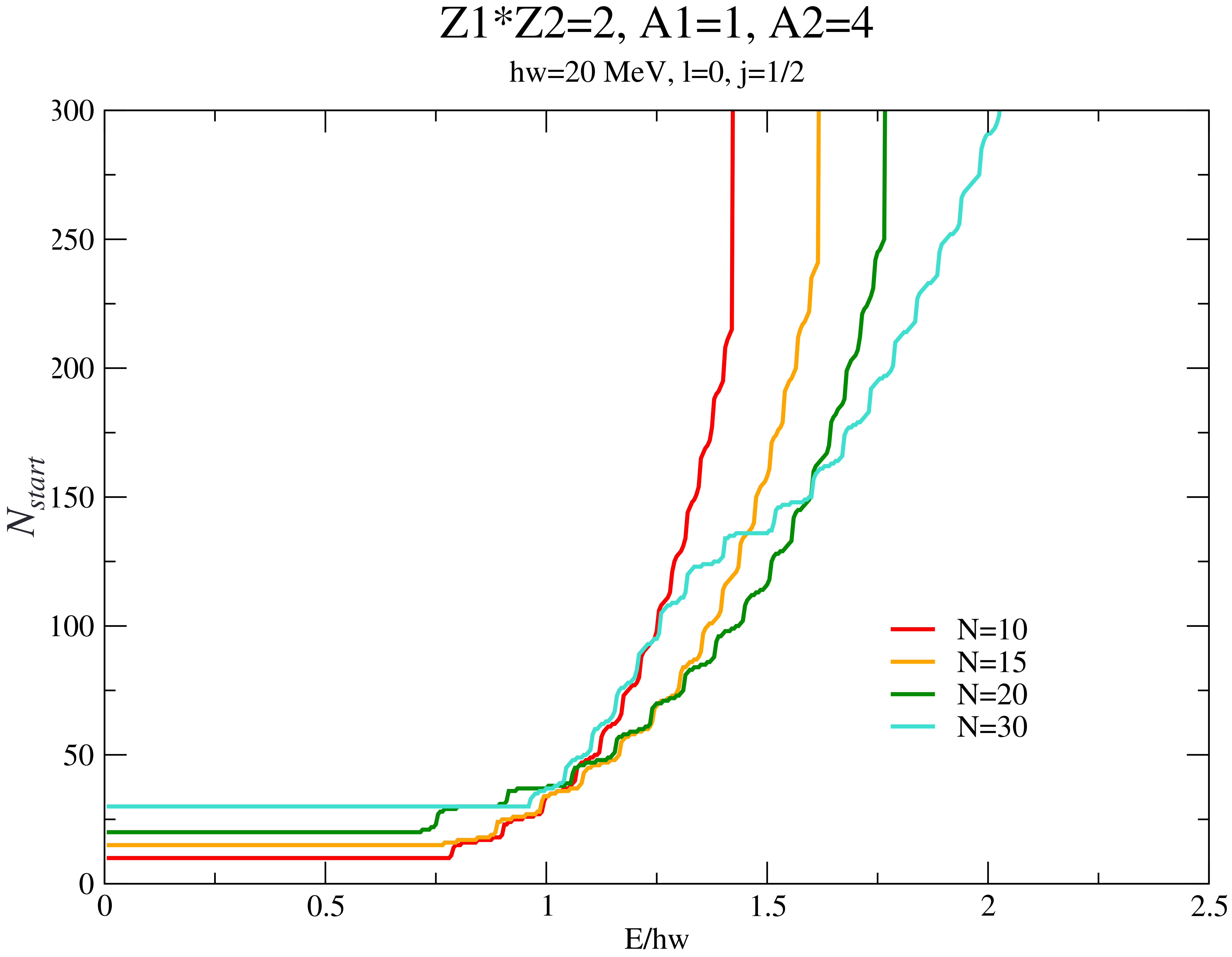
J. Révai, M. Sotona, and J. Žofka, J. Phys. G 11, 745 (1985).

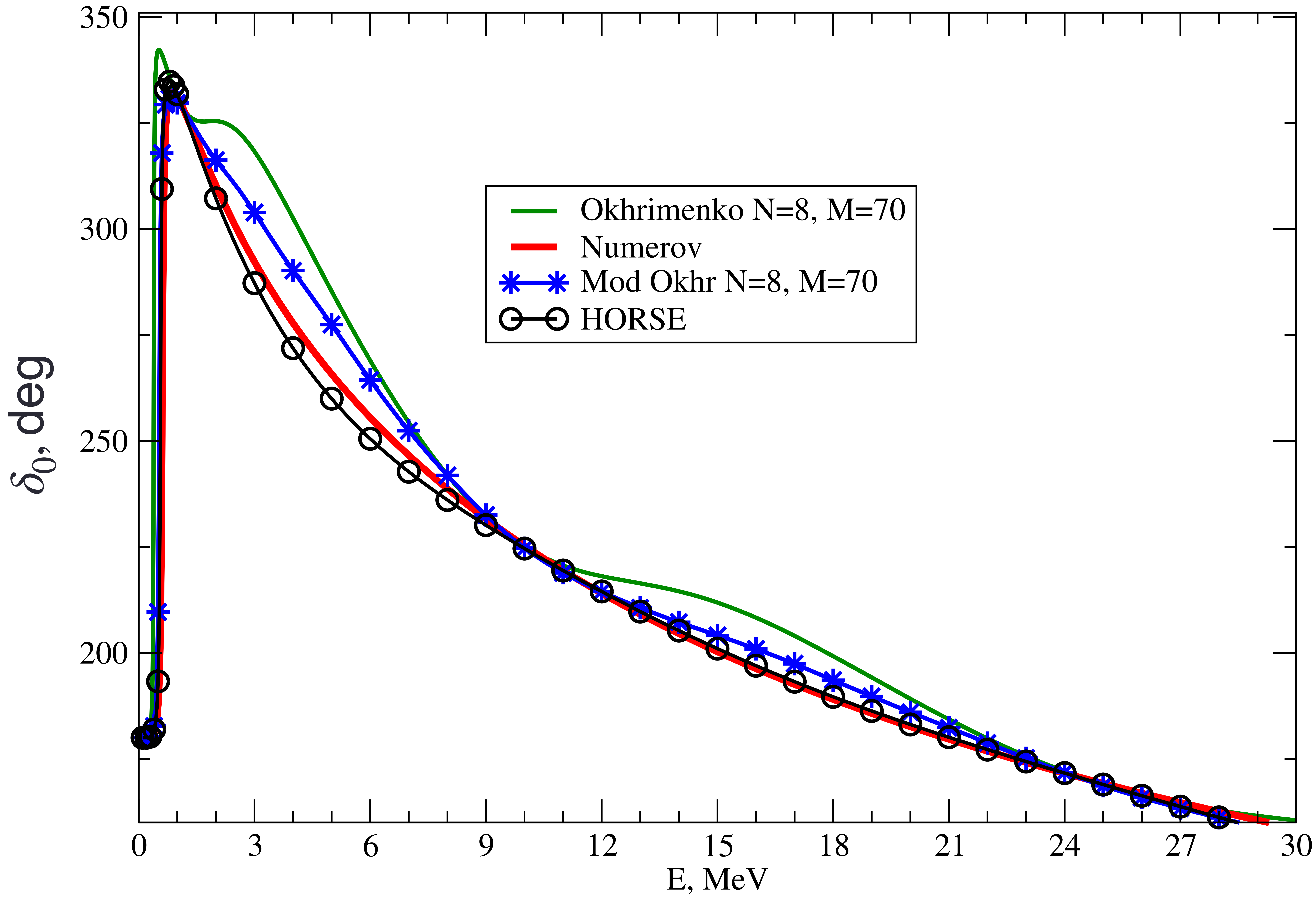


$N = 10$
Numerov
HORSE
HORSE (WS HC)
HORSE (WS+C HC)
δ_1, deg
E, MeV
0
15
30
45
60
75
90
105
120
0
5
10
15
20
25
30



$N = 10$
δ_1, deg
E, MeV
Numerov
HORSE
HORSE (WS HC)
HORSE (WS+C HC)
115
110
105
100
95
2
3
4
5
6
7
8


Z1*Z2=2, A1=1, A2=4
hw=20 MeV, l=0, j=1/2
N_start
E/hw
0
0.5
1
1.5
2
2.5
0
50
100
150
200
250
300
N=10
N=15
N=20
N=30



Okhrimenko N=8, M=70
Numerov
Mod Okhr N=8, M=70
HORSE
δ_0, deg
E, MeV
350
300
250
200
0
3
6
9
12
15
18
21
24
27
30

Summary

- We modified the method of I. P. Okhrimenko, there is no need in different dimension for Coulomb matrix

- We checked the proposed TRR, comparing the expansion coefficients obtained from it with the exact values, it turns out that the asymptotic formula works in a wide range of n

- This approach is further compatible with the Efros method, which allows the use of an even smaller potential matrix

Thank you for your attention!