First approach to the bond energy levels broadening in dense hydrogen plasma

Simplified approach in the frame of Cut-off potentials

Nenad M. Sakan[1], Zoran Simić[2], Vladimir A. Srećković[1], Momchil Dechev[3]

[1]University of Belgrade, Institute of Physics, PO Box 57, 11001 Belgrade, Serbia,
[2]Astronomical Observatory, Volgina 7, 11060 Belgrade, Serbia,
[3]Institute of Astronomy and National Astronomical Observatory, Bulgarian Academy of Sciences, 72, Tsarigradsko chaussee Blvd. Sofia, Bulgaria

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Outline

Dense plasma.

Our modeling methods

Why there is a interest in a simple model broadening of dense plasma?

Modeling idea!

Conclusions

Dense plasma

Anatoly A. Mihajlov (1941-2017)

- Small interionic distance $r_{s;i} = \left(\frac{3}{4\pi N_e}\right)^{1/3}$ - ionic Wiegner-Saitz radius
- Large intristic plasma field
- Strongly coupled Coulomb systems
- The model for plasma of small and moderate nonideality are not applicable

Strongly coupled coulomb systems!

$$\Gamma = \frac{E_{pot}}{E_{kin}} \in [0.1, 2] \tag{1}$$

Dense plasma

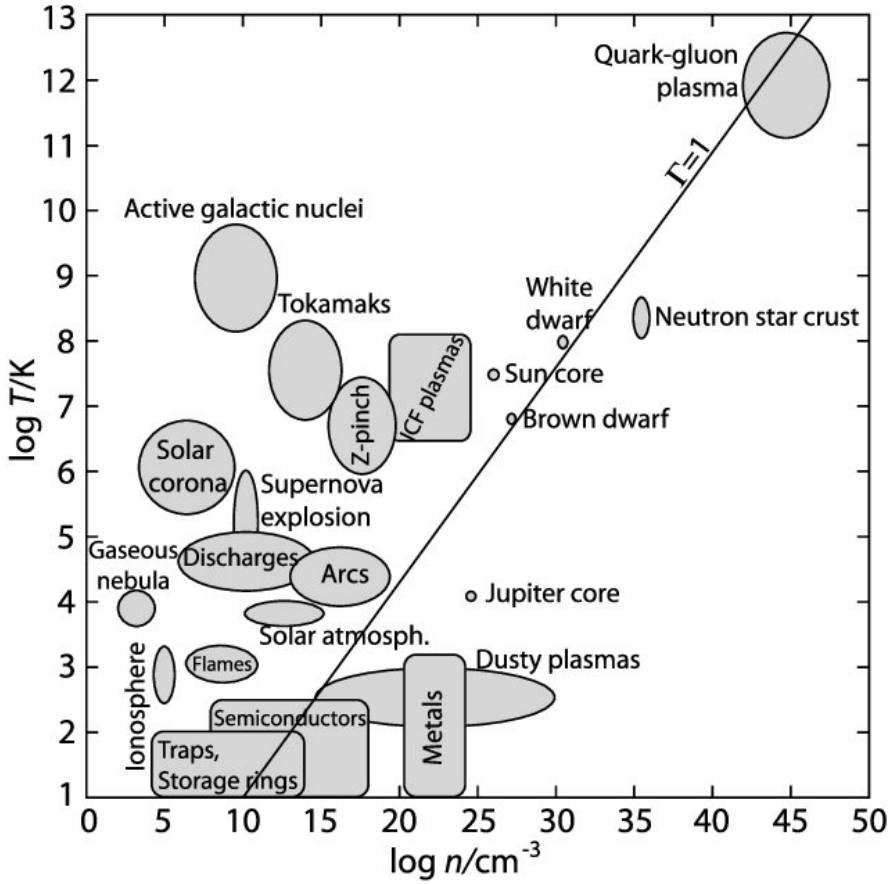


Figure: Different types of plasmas over the density-temperature plane. Note the extremely wide range of these parameters. Strongly coupled plasmas are located right from the $\Gamma = 1$ line.

"Strongly Coupled Plasma Liquids" Z. Donko, P. Hartmann, G. J. Kalman, https://doi.org/10.48550/arXiv.0710.5229

Our modeling methods

Hydrogen model without plasma influence.

$$U_{Coul}(r) = -\frac{e^2}{r}, \tag{2}$$

Hydrogen model with plasma influence

$$U_0(r; r_{cut}) = \begin{cases} -\frac{e^2}{r} + \frac{e^2}{r_{cut}} & : \quad 0 < r \leq r_{cut} \\ \vdots & \\ 0 & : \quad r_{cut} < r \end{cases}, \tag{3}$$

Our modeling methods

Complex atom without plasma influence.

$$U_{Cplx}(r; r_{ion}) = \begin{cases} -\dfrac{Z(l)e^2}{r} & : \quad 0 < r \leq r_{ion} \\ & : \\ -\dfrac{e^2}{r} & : \quad r_{ion} < r \end{cases}, \qquad (4)$$

Complex atom with plasma influence.

$$U^{Plas}_{Cplx}(r; r_{ion}; r_{cut}) = \begin{cases} -\dfrac{Z(l)e^2}{r} + \dfrac{e^2}{r_{cut}} & : \quad 0 < r \leq r_{ion} \\ & : \\ -\dfrac{e^2}{r} + \dfrac{e^2}{r_{cut}} & : \quad r_{ion} < r \leq r_{cut} \\ 0 & : \quad r_{cut} < r \end{cases}, \qquad (5)$$

Our modeling methods

- Drifting awway from analyticaly solvable systems $\rightarrow$ faster calaculations with acceptable error ($\delta < 10^{-5}$)
- Possibility of inclusion of more complex forms of potentials
- Less possibility of numerical instabilities as well as explsions of solutions

The usage of norm conserving pseudoppotentilas for describing of H, He, and preparation for Ar atom.

Interest in broadening

In the frame of presented model the plasma-emitter iteraction was described as a simple cutting off a upper bond energy of pseudoppotential.
It s a good approximation in a close vicinity of emmiter as well as in estreme far field. There is a need for good plasma-emiter interraction modeling
Correct method should include the coupling of ab-initio quantuum model solver with the molecular dynamic simulation (e.g. Quantuum Espresso coupled to LAMMPS)
There is s need for a simple enough model that could be solved without special effort with simple personal computer in normal computation time.

Modeling idea

The plasma is dense and locked in crystal like structure.

DENSE PACKING OF THE SPHERES!

Figure: Stack of cannonballs

Modeling idea

From adequate distribution of emiters per energy $f(E)$ the portion of the selected energy particles as well as adequate plasma parameters are calculated.
Then the averaged radial potential is used for solving of a quantuum mechanical radila function for the emmiter under the modified conditions.
In such way a set of energy detuning along with calculated potential an realised wave functions are calculated

Modeling idea

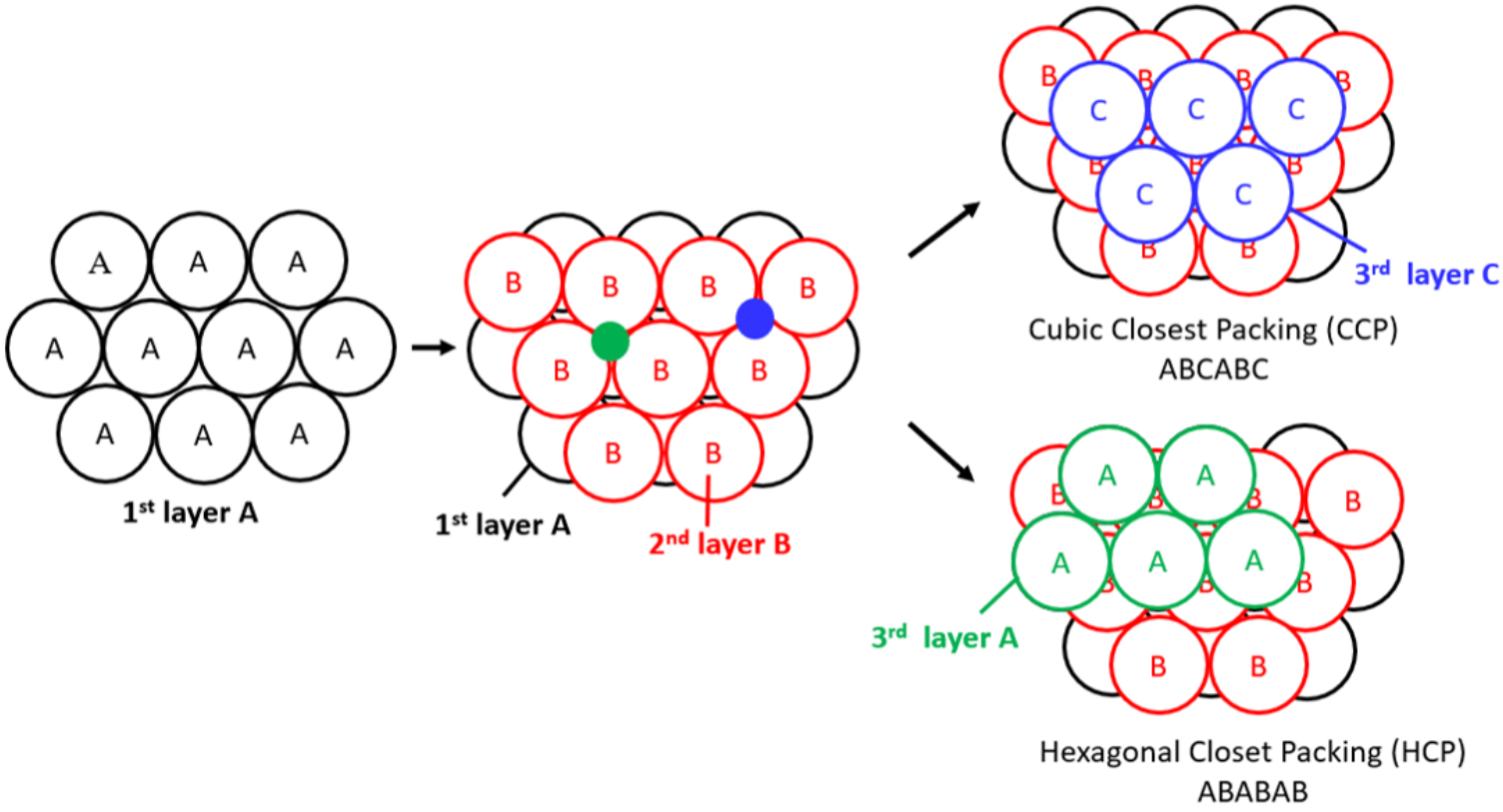
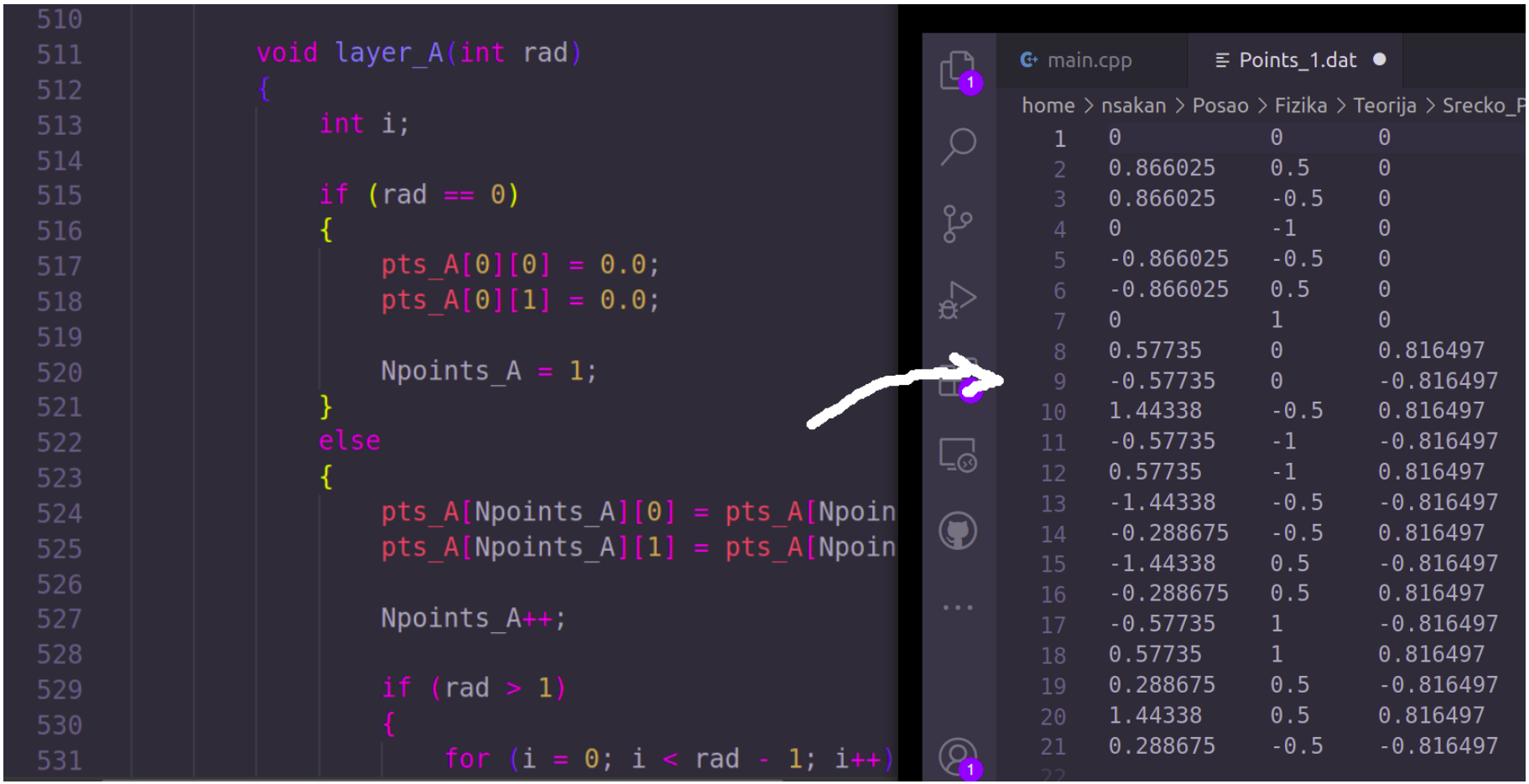


Figure: Dense packing of identical spheres

Modeling idea



```
510
511     void layer_A(int rad)
512     {
513         int i;
514
515         if (rad == 0)
516         {
517             pts_A[0][0] = 0.0;
518             pts_A[0][1] = 0.0;
519
520             Npoints_A = 1;
521         }
522         else
523         {
524             pts_A[Npoints_A][0] = pts_A[Npoin
525             pts_A[Npoints_A][1] = pts_A[Npoin
526
527             Npoints_A++;
528
529             if (rad > 1)
530             {
531                 for (i = 0; i < rad - 1; i++)
```

main.cpp | Points_1.dat

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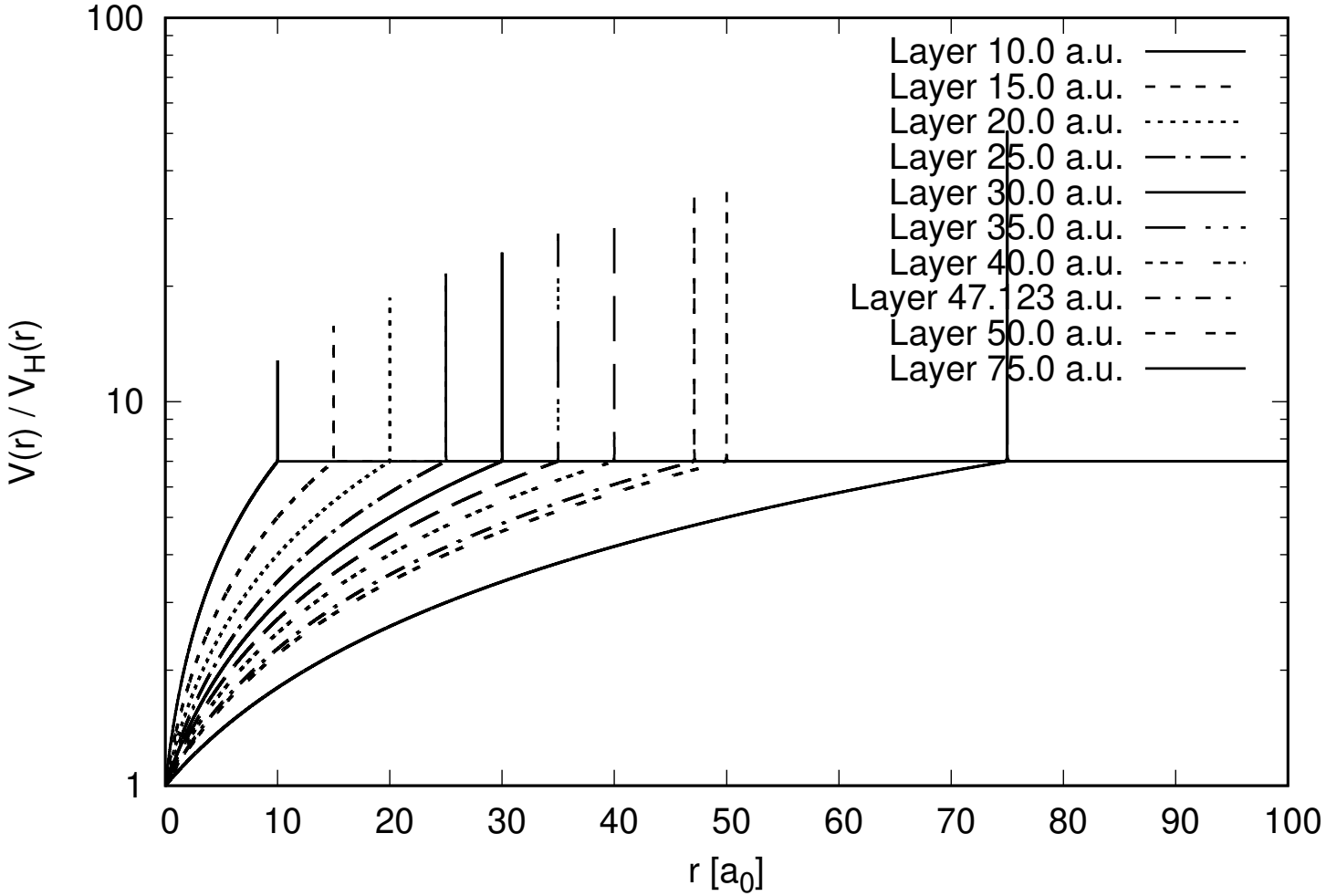
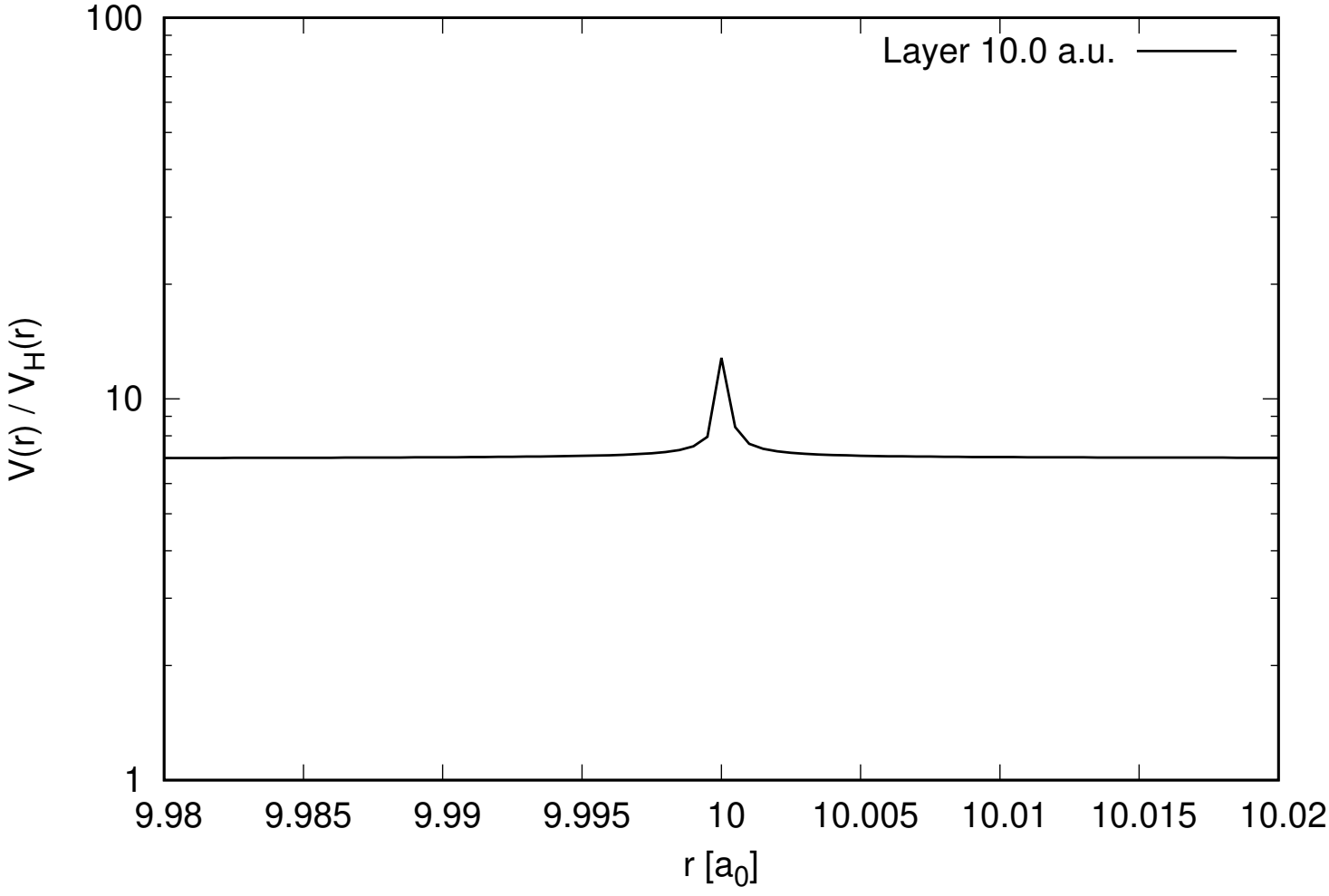
1	0	0	0
2	0.866025	0.5	0
3	0.866025	-0.5	0
4	0	-1	0
5	-0.866025	-0.5	0
6	-0.866025	0.5	0
7	0	1	0
8	0.57735	0	0.816497
9	-0.57735	0	-0.816497
10	1.44338	-0.5	0.816497
11	-0.57735	-1	-0.816497
12	0.57735	-1	0.816497
13	-1.44338	-0.5	-0.816497
14	-0.288675	-0.5	0.816497
15	-1.44338	0.5	-0.816497
16	-0.288675	0.5	0.816497
17	-0.57735	1	-0.816497
18	0.57735	1	0.816497
19	0.288675	0.5	-0.816497
20	1.44338	0.5	0.816497
21	0.288675	-0.5	-0.816497

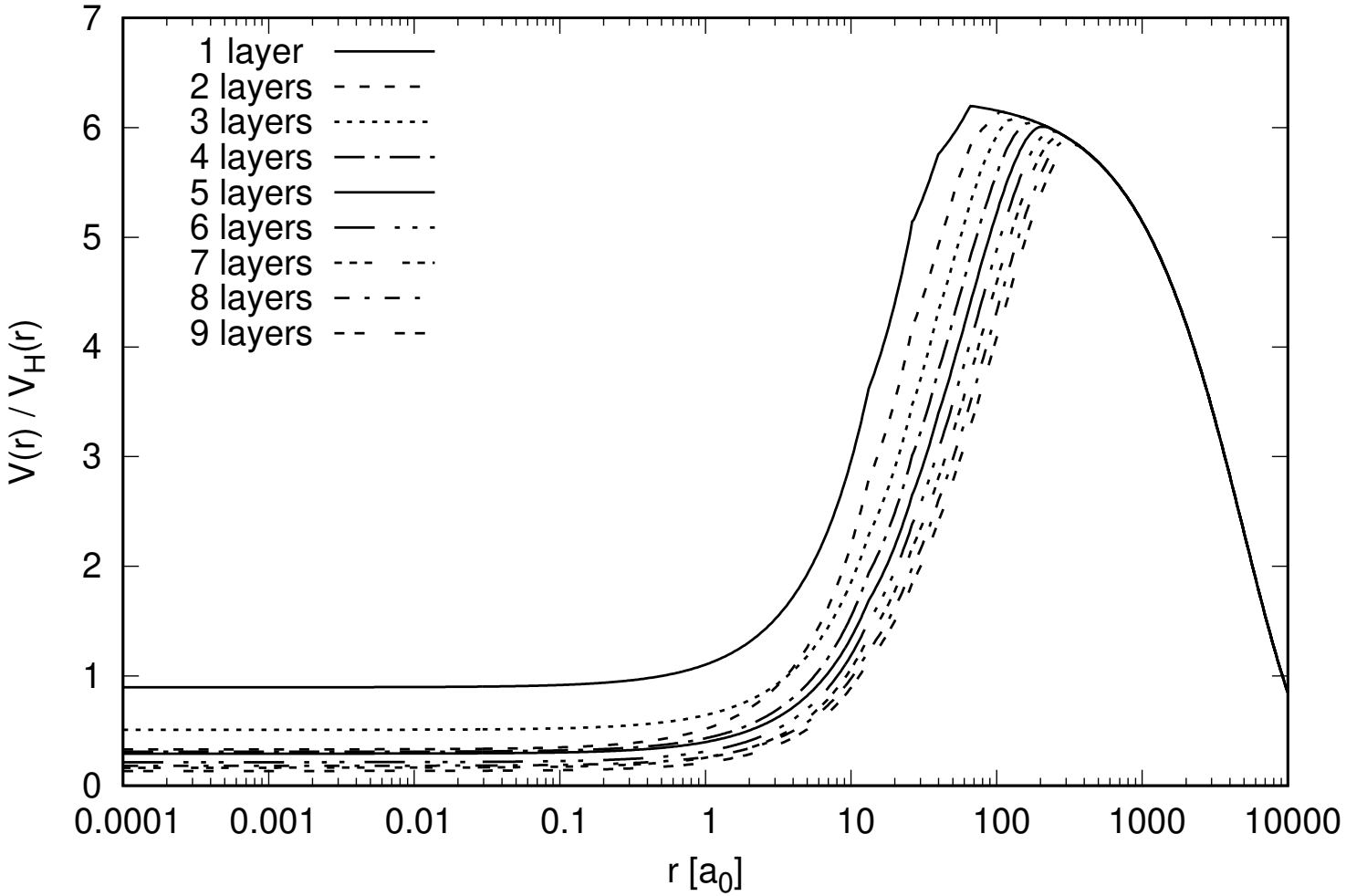
Modeling idea



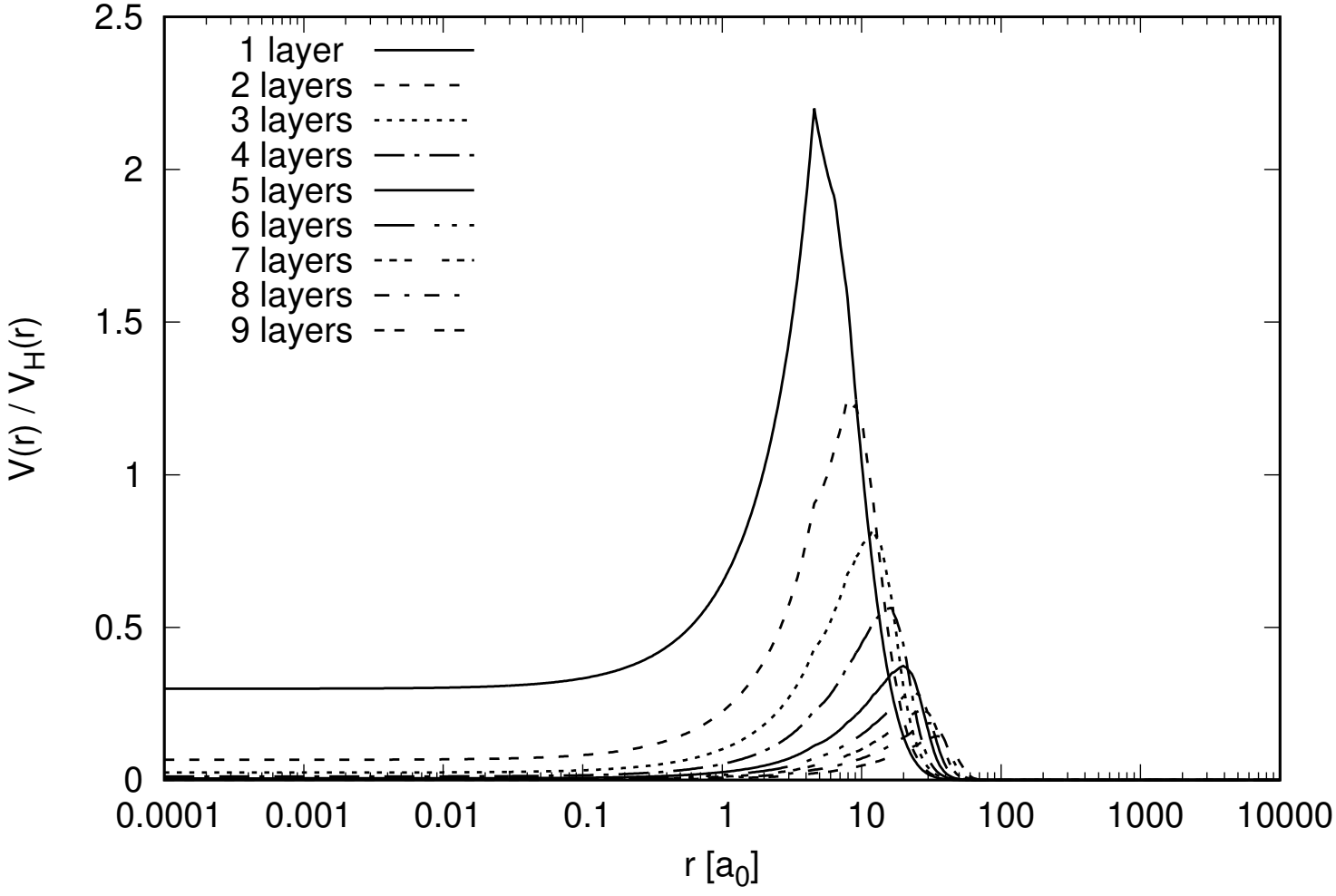
Modeling idea



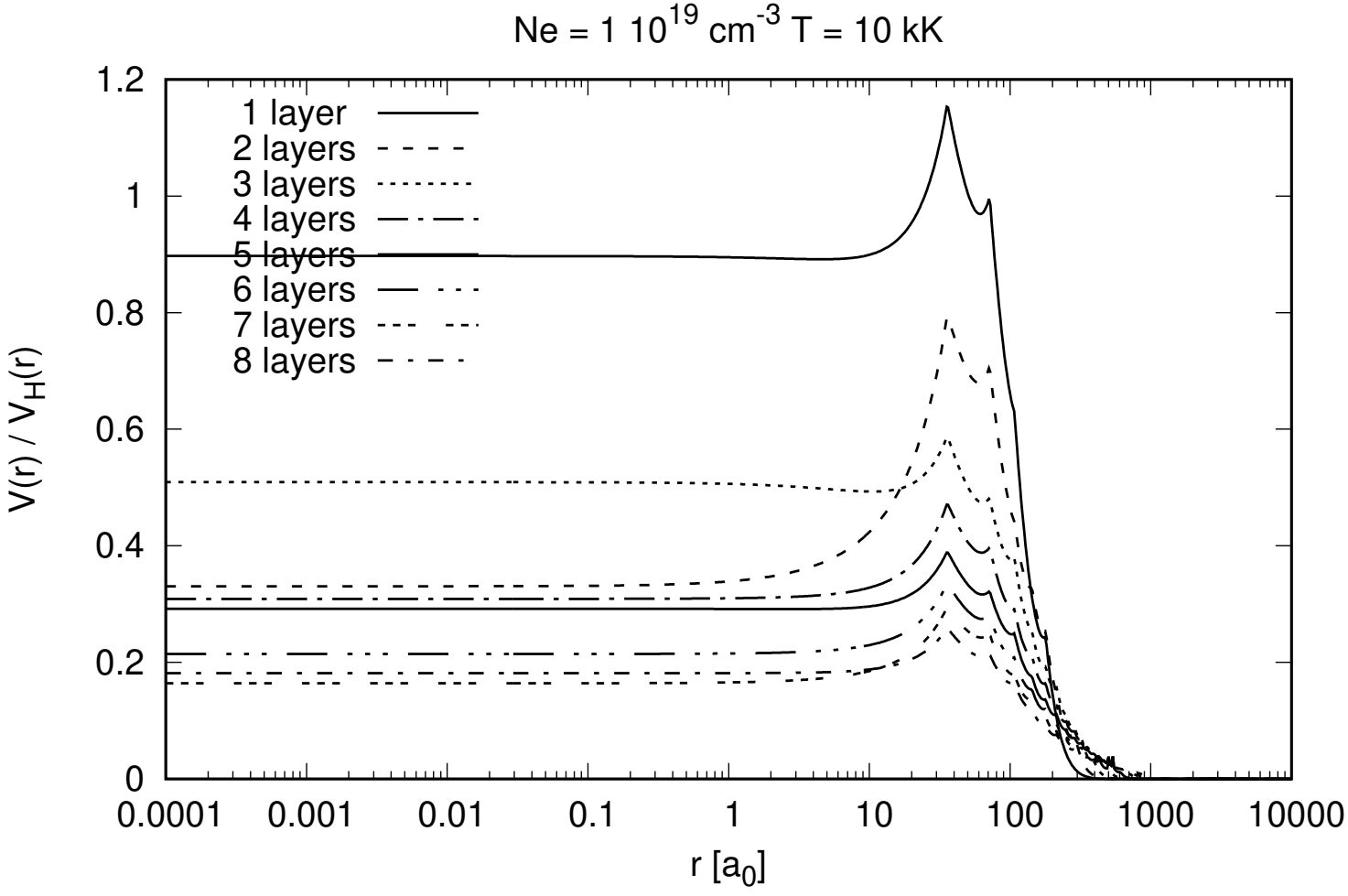
Modeling idea



Modeling idea



Modeling idea



Conclusions

- Step forward in making more precise plasma describing in frame of used model.
- Simple model could again be proven usable.
- This type of plasma influence calculation could be fast as well as promissing for dense plasma.
- Testing is needed.

Thank You for the attention