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Potential Candidates for Cut-off Dense Plasma Modeling

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Abstract

The modeling of plasma behavior from mid up to strong non-ideality, e.g. plasma with a dominant Coulomb interaction is of interest. The micro field is strongly dependent on a form of used pseudo-potential. It is important to have in mind that the plasma behavior is considered as a variation to the main form of a potential. It was obvious from previous papers that the pseudo-potentials used in solid state physics, e.g. ab-initio ones, could be used successfully in describing of a dense plasma. Here we present the candidates potentials calculated with ab-initio method that should be analyzed in order to be used for describing a dense plasma. As a result, after studying of the potentials, it is expected to have a method of introducing a more complex atoms and ions in existing plasma model.

Keywords: astrophysical plasma modeling; dense plasma; optical properties.

Introduction

In the dense plasma the inter-particle Coulomb interaction becomes dominant over the thermal kinetic energy (Fortov et al. 2006). In such conditions a coupled system of particles behaves partially like a crystal. The simplified version, for hydrogen case, of non-ideality parameter **Γ** is given by:

$$\Gamma = \frac{E_p}{E_k} = \frac{e^2}{kTr_{WS}} \sim e^2 N_e^{1/3} \beta \quad (1)$$

Where $\beta = 1/(kT)$, and r_{WS} is a Wiegner Seits radius given by:

$$r_{WS} = \left(\frac{3}{4\pi N_e}\right)^{1/3}$$

The plasma interaction, cut-off Coulomb potential, was used successfully previously for describing of dense plasma in Vitel Y. (2004), and for more details see later papers for example Dimitrijević, et al (2018), Srećković, et al. (2018), Mihajlov, et al. (2015), Ignjatović, et al. (2009). Although the expected plasma influence should be governed in the far field concerning a ionic core radius, it is expected to have a strong influence of the form of a ab-initio yielded pseudopotential. The area of interest in Hydrogen model is in range of $0.1 < \Gamma < 1.5$, while for other species the thourough investigation of model behavior is needed.

Pseudopotentials, link between the dense plasma and condensed matter

The describing plasma depends of two parts, the atom/ion content, as well as plasma influence. While the plasma influence is described as a collective phenomenon, the atom and ion influence is described with the help of pseudo-potential. The idea of describing a complex atom dense plasma as well as describing of complex atom mixtures plasma arises. The atom

and ion influence should be described by the ionic core of the adequate complex atom and ion, while the plasma influence is described with the collective phenomena modeling

There are several ab-initio calculations that are potential candidates for generating a pseudo-potentials capable for being used in dense plasma modeling. Our choice was ATOM, the program originally written by Sverre Froyen at the University of California at Berkeley, and now maintained by Alberto Garcia, see Soler et al. (2002).

It is expected that this approach could enable an inclusion of more complex atom and ion plasma models. A first step the comparison of exact model for Hydrogen with previously used Opium code generated one as well as ATOM generated should be carried out.

Results

The investigation of usability of ab-initio calculated pseudo-potentials is still work in progress. Two ab-initio programs were used in the presented topic, Opium, pseudo potential generation code, and the mentioned ATOM. The simplicity of inclusion ions as well as maturity of the code is leading towards ATOM. At this moment a intensive check of the ability of using ab-initio generated pseudo-potentials is a work in progress. Since now, the Opium generated ones are in focus.

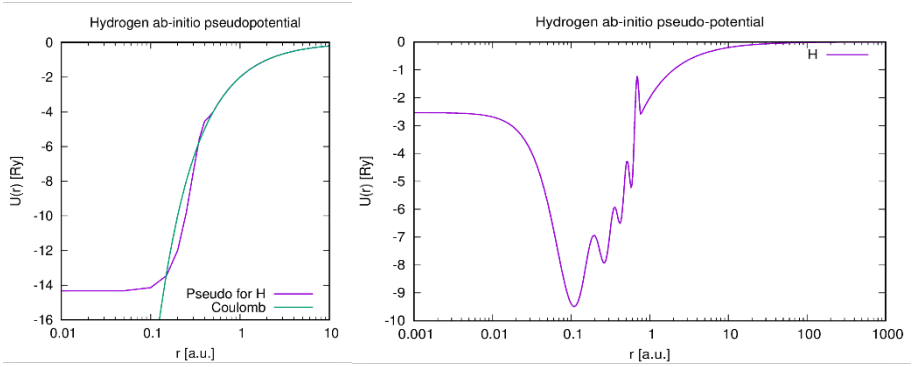

Figure 1. *Comparison of hydrogen pseudo-potential generated with ATOM code, left side figure, with opium generated one, on the right*.

As it could be seen from the Figure 1. the two different forms of the pseudo-potential yields a entirely good solution for the bond states for hydrogen atom. All bind energies are well within expected 0.1% error, that was expected with the solving procedure. Similarly, on Figure 2. a set of pseudo-potentials for He are given.

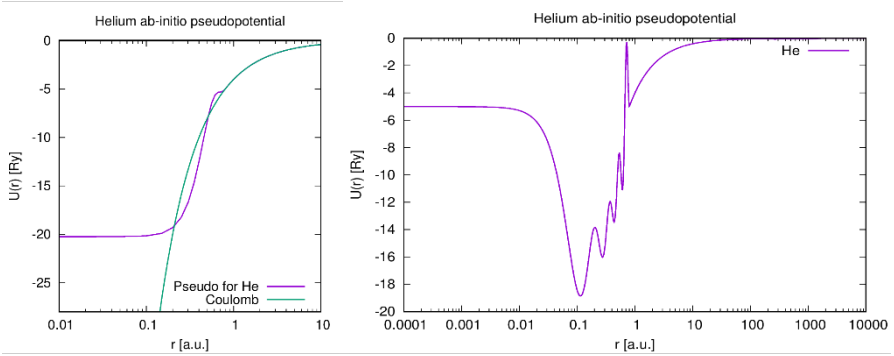

Figure 2. *Comparison of He pseudo-potential generated with ATOM code, left side figure, with opium generated one, on the right*.

The form of pseudo-potentials generated by the opium code for both hydrogen as well as helium is similar in form, but complex. It led to the conclusion that much more precaution should be taken before promoting final results. The experience in both varying parameters of the initial guess fir the levels as well as a form of ab-initio potentials is needed.

The next step is the simulation of the influence of ionic component in plasma, one of the collective plasma effect. It is simulated by the means of dense packing model. The ions are considered motionless, and their inter-ionic distance is exact Wiegner-Seits one. The screening is modeled as Debye one, although the model is not applicable to dense plasma the results are good enough, the work on better screening model is in progress. This step is step further in comparison to previous work. In this step a electron density and electron temperature are converted to inter-ionic distance, e.g. the Wiegner-Seitz radius. Based on those facts a averaged potential of emmiter is calculated.

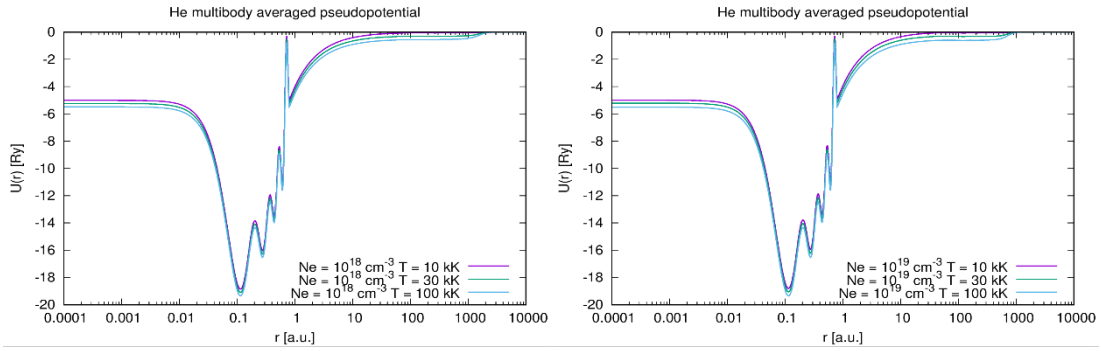

Figure 3. *The generation of cut-off platou as a consequence of multiple coupled ionic fields in plasma, left figure Ne = 10^{18} cm^{-3}, right Ne=10^{19} cm^{-3}, various temperatures*.

From Figure 3. it could be seen that the cut-off radius, that exists as the consequence of the mean plasma interaction is generated by the means of simple model. Also the other effect of additional lowering of the bound energy could be observed as a lowering of potential well, especially in a area of small radii. Previously this effect was a parameter in model, and now it is expected to have not only physical meaning but also a model for it's estimating.

It is obvious that there is a need for further describing of inclusion of more precise screening model as well as modeling of the influence of the thermal energies of each of plasma components. The presented potentials are solvable by the means of numerical integration of Schrodinger equation. Since a work on test procedure for the final results is also a work in progress it is expected to have the data on dipole matrix elements as well as oscillator strengths for complex emitters in dense plasma presented in near future.

Conclusion

From presented results it is obvious that the proposed method of inclusion of complex atoms and ions in plasma could lead to a usable model potential. The benefits of proposed model in contrast to the more widely used, molecular dynamics coupled with the exact Schrodinger solver, is a computing power relaxed calculations that are applicable on any desktop system and could be used as such. After this test of the code the inclusion of bond-free and free-free transitions should take place.

A describing of broadening mechanisms for described plasma are still needed, and it is expected to be a one of the further steps. After all the presented research shows that the simplified approach could lead to good, applicable results for both experimental as well as stellar/Solar plasma in areas of moderate as well as relatively high densities. The automatic generation of mean plasma influence as a mean of multi-body averaged potential gives an idea of introducing more complex models of influence of separate plasma components

The test and inclusion of model for helium, that is a first step in progress, could lead to a better modeling of a Solar and stellar dense plasmas.

It is expected that in further work an method for describing a plasma in initial LIBS breakdown of complex targets and mixtures could help with better understanding of laboratory plasma as well as diagnostic one, like in NOVA2LIBS4fusion project.

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