Modeling optical processes in dense astrophysical and laboratory plasmas: dipole moment and pseudo potential

N.M. Sakan¹⁰, V.A. Srećković¹⁰, Z. Simić² and M. Dechev³⁰

¹ University of Belgrade, Institute of Physics Belgrade, PO Box 57 (E-mail: nsakan@ipb.ac.rs, vlada@ipb.ac.rs)

² Astronomical Observatory, Volgina 7, 11060 Belgrade, Serbia (E-mail: zsimic@aob.rs)

³ Institute of Astronomy and National Astronomical Observatory, Bulgarian Academy of Sciences, 72, Tsarigradsko chaussee Blvd. Sofia, Bulgaria (E-mail: mdechev@nao-rozhen.org)

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Abstract. This manuscript deals with aspects of dense plasma behavior and modeling in a cut-off pseudo-potential figure. The method of cut-off pseudo potentials, both Coulomb and Hartree-Fock ones, has been used e.g. in a description of dense astrophysical plasma. Here are presented some of the aspects of the model and analysis of the behavior of dipole moments. The presented results are important for the estimation of the optical properties of moderate and high density hydrogen astrophysical plasma. The behavior of such plasma is also of interest in fusion experiments and various laboratory research.

Key words: astrophysical plasma – fusion plasma – dense plasma – optical characteristics – modeling – stellar atmospheres – dipole approximation

1. Introduction

Both theoretical and experimental studies are interested in the issues of radiative transfer, energy transport, and plasma opacity under moderate and strong nonideality (van Horn, 1991; Treumann & Baumjohann, 1997; Rogers & Iglesias, 1998; Vitel, 2004; Mihajlov et al., 2011a; Khrapak & Khrapak, 2020). In recent decades, a large number of theoretical and experimental investigations have focused on the strong coupling and density effects in plasma radiation (Kobzev & Popovich, 2013; Remington, 2005; Uzdensky & Rightley, 2014). Moreover, Machine learning (ML) was used in order to estimate plasma parameters and characteristics of such systems (Akçay et al., 2021; Trieschmann et al., 2023). The plasma of the inner layers of the solar atmosphere and partially ionized layers of other stellar atmospheres, such as the atmospheres of DA white dwarfs are taken into consideration (Bodmer & Bochsler, 2000; Srećković et al., 2017; Chabrier et al., 2006; Somov, 2006). In many-particle systems it is common to make a switch from a variety of particles in a system toward a model particle, the so-called pseudo particle, (Fortov et al., 2006; Mihajlov et al., 2011b; Douis & Meftah, 2013; Srećković et al., 2018). The virtual particle that possesses the average behavior of all of the system particles in a form of averaged one. That behavior is described with the help of averaged, pseudo-potential (see e.g. Ignjatović et al., 2017, and references therein). The usage of pseudo-potentials relaxes a numerical requirement, since the solution methods are simpler than for the system of particles and as such code is capable of running on a desktop computer, e.g. it does not need extensive computing power.

It is well known that Coulomb collisions between charged particles have the ability to transfer energy and cause the plasma to heat or cool. The control of the electron heat flux in the solar wind appears to be influenced by Coulomb collisions (Kalman et al., 2006; Salem et al., 2003). Additionally, the stability or instability of plasma configurations can be influenced by Coulomb forces. For instance, stable or unstable magnetic structures may arise as a result of the equilibrium between Coulomb and magnetic forces. In addition to influencing the transport of charged particles in solar plasma, which can alter their speed and distribution, Coulomb forces can also contribute to the acceleration of particles in solar plasma, as in the case of solar flares or coronal mass ejections (see e.g. Bodmer & Bochsler, 2000; Gordovskyy et al., 2005).

2. Theory

In order to have some adequate representation of the plasma characteristics one of the most common parameters is a non-ideality parameter, Γ , given in simplest form applicable for hydrogen plasma given by

$$\Gamma = \frac{E_{pot}}{E_{kin}} = \frac{q_e^2}{4\pi\varepsilon_0 \langle r \rangle kT_e} = \frac{q_e^2}{4\pi\varepsilon_0 kT_e} \sqrt[3]{\frac{4\pi n_e}{3}}.$$
 (1)

It presents a ratio of the intrinsic potential energy pf plasma divided by thermal energy, that could be related to the kinetic energy of plasma constituents (Tkachenko et al., 2006; Adamyan et al., 2009; Sakan et al., 2018). Here we are dealing with describing of plasma of mild nonideality, up to strongly nonideal plasma, $0.1 \leq \Gamma \leq 2$.

To calculate the optical properties of plasma the Schroedinger equation that introduces the collective plasma pseudo-potential should be solved (Prandini et al., 2018). For the case of hydrogen atom in plasma the simple form of pseudopotential, cut-off Coulomb one, possesses the ability to have an analytical solutions in entire radial space as well as all bond as well as free solutions.

$$U_0(r; r_{cut}) = \begin{cases} -\frac{e^2}{r} + \frac{e^2}{r_{cut}} & : & 0 < r \le r_{cut} \\ 0 & : & r_{cut} < r \end{cases}$$
(2)

where r_{cut} is cut off radius (see e.g. Mihajlov et al., 2011a).

In later work it has been proven that the Hartree-Fock potential could be used instead of physically more correct Coulomb one. So the potential, could be substituted with the Hartree-Fock one shifted by the average plasma energy $1/r_{cut}$. It also relaxes the numerical complexity of the calculations, and in case of hydrogen the overall relative error is comparable or smaller than $1 \cdot 10^{-7}$.

In dipole approximation, that is valid for high density plasma, the radial part of equation is of interest. By the introduction of the substitution R(r) = P(r)/r it becomes

$$\frac{d^2P}{dr^2} + \left[\frac{2m}{\hbar^2}\left(E - U(r)\right) - \frac{l(l+1)}{r^2}\right]P = 0.$$
(3)

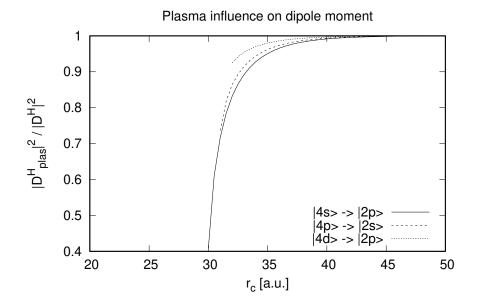


Figure 1. The plasma influence onto dipole matrix element for the transitions from main quantum number n = 4 onto states with n = 2.

In this contribution, we will present computed quantities, i.e. a dataset, and explain the results and future perspectives.

3. Results and discussion

Here, a behavior of plasma influence onto the dipole matrix elements is discussed. In Fig. 1 a influence of average plasma potential $1/r_c$ on the dipole

matrix element is shown. It could be seen that for the same main quantum number transition, from n = 4 to n = 2 the From Fig. 2 the influence of the enlarged plasma potential energy, e.g. diminishing of r_c , the influence of plasma is dominant onto the far most outer shell. This is expected behavior, but with the

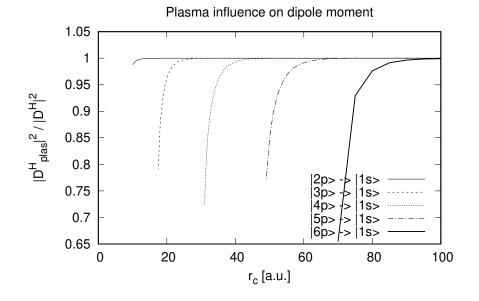


Figure 2. The plasma influence onto dipole matrix element for the transitions onto 1s state.

further steps that have been carried out it is expected to have a more adequate pseudo-potential model for describing of plasma influence.

The presented results could show a behavior of the dipole matrix elements inside plasma. As such they could be used as a mark of the real behavior of emitter in plasma. The work on calculating a more adequate pseudo-potentials that could characterize a better plasma influence onto the emitter is in progress. The results presented here could be of interest in describing of hydrogen astrophysical plasma optical properties in area of plasmas of moderate and high non-ideality. The behavior of such plasma is also of interest in fusion experiments and various laboratory research.

4. Final remarks and future work

This work examines dense plasma behavior and modeling in a cut-off pseudopotential figure. Cut-off pseudopotentials, including Coulomb and Hartree-Fock models, have been used to describe dense astrophysical plasma. The given results are crucial for estimating the optical characteristics of moderate and high density hydrogen astrophysical plasma. Plasma behavior is relevant to fusion experiments and laboratory research using ML (see e.g. Sakan et al., 2022; Lemishko et al., 2024, and references therein).

The findings and their analysis demonstrate the applications' interdisciplinary nature. This work's perspective and short-term goal is to use machine learning for astrophysical plasma research.

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References

- Adamyan, V. M., Mihajlov, A. A., Sakan, N. M., Srećković, V. A., & Tkachenko, I. M., The dynamic conductivity of strongly non-ideal plasmas: is the Drude model valid? 2009, Journal of Physics A Mathematical General, 42, 214005, DOI:10.1088/1751-8113/42/21/214005
- Akçay, C., Finn, J. M., Brennan, D. P., Burr, T., & Kürkçüoğlu, D. M., Machine learning methods for probabilistic locked-mode predictors in tokamak plasmas. 2021, *Phys. Plasmas*, 28, DOI:10.1063/5.0053670
- Bodmer, R. & Bochsler, P., Influence of Coulomb collisions on isotopic and elemental fractionation in the solar wind acceleration process. 2000, Journal of Geophysical Research, 105, 47, DOI:10.1029/1999JA900434
- Chabrier, G., Saumon, D., & Potekhin, A. Y., Dense plasmas in astrophysics: from giant planets to neutron stars. 2006, J. Phys. A, 39, 4411, DOI:10.1088/0305-4470/39/17/S16
- Douis, S. & Meftah, M. T., Correlation Function and Electronic Spectral Line Broadening in Relativistic Plasmas. 2013, Serbian Astronomical Journal, 186, 15, DOI: 10.2298/SAJ130218002D
- Fortov, V., Iakubov, I., & Khrapak, A. 2006, Physics of Strongly Coupled Plasma, International Series of Monographs on Physics (OUP Oxford), ISBN: 9780199299805
- Gordovskyy, M., Zharkova, V. V., Voitenko, Y. M., & Goossens, M., Proton versus electron heating in solar flares. 2005, *Advances in Space Research*, **35**, 1743, DOI: 10.1016/j.asr.2005.07.004
- Ignjatović, L., Srećković, V., & Dimitrijević, M., The Screening Characteristics of the Dense Astrophysical Plasmas: The Three-Component Systems. 2017, Atoms, 5, 42, DOI:10.3390/atoms5040042

- Kalman, G. J., Rommel, J. M., & Blagoev, K. 2006, Strongly Coupled Coulomb Systems (Springer Science & Business Media)
- Khrapak, S. A. & Khrapak, A. G., On the conductivity of moderately non-ideal completely ionized plasma. 2020, *Results in Physics*, **17**, 103163, DOI:10.1016/j.rinp. 2020.103163
- Kobzev, G. & Popovich, M. 2013, Transport and optical properties of nonideal plasma (Springer Science & Business Media)
- Lemishko, K., Armstrong, G. S. J., Mohr, S., et al., Machine learning-based estimator for electron impact ionization fragmentation patterns. 2024, *Journal of Physics D: Applied Physics*
- Mihajlov, A. A., Sakan, N. M., Srećković, V. A., & Vitel, Y., Modeling of the Continuous Absorption of Electromagnetic Radiation in Dense Hydrogen Plasma. 2011b, *Baltic Astronomy*, 20, 604, DOI:10.1515/astro-2017-0345
- Mihajlov, A. A., Sakan, N. M., Srećković, V. A., & Vitel, Y., Modeling of continuous absorption of electromagnetic radiation in dense partially ionized plasmas. 2011a, J. Phys. A, 44, 095502, DOI:10.1088/1751-8113/44/9/095502
- Prandini, G., Marrazzo, A., Castelli, I. E., Mounet, N., & Marzari, N., Precision and efficiency in solid-state pseudopotential calculations. 2018, npj Computational Materials, 4, 72, DOI:10.1038/s41524-018-0127-2
- Remington, B. A., High energy density laboratory astrophysics. 2005, Plasma Physics and Controlled Fusion, 47, A191, DOI:10.1088/0741-3335/47/5A/014
- Rogers, F. J. & Iglesias, C. A., Opacity of Stellar Matter. 1998, *Space science reviews*, **85**, 61, DOI:10.1023/A:1005132518820
- Sakan, N. M., Srećković, V. A., Simić, Z. J., & Dimitrijević, M. S., The Application of the Cut-Off Coulomb Model Potential for the Calculation of Bound-Bound State Transitions. 2018, Atoms, 6, DOI:10.3390/atoms6010004
- Sakan, N. M., Traparić, I., Srećković, V. A., & Ivković, M., The usage of perceptron, feed and deep feed forward artificial neural networks on the spectroscopy data: astrophysical & fusion plasmas. 2022, Contributions of the Astronomical Observatory Skalnate Pleso, 52, 97, DOI:10.31577/caosp.2022.52.3.97
- Salem, C., Hubert, D., Lacombe, C., et al., Electron Properties and Coulomb Collisions in the Solar Wind at 1 AU: Wind Observations. 2003, *The Astrophysical Journal*, 585, 1147, DOI:10.1086/346185
- Somov, B. V. 2006, Plasma Astrophysics, Part I: Fundamentals and Practice (Springer New York, NY)
- Srećković, V. A., Šulić, D. M., Ignjatović, L. M., & Dimitrijević, M. S., A study of high-frequency properties of plasma and the influence of electromagnetic radiation from IR to XUV. 2017, Nucl. Techn. & Rad. Protect., 32, 222, DOI: 10.2298/NTRP1703222S
- Srećković, V. A., Sakan, N., Šulić, D., et al., Free-free absorption coefficients and Gaunt factors for dense hydrogen-like stellar plasma. 2018, Mon. Not. R. Astron. Soc., 475, 1131, DOI:10.1093/mnras/stx3237

- Tkachenko, I. M., Adamyan, V. M., Mihajlov, A. A., et al., Electrical conductivity of dense non-ideal plasmas in external HF electric field. 2006, Journal of Physics A Mathematical General, 39, 4693, DOI:10.1088/0305-4470/39/17/S58
- Treumann, R. A. & Baumjohann, W. 1997, Advanced space plasma physics (Imperial College Press: London, UK), DOI:10.1142/p020
- Trieschmann, J., Vialetto, L., & Gergs, T., Review: Machine learning for advancing low-temperature plasma modeling and simulation. 2023, J. Micro/Nanopatterning Mater. Metrol., 22, 041504, DOI:10.1117/1.JMM.22.4.041504
- Uzdensky, D. A. & Rightley, S., Plasma physics of extreme astrophysical environments. 2014, *Reports on Progress in Physics*, **77**, 036902, DOI:0.1088/0034-4885/77/3/036902
- van Horn, H. M., Dense Astrophysical Plasmas. 1991, *Science*, **252**, 384, DOI:10.1126/ science.252.5004.384
- Vitel, Y., Spectra of dense pure hydrogen plasma in Balmer area. 2004, J. Quant. Spectrosc. Radiat. Transf., 83, 387, DOI:10.1016/S0022-4073(02)00380-1