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Dataset for Optical Processes in Dense Astrophysical and Laboratory Plasmas

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Abstract: The interest in the modeling of laboratory and astrophysical plasma behavior from mid up to strong non-ideality (NI), e.g., plasma in which a Coulomb interaction becomes dominant, led us to further investigate the optical properties of such systems. An expanded set of results and properties like wave functions, dipole matrix elements, etc., for such systems is presented in this submission. The methodologies of our research, as well as the current and future elements of their applications, are explained. In addition to being helpful to other researchers for achieving a variety of goals, the data from this study could be useful the interdisciplinary fields of machine learning, astrochemistry and fusion physics. The dataset is available online at the repository Figshare.

Keywords: atomic data; astrophysical plasma; fusion plasma; coupled system; optical characteristics; modeling; stellar atmospheres

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1. Introduction

Data and databases for atomic processes are essential in many areas of astrophysics, fusion science, etc., and modeling codes for such processes require accurate data [1–6]. Data for hydrogen are important as hydrogen is one of the most abundant species in the universe. Moreover, the description and modeling of and data connected with the interactions in mid up to strong non-ideal (NI) plasmas are important for modeling such environments because of the relatively rarity of experiments and experimental data [7–11].

This trend involves using data directly to produce predictions, either alone or in combination with models, resulting in a controllable level of agreement with the data [12,13]. It is know that Coulomb collisions between charged particles can transfer energy and contribute to the heating or cooling of plasma. For example [14] showed that Coulomb collisions seem to play a part in the regulation of electron heat flux in solar wind. Also, Coulomb forces can contribute to the stability or instability of plasma configurations. For example, the balance between Coulomb forces and magnetic forces can lead to the formation of stable or unstable magnetic structures. Coulomb forces can not only play a role in the acceleration of particles in solar plasma, such as in the case of solar flares or coronal mass ejections, but can also influence the transport of charged particles in solar plasma, affecting their motion and distribution. Our aim is to collect spectroscopic information, i.e., data, on such systems.

The set of results presented here is a comprehensive dataset of solutions of a purely quantum mechanical system that describes the behavior of the hydrogen emitter in plasma with the help of two types of model potential. The influence of plasma is described as the cutting off of the potential that is above the average plasma energy. The advantage of this approach is that it is a straightforward approach without a robust procedure with results applicable to the plasma of mid to strong non-ideality. It should be noted that our research started with the work [15] as case study.

This submission presents a comprehensive set of results for hydrogen plasma wave functions and dipole matrix elements. Also, a set of pseudo-potentials that are utilized in computation form part of the given data. In addition to being useful to other researchers for a variety of purposes, these data could serve as material in the interdisciplinary fields of machine learning, astrophysics, and fusion physics [16–19]. Moreover, the data could be useful in technological facilities, power-generating facilities, attosecond laser experiments like in extreme light infrastructure (ELI) beamline facilities [20–22], etc.

In this contribution we will present computed quantities, i.e., a dataset, and discuss the results (in Section 2). We will present some illustrative examples. In Section 3, we present our conclusions and further directions for research. Needed relations and formulas are presented in the Appendix A. The dataset is available online at the repository Figshare.

2. Results and Discussion

A complete set of results for dipole matrix elements and hydrogen plasma wave functions is presented in this contribution. The provided data also include a collection of pseudo-potentials that are used in the calculations.

2.1. Calculated Quantities

In order to obtain the results, the shooting method was coupled with the Numerov radial Schrodinger equation solver [23–26]. The convergence towards unperturbed states in both the energy level values and wave function form was carried out earlier.

With the aim of defining the area in which it is expected to have good usability of the presented data, an NI parameter Γ is introduced. This parameter is generally used for describing the properties of plasma with an enlarged inter-particle Coulomb interaction. Here, it is presented in its hydrogen case form: $\Gamma = e^2/(kTr_{WS}) \sim e^2 N_e^{1/3}/kT$, $r_{WS} = (3/(4\pi N_e))^{1/3}$. From the knowledge of the applied quantum model [27–30], it is expected that the validity of its results will be in the area of $0.1 \leq \Gamma \leq 4$. Also, it is supposed to give a better description of plasma in comparison to other models.

The cut-off radius is used as a measure of the average plasma influence, and in atomic units, can be obtained with the relation $< E_p >= -e^2/r_c$. So, the modified potential that includes a plasma influence is cut off at the r_c radius and shifted upwards to have a zero value at large radii. The simplest potential, the Coulomb form, can be described mathematically, while the Hartree–Fock potential is based on the Pseudo Dojo database [31,32] (see Figure 1).

$$V(r) = -\frac{e^2}{r}, \qquad V_c(r) = \begin{cases} -\dfrac{e^2}{r} + \dfrac{e^2}{r_c} & , \quad 0 < r \leq r_c, \\ 0 & , \quad r_c < r < \infty \end{cases}. \tag{1}$$

Although the difference in the forms of the potential and the unperturbed potential is small, the difference still affects the dipole matrix element. From Figure 1, it is obvious that even for plasma with strong Coulomb coupling, the pseudo-potential is barely visible, unlike that in an unperturbed state. Although the cut-off does not fully describe plasma behavior in the vicinity of r_c, it is very good at describing the ionic core area, $r < r_c$, as well as the far area where plasma's influence behaves like a continuum, with the effective plasma influence having an average plasma energy of $E = 1/r_c$. All of the complex processes, as well as the dynamic ones, could be included within this model as a variation. It is necessary to mention that this approach is good at describing dense-plasma phenomena. The potentials are used to solve the radial Schrodinger equation and yield a solution for the radial wave function $P(r) = rR(r)$.

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

An example of wave function $P(r)$ for both perturbed and unperturbed potential for simple Coulomb potential and Hartree–Fock potential is given in Figure 2. The cut-off radius $r_c = 29.8507$ a.u. is used since this is the smallest out of the calculated ones, where a bond level of $|n = 4, l = 0>$ is realized. It can be seen that in such cases, the wave function differs significantly from the unperturbed cases. Also, the Coulomb potential (CP), solution is almost identical to the HF one, which can be seen in Figure 2. The sets of wave functions are calculated here using the Numerov method of numerical integration, and are given for the unperturbed CP and HF potentials, as well as the cut-off ones (as a part of the dataset).

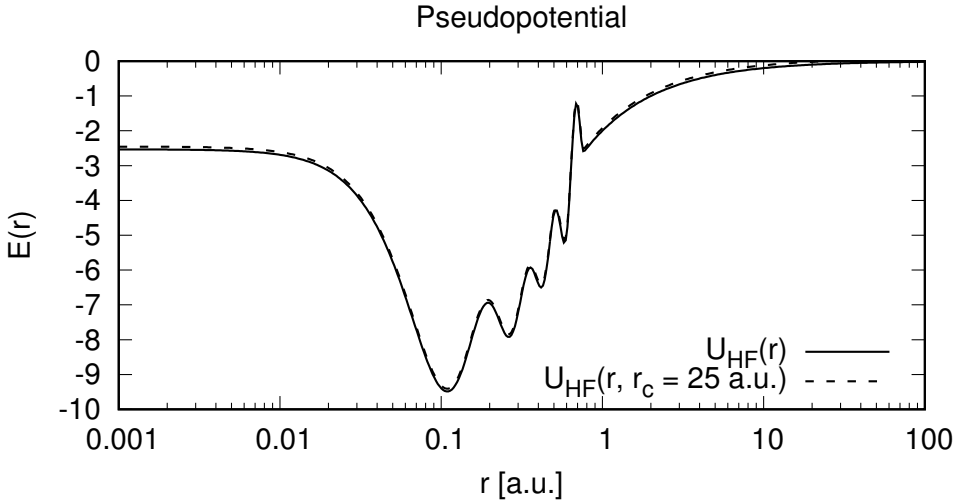


Figure 1. Hartree–Fock (HF) pseudo-potential for hydrogen atoms and hydrogen atoms in plasma in case of cut-off radius of 25 a.u.

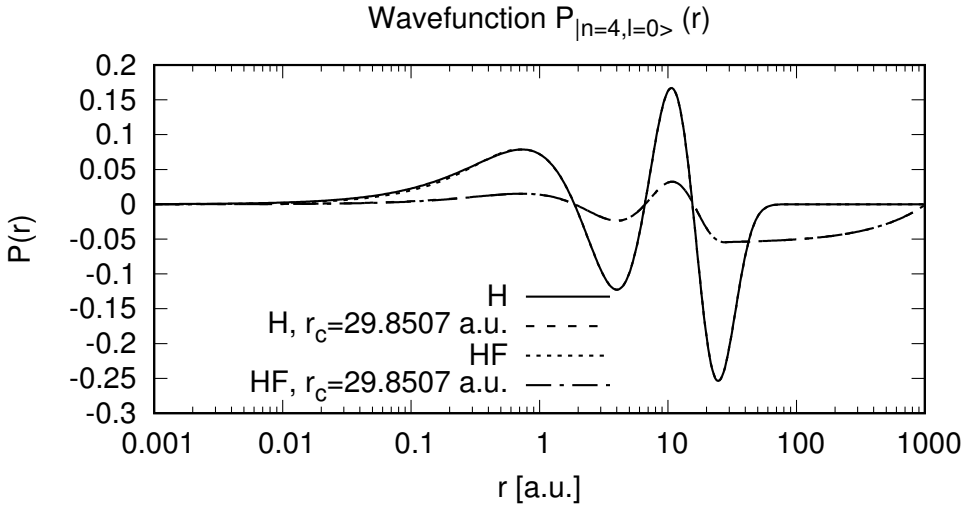


Figure 2. Wave functions for hydrogen atoms in case of CP and HF potential, with and without plasma influence.

These data are further used to obtain the dipole matrix elements

$$\hat{D}_{|n,l>;\,|n',l'>} = \int P_{|n',l'>} r P_{|n,l>} dr \tag{3}$$

A set of dipole matrix elements for all allowed transitions for unperturbed states, as well as those achieved when perturbed by plasma, are given in the presented dataset. Through the direct use of dipole matrix elements, users can calculate the oscillator strength, absorption cross-sections, absorption coefficients and spectral line profiles [33–36].

A detailed description of the method and the necessary relations can be found in Appendix A.

It is important to note that the procedure of calculating pseudo-potential concerning collective phenomena took more than five hours on a powerful PC for nine layers of potentials. The calculation of bond states with the help of special function models took about half a day per model, while the purely numerical calculation of a bond state took seconds. Thus, the calculation time is shortened by several orders of magnitude. Also, it is good to have in mind that all of the mentioned calculation times are much shorter than molecular dynamic ones.

In today's scientific literature, artificial intelligence (AI) and data science approaches are being used more and more, where data can now be directly employed in generating models [12,37]. One example is atomic physics, where machine learning (ML) is used to determine plasma parameters through emission spectroscopy. Recently, the open access, Python-based Sikit-Learn ML framework https://scikit-learn.org, accessed on 19 January 2024 was used to assess line intensities in order to estimate plasma electron concentrations and temperatures under conditions relevant to tokamak divertors. The perspective of this work and planned work in the near future is the use of the ML for NI plasma parameter determination.

2.2. Computation and Datasets

The extensive set of results for the hydrogen wave functions and dipole matrix elements in plasma from mid up to strong NI are presented in this submission and can be accessed in the online open access repository https://doi.org/10.6084/m9.figshare.25359088.v1 (accessed on 1 October 2024). Furthermore, Figures 1 and 2 also present the results.

The repository data are sorted into three directories/folders with the presented dataset and a fourth one with a detailed description of the data:

```
|-- D/
|-- Description/
|-- Pot/
|-- Psi/
```

The directory `Pot/` contains files with the used pseudo-potentials for the calculation of the wave functions and dipole matrix elements. All of them contain a header compatible with gnuplot software [38] (http://www.gnuplot.info/, accessed on 1 September 2024.) and two columns of data on the radius and the potential. There are three types of filenames: a file that contains the Hartree–Fock (HF) potential of the unperturbed hydrogen atom that is used in calculations, and files where the potentials for the plasma-perturbed potentials are given for the mentioned cut-off radius.

The directory `Psi/` contains files with the calculated wave functions, and the header of each file consists of three comment lines compatible with the `gnuplot` software. The directory `D/` contains the calculated data for the dipole matrix elements for allowed transitions. The directory `Description/` contains the file `README.text` with a more detailed description of the results, as well as the calculations.

3. Conclusions and Further Directions

A complete set of results for dipole matrix elements and hydrogen plasma wave functions is presented in this contribution. The provided data also include a collection of pseudo-potentials that are used in the calculations. The new dataset is displayed in the Figshare repository and is ready for future use: https://doi.org/10.6084/m9.figshare.25359088.v1 (accessed on 1 October 2024). The provided data and information have multiple practical applications across various scientific domains:

- For laboratory research (laser-driven plasma, spectroscopic investigation, fusion experiments, etc.);
- For use in technology and industry;

- For potential astrophysical use (the modeling of different atmospheres, AGNs);
- For different theoretical investigations (in confined systems in the generation of new materials and investigating stars).

The data and their analysis illustrate the multidisciplinary nature and applications of our results. Since these studies concern fusion research, our plan is to expand this investigation in the future, but with data related to tungsten (see e.g., [39,40]). The perspective of this work and the aim of work carried out in the near future aim is the employment of ML for NI plasma parameter determination.

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Abbreviations

The following abbreviations are used in this manuscript:

AI	Artificial intelligence
CP	Coulomb potential
ELI	Extreme light infrastructure
HF	Hartree–Fock
ML	Machine learning
NI	Non-ideality

Appendix A. The Method and Important Quantities

In order to calculate the optical properties of plasma, the Schroedinger equation, which introduces the collective plasma pseudo-potential, should be solved. For the case of hydrogen plasma, the form of the pseudo-potential can have analytical solutions in the entire radial space as well as all bonds and free solutions.

$$U_0(r;r_{cut}) = \begin{cases} -\dfrac{e^2}{r} + \dfrac{e^2}{r_{cut}} & : \quad 0 < r \leq r_{cut} \\ 0 & : \quad r_{cut} < r \end{cases}, \tag{A1}$$

In the dipole approximation, for high-density plasma, the radial part of the equation is

$$-\left[\frac{\hbar^2}{2m}\nabla^2 + U(r)\right]\Psi = E\Psi \tag{A2}$$

with the complete solution given by

$$|\Psi(r,\theta,\varphi)\rangle = |R_l(r)\rangle \cdot |Y_l^m(\theta,\varphi)\rangle, \tag{A3}$$

The radial part of the Schroedinger equation is

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \frac{2m}{\hbar^2}[E - U(r)]R - \frac{l(l+1)}{r^2}R = 0. \tag{A4}$$

and through the introduction of the substitution

$$R(r) = P(r)/r. \tag{A5}$$

it can be presented by equation

$$\frac{d^2P}{dr^2} + \left[\frac{2m}{\hbar^2}(E - U(r)) - \frac{l(l+1)}{r^2}\right]P = 0. \tag{A6}$$

In case of the cut-off Coulomb pseudo-potential, Equation (A1), in every part of the space and all of the realized energetic states, the solutions for the wave function are a combination of special functions.

The normalization of the wave function should be carried out as follows:

$$\int \langle \Psi | \Psi \rangle dV = 1, \tag{A7}$$

such that in a case of radial functions, $R(r)$ and $P(r)$ become

$$\int_0^\infty R(r)R(r)r^2dr \equiv \int_0^\infty P(r)P(r)dr = 1. \tag{A8}$$

With the help of the calculated wave functions, a dipole matrix element is calculated:

$$\hat{D}_{n,l;\,E,l'} = \int P_{nl}rP_{El'}dr,$$

and it is used to calculate the measurable optical properties of plasma, like cross-sections, oscillator strengths, Einstein coefficients, or absorption coefficients.

$$\sigma(nl;E) = \frac{4\pi^2e^2k}{3(2l+1)}\sum_{l'=l\pm1} l_{max}\left(\int P_{nl}rP_{El'}dr\right)^2, \tag{A9}$$

$$\sigma(E;E') = \frac{8\pi^4}{3}\frac{\hbar e^2k}{q^2}\sum_{l'=l\pm1} l_{max}\left(\int P_{E'l'}rP_{El}dr\right)^2, \tag{A10}$$

The emission and absorption cross-sections are related to each other according to the following equations:

$$q^2\sigma(E;nl) = 2(2l+1)k^2\sigma(nl;E), \qquad q^2 = \frac{2mE}{\hbar^2}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}. \tag{A11}$$

$$q'^2\frac{d\sigma(E';E)}{d\omega} = q^2\frac{k^2}{\pi^2}\sigma(E;E'). \tag{A12}$$

The measurable quantities in dense plasma are the absorption coefficients. They may be of interest for some astrophysical plasmas, such as the plasma of the inner layers of the solar atmosphere and the plasmas of partially ionized layers in other stellar atmospheres (for example, some DA and DB white dwarfs).

$$\kappa_{bf}(\omega;N_e,T) = \sum_{n,l} N_{nl}\sigma(nl;E), \tag{A13}$$

$$\kappa_{ff}(\omega;N_e,T) = N_iN_e\int_0^\infty \sigma(E;E')vf(v)dv. \tag{A14}$$

$$\kappa(\omega;N_e,T) = \kappa_{ff}(\omega;N_e,T) + \kappa_{bf}(\omega;N_e,T), \tag{A15}$$

$$\kappa^{tot}(\omega; N_e, T) = \kappa(\omega; N_e, T)\left[1 - \exp\left(-\frac{\hbar\omega}{kT}\right)\right]. \quad \text{(A16)}$$

Let us remark that, with minor modifications, the current method can be extended to various types of laboratory dense hydrogen-like plasmas. We mostly refer to alkali metals, helium and other rare-gas plasmas.

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