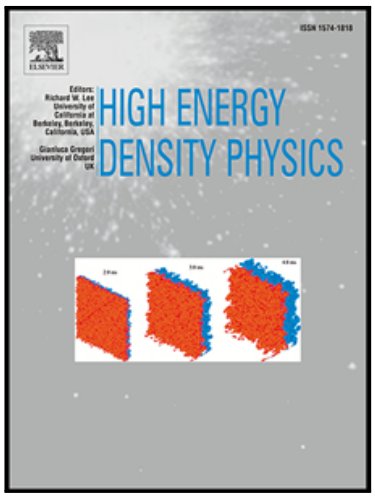

Free-free opacity in dense plasmas with an average atom model

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Free-free opacity in dense plasmas with an average atom model

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A model for the free-free opacity of dense plasmas is presented. The model uses a previously developed average atom model, together with the Kubo-Greenwood model for optical conductivity. This, in turn, is used to calculate the opacity with the Kramers-Kronig dispersion relations. Comparisons to other methods for dense deuterium results in excellent agreement with DFT-MD simulations, and reasonable agreement with a simple Yukawa screening model corrected to satisfy the conductivity sum rule. Comparisons against the very recent experiments of Kettle et al for dense aluminum also reveal very good agreement, in contrast to existing models. Weaknesses in the model are also highlighted.

Keywords: opacity, warm dense matter, average atom model

I. INTRODUCTION

In the regime of dense plasmas, the influence of the plasma environment on the opacity becomes significant. Recently there has been a particular focus on the free-free contribution to opacity [1–5]. This is driven in part by its relevance for Inertial Confinement Fusion (ICF) modeling [3] but also due its astrophysical relevance in the solar core [6] and the accuracy of astrochonology with white dwarf stars [7, 8], as well as the possibility of its direct measurement at free electron laser facilities such as the FLASH XUV-FEL at Hamburg [1]. Very recently, measurements of the free-free contribution to opacity for solid density aluminum at 1 eV and room temperature have been published [4]. These latest experiments were found to disagree with recent efforts to improve modeling of this feature [1, 2].

The free-free component of opacity has traditionally been modeled using Kramers' classical cross section [9] modified by a so-called Gaunt factor to account for quantum effects [10]. The quality of the approximation for the Gaunt factor then determines the accuracy of the free-free opacity. The Gaunt factor should, in principle, be calculated directly from free (or continuum) wavefunctions in the presence of the nucleus and bound electrons, with density and temperature effects incorporated through the ionic structure factor and partial ionization fraction of the plasma. Relatively crude approximations for each of these dense plasma effects are often used [2, 5, 11, 12]. For example, the ionic structure factor $S(k)$ is taken to be its ideal gas value ($S(k) = 1$) [2], or the scattering potential can be purely Yukawa with bound states taken into account through an average ionization [5].

In this paper we calculate the free-free opacity of dense plasmas with an average atom model [13, 14]. The average atom model incorporates dense plasma effects self-consistently. It takes into account a realistic ionic structure factor, treats bound and free electrons equally, predicts average ionization and has no ad hoc continuum lowering model. The average atom model is first used to calculate the electronic structure of an atom in the plasma, and then the optical conductivity is calculated using the Kubo-Greenwood formalism [15–18]. The Kramers-Kronig dispersion relations are then used to calculate an index of refraction and hence the opacity.

Calculations based on this model are compared to Density Functional Theory Molecular Dynamics (DFT-MD) simulations for warm dense deuterium at conditions relevant to ICF experiments [3]. We also compare to a recent model [5] that assumes Yukawa screening, sets $S(k) = 1$, and determines the screening length based on an average ionization model [19]. This model is relevant because it is used in the Los Alamos ATOMIC code [20, 21] and recent opacity tables. ATOMIC is a multi-purpose opacity and kinetics code that has been recently used to generate new Los Alamos OPLIB opacity tables for hydrogen through zinc [22]. ATOMIC uses atomic data from the Los Alamos suite of atomic physics codes [23] and an equation-of-state (known as ChemEOS) based on a chemical picture [19]. The generated opacity tables are required to cover very large ranges of temperature and density and thus need to use atomic structure and EOS models that are robust and reasonably well-behaved over a number of regions in which different pieces of physics are important.

We also use the present average atom model to calculate the opacity of dense aluminum. We compare to experimental measurements of the opacity of solid density aluminum that are sensitive to the free-free opacity. Under the conditions considered, aluminum is not fully ionized and has significant bound structure. The average atom model used is based on DFT and suffers from the well known band gap problem of DFT. This means that the bound state energies are known to be incorrect. This could presumably be fixed in the usual way with the

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