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Equation of state of high density plasmas

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Abstract

We present results on the equation of state (EOS) of high density hydrogen plasmas. We use a hybrid first principles method capable of describing fully ionized plasmas. Electrons as well as the electron–ion interactions are described with Green's functions technique which includes dynamic screening and degeneracy effects. The properties of the proton subsystem are calculated using classical integral equations (HNC) which take strong correlations into account. We compare our results to a variety of analytic approaches and simulation techniques.

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1. Introduction

Today there exists a great variety of methods to determine the equation of state (EOS) of nonideal plasmas. Many of them are based on first principles but differ strongly in their physical and technical approximations [1–7]. As none of these methods and none of further ones (DFT, DFT-MD, etc) is able to describe the whole parameter space, hybrid techniques, which are sophisticated combinations of some of the above, become more and more important. In particular, the description of the complex interplay of correlations, screening and degeneracy in dense plasmas needs to be studied. We report here a hybrid technique based on first principle calculations which is capable of describing fully ionized high density plasmas. We show its capabilities and shortcomings in comparison with other methods.

2. EOS for weakly coupled systems

We consider a multi-component, many-body system consisting of charged particles. In quantum statistical theory, the pressure p is given by the charging formula [1]

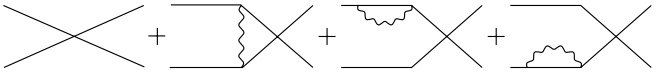
$$(p - p_0)\Omega = -\int_0^1 \frac{\mathrm{d}\lambda}{\lambda}\langle \lambda V \rangle, \tag{1}$$

with $\langle \lambda V \rangle$ being the mean value of the potential energy in the thermodynamic limit, p_0 the ideal pressure and Ω the volume of the system. The charging parameter λ changes the interaction strength from no correlations ($\lambda = 0$) to full correlations ($\lambda = 1$). In Coulomb systems, the elementary interaction is modified due to screening. An exact expression for $\langle \lambda V \rangle$ is therefore given by [1]

$$\langle \lambda V \rangle = \frac{1}{2} \sum_{a\sigma_a, b\sigma_b} \int d\mathbf{1} d\mathbf{r_2} \left\{ \lambda V_{ab}(\mathbf{12}) G_a(\mathbf{11}^{++}) G_b(\mathbf{22}^{+}) + V^s_{ab}(\mathbf{12}, \lambda) \Pi_{ab}(\mathbf{121}^{++}\mathbf{2}^{+}) \right\}, \tag{2}$$

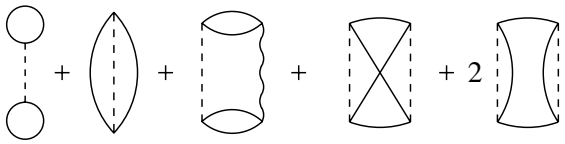
where V^s_{ab} is the dynamically screened potential, Π_{ab} is the polarization function and G_a is the one-particle Green's function.

Using Feynman diagrams, the following weak coupling expansion for the polarization function can be given in terms of the dynamically screened potential V^s (waved line) [2]

$\Pi_{ab}(12) \approx$  . (3)

This expansion has its origin in the dynamically screened ladder approximation of the polarization function which in principle avoids the known Coulomb divergencies. All terms that include up to one screened potential are considered: from left to right, we have the well-known RPA term, the vertex term as the first ladder contribution, and two topologically equivalent self-energy terms (self-energy corrections to the RPA). According to the nature of this expansion all Green's functions of equations (2) and (3) are now substituted by free single particle Green's functions.

The expansion (3) leads to the following expression for the potential energy (2)

$\langle \lambda V \rangle \approx$  . (4)

From left to right, we have the following contributions: the mean field Hartree (H) term, the quantum exchange or Hartree–Fock (HF) term, the Montroll–Ward (MW) term which includes screening effects and first nonideality contributions, the normal e^4, and anomal e^4 exchange terms. This expansion contains all terms up to the order e^4. The MW term includes the Debye–Hückel (DH) law as the high temperature limit. The last two terms describe exchange effects of the order e^4. They originate from terms with dynamically screened potentials.

Up to now, electrons and ions are treated equally as quantum mechanical particles. In this way, only the coupling strength but not the degeneracy of the particles limits the applicability of this approach. For weakly coupled plasmas, this approach is exact; for moderately coupled systems, it can be considered as a good approximation. The advantages are especially noticeable for higher densities where the ions (protons) must be described quantum mechanically, too.

3. EOS including strong ion–ion correlations

Caused by the highly degenerate electrons, plasmas remain fully ionized even for higher densities. Nevertheless, the ions are often nondegenerate. Since their interaction might be strong, they must be treated as a liquid embedded in (degenerate) electrons rather than as a gas. The effect of strong ion–ion correlations is still missing in our EOS.

We include the latter by applying techniques of classical fluid theory for the ion subsystem. In particular, we solve the Ornstein–Zernicke equation with the hypernetted chain (HNC)

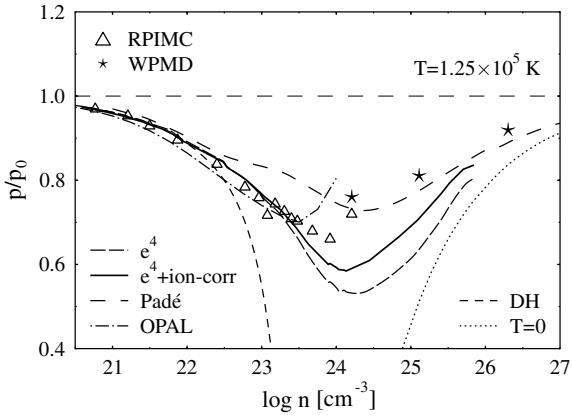


Figure 1. Pressure of a hydrogen plasma normalized to the ideal pressure as a function of the density. Our results (e^4 – equation (4), e^4 + ion-corr – equation (4) + strong proton–proton corr.) compared to RPIMC results [4], WPMD data [3], OPAL [6], Padé formula [7] and limiting results.

closure relation for a pure one component plasma to get a binary distribution function that contains strong ion–ion interactions. From the binary distribution function, thermodynamic variables of state such as pressure or internal energy can be calculated [1]. This ionic contribution is added to the EOS of the last section (equations (1) and (4)). Since the nondegenerate weak coupling limit for the ions (Debye–Hückel) is contained in both of the summands, the DH term is subtracted to avoid double counting.

It turns out that the normal e^4 exchange term for the ions as second order contribution is by far not able to give a good approximation in the case of strong coupling. Moreover, it leads to an overall poor quality of the expansion whereas the inclusion of only the electron e^4 term gives rather good results. Therefore, we keep the electron e^4 term to allow for the best description of degeneracy and coupling in the electron system and add an HNC based ion term whereas only first and second order quantum effects for the ions are kept in the weak coupling EOS (equation (4)).

4. Results and comparisons

We discuss the behaviour and the properties of a hydrogen plasma on the basis of the 1.25×10^5 K isotherm of the pressure (figure 1) and the 5×10^4 K isotherm of the internal energy (figure 2). At low and at very high densities, the thermodynamic functions approach the ideal gas values for classical and highly degenerate systems, respectively. In the low density limit, this behaviour is reproduced by most of the methods with satisfactory agreement. However, such results are not easily achieved at high densities. In this region, our weak coupling EOS (equations (1) and (4)) can serve as a benchmark for simulations and hybrid models. Techniques aimed to describe the intermediate density region in a sufficient way suffer at very high densities from the treatment of the ions as classical particles (e.g., our EOS including strong ion–ion correlations, wave packet molecular dynamics (WPMD), [3]) are restricted to not so high electron degeneracy (e.g., RPIMC [4], DPIMC [5]) for computer technical reasons, or are by derivation restricted to lower densities (e.g., OPAL [6]).

At intermediate densities, nonideality contributions to the EOS lower the isotherms. This behaviour results from a complex interplay of degeneracy, screening and correlations within all

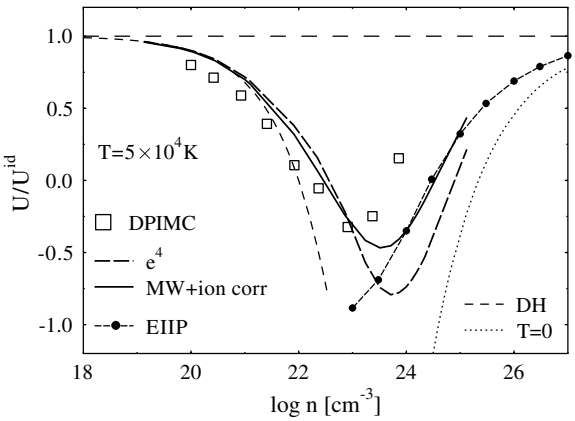


Figure 2. Internal Energy of a hydrogen plasma normalized to the ideal law as function of the density. Our results (e^4—equation (4), MW + ion correlation—equation (4) + strong proton–proton correlation) compared to DPIMC results, EIIP (all from [5]) and limiting results.

of the particles. Due to the inclusion of strong ion–ion correlations, we reduce the depth of the pressure/internal energy minimum of our EOS and achieve better agreement with direct path integral Monte Carlo (DPIMC) and restricted path integral Monte Carlo (RPIMC) simulations in the descending branch of the isotherm. Additionally, we are able to calculate our EOS for higher densities than PIMC as long as the protons behave classically, and we reach surprisingly good agreement with the effective ion–ion potential method (EIIP) of Trigger *et al* [5] as shown in figure 2.

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