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Nonlinear Screening in Moderate-Z Hot Dense Matter

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Abstract. In this paper we show that linear (Debye-Hückel) electrostatic screening is not accurate for solid density, moderate-Z (Z >10)materials in the hot dense matter regime ($T > 100$eV). The disparity between linear and nonlinear descriptions will easily exceed 50%, and in some cases can exceed a factor of two. The effect is most strongly dependent on Z and T with lower temperatures and higher Z favouring stronger nonlinear effects. Our conclusions are reached via fully nonlinear calculations performed using a Poisson-Boltzmann model that has been modified to account for quantum diffraction.

1. Introduction

In the past few years there has been a resurgence of interest in the problem of microphysical properties of hot dense plasmas. This has been driven by the completion of a number of new facilities, thus expanding the capabilities of experimental researchers. The inertial fusion studies on the National Ignition Facility have raised a number of questions about plasma microphysics including both Equation of State and transport. On the other hand, experiments on both XFELs and optical laser facilities (e.g. Orion [1]), have reinvigorated interest in *ionization potential depression* (IPD; or *continuum lowering*) [2] The recent results from both XFELs and optical high-powered lasers (e.g. [3]) indicate that no single framework or model appears to be capable of describing all of the experimental results, although considerable progress has since been made on the theoretical front [4]. The long established models that these new results have been compared to include the model of Ecker and Kröll [5], the Stewart-Pyatt model [6], as well as the Ion Sphere, and Debye-Hückel models.

The problem of IPD emerges in plasmas because the plasma collectively responds to the presence of any charged particle, resulting in screening of the particle's field. Thus the microfield around the particle is no longer identical to the bare Coulomb field. If we generically represent this microfield via the screened form,

$$\phi(r) = \frac{Ae^{-\kappa r}}{r}, \tag{1}$$

then an examination of the behaviour at radii much smaller than the screening length reveals that,

$$\phi \approx \frac{A}{r} - \kappa A. \tag{2}$$

Thus from the point of view of solving the quantum mechanical problem of the energy levels of an ion, all of the energy levels will be shifted by κA. This means that, unlike an isolated atom or ion, there will only be a finite number of energy levels. Clearly the IPD needs to be calculated accurately, if the atomic physics is to be modelled correctly. It is because of this that the IPD problem remains such an important outstanding problem.

Having said this, it is important to note that electrostatic screening affects many other aspects of plasma behaviour [7]. It introduces a correction to the internal energy and equation of state [8]. It is an important factor in determining transport properties such as electrical resistivity and thermal conductivity (as well as plasma composition) [9], and it is also important in determining the energy exchange rates [10]. Screening also affects low-energy nuclear reactions both in nature and the laboratory (see [11] and references therein), and other processes [12].

In non-degenerate, weakly-coupled plasmas it is generally assumed that Debye-Hückel (DH) or linear screening ‡is the most correct description of electrostatic screening. However the foundational equation for Debye-Hückel screening — the Poisson-Boltzmann equation — is a rather nonlinear equation, and the extent to which DH screening applies is not very thoroughly discussed in the literature.

In this paper we show that the electrostatic screening of moderate Z ions enters a nonlinear regime in hot dense matter. We are guided to this conclusion by the analysis of the hydrogenic plasma by Lampert and Crandall. To illustrate this we use

‡ In this paper we will use 'Debye-Hückel' interchangeably with 'linear'. However 'linear' screening is a more general term that does not apply exclusively to situations where DH screening is appropriate.

the specific case of solid density Al in the temperature range of 200$\geq T_e \geq$ 500 eV, and consider the effect on the Al^{10+} ion. The nonlinear effects primarily introduce a uniform shift in the screened potential. Therefore this is particularly important for the IPD problem, as established models such as the Debye-Hückel model, the Stewart-Pyatt model [6] , and Crowley's model [13], have generally adopted a linear treatment of screening. Here we show that a linear treatment of screening is likely to be inadequate for ions with $Z^\star > 10$ in hot dense plasmas. In some cases the difference between linear and nonlinear screening can reach a factor of 5 in the IPD. Even in the case of $Z^\star = 10$, at solid density, linear screening is not particularly accurate even at 500eV, so very high temperatures need to be reached before the linear screening model becomes accurate.

The paper is organized as follows : (i) In Section 2, we describe the modified Poisson-Boltzmann model that we use which accounts for quantum diffraction of the electrons, (ii) in Section 3 we examine the conditions under which nonlinear screening effects might be expected, and conclude that this this will only be possible in HDM conditions for Z >10, (iii) in Section 4 we describe how we carried out the full nonlinear solution of the Poisson-Boltzmann equation to verify this, (iv) in Section 5 we present the results of these calculations. In the following two Sections we discuss the results and state our conclusions.

2. Model

For the purpose of showing the importance of non-linear electron screening, we will work in a framework where the base model is the Poisson-Boltzmann equation. This requires that the plasma has reached sufficiently high temperature that the effects of degeneracy can be neglected. The corresponding linear model is the Debye-Hückel model, and we will compare our results to this. We adopt the following normalizations to cast the core equation in dimensionless form : $\tilde{\phi} = e\phi/k_BT$, and $\tilde{r} = r/\lambda_D$ (where λ_D is the (electron) Debye length). With these normalizations, the Poisson-Boltzmann equation becomes :

$$\tilde{\nabla}^2\tilde{\phi} = e^{\tilde{\phi}} - e^{-Z_p\tilde{\phi}}, \tag{3}$$

where we use Z_p to denote the charge state of the ions in the plasma. As it is also of interest to examine the case where the ions are replaced by a uniform neutralizing positive background, the equation,

$$\tilde{\nabla}^2\tilde{\phi} = e^{\tilde{\phi}} - 1, \tag{4}$$

will also be considered.

The Poisson-Boltzmann model does require some modifications to include physics that Eq.s 3 and 4 do not naturally account for. On length-scales approaching the de Broglie wavelength of an electron, quantum diffraction can no longer be neglected. The net effect of this is to put a limit on how close an electron can "approach" an ion. This 'softens' the electron-ion interaction, effectively removing the Coulomb singularity which might otherwise be problematic. Early work on this effect in plasmas was done by Kelbg [14]. To incorporate this into the Poisson-Boltzmann model, we use an approach suggested by Ebeling [8]. In Ebeling's "Quantum Debye-Hückel Approximation" an inner radius given by,

$$a(T) = \frac{h}{8\sqrt{2\pi m k_B T}}, \tag{5}$$

which is a hard barrier for the electrons. Since the potential is repulsive for the ions, in the cases where the ions are mobile we also regard $r = a$ as a hard barrier for the ions as well, as any error this will introduce will be negligible. Although this can be seen as important in terms of addressing quantum corrections, it is also important in terms of ensuring that the Poisson-Boltzmann equation is tractable (even numerically) when the central charge is effectively point-like. Imposing this barrier imposes an inner boundary condition by stating that the electric field must be given by,

$$\tilde{E}_r = \frac{\Gamma}{\tilde{a}^2}, \tag{6}$$

where,

$$\Gamma = \frac{Ze^3 n_0^{1/2}}{4\pi\varepsilon_0^{3/2}(k_B T)^{3/2}} \tag{7}$$

If we then linearize the model with this inner boundary condition, and seek the analogue of the Debye-Hückel solution (for immobile ions; which we will denote as the QDH potential), then we find,

$$\phi_{QDH} = \frac{\Gamma e^a}{(1+a)} \frac{e^{-r}}{r}, \tag{8}$$

note that here (and henceforth) we have dropped using the tilde to denote normalized quantites, and thus all quantities should be regarded as being normalized unless stated otherwise.

3. Onset of Nonlinear Screening

It is now clear that the screening behaviour is determined by two dimensionless quantities — Γ and a. However it is well known that the linearized, or Debye-Hückel, solution is a very good approximation to the actual solution of the Poisson-Boltzmann equation [15] for a wide range of conditions. It is therefore necessary to determine the conditions under which the linear approximation breaks down, and thus where screening may be stronger than expected. In general, this is an unsolved problem. However, Lampert and Crandall [16] established an absolute upper bound on the solution to Eq. 3 for the specific case of Z =1, which can be written as,

$$\phi_{LC} = U(a, \alpha) \frac{e^{-r}}{r}, \tag{9}$$

and,

$$U(a, \alpha) = 2(1+\alpha) a e^{(1+\alpha)a} \ln\left[\frac{1+e^{-\alpha a}}{1-e^{-\alpha a}}\right], \tag{10}$$

which applies for $r \geq (1+\alpha)a$, with $\alpha > 0$. So for a given choice of α we can compare this absolute upper bound to Eq. 8. Since they are both Debye-Hückel functions, this means that only the pre-factors need to be compared. If $\phi_{QDH} > \phi_{LC}$,i.e.,

$$\frac{\Gamma}{1+a} > 2(1+\alpha) a e^{\alpha a} \ln\left[\frac{1+e^{-\alpha a}}{1-e^{-\alpha a}}\right]. \tag{11}$$

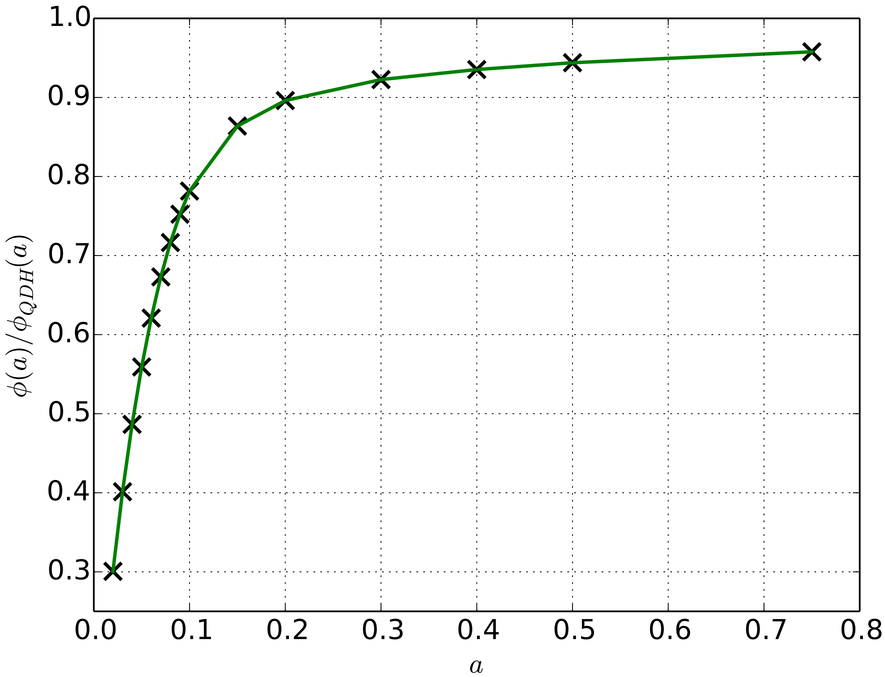

Figure 1. Results of solution of Poisson-Boltzmann equation for different a with Γ =1 in terms of $\phi(a)/\phi_{QDH}(a)$.

On carrying out a number of numerical tests, it was found that choosing α = 1 was adequate for converting Eq. 11 into a relation for indicating the onset of the non-linear regime, i.e.

$$f = \frac{\Gamma}{1+a} - 4ae^{a}\ln\left[\frac{1+e^{-a}}{1-e^{-a}}\right], \tag{12}$$

where $f > 0$ indicates that the screening has become non-linear, and f <0 indicates the linear regime. This equation was found to work well for both the immobile and mobile ion cases, as well as for Z >1.

In the numerical tests, we observed a continuous transition from the linear screening regime into the non-linear screening regime (also observed in [15]) as a or Γ was varied. Thus a substantial departure from the linear regime can occur before the point indicated by Eq.12. Examples of these numerical tests (for the case of immobile ions) are shown in figs. 1 and 2 for the cases of Γ =1, and Γ =0.1 respectively. In fig.s 1 and 2, the ratio $\phi(a)/\phi_{QDH}(a)$ is plotted against a, where ϕ_{QDH} is given by Eq. 8. For Γ =1, Eq. 12 predicts a transition for a =0.064, and for Γ =0.1, Eq. 12 predicts a transition for a =0.004. In both cases these points lie in a steep region on the curve, and thus Eq. 12 is a good indicator of where the nonlinear regime lies. The numerical details of how these calculations were performed is covered in Sec. 4.

Eq. 12 can also be used to determine which regions of parameter space are susceptible to nonlinear screening. In fig. 3, we plot f as a function of temperature for the cases of Z =10 and Z = 6 respectively, under the assumption of n_e =6×10^{29}m^{-3}.

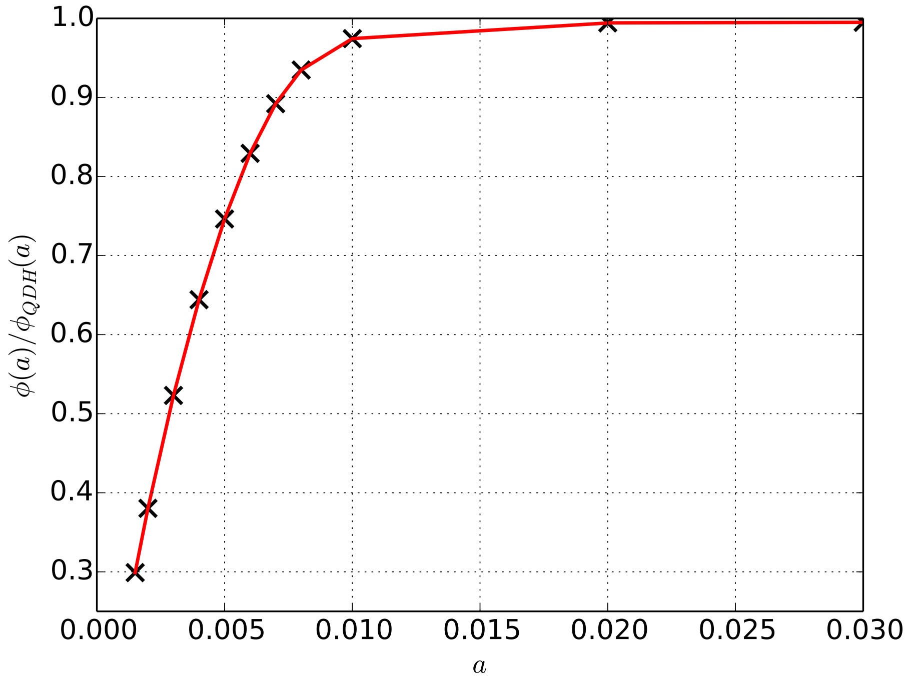

Figure 2. Results of solution of Poisson-Boltzmann equation for different a with Γ =0.1 in terms of $\phi(a)/\phi_{QDH}(a)$.

By examining fig. 3 we find that, in the case of Z =6, the temperature at which one enters the non-linear regime is so low that correspondingly high ionization will not be achieved at that temperature. This conclusion gets stronger if Z is reduced even further. In contrast for Z >10, the transition temperature is in excess of 100eV, which means that, at solid density, sufficiently high degrees of ionization can be achieved at temperatures close to this. This means that both ionization to $Z > 10$ would be expected and that the electrons would be far from degenerate ($\Theta > 5$). Note that, because of the continuous transition between the linear and non-linear screening regimes, one can expect quite substantial departures from the Debye-Hückel model even at temperatures in the range of 200–500 eV.

4. Nonlinear Calculations — Setup

In order to quantitively determine the strength of the non-linear screening, we carried out a set of calculations in which we numerically solved the Poisson-Boltzmann equation (both mobile (Eq. 3) and immobile ions (Eq.4)) for the problem of a single central ion. For this we used a Newton-Kantorovich method. To clarify : by 'Newton-Kantorovich', we mean a method that is also often called 'Quasilinearization', and is often attributed specifically to Bellman and Kalaba [17]. A convergence criterion of 10^{-6} was set. This was done on a radial grid of 80000 cells, with a cell spacing of 10^{-4}. For the inner boundary condition, we enforced Eq. 6, and for the outer

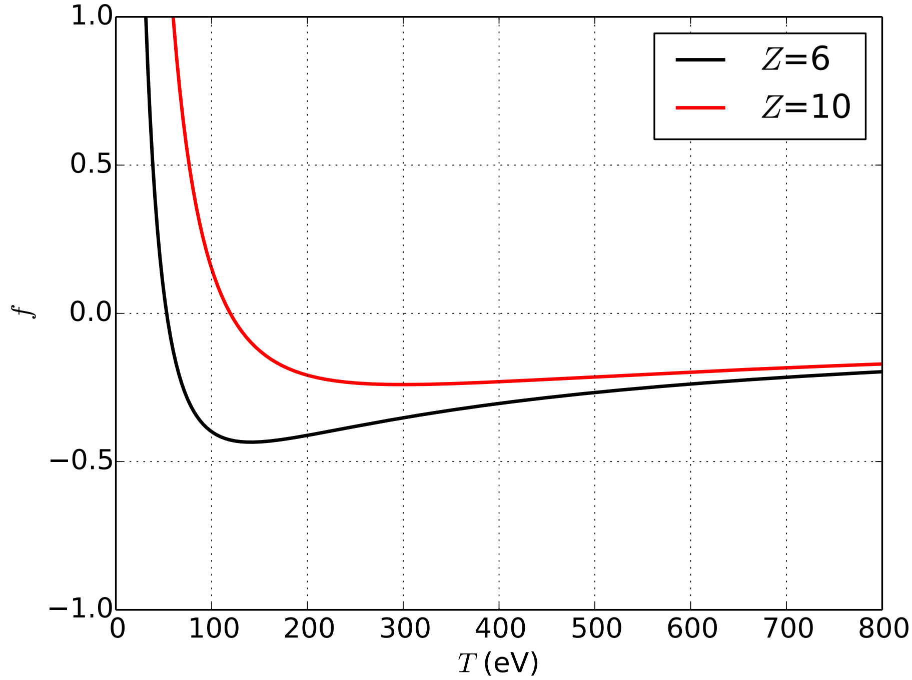

Figure 3. Plot of f (Eq. 12) against T for both Z =10 (red) and Z =6 (black) , assuming $n_e = 6\times10^{29}\mathrm{m}^{-3}$.

boundary condition we enforced $\phi = 0$. For each temperature, we assumed a fixed electron density of 6×10^{29} m^{-3}. The central ion was taken to have an effective charge of $Z^{\star}$ =10, and the ions in the surrounding plasma were assumed to have Z_p =10.

We have checked this method by comparing its results to those obtained by scipy's `solve_bvp` routine [18], which implements a 4th order collocation algorithm [19], and the `scikits.bvp1lg` package, which calls Bader and Ascher's collocation at Gaussian points solver `colnew` [20]. Both of these solvers were called with an initial radial grid of 50 cells, which was refined by the solvers until the tolerance of 10^{-10} was reached. The results from the Newton-Kantorovich method were in excellent agreement with those obtained by these established solvers.

5. Nonlinear Calculations — Results

The results of the calculation yield ϕ over the entire grid. For an overview of the results, we can look at the screening energy at small radii, U_s. In a pure Poisson-Boltzmann model of this type, this screening energy also corresponds to the IPD. From $\phi(a)$, U_s is calculated via $U_s = \Gamma/a - \phi(a)$. A subset of these results are tabulated in Table 1 where we compare the computed result to the Debye-Hückel screening energy, $U_{s,DHe} = Ze^2/4\pi\varepsilon_0\lambda_{D,e}$.

For the case of mobile ions, the corresponding results are tabulated in Table 2 where they are compared to $U_{s,DH} = \sqrt{1+Z_p}Ze^2/4\pi\varepsilon_0\lambda_{D,e}$. Note that the values of

T (eV)	a	Γ	U_s (eV)	$U_{s,DHe}$ (eV)
130	0.069	1.012	723.8	131.4
150	0.06	0.816	674.1	122.3
200	0.045	0.5296	552	105.9
225	0.04	0.444	488.1	99.9
250	0.036	0.379	427.9	94.8
275	0.033	0.329	373.3	90.4
300	0.03	0.288	324.1	86.5
350	0.026	0.229	243.3	80.1
400	0.023	0.187	188	74.9
450	0.02	0.157	150.8	70.6
500	0.018	0.134	125.2	67.0

Table 1. Results for U_s from solution of Poisson-Boltzmann equation for the case of immobile ions.

T (eV)	U_s (eV)	$U_{s,DH}$ (eV)
200	562.4	351.4
225	504.2	331.3
250	446.2	314.3
275	393.5	299.7
300	351.0	286.9
325	314.2	275.7
350	281.6	265.6
375	252.5	256.6
400	230.4	248.5
500	176.2	222.3

Table 2. Results for U_s from solution of Poisson-Boltzmann equation for the case of mobile ions (Z_p =10).

a and Γ will be the same as those given in Table 1 for the same temperature.

The results for both the immobile and the mobile ion cases are also plotted in fig.s 4 and 5 respectively. In terms of the actual screening potentials that have been calculated, we present in fig.s 6 and 7 the potentials that are calculated for T_e =200eV (a=0.045,Γ=0.5296) in the immobile and mobile ion cases respectively. Alongside the numerical solutions we have also plotted the bare Coulomb potential and the corresponding Debye-Hückel solution.

6. Discussion

From Tables 1 and 2 (and fig.s 4 and 5) it can be seen that the conclusions we reached via Lampert and Crandall's theory are born out — there is clearly a strong non-linear screening effect that leads to a significantly higher screening energy than would be predicted by linear theory. In the case of immobile ions, it can be seen that the deviation from linear theory can become very strong (over a factor of 5), and a difference of nearly a factor of 2 persists even at 500eV. In the case of mobile ions, the

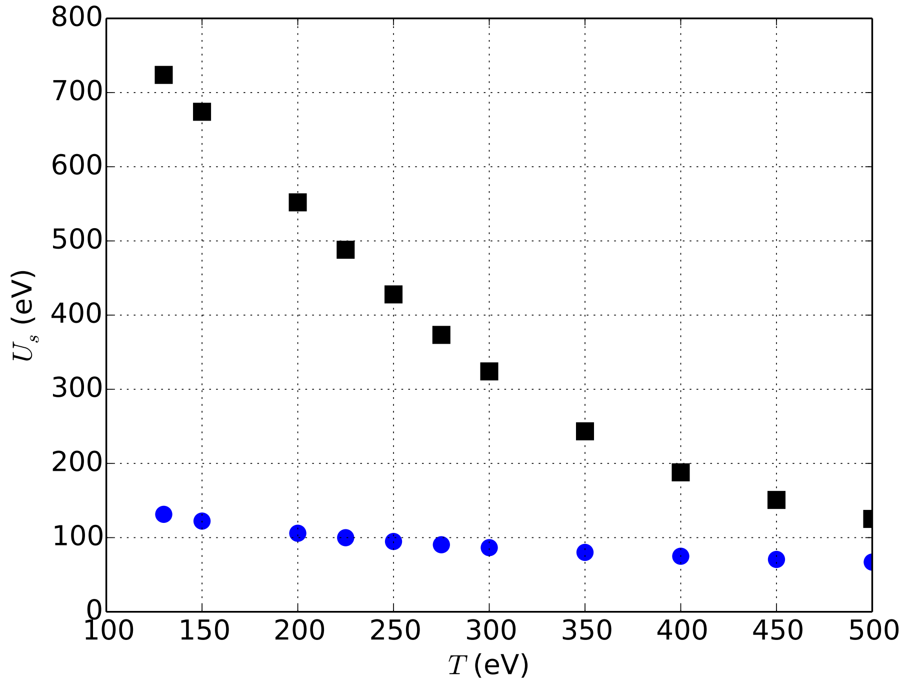

Figure 4. Plot of results for the screening energy at small radii (U_s) from solution of Poisson-Boltzmann equation (black squares) for the immobile ion case (see Table 1). Values for Debye-Hückel screening are also plotted (blue circles).

deviation from linear theory is much less strong, but still amounts to a difference of 60% at 200eV.

Interestingly, in the 200–500 eV range, the difference between the screening energy in the mobile and immobile ions case is not large. This is in stark contrast with the corresponding linear theories (Debye-Hückel) for this problem which differ by a factor of $\sqrt{1+Z_p}$ =3.32. Both this observation, and the deviations from linear theory, are indicative of the electron screening being dominant in this parameter range. In Crowley's model [13], the ionic contribution is usually dominant, which also underlines why these results may be surprising. This can only occur because, in this parameter range, we have entered the regime of non-linear electron screening.

Interestingly, we find that in the immobile ion case, the disparity in the screening energy between the linear and nonlinear calculations is 46% at 500eV. In the mobile ion case the disparity at 500eV is 21%. We therefore find that, the linear theory is still fairly inaccurate even at quite high temperatures, and thus very high temperatures need to be achieved before the linear theory becomes a highly accurate description of the screening.

In fig.s 6 and 7 we show two examples of the actual potentials as a function of radius, i.e. the raw output of the numerical calculation. Also shown in these figures is the bare Coulomb potential and the corresponding linear screening solution. These plots give a better idea of how non-linear screening manifests itself. In both figures

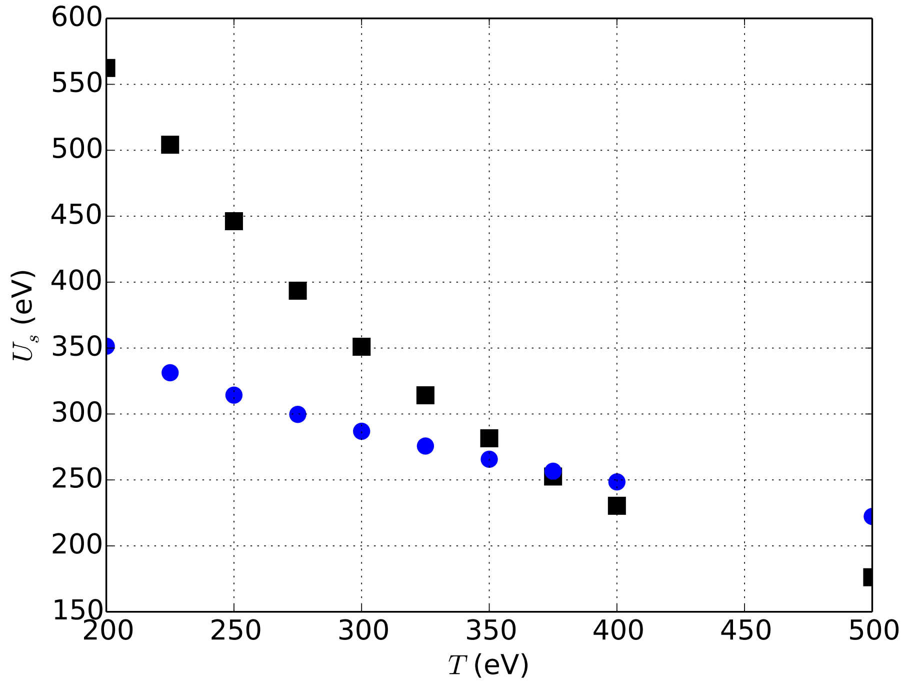

Figure 5. Plot of results for the screening energy at small radii (U_s) from solution of Poisson-Boltzmann equation (black squares) formobile ion case (see Table 2). Values for the corresponding Debye-Hückel screening are also plotted (blue circles).

we see that the non-linear solution follows the linear solution, i.e. is essentially the same function, but appears to be offset from the linear solution in an almost uniform fashion. Thus the characteristic scale-length, the Debye length, does not appear to be affected, nor is the DH function. In the immobile ion case this offset simply appears to a uniform reduction in the potential (relative to the DH potential) at all r.

The mobile ion case (for $Z_p = 10$) is rather more interesting, and shows stronger deviation from the DH function. At very small r the nonlinear potential is indeed smaller than the DH potential, however we find that at some point the nonlinear potential becomes larger than the DH potential, and remains larger than the DH potential. This does not necessarily conflict with Lampert and Crandall's results as these were obtained for the case of $Z_p = 1$ only. In fact if we repeat the calculation with Z_p =1 then this behaviour vanishes and the nonlinear potential is always less than the DH potential.

Furthermore, when the calculation with mobile ions is repeated for Z_p =1, we find that the screening energies are very close to the immobile ion case. These are shown in fig. 8, in which we see that the results of the mobile, Z_p =1 calculation (in terms of screening energy) virtually coincide with the results of the immobile ion calculation. Thus in a dense hydrogenic plasma doped with Al, it may well be possible to achieve rather large screening energies. In terms of experimentally investigating nonlinear screening this may be the most interesting strategy to pursue, as the results

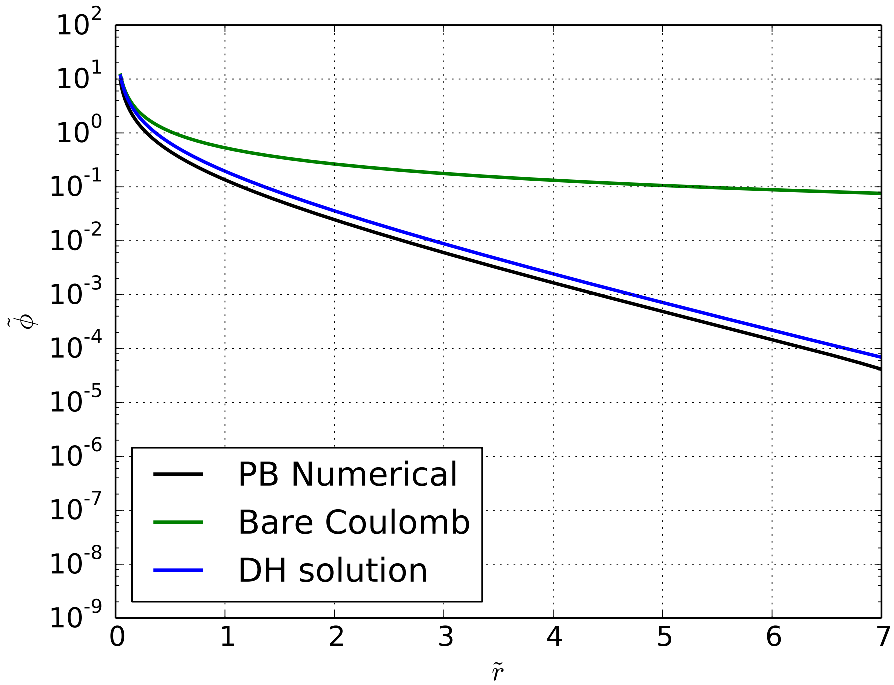

Figure 6. Plot of the potential numerically calculated from the nonlinear PB equation for the immobile ion case with T_e =200eV, a=0.045,Γ=0.5296. Also shown is the corresponding Debye-Hückel solution, and the bare Coulomb potential.

of this study indicate that this system would show the greatest deviations from linear screening theory.

7. Conclusions

In this paper we have proposed a model for examining the effects of nonlinear screening in hot dense matter. This consists of the Poisson-Boltzmann equation with an inner boundary condition on the electrons based on Ebeling's 'Quantum Debye-Hückel Approximation' [8] which accounts for quantum diffraction. We then combined this model with Lampert and Crandall's analysis to estimate the conditions under which nonlinear screening effects should be expected. We concluded that this would occur in hot dense matter (solid density) for a few hundred eV, but only for Z >10.

Finally we carried out a set of fully nonlinear numerical calculations which demonstrated this for the case of a hot dense Al plasma. We showed that the screening energy strongly deviated from the prediction of linear screening theory, and how the nonlinear effects manifest as a quasi-uniform shifting of the screened potential.

Since the nonlinear effects manifest in this way, the implication is that nonlinear screening will primarily affect Ionization Potential Depression, and thus could have very substantial implications for the radiative and atomic physics of these plasmas. It already appears to be the case that the radiative and atomic physics of these plasmas is

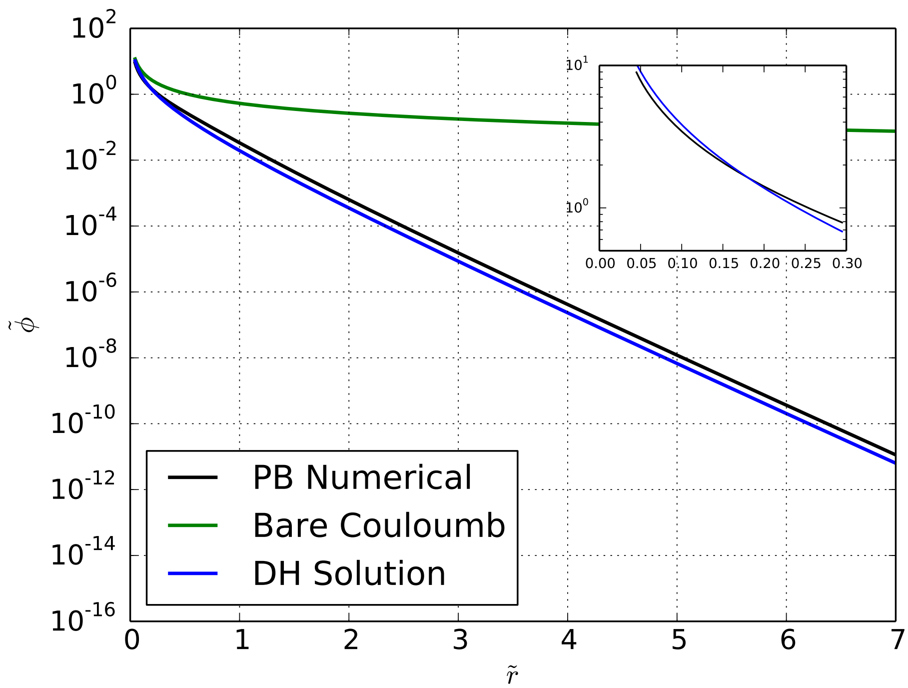

Figure 7. Plot of the potential numerically calculated from the nonlinear PB equation for the mobile ion case with T_e =200eV, a=0.045,Γ=0.5296, and Z_p =10. Also shown is the corresponding Debye-Hückel solution, and the bare Coulomb potential. Inset shows zoomed view at small radius to show curves crossing.

not as well understood as had been previously thought. We therefore suggest, based on the study presented in this paper, that serious consideration is given to incorporating nonlinear screening into future studies of IPD, and the radiative and atomic physics of moderate-Z HDM. It is likely that this could influence a number of different areas of study in ultra-intense laser-matter interactions including x-ray spectroscopy of HDM [21], fast electron transport [22, 23, 24, 25], and fast electron heating to produce HDM [26, 27].

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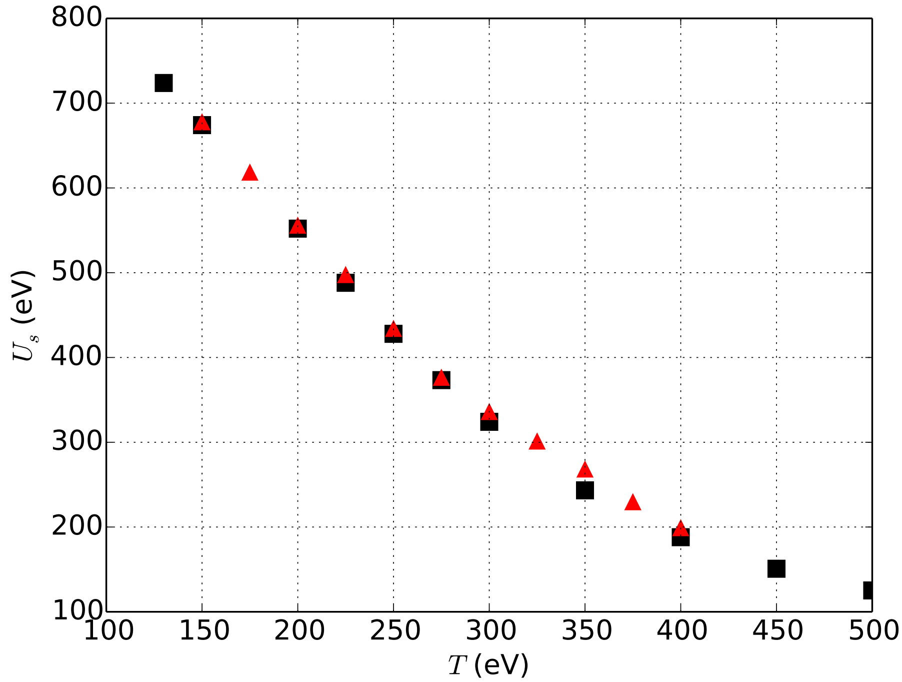

Figure 8. Results of mobile ion calculation with Z_p =1 in terms of screening energy against temperature (Red triangles). Also shown are the corresponding results from the immobile ion calculation (black squares).

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