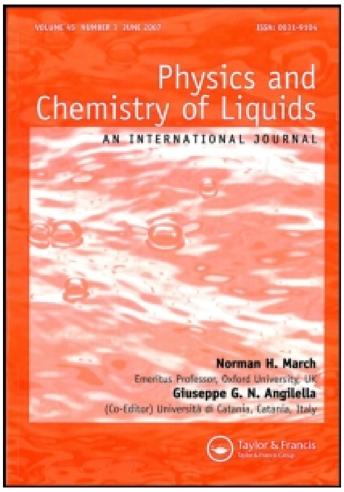

Physics and Chemistry of Liquids
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713646857

Inhomogeneous Electron Liquid in Intense Electric Fields

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To cite this Article Pfalzner, S. and March, N. H.(1994) 'Inhomogeneous Electron Liquid in Intense Electric Fields', Physics and Chemistry of Liquids, 27: 2, 77 — 82
To link to this Article: DOI: 10.1080/00319109408029512
URL: http://dx.doi.org/10.1080/00319109408029512

Phys. Chem. Liq., 1994, Vol. 27, pp. 77–82
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INHOMOGENEOUS ELECTRON LIQUID IN INTENSE ELECTRIC FIELDS

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(Received June 30, 1992)

The partition function of an inhomogeneous liquid in an intense electric field is first calculated, for various one-body potentials which contribute to the spatial variation of the electron density. This latter quantity is then sampled by taking, essentially, the inverse Laplace transform of the generalized partition function or Slater sum. Conclusions are thereby drawn as to the sensitivity of the above physical quantities to (a) the choice of one-body potential and (b) the intensity of the electric field.

KEY WORDS: Slater sum, Laplace transform, atoms in electric fields.

1. INTRODUCTION

In earlier works, the partition function $Z(\beta)$ and the Slater sum $C(\mathbf{r}, \beta)$, with $\beta = (k_B T)^{-1}$ were studied for confined atoms, with inhomogeneous ground-state electron density $\rho(\mathbf{r})$, in an intense but constant electric field $\mathbf{E}$. As stressed in Ref. 1, the long-term aim must be to bring such calculations into contact with a body of experimental data on atomic ions "confined" in plasmas, and in particular with data on multiphoton ionization.

The purpose of the present work is first of all to extend the above study[1] by considering different one-body potentials $V(\mathbf{r})$ leading to the inhomogeneous electron liquid with density $\rho(\mathbf{r})$. Secondly, and the most important focal point of our paper, results will then be obtained from the Slater sum $C(\mathbf{r}, \beta)$ for the electron density $\rho(\mathbf{r}, \varepsilon)$. This is related to $C(\mathbf{r}, \beta)$ through the Laplace transform relation[2]

$$C(\mathbf{r}, \beta) = \beta \int_0^\infty \exp(-\beta\varepsilon)\rho(\mathbf{r}, \varepsilon)\, d\varepsilon. \tag{1.1}$$

The outline of the paper is then as follows. In Section 2, results are reported for the Slater sum for different choices of one-body potential $V(\mathbf{r})$, as a function of both temperature T and plasma density n, for three different values of electric field strength. In Section 3, use is made of the relation (1.1) to extract, by numerical Laplace transform inversion, the energy dependence of the electron density $\rho(\mathbf{r}, \varepsilon)$, again for different values of the electric field strength. Section 4 constitutes a summary, plus some proposals for future work.

2. SLATER SUM: DEPENDENCE ON $V(\mathbf{r})$, TEMPERATURE T AND PLASMA DENSITY n

Following the model employed in Ref. 1, $C(\mathbf{r}, \beta)$ has been calculated for three forms of one-body potential $V(\mathbf{r})$:

i) $V(\mathbf{r}) = \text{constant}$

ii) The Coulomb form $V(\mathbf{r}) \sim 1/r$ and

iii) The neutral atom (zero electric field) Thomas-Fermi self-consistent potential energy[3].

Figure 1 shows the dependence of $C(\mathbf{r}, \beta)/\beta$, at two distances ($z$) from the atomic nucleus, along the electric field direction (z axis), as a function of inverse temperature $\beta = (k_B T)^{-1}$, for two different choices of plasma density and two different electric field strengths. Comparison of the uppermost and the lowest parts of Figure 1 reveals that there is marked dependence on the choice of $V(\mathbf{r})$, but that the effect of varying the density is not a prominent feature over the range shown in the Figure except for the constant potential case (solid curves). Furthermore, Figure 1 leads to the conclusion that the electric field has its strongest influence for low temperatures and densities.

Figure 2 likewise shows C/β, but now as a function of density and makes the point noted above about the relative insensitivity to density variation more explicitly. For a given β, there is seen to be a considerable range of plasma density over which there is insensitivity to density.

These calculations of C/β serve to extend somewhat the results of the model used in Ref. 1. However, we turn next to the main objective of this present study; namely to extract the energy (ε) dependence of $\rho(\mathbf{r}, \varepsilon)$ in Eq. (1.1). This we do, as noted earlier, by inverting the Laplace transform of C/β numerically. The results thus obtained from the calculations recorded in Figures 1 and 2 will be presented in Section 3 immediately below.

3 ELECTRON DENSITY $\rho(\mathbf{r}, \varepsilon)$ FOR DIFFERENT VALUES OF PLASMA DENSITY n AND ELECTRIC FIELD STRENGTH E

Of course, the ground-state electron density $\rho(\mathbf{r}, \varepsilon)$ in the model of Ref. 1 depends on (a) the plasma density n and (b) the strength E of the electric field, in addition of course to the variables $\mathbf{r}$ and ε displayed explicitly. As samples of our results obtained

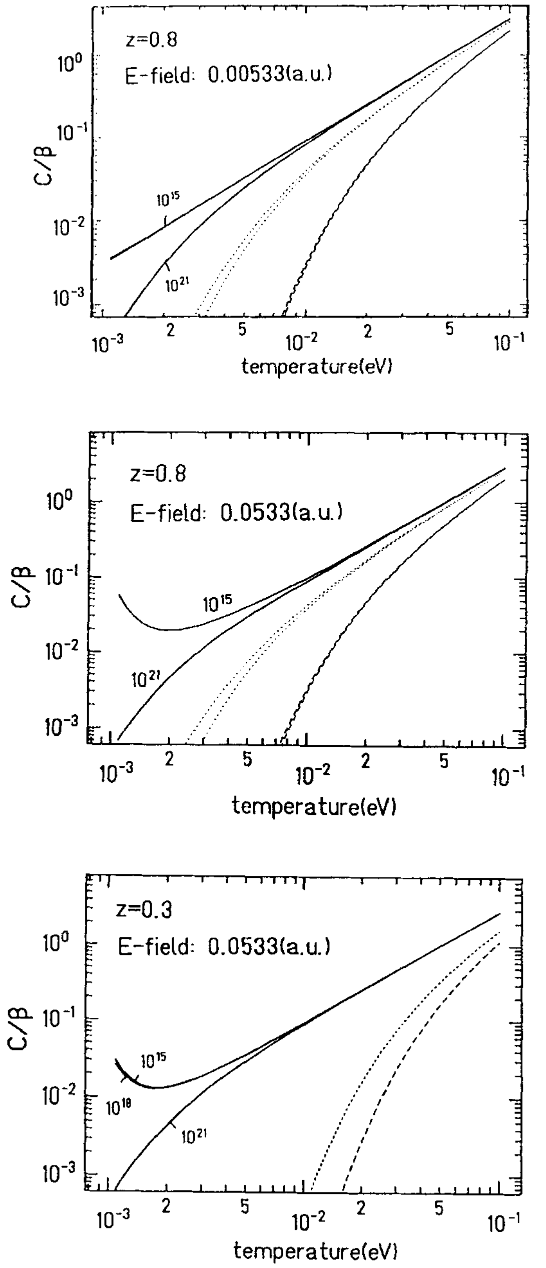

Figure 1 Shows Slater sum C divided by β vs temperature. Solid curves correspond to one-body potential $V(\mathbf{r})$ = constant. Dashed curves are for bare Coulomb potential. Dotted curves correspond to self-consistent neutral atom Thomas-Fermi potential (zero electric field). Curves are labelled with plasma densities n. Note that uppermost and middle parts of the Figure correspond to same value of distance z from nucleus but to electric field strengths differing by a factor of 10. Lowest plot is for a smaller value of z but for same electric field strength as for middle part of Figure.

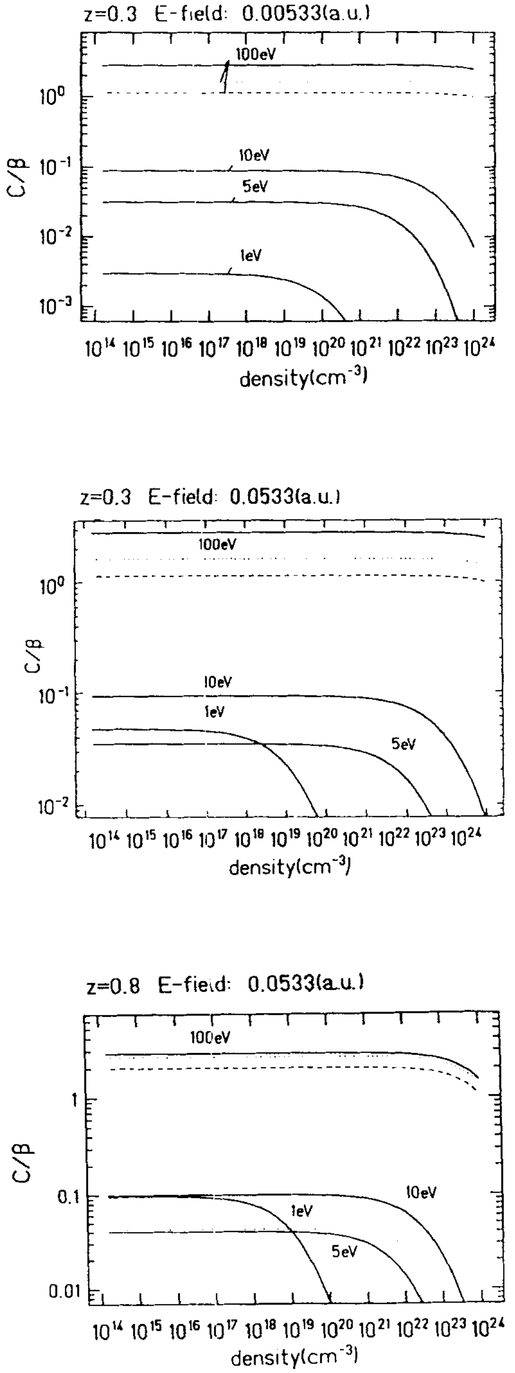

Figure 2 Ordinate is same as Figure 1. But independent variable is now the plasma density n while the curves are labelled by the temperature in eV.

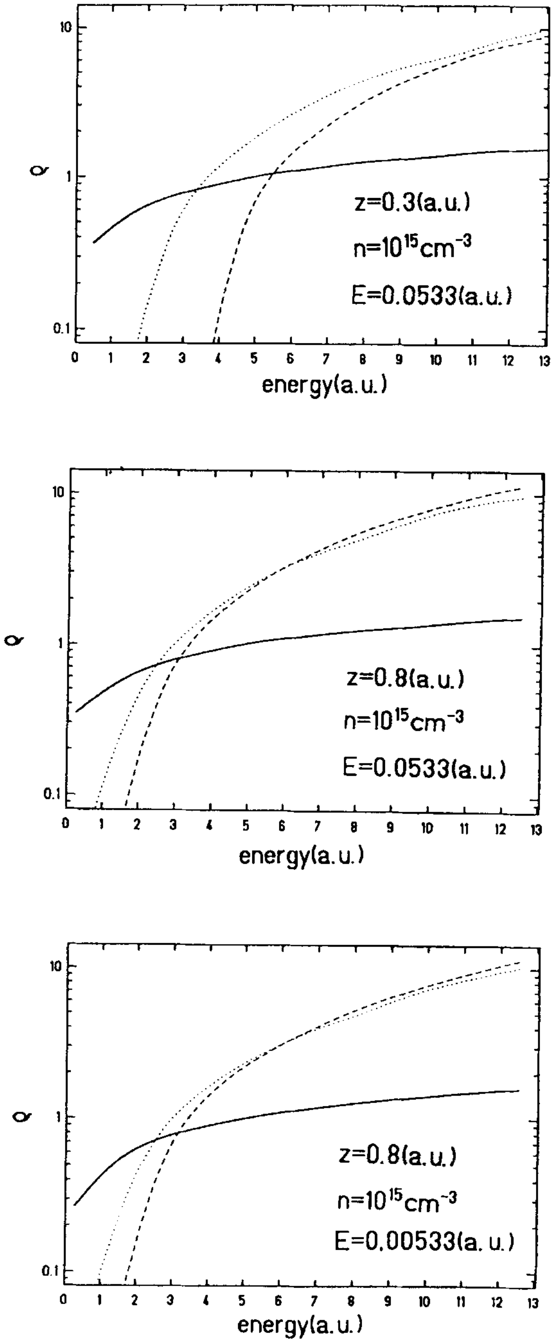

Figure 3 Electron density $\rho(\mathbf{r}, \varepsilon)$ as calculated from C/β in Figures 1 and 2 by numerical inversion of Laplace transform entering Eq. (1.1). Values of z, n and E are shown explicitly for each of three parts of this Figure.

by numerical Laplace inversion, we show in the uppermost part of Figure 3, $\rho(\mathbf{r}, \varepsilon)$ as a function of energy for $n = 10^{15}$, $E = 0.0533$ and for the distance z measured from the nucleus taken as $z = 0.3$. The middle part of Figure 3 corresponds to a change solely in the value of z. Whereas the constant potential case does not therefore change, there is seen to be considerable dependence on the distance from the nucleus, as might have been anticipated, especially at the lower values of energy.

However, comparing the middle and lowest parts of Figure 3, after changing the strength of the electric field by a factor of 10, but keeping z and plasma density n fixed, the sensitivity to electric field is found to be relatively small.

4 SUMMARY AND DIRECTIONS FOR FUTURE WORK

The main aim of the present paper has been to utilize the model of Ref. 1 to study the ground state density $\rho(\mathbf{r}, \varepsilon)$, through Eq. (1.1), starting from $C(\mathbf{r}, \beta)/\beta$. This study has displayed the electron density as a function not only of the variables **r** and energy ε exhibited explicitly but also as a function of plasma density n and electric field strength E. Conclusions are thereby drawn as to the sensitivity of $\rho(\mathbf{r}, \varepsilon)$ to variations in the plasma density and field strength.

One fairly obvious extension of the present work would be to calculate the electron density in the regime of intermediate degeneracy. This can also be done from $C(\mathbf{r}, \beta)$, but now incorporating also the Fermi-Dirac distribution function, as set out in the early work of March and Murray[2]. We intend to explore this generalization in future work, as well as to study the effects of allowing the one-body potential $V(\mathbf{r})$ to depend on β and electric field strength E, as it should in fully self-consistent theory.

Of course, all the results of the present study are within the framework of the admittedly simple model developed in Ref. 1. Basic steps that remain to be taken beyond that model are:

i) To deal more realistically with confinement of the inhomogeneous electron liquid in electric fields.

ii) To treat time-dependent electric fields. This would then complement the studies of Kulander *et al.*[4], where a method of solving the time-dependent Schrödinger equation for an atom or molecule in an intense pulsed-laser field is employed to study multiphoton emission processes. Time-dependent electron density theory would then be the tool to use to extend the present work; this has been reviewed elsewhere by Bartolotti[5].

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