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AND SOLID STATE PLASMAS AT ANY DEGENERACY***

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1. INTRODUCTION

A precise knowledge of multi component Fermi plasmas at any degree of degeneracy is a question of both fundamental and practical interest. For instance, the one component (OCP) and the two component plasmas serve as standard models for electrons in metals, for electron hole systems in semiconductors, for white dwarfs, for the solar core and for fusion plasmas.

Great progress has been made in giving thermodynamic functions for the OCP; here we mention only the recent work by Dandrea, Ashcroft and Carlson [1] and by Tanaka et al. [2] and refer to papers quoted therein. The main progress of the last years is due to the inclusion of local field corrections in order to proceed from the highly degenerate or nondegenerate situations, respectively, towards a stronger coupling. The improvements dealt with in [1] in order to go beyond the random phase approximation (RPA) were achieved by using the (static) STLS [3], or by the dynamical Holas et al. [4] theories, respectively. For a comparison, see [18].

In this paper we give the results of thermodynamical calculations for two component plasmas which are of interest for dense hydrogen, noble gas and alkali plasmas and for electron hole plasmas in optically excited semiconductors as well. So far we consider the coupling to be not too strong, i.e., we consider only approximations up to the Montroll-Ward contribution of the thermodynamic quantities such as pressure and chemical potential. In this way we are restricted to systems at high temperatures (and any density) and to systems at high densities (and any temperature), i.e. to systems in which nonideality effects are not too important. If we further neglect bound states, we exclude certain rectangular area in the density-temperature plane (see e.g., [1],[5]). We mention the need of thermodynamic potentials in the density functional technique [6],[7] and for the construction of Padé formulas at finite temperatures [1],[2],[5],[6],[8],[9]. Especially, such formulas are needed for the discussion of phase diagrams and the determination of critical points in connection with partial ionization [10]-[12]. Of special interest is the hydrogen plasma for its abundance in the universe and for technical reasons [13]-[15].

2. BASIC EXPRESSIONS

In the framework of the grand canonical ensemble, we obtain the pressure as a function of the chemical potential μ_n for given temperature and volume Ω according to a charging procedure over the potential energy with respect to the coupling constant [5],[16]. The final result for the Montroll-Ward, or ring sum part is (for the correlation part of the pressure)

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$$p^{corr} = -\hbar \int \frac{d\vec{p}}{(2\pi)^3} \int_0^\infty \frac{d\omega}{2\pi} \coth\left(\frac{\beta\hbar\omega}{2}\right) * \{ \arctan(\varepsilon''(p\omega)/\varepsilon'(p\omega)) - \varepsilon''(p\omega) \}. \quad (1)$$

The pressure consists then of three parts (p_x -exchange)

$$p(\Omega T\{\mu_a\}) = p_0(\Omega T\{\mu_a\}) + p_x(\Omega T\{\mu_a\}) + p^{corr}(\Omega T\{\mu_a\}) + \text{higher orders of exchange and coupling}. \quad (2)$$

From (2) we get the equation of state

$$p = p(n)$$

using

$$\begin{aligned} n_a &= z_a \frac{\partial}{\partial z_a} [p(\Omega T\{\mu_a\})/kT], \\ z_a &= \exp(\mu_a/kT), \end{aligned} \quad (3)$$

on inversion of $n = n(\mu)$ to $\mu = \mu(n)$.

We have thus the chemical potential and the pressure according to (2), see e.g., [1],[6],[17]. In place of (1), we may also use a formula, in which instead of the continuous frequency integration over ω , there remains a summation over discrete Matsubara frequencies [6],[7],[16],[18],[19], of course with a slightly changed integrand. While the Matsubara frequency formula numerically works faster at high degeneracy (the summation may be transformed into a continuous integral at $T = 0$), formula (1) is less time consuming in the weakly degenerate limit, and vice versa.

In order to get numerical data for the chemical potentials, we may proceed as described above; instead we may start from the free Helmholtz energy

$$F = \sum \mu_a N_a - p\Omega \quad (4)$$

from which we get the correlation part of the chemical potential

$$\mu_e^{corr} = -\frac{\partial}{\partial n_e} p^{corr}(\Omega T\{\mu_a\}), \quad (5)$$

where we now have to adopt the following connection between $\alpha_a = \exp(\mu_a/kT)$ and n_a according to the discussion on inversion given in [1],[6],[17],[18]

$$n_a(\alpha_a, T) = \frac{2s_a + 1}{\Lambda_a^3} I_{1/2}(\alpha_a); \quad (6)$$

Λ_a -thermal wavelength, s_a -spin, $I_{1/2}$ -Fermi integral.

3. RESULTS

We evaluated (1) numerically using the exact RPA dielectric function for ε' and ε'' . At higher degeneracy (larger α) the integration becomes more and more time consuming due to the plasmon peak behaviour of the integrand, the latter does not exist in the Matsubara frequency summation technique [6],[7],[18]. Both electrons and ions are dealt with on the same footing. Of course, in improved theories, the ions should be handled more carefully.

In Fig. 1 we gave the results for hydrogen. There is good agreement with [6] and [18] see also [20],[21].

The correlation part of the chemical potential of an electron proton pair is given in Fig. 2. Here the connection between temperature for a given value of α is fixed according to Eq.(6). Again we have excellent agreement with [6] and [18].

It should be remarked that the high degeneracy results coincide with the $T=0$ two component calculations given in [22], which read for the correlation part of the chemical potential of an e - p part

$$\begin{aligned} \mu_{ep}^{corr} &= A \ell n r_s + B [Ryd], \\ A &= 114.53, \quad B = 558.01. \end{aligned} \quad (7)$$

The results given in [23] are slightly inaccurate at intermediate α -values due to an unjustified cut-off in the limits of integration. Finally we give the correlation parts of the pressure (Fig. 3) and of the chemical potential of an electron hole pair (Fig. 4) in GaAs with the effective masses $m_e^{eff} = 0.067m_e$, $m_h^{eff} = 0.62m_e$, and with $\varepsilon_0 = 12,9$; no multi-valley degeneracy.

In the latter case there is agreement with the two component $T = 0$ calculations [22] which yielded for GaAs if we write the result in the shape of (7)

$$A = 3,558 \cdot 10^{-4}, \quad B = -2,033 \cdot 10^{-3} [Ryd].$$

For germanium we have with $m_e^{eff} = 0,22m_e$, $m_h^{eff} = 0,2245m_e$, $\varepsilon_0 = 15,36$ and the multivalley degeneracy $g_e = 4$, $g_h = 2$

$$A = 6,802 \cdot 10^{-4}, \quad B = -3,201 \cdot 10^{-3} [Ryd].$$

For thermodynamic functions of semiconductors see also [9],[24],[25]. Especially in [25] a Sommerfeld expansion was given for thermodynamic quantities of GeSi and GaAs.

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Figure Captions

- Fig. 1 Correlation part (Montroll Ward) of the pressure as a function of the fugacity (of the electron component) for hydrogen. Eq. (6) was used, see text.
- Fig. 2 Correlation part (Montroll Ward) of the chemical potential of an electron proton pair as a function of the fugacity of electrons. Eq.(6) was used.
- Fig. 3 Same as Fig. 1, but for optically excited electrons and holes in GaAs. DH - Debye - Hückel approximation.
- Fig. 4 Correlation part of the chemical potential for an electron hole pair, according to (5) and (6), for GaAs.

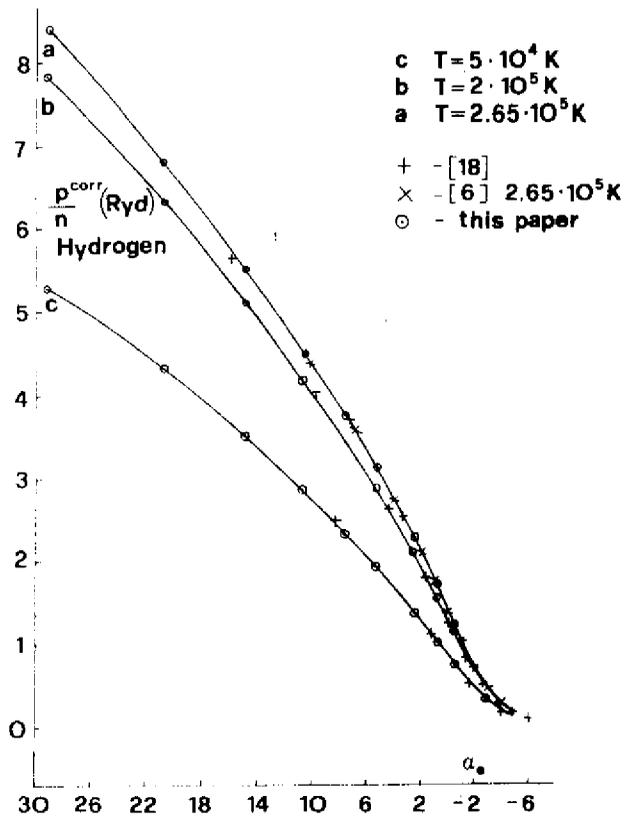


Fig. 1

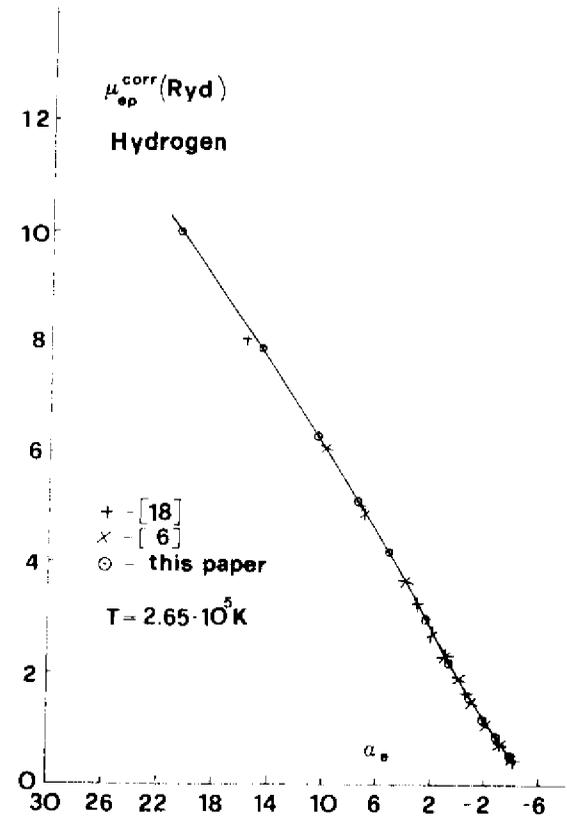


Fig. 2

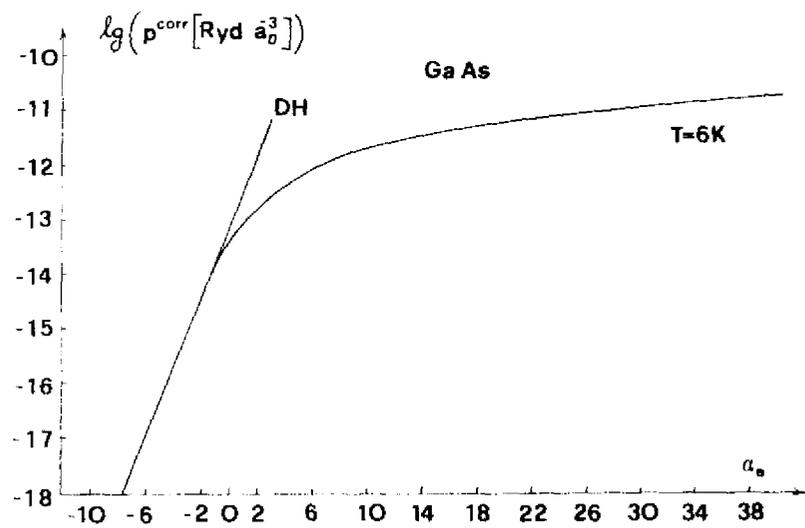


Fig. 3

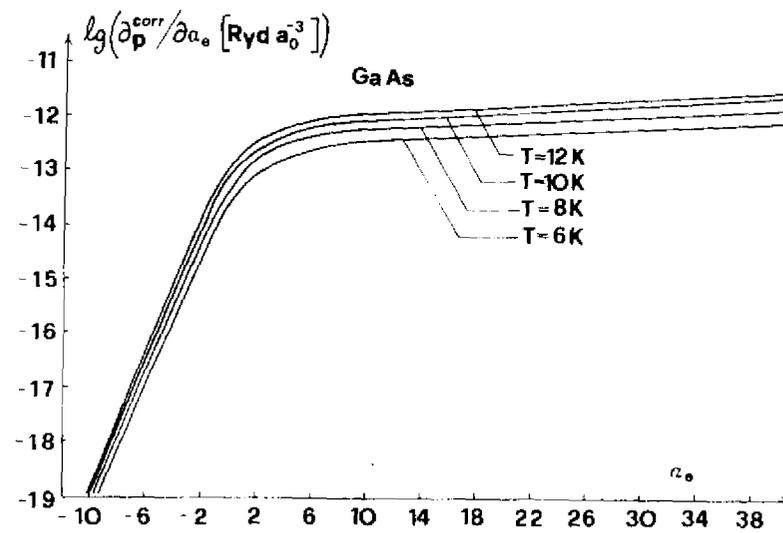
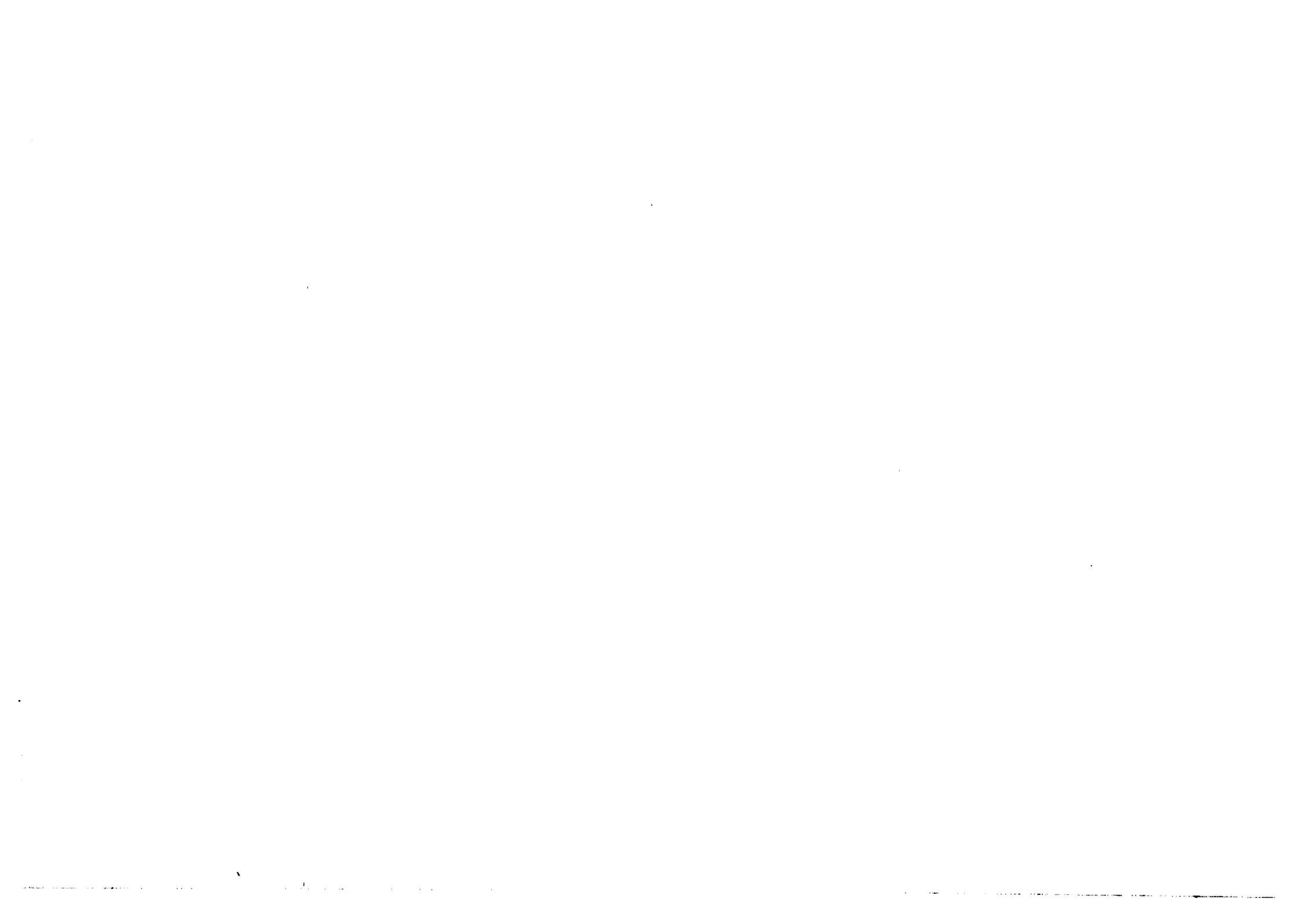


Fig. 4



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