

# The Thermodynamics of White Dwarf Matter. II.

G. SHAVIV

Department of Physics and Astronomy  
Tel Aviv University, Ramat Aviv, Israel

A. KOVETZ\*

Centre de recherches mathématiques  
Université de Montréal, Canada

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An equation of state is constructed for a dense plasma in which the electrons are strongly degenerate. In addition to the perfect gas and non-interacting fermion terms for the ions and electrons, respectively, we have the classical Coulomb and the Thomas-Fermi corrections; these are of first and second order in  $Z^{2/3}\alpha$ , where  $Z$  is the charge number and  $\alpha$  the fine structure constant. In addition, there is the exchange interaction between the electrons and a quantum correction due to the non-commutation of the ionic coordinates and momenta; the latter is the counterpart, in a disordered state, of the harmonic vibration terms (Kovetz and Shaviv, 1970, Paper I) in a lattice.

This equation of state is used together with the one obtained in Paper I to determine the conditions for a phase transition between liquid and solid. Some numerical examples for this are given.

*Key words:* white dwarfs — stellar thermodynamics

## 1. Introduction

In a previous paper (Kovetz and Shaviv, 1970) thermodynamical quantities were derived for a model of white dwarf matter consisting of an ionic lattice embedded in a uniform electronic space charge. The purpose of this paper is to give a similar treatment (in Section 2) for the “liquid” phase and to determine (in Section 3) the transition between the two phases.

## 2. The Liquid Phase

### a) The Coulomb Correction

At temperatures and densities at which the electrons are strongly degenerate, so that their electrical interaction energy is small compared to their Fermi energy, we may take them to be uniformly distributed, to a first approximation. Intensive thermodynamic quantities for such a system of positive ions in a uniform negative background, apart from the kinetic (perfect gas) part, depend on temperature and density through the combination  $\Gamma = (Ze)^2/\langle r \rangle kT$ , where  $Ze$  is the ionic charge,  $k$  is Boltzmann’s constant and  $\langle r \rangle$  is related to the ionic number density  $n$  through  $4\pi \langle r \rangle^3/3 = n^{-1}$ . If, therefore, the internal Coulomb

energy is  $E_c = NkT f(\Gamma)$ , then the corresponding free energy is  $F_c = NkT \int_0^\Gamma dx f(x)/x$ , from which all

other thermodynamic quantities can be obtained by differentiation. For small  $\Gamma$  ( $\leq 0.05$ ) Debye-Huckel theory (e.g. Landau and Lifshitz, 1958) gives  $f(\Gamma) = - (3^{1/2}/2) \Gamma^{3/2}$ . For sufficiently large  $\Gamma$  ( $\sim 100$ ) the ions arrange themselves in a lattice and then the Wigner-Seitz approximation gives  $f(\Gamma) = - .9 \Gamma$  (Salpeter, 1961). For intermediate values of  $\Gamma$  resort must be had to numerical methods. The Broyles-Sahlin-Carley method (1963) has given reliable results for  $\Gamma \leq 2.5$ . Brush *et al.* (1966) obtained values of  $f(\Gamma)$  for  $0.05 \leq \Gamma \leq 100$  by using a Monte-Carlo technique (Metropolis *et al.*, 1953) to obtain a canonical average for a system of  $N$  ions ( $32 \leq N \leq 500$ ) in a cube with periodic boundary conditions. They calculated the interaction energies only approximately, and the precise effect of this on their results is not clear. We have therefore carried out a similar Monte-Carlo calculation for  $N$  ions in a sphere. For a given configuration of  $N$  ions in a sphere of radius  $R$  filled with a uniform charge  $-NZe$ , the energy is

$$E = \Gamma k T N^{-1/3} \left( - .9 N^2 + .5 N R^{-2} \sum_{i=1}^N |r_i|^2 + R \sum_{i \neq j} |r_i - r_j|^{-1} \right) \quad (1)$$

\* On leave of absence from Tel Aviv University.

Table. 1 *The Coulomb correction to the total energy per ion, in units of  $kT$ , vs.  $\Gamma$*

Columns 2 and 3 give the Broyles-Shalin-Carley and the Brush-Sahlin-Teller results; the last three columns give the results of Monte-Carlo calculations for 100 and 200 ions in a sphere, and the values obtained from these by extrapolation.

$\Gamma$	SC	BST	$N=100$	$N=200$	Extp.
0.05	0.0094	0.0128			
0.1	0.0258	0.0270			
1	0.577	0.579			
2	1.321	1.338			
2.5	1.723	1.729			
5		3.774	3.625	3.632	3.658
10		8.069	7.786	7.838	8.040
25		21.113	20.73	20.78	20.97
50		43.221	42.75	42.82	43.09
75		65.572	64.84	64.87	65.04
100		87.82	87.05	87.07	87.12
125			109.2	109.2	109.2
150			131.4	131.4	131.4

where  $r_i$  is the position of the  $i$ -th ion. The results of canonical averages for  $N=100$  and  $N=200$  are given in Table 1. The error in  $f(\Gamma)$  due to the finite number of ions in the sphere varies as  $N^{-1/3}$ . The results for  $N=100$  and  $N=200$  can therefore be used to obtain an extrapolated value of  $f(\Gamma)$  for large  $N$  which is probably accurate to within 1% (Table 1, column 6).

In numerical calculations we have used for the equation of state the Broyles-Sahlin-Carley values (taken from Brush *et al.*, 1966) for  $\Gamma \leq 2.5$  and the values in column 6 for  $\Gamma > 2.5$ . Between each pair of values  $f(\Gamma)$  was obtained by taking it to be of the form  $f(\Gamma) = a\Gamma^{3/2}/(\Gamma^{1/2} + b)$  with constant  $a$  and  $b$ .

### b) *The Thomas-Fermi Correction*

In the foregoing subsection the electrons were assumed to form a uniform background. Clearly, however, they will have a tendency to crowd around the ions. The resulting small effect on the free energy is obtained as follows.

In the unperturbed state the electron chemical potential  $\mu_0$ , number density  $n_0 = n_e(\mu_0, T)$  and free energy density  $f_0 = f_e(\mu_0, T)$  are all uniform. The Coulomb interaction potential  $\phi$  then causes the electrons to arrange themselves in such a way that  $\mu_0 \rightarrow \mu + e\phi$ , where  $\mu$  is a new *constant*. The difference  $\mu - \mu_0$  is of order  $e\phi$  and is determined by the requirement that the total charge  $\int n_e(\mu + e\phi, T)dV$

equal  $\int n_e(\mu_0, T)dV$ . This gives

$$\mu - \mu_0 = -V^{-1} \int e\phi dV \equiv -e\phi_{av}. \quad (2)$$

The resulting *change* in the free energy is

$$\begin{aligned} \int (f_e - f_0) dV &= \int [\partial f_e / \partial n_e] \delta n_e \\ &+ \frac{1}{2} (\partial^2 f_e / \partial n_e^2) (\delta n_e)^2 dV \\ &= \frac{1}{2} \frac{\partial^2 f_e(n_e, T)}{\partial n_e^2} \left( \frac{\partial n_e(\mu_0, T)}{\partial \mu} \right)^2 \int (\phi - \phi_{av})^2 dV \\ &= \frac{1}{2} e^2 \frac{\partial n_e(\mu_0, T)}{\partial \mu} \text{Var}(\phi) \end{aligned} \quad (3)$$

where  $\text{Var}(\phi)$  is the variance  $\int (\phi - \phi_{av})^2 dV$  of  $\phi$  throughout the volume of the system. To this we must add the change in electrical energy produced by a change  $-e\delta n_e$  in charge density in the presence of a potential  $\phi$ :

$$\begin{aligned} - \int \phi e \delta n_e dV &= -e^2 \frac{\partial n_e(\mu_0, T)}{\partial \mu} \int \phi (\phi - \phi_{av}) dV \\ &= -e^2 \partial n_e(\mu_0, T) / \partial \mu \text{Var}(\phi), \end{aligned} \quad (4)$$

So that the total change is

$$-(e^2/2) \partial n_e(\mu_0, T) / \partial \mu \text{Var}(\phi). \quad (5)$$

Introducing non-dimensional quantities by  $\phi = (Ze / \langle r \rangle) \tilde{\phi}$ ,  $V = (4\pi \langle r \rangle^3 / 3) N \tilde{V}$ ,  $\tilde{\text{Var}}(\tilde{\phi}) = \int (\tilde{\phi} - \tilde{\phi}_{av})^2 d\tilde{V}$ , we find that the change in free energy is

$$F_{TF} = -\frac{e^2}{2} N \Gamma k T \partial n_e(\mu_0, T) / \partial \mu \langle r \rangle^2 \overline{\text{Var}}(\tilde{\phi}) \quad (6)$$

where the bar denotes averaging over a canonical ensemble of ion configurations. Since the ensemble is determined by  $\Gamma$  (we are dealing with a perturbation of the Coulomb correction), the product  $\Gamma \overline{\text{Var}}(\tilde{\phi})$  is a function  $g(\Gamma)$  of  $\Gamma$ . For large  $\Gamma$ , when the system is in the ground state, we obtain from the Wigner-Seitz approximation  $g(\Gamma) = (108/175) \Gamma = .6175 \Gamma$  (in agreement with Salpeter, 1961); in the limit of small  $\Gamma$  we find from Debye-Huckel theory (e.g. Landau and Lifshitz, 1958) that  $g(\Gamma) = (\Gamma/3)^{1/2}$ . Rather than interpolate between these, we have chosen for the purpose of numerical calculations the large- $\Gamma$  form

$$\begin{aligned} F_{TF} &= -(e^2/2) N k T \partial n_e(\mu_0, T) / \partial \mu \langle r \rangle^2 g(\Gamma), \\ g(\Gamma) &= .6175 \Gamma. \end{aligned} \quad (7)$$

This is expected to be correct in the neighbourhood of the phase transition. It is incorrect at low  $\Gamma$ , but there the whole Thomas-Fermi correction is anyway

small, so that we can afford a large error in it without any ill effects. From (7) we obtain in the usual way the Thomas-Fermi correction to the various thermodynamic quantities. In this connection it should be noted that  $\mu_0$  is a function of  $N$ ,  $V$  and  $T$  via  $n_0 = n_e(\mu_0, T)$ .

### c) The Exchange Effect

The effect of the Pauli exclusion principle on the electromagnetic interaction of the electrons is not included in the Coulomb correction of subsection a) and so must be handled separately. It has been shown by Zapolsky (1960) that the exchange interaction energy between two electrons with momenta  $\mathbf{p}_1$ ,  $\mathbf{p}_2$  and energies  $\varepsilon_i^2 = m_e^2 c^4 + \mathbf{p}_i^2 c^2$  in a volume  $V$  is

$$E_{\times 12} = \frac{2\pi(e\hbar c)^2}{V\varepsilon_1\varepsilon_2} \left( 1 - \frac{m_e c^4}{\varepsilon_1\varepsilon_2 - m_e^2 c^4 - \mathbf{p}_1 \cdot \mathbf{p}_2 c^2} \right) \quad (8)$$

To obtain the resulting perturbation of the perfect fermion free energy of  $N_e$  electrons in a volume  $V$  at temperature  $T$  we must take a statistical average of (8) (Peierls, 1932). Recalling that the number of electrons in state  $\alpha$  with energy  $\varepsilon_\alpha$  is  $n_\alpha = (e^{(\varepsilon_\alpha - \mu)/kT} + 1)^{-1}$ , we obtain

$$\begin{aligned} F_{\text{ex}}(N_e, V, T) &= \frac{\alpha}{4\pi^3} m_e c^2 (m_e c/\hbar)^3 V \\ &\cdot \int_1^\infty \frac{dx_1}{e^{(m_e c^2 x_1 - \mu)/kT} + 1} \int_1^\infty \frac{dx_2}{e^{(m_e c^2 x_2 - \mu)/kT} + 1} f(x_1, x_2), \\ f(x_1, x_2) &\equiv 2\sqrt{x_1^2 - 1}\sqrt{x_2^2 - 1} \\ &+ \log \left( \frac{x_1 x_2 - 1 - \sqrt{x_1^2 - 1}\sqrt{x_2^2 - 1}}{x_1 x_2 - 1 + \sqrt{x_1^2 - 1}\sqrt{x_2^2 - 1}} \right). \quad (9) \end{aligned}$$

It should be noted that in (9)  $\mu$  is to be considered a function of  $N_e$ ,  $V$  and  $T$  defined by the usual relation  $N_e/V = n_e(\mu, T)$  for non-interacting fermions. With this understanding we can use  $F_{\text{ex}}$  to obtain in the standard way the exchange contribution to the various thermodynamic quantities. It is, however, simpler to recall that a small change in the free energy at given  $N_e$ ,  $V$ ,  $T$  is a small change in the thermodynamic potential  $H = -PV$  at given  $T$ ,  $\mu$  and  $V$ . We can therefore say that the correction  $H_{\text{ex}}(T, \mu, V)$  to  $H$  due to exchange effects is also given by Eq. (9) and obtain the effect on other quantities from  $N_{e, \text{ex}} = -\partial H_{\text{ex}}/\partial \mu$ ,  $P_{\text{ex}} = -\partial H_{\text{ex}}/\partial V = -H_{\text{ex}}/V$ ,  $S_{\text{ex}} = -\partial H_{\text{ex}}/\partial T$ .

Since we are interested in strongly degenerate electrons we shall use the form taken by (9) when the

fermi parameter  $(\mu - m_e c^2)/kT$  is large:

$$\begin{aligned} H_{\text{ex}}(T, \mu, V) &= \alpha/(4\pi)^3 m_e c^2 (m_e c/\hbar)^3 \{ \phi(\tau) \\ &+ \beta^{-2}(4g_2 - 8g_1) + 4c_2 \beta^{-2}[1 + x^2 + 2\log 2\beta x^2 \\ &- 3x^{-1}(x^2 + 1)^{1/2} \log \tau] - 12c_4 \beta^{-4}[x^{-2} + 2x^{-4} \\ &+ 3x^{-5}(x^2 + 1)^{1/2} \log \tau] + 4c_2^2 \beta^{-4}(2 + 2x^{-2} + x^{-4}) \} \quad (10) \end{aligned}$$

(Kovetz *et al.*, 1971), where

$$x^2 = (\mu/m_e c^2)^2 - 1, \beta = m_e c^2/(kT), \tau = x + (x^2 + 1)^{1/2},$$

$$c_2 = \pi^2/12, c_4 = 7\pi^4/120,$$

$$g_1 = \int_0^\infty \frac{t \log t dt}{e^t + 1} = .449,$$

$$g_2 = \int_0^\infty \frac{ds}{e^s + 1} \int_0^\infty \frac{dt}{e^t + 1} \log \left| \frac{s-t}{s+t} \right| = -.504,$$

$$\begin{aligned} \phi(\tau) &= \frac{1}{32} \left( \tau^4 + \frac{1}{\tau^4} \right) + \frac{1}{4} \left( \tau^2 + \frac{1}{\tau^2} \right) \\ &- \frac{9}{16} - \frac{3}{4} \left( \tau^2 - \frac{1}{\tau^2} \right) \log \tau + \frac{3}{2} (\log \tau)^2. \end{aligned}$$

### d) The Ionic Quantum Correction

When the ions form a lattice the non-commutation of their coordinates and momenta results in a spectrum of vibrations (Paper I). Were we to neglect the corresponding effect in the liquid phase, an asymmetry would result which would prevent any reasonable determination of conditions for a phase transition between liquid and solid.

The perturbation in the free energy due to this effect is (Landau and Lifshitz, 1958, § 33)

$$\begin{aligned} F_q &= -\frac{\hbar^2}{24(kT)^2} \sum_i \overline{m_i^{-1} (\text{grad}_i U)^2} + \\ &\frac{\hbar^2}{12kT} \sum_i \overline{m_i^{-1} \Delta_i U} \quad (11) \end{aligned}$$

where the gradient and laplacian of the energy  $U$  are taken with respect to the coordinates of the  $i$ -th ion (which has mass  $m_i$ ), and the bars denote canonical averages. Proceeding as we have done in subsection b) we obtain

$$F_q/(NkT) = (\hbar \Omega_p/kT)^2 h(\Gamma)/36, \quad (12)$$

where  $\Omega_p$  is the ion plasma frequency

$$\Omega_p^2 = 4\pi Z^2 e^2 n/m_i \quad (13)$$

and  $h(\Gamma)$  is a function determined by non-dimensional averages corresponding to those of Eq. (11). For large  $\Gamma$  the Wigner-Seitz approximation gives  $h(\Gamma) = 3$  and for small  $\Gamma$  Debye-Huckel theory gives  $h(\Gamma) \propto \Gamma^{3/2}$ .

In numerical calculations we use the high- $\Gamma$  form

$$F_q/(NkT) = (\hbar \Omega_p/kT)^2/12 = (\Theta/T)^2/12 \quad (14)$$

where  $\Theta$  is the Debye temperature defined by  $\hbar \Omega_p = k\Theta$ . This again introduces errors at low densities and high temperatures, where the correction itself is unimportant.

To sum up, we describe the liquid phase by the usual perfect and non-interacting fermion expressions for the ions and electrons, respectively, and then add the corrections resulting from  $F_c, F_{TF}, F_{ex}$  (or rather  $H_{ex}$ ) and  $F_q$ . We call rather arbitrarily the corrections resulting from  $F_{TF}$  and  $H_{ex}$ , which are the same for the liquid and solid phases, "electronic", and those resulting from  $F_c$  and  $F_q$ , which have different forms in the two phases, "ionic".

### 3. The Phase Transition

Having determined, in the previous section, the corrections that are necessary for the description of the liquid phase, it remains to determine the conditions under which a transition between this phase and the solid phase will occur. In a star the gravitational field will effect a separation of the two phases, and the equilibrium conditions for this are the continuity of pressure,

$$P_{is}(\rho_s, T) + P_e(\rho_s, T) = P_{il}(\rho_l, T) + P_e(\rho_l, T) \quad (15)$$

and of chemical potential (referred to an ion)

$$\mu_{is}(\rho_s, T) + Z \mu_e(\rho_s, T) = \mu_{il}(\rho_l, T) + Z \mu_e(\rho_l, T), \quad (16)$$

where the subscripts i, e, s, l refer to ionic, electronic, solid and liquid, respectively; the factor  $Z$  multiplying  $\mu_e$  in (16) ensures the electrical neutrality at the phase transition. Equations (15)–(16) determine  $\rho_l$  and  $\rho_s$  as functions of  $T$  at the transition. For the purpose of a numerical calculation, however, they are useless, because the small ionic terms which are discontinuous between the phases are overshadowed by the large electronic terms which are continuous but very sensitive to the difference  $\rho_s - \rho_l$ : when the electrons are strongly degenerate the ions have only a small effect on the equation of state.

The necessary modification of Eqs. (15)–(16) is obtained by assuming that  $|\rho_s - \rho_l| \ll \rho_l$ . A first order expansion in Eq. (15) then gives

$$\rho_s - \rho_l = (P_{il} - P_{is})/(\partial P_{is}/\partial \rho + \partial P_e/\partial \rho); \quad (17)$$

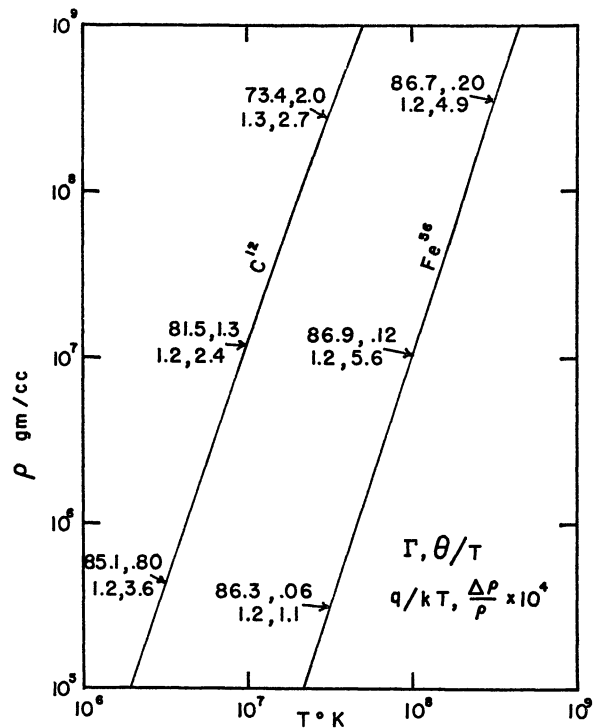


Fig. 1. Transition lines for C<sup>12</sup> and Fe<sup>56</sup>. The values of the Coulomb parameter  $\Gamma$ , the ratio  $\theta/T$  of Debye temperature to temperature, the latent heat per ion in units of  $kT$  and the fractional density change  $(\rho_s - \rho_l)/\rho_l$  are shown at selected points along the transition lines

the derivatives here are at constant temperature and the r.h.s. is evaluated at  $(\rho_l, T)$ . Since  $\partial P_e/\partial \rho = \gamma_T P_e/\rho$ , where  $\gamma_T \sim 1$ , and  $P_i/P_e \sim Z^{2/3} \alpha$  it follows that  $(\rho_s - \rho_l)/\rho_l \sim Z^{2/3} \alpha$ . But at the phase transition  $|P_{is} - P_{il}| \ll P_{il}$ , so that the fractional density change is in fact much smaller ( $\sim 10^{-4}$ ). Carrying out a similar expansion in Eq. (16) and using Eq. (17) and  $(\partial \mu/\partial \rho)_T = n^{-1}(\partial P/\partial \rho)_T$ , we obtain

$$f_{is}(\rho_l, T) = f_{il}(\rho_l, T), \quad (18)$$

where  $f_i = \mu_i - P_i/n$  is the free energy per ion. Eqs. (17)–(18) determine  $\rho_l(T)$  and  $\rho_s(T)$ . The basic reason behind the simple result (18) is that, because the (total) pressure-density relation is hardly affected by the ions, we essentially have a system at given temperature and density. Such a system attains thermodynamic equilibrium when the free energy per ion is a minimum. Hence the actual phase will be that with lower  $f_i$  ( $f_e$  being continuous) and the transition will occur when  $f_{is} = f_{il}$ .

Equation (18), together with the relation  $f_i = u_i - T s_i$  between the ionic free energy, total

energy and entropy, determines the latent heat:

$$q = T(s_{\text{is}} - s_{\text{II}}) = u_{\text{II}} - u_{\text{is}} \quad (19)$$

Results of actual solutions of Eq. (18) for  $\text{C}^{12}$  and  $\text{Fe}^{56}$  are shown in Fig. 1. The competition along the transition lines between the Coulomb effects and the quantum correction is brought out clearly: the former are important at low densities and the latter gets the upper hand at high densities. We should, however, keep in mind the fact that the equations of state for the two phases are approximate: the Thomas-Fermi procedure is essentially an expansion in  $Z^{2/3} \alpha$  and the quantum corrections for the ions are of the first order ("unharmonic terms" not having been taken into account). And when these approximations are joined by Eq. (18) one cannot expect a smooth transition, quite apart from the fact that we *know* that an order-disorder transition is involved. The difference between the errors in the two approximations is, of course, included in the latent heat, Eq. (19). It is remarkable that the values of  $T$  at the transition seem to vindicate the empirical Lindemann rule [Eq. (46) of Mestel and Ruderman, 1967].

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G. Shaviv  
 A. Kovetz  
 Université de Montréal  
 Centre de recherches mathématiques  
 Case postale 6128  
 Montréal 101, Canada