

for the change in sign. The solution can therefore be written

$$\phi_-(x) = \sum b_i x^{i/2}, \quad (49)$$

where

$$b_0 = -1/Z,$$

$$b_1 = 0,$$

$$b_2 = \phi'_-(0) = \text{arbitrary},$$

$$b_i = -a_i, \quad i \geq 3.$$

At large x , (28) can be written

$$\phi_-''(x) \cong K_-^2(\phi_- - \phi_+),$$

the solution to which is

$$\phi_-(x) = x(\phi/x)_\infty - K_-^2(K_+^2 - K_-^2)^{-1} A e^{-K_+ x} + B e^{-K_- x}, \quad (50)$$

where

$$K_-^2 = 6\epsilon\theta^2 [dI_2(\eta)/d\eta]_{\eta_\infty}. \quad (51)$$

The value of b_2 was iterated on until (50) matched the numerical solution both as to value and slope at some suitably large x .

The uniqueness of the solution can again be seen from a qualitative examination of the differential equation, though the situation is somewhat more complicated than before in that two qualitatively different forms of the solution are possible: (1) $\phi_-(x) < x\phi_\infty'$, $\phi_-'(x) > \phi_\infty'$, and $\phi_-''(x) < 0$ for all x ; (2) $\phi_-(x)$ not only crosses the line $x\phi_\infty'$, but also crosses the curve $\phi_+(x)$ at some point x_1 with a slope such that $\phi_+'(x_1) < \phi_-'(x_1) < \phi_\infty'$, with $\phi_-''(x) < 0$ for $x < x_1$ and $\phi_-''(x) > 0$ for $x > x_1$. For $Z=1$, only the first type solution has been observed; for $Z=2$, either type may occur, depending on the density and temperature; and for somewhat larger Z , only the second type has been found. The reason for this will be discussed in Sec. 4b.

In all cases, the numerical results checked Eq. (30) with about the same accuracy as for Eq. (19).

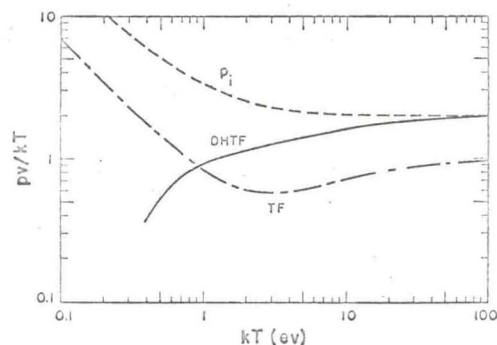


FIG. 1. Variation of pressure with temperature according to the DHTF and TF theories of the atom for deuterium at normal liquid density, $\rho = 0.17$ g/cc (or for hydrogen at $\rho = 0.085$ g/cc). p_i is the pressure of a mixture of uncharged (Boltzmann) nuclei and (quantum-degenerate) electrons.

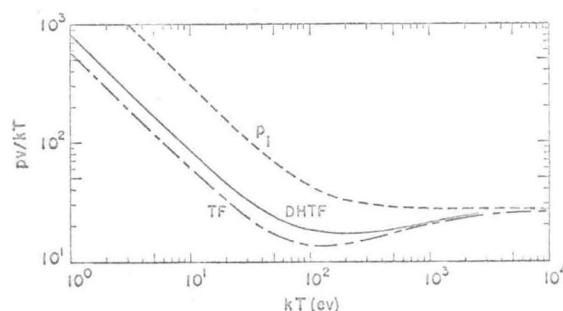


FIG. 2. Variation of pressure with temperature for iron at ten times normal density ($\rho = 78.5$ g/cc).

c. Evaluation of the Thermodynamic Functions

As pointed out earlier, the integrands of the expressions (34) and (35) for A_e can be considered as functions of only the two parameters vT^2 and $T\lambda^{-4}$. However, A_e was actually computed by the more time-consuming but more straightforward procedure¹² of integrating the differential equations for the desired v and T and for each of twelve values of λ^2 , and evaluating the λ^2 integrals with the aid of Simpson's rule.

In order to evaluate p and E , calculations were not actually done at the $v = \rho^{-1}$ and T of interest but rather at $[(1 \pm 0.1)\rho, T]$ and at $[\rho, (1 \pm 0.1)T]$, and p and S calculated from (36) by numerical differentiation in a linear approximation. The associated error is roughly one percent, compared with which the errors in Simpson's rule and in integrating the differential equations are negligible.

In a few cases, the pressure was also evaluated from the virial theorem (37). In each case, the result agreed with that obtained from (36) within the one percent uncertainty in the latter.

4. RESULTS

a. Pressure

Some numerical results for the pressure are shown in Figs. 1-4, which include for comparison curves showing the pressure of the uncharged ideal gas⁸

$$\begin{aligned} p_i v &= -v(\partial A_i / \partial v)_T \\ &= kT + \frac{2}{3} Z k T I_2(\eta_\infty) / I_2(\eta_\infty) \end{aligned} \quad (52)$$

(where v is volume per atom), and also curves showing the electronic pressure as calculated from the TF theory of the atom.¹

It may be seen, especially from Fig. 1, that at high temperatures, the value of pv/kT for the DHTF theory is greater than that for the TF theory by approximately unity, as is to be expected since the one theory includes the nuclear contribution to the pressure whereas the other does not.

¹² This procedure is almost essential to insure consistent values of A_e for use in evaluating the derivatives $(\partial A_e / \partial v)$ and $(\partial A_e / \partial T)$.