We first note from (15)–(17) and (27)–(29) that (for given Z) the solutions $\phi_+(x)$ and $\phi_-(x)$ do not depend on v, T, and λ independently, but only on the two quantities η_∞ and θ, or from (38) and (13), only on

$$vT^{\frac{3}{2}} \quad \text{and} \quad T\lambda^{-4}. \tag{40}$$

Thus if v_1 and T_1 are some fixed volume (per atom) and temperature and if v and T are quantities related to v_1 and T_1 through a scale factor c such that

$$v=c^6v_1 \quad \text{and} \quad T=c^{-4}T_1, \tag{41}$$

then A_e may be written

$$A_e(v,\,T)=K\int_0^1 \lambda^2[\phi_+'(0)-\phi_-'(0)]_{v,T,\lambda}d(\lambda^2)$$

$$=Kc^{-4}\int_0^{c^2}(c\lambda)^2[\phi_+'(0)-\phi_-'(0)]_{v_1,T_1,c\lambda}d(c^2\lambda^2)$$

where K is the constant before the integral sign in (34). Differentiation of this expression gives

$$\left(\frac{dA_e}{dc}\right)_{v_1,T_1}=-\frac{4}{c}A_e+\frac{2}{c}K[\phi_+'(0)-\phi_-'(0)]_{v_1,T_1,c}$$

$$=-\frac{4}{c}A_e+\frac{2}{c}K[\phi_+'(0)-\phi_-'(0)]_{v,T,1}. \tag{42}$$

But from (36) and (41),

$$\left(\frac{dA_e}{dc}\right)_{v_1,T_1}=\left(\frac{\partial A_e}{\partial v}\right)_T\left(\frac{dv}{dc}\right)_{v_1}+\left(\frac{\partial A_e}{\partial T}\right)_v\left(\frac{dT}{dc}\right)_{T_1}$$

$$=-6\frac{v}{c}p_e+4\frac{T}{c}S_e, \tag{43}$$

and combining this with (42) and (39) gives

$$p_ev=\tfrac{2}{3}(A_e+TS_e)-\tfrac{1}{3}E_p$$

$$=\tfrac{2}{3}(E_e-E_p)+\tfrac{1}{3}E_p, \tag{44}$$

which completes the proof of (37). (In the singular case $T=0$, the proof can be carried out in a manner entirely analogous to that which has been given for a modified DHTF theory.[4])

3. NUMERICAL METHODS

The differential equations (16) and (28) were integrated numerically with the aid of IBM Type 704 digital computers, using numerical methods similar to those employed elsewhere.[2,4]

a. Integration of the Equation for ϕ_+

For small x, it may be seen from (15) and (17) that $\eta_+\gg 1$, so that the second term in (16) is negligible compared with the first, the differential equation thus reducing to that for the temperature-dependent TF atom. The solution can, therefore, be written in series form:

$$\phi_+(x)=\sum a_ix^{i/2}, \tag{45}$$

the values of the first few coefficients being[11]

$$a_0=1, \qquad a_1=0,$$

$$a_2=\phi_+'(0)=\text{arbitrary}, \qquad a_3=\tfrac{4}{3}$$

$$a_4=0, \qquad a_5=2a_2/5,$$

$$a_6=\tfrac{1}{3}, \qquad a_7=3a_2^2/70+O(T^2).$$

For $i\geq 7$, the a_i contain temperature-dependent terms, which however are of no importance provided (45) is used only to sufficiently small values of x.

Using an estimated value of a_2, integration of (16) was started with the aid of (45), and then continued by a difference method. Because of the boundary condition (17), at large x Eq. (16) can be written with the aid of Taylor series expansions and Eq. (15) in the form

$$\phi_+''(x)\cong K_+^2[\phi_+-x(\phi/x)_\infty]$$

or

$$\phi_+(x)=x(\phi/x)_\infty+Ae^{-K_+x}, \tag{46}$$

where

$$K_+^2=6\epsilon\theta^{\frac{1}{2}}[dI_{\frac{1}{2}}(\eta)/d\eta+ZI_{\frac{1}{2}}(\eta)]_{\eta_\infty}. \tag{47}$$

At some large x, then, the constant A was evaluated so as to match (46) to the numerical solution, and the slopes of the two solutions were then compared. The value of a_2 was then modified, and an iterative procedure carried out until the two slopes were equal to the desired accuracy.

It may easily be seen that this solution of (16)–(17) is a unique one (barring solutions with singularities at finite x): for any integral of (16), the curvature is positive for $\eta_+>\eta_\infty$, and negative for $\eta_+<\eta_\infty$; if ϕ_1 and ϕ_2 are two integrals satisfying the boundary conditions at the origin with $\phi_1'(0)>\phi_2'(0)$, then for all x, $\phi_1(x)>\phi_2(x)$, $\phi_1'(x)>\phi_2'(x)$, and $\phi_1''(x)>\phi_2''(x)$. The solution (which satisfies both boundary conditions) has the properties $\phi_+(x)>x\phi_\infty'$, $\phi_+'(x)<\phi_\infty'$, and $\phi_+''(x)>0$ for all x.

As a check on the integration of the differential equation, the results were used for a numerical evaluation of the integral (19); the value of q_+ thus obtained was generally equal to $-\lambda Ze$ within one-twentieth percent, except at large Z and low θ where the function (18) changes very rapidly with x.

b. Integration of the Equation for ϕ_-

With η_+ being a known function from the solution of (16)–(17), the integration of (28) can be carried out in a similar manner. At small x, $\eta_-\ll 0$ from (27) and (29), and (28) reduces to

$$\phi_-''(x)=-\tfrac{3}{2}(4\epsilon)^3\theta^{\frac{1}{2}}xI_{\frac{1}{2}}(\eta_+), \tag{48}$$

which is identical with the small-x form of (16) except

[11] Reference 5, Sec. II.