

# MORE MANY-BODY PERTURBATION THEORY FOR AN ELECTRON-ION SYSTEM

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## ABSTRACT

From previous finite-temperature, quantum, many-body perturbation theory results for the grand partition function of an electron-ion fluid through order  $e^4$ , we compute the electron and ion fugacities in terms of the volume per ion and the temperature to that same order in perturbation theory. From these results we also give the pressure, again to the same order in perturbation theory about the values for the non-interacting fluid.

## I. INTRODUCTION AND SUMMARY

There has been, and there continues to be, strong interest in the computation of as much as possible in the way of exact results for the equation of state of matter under extreme conditions. In stellar interiors, in plasma fusion, and in some other applications, the familiar regime of solids, liquids and gases ceases to be germane. Rather the fluid state in which liquids and gases are not distinguishable is what is important. In this paper we will be concerned with a hot and/or dense system of electrons and ions. In a previous paper [1] we have begun the computation of the expansion in powers of the charge on the electron  $e$  of the thermodynamic functions about the ideal Fermi gas or “hot-curve” limit. In that paper Matsubara, many-body perturbation theory [2] was carried through the second exchange correction (order  $e^4$ ). And all the terms necessary for the expression of the grand partition in terms of the fugacity were obtained to that order. In this paper we extend that effort by solving for the electron and ion fugacities in terms of the volume per ion and the temperature. From these solutions, we are able to express the perturbation coefficients, in principle exactly, in the same terms, through order  $e^4$ . As a practical matter we will however use various representations which have a maximum error of the order of one tenth of a percent.

In the second section, we recapitulate the results of our previous work [1], recasting it in the process explicitly as the logarithm of the grand partition function in terms of the volume, temperature, and the parameters electron and ion fugacity. From the standard quantum statistical mechanical equations [3] we have the equations necessary to eliminate the fugacities. In the third section, we solve these equations

and use the solutions to give pressure as a function of temperature and density. From the pressure, one can, by standard thermodynamics, derive expressions for the other thermodynamic quantities, but we have not done so. In the fourth section we obtain the necessary representations for the functions of the de Broglie density, to an accuracy of the order of one-tenth of a percent or better, necessary to actually evaluate the expansion coefficients. These expressions are good over the full range from an ideal gas to a degenerate Fermi gas. A limiting version of the expansion is given which indicates the behavior for low densities and high temperatures. In the fifth section, we examine the actual values of the expansion coefficients. Some further limiting versions of the expansion are given which address the region of high density.

## II. FUGACITY EXPANSION OF THE COEFFICIENTS

In this paper we will treat the electrons as Fermions, but will treat the ions as Maxwell-Boltzmann particles. The treatment of the ions could be improved, if required. The pressure we will be concerned with is the total pressure. We start with the electrically neutral Hamiltonian,

$$H = \sum_{i=1}^{ZN} \frac{p_i^2}{2m} + \sum_{j=1}^N \frac{P_j^2}{2M} + \sum_{i<j}^{ZN} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \sum_i^{ZN} \sum_j^N \frac{Ze^2}{|\vec{r}_i - \vec{R}_j|} + \sum_{i<j}^N \frac{Z^2e^2}{|\vec{R}_i - \vec{R}_j|}, \quad (2.1)$$

where  $\vec{r}$ ,  $\vec{p}$  are the position and momentum for the electrons and  $\vec{R}$ ,  $\vec{P}$  are for the ions of charge  $Z$ . Although not expressed in exactly this way, we [1] have previously obtained by means of Matsubara perturbation theory [2] the necessary information for the grand partition function for an electron-ion fluid with the coefficients expressed as a function of the volume  $\Omega$ , the temperature  $T$ , the electron fugacity  $z$ , and the ion fugacity  $z_{\text{ion}}$ . It is useful to recapitulate these results here. First we introduce the notation,

$$I_n(z) = \int_0^\infty \frac{zy^n e^{-y} dy}{1 + ze^{-y}} = \Gamma(n+1) \sum_{j=1}^\infty \frac{(-1)^{j+1} z^j}{j^{n+1}}, \quad n > -1. \quad (2.2)$$

These functions have the property,

$$z \frac{d}{dz} I_n(z) = n I_{n-1}(z), \quad (2.3)$$

which will be useful. Thus, taking account of the sign error in (2.3) *et seq.* of reference [1], and without including the missing  $e^4$  term in the sum of the ring diagrams, we may write,

$$\begin{aligned} \log \mathcal{Q}(\Omega, T, z, z_{\text{ion}}) = & z_{\text{ion}} \Omega \left( \frac{2\pi M k T}{\tilde{h}^2} \right)^{\frac{3}{2}} + 2\Omega \left( \frac{2\pi m k T}{h^2} \right)^{\frac{3}{2}} \left\{ \frac{I_{\frac{3}{2}}(z)}{\Gamma(\frac{5}{2})} \right. \\ & + \frac{1}{\pi} \left( \frac{2\pi m e^4}{h^2 k T} \right)^{\frac{1}{2}} \hat{X}(z) + \frac{\sqrt{\pi}}{3} \left( \frac{2\pi m e^4}{h^2 k T} \right)^{\frac{3}{4}} \left[ Z^2 \left( \frac{h^2 M}{\tilde{h}^2 m} \right)^{\frac{3}{2}} z_{\text{ion}} + \frac{2}{\sqrt{\pi}} I_{-\frac{1}{2}}(z) \right]^{\frac{3}{2}} \\ & \left. - \left( \frac{2\pi m e^4}{h^2 k T} \right) \left( \frac{1}{2} \hat{T}(z) + \hat{\Theta}(z) \right) + o(e^4) \right\}, \quad (2.4) \end{aligned}$$

where  $h$  is Planck's constant, the 2 in front of  $I_{-\frac{1}{2}}(z)$  is because of the two electron spin states, and  $\tilde{h}$  is an arbitrary constant with the same dimensions as Planck's

constant. An alternate expression for the Debye-Hückel term [the coefficient of  $e^3$  in (2.4)] which facilitates comparison with other work [4] is

$$\frac{2\sqrt{\pi}}{3}\Omega\left(\frac{e^2}{kT}\right)^{\frac{3}{2}}\left[Z^2\frac{z_{\text{ion}}}{\Omega}\frac{\partial N_{\text{ion}}}{\partial z_{\text{ion}}}+\frac{z}{\Omega}\frac{\partial(ZN)}{\partial z}\right]^{\frac{3}{2}}. \quad (2.5)$$

The fugacity expansions of the other functions in (2.4) are given by Baker and Johnson [1] as,

$$\hat{X}(z) = \pi \sum_{n_1, n_2=1}^{\infty} \frac{(-z)^{n_1+n_2}}{\sqrt{n_1 n_2 (n_1 + n_2)}}. \quad (2.6)$$

$$\hat{\Theta}(z) = \sum_{J=3}^{\infty} \frac{-(-z)^J}{\sqrt{J}} \sum_{j_1=1}^{J-2} \sum_{j_2=1}^{J-j_1-1} \frac{J-j_1-j_2}{j_1 j_2} \sin^{-1} \left( \sqrt{\frac{j_1 j_2}{(J-j_1)(J-j_2)}} \right), \quad (2.7)$$

$$\hat{T}(z) = \sum_{j_1, j_2, j_3, j_4=0}^{\infty} \frac{(-1)^{j_1+j_2+j_3+j_4} z^{2+j_1+j_2+j_3+j_4}}{b\sqrt{2+j_1+j_2+j_3+j_4}} \int_{-1}^1 \frac{b d\lambda}{a+b\lambda} \sin^{-1} \left( \frac{a+b\lambda}{\sqrt{AC}} \right), \quad (2.8)$$

where

$$\begin{aligned} AC &= (1+j_1+j_2)(1+j_3+j_4)(1+j_1+j_4)(1+j_2+j_3), \\ B &= a+b\lambda, \\ a &= (2+j_1+j_2+j_3+j_4)\left(\frac{1}{2}+j_4\right) - (1+j_1+j_4)(1+j_3+j_4), \\ b &= \frac{1}{2}(2+j_1+j_2+j_3+j_4). \end{aligned} \quad (2.9)$$

From standard quantum statistical mechanics the required functions may be deduced from equation (2.4) by means of

$$\frac{P\Omega}{kT} = \log \mathcal{Q}(\Omega, T, z, z_{\text{ion}}), \quad (2.10)$$

$$ZN = z \frac{\partial}{\partial z} \log \mathcal{Q}(\Omega, T, z, z_{\text{ion}}) \Big|_{\Omega, T, z_{\text{ion}}}, \quad (2.11)$$

$$N_{\text{ion}} = z_{\text{ion}} \frac{\partial}{\partial z_{\text{ion}}} \log \mathcal{Q}(\Omega, T, z, z_{\text{ion}}) \Big|_{\Omega, T, z}, \quad (2.12)$$

where  $N_{\text{ion}} = N$  for system neutrality.

To implement (2.11) we need the function,  $I_{\frac{1}{2}}(z)$  whose expansion is given above, and

$$z \frac{d}{dz} \hat{X}(z) = \pi \sum_{n_1, n_2=1}^{\infty} \frac{(-z)^{n_1+n_2}}{\sqrt{n_1 n_2}} = \left[ \sqrt{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1} z^n}{\sqrt{n}} \right]^2 = [I_{-\frac{1}{2}}(z)]^2, \quad (2.13)$$

$$z \frac{d}{dz} \hat{\Theta}(z) = \sum_{J=3}^{\infty} -(-z)^J \sqrt{J} \sum_{j_1=1}^{J-2} \sum_{j_2=1}^{J-j_1-1} \frac{J-j_1-j_2}{j_1 j_2} \sin^{-1} \left( \sqrt{\frac{j_1 j_2}{(J-j_1)(J-j_2)}} \right), \quad (2.14)$$

$$z \frac{d}{dz} \hat{T}(z) = \sum_{j_1, j_2, j_3, j_4=0}^{\infty} \frac{2(-1)^{j_1+j_2+j_3+j_4} z^{2+j_1+j_2+j_3+j_4}}{\sqrt{2+j_1+j_2+j_3+j_4}} \int_{-1}^1 \frac{b d\lambda}{a+b\lambda} \sin^{-1} \left( \frac{a+b\lambda}{\sqrt{AC}} \right), \quad (2.15)$$

The function  $I_{-\frac{1}{2}}$  has been studied by Baker and Johnson [1], but we need to investigate the second two functions. They have found the asymptotic behaviors,

$$\hat{\Theta}(z) \asymp \frac{2}{\pi^{\frac{3}{2}}} (\log z)^{\frac{3}{2}}, \quad \hat{T}(z) \asymp (0.2276 \pm 0.0003) (\log z)^{\frac{3}{2}}, \quad z \rightarrow \infty. \quad (2.16)$$

Thus we can deduce, in a straightforward manner,

$$z \frac{d}{dz} \hat{\Theta}(z) \asymp \frac{3}{\pi^{\frac{3}{2}}} (\log z)^{\frac{1}{2}}, \quad z \frac{d}{dz} \hat{T}(z) = (0.3413 \pm 0.0004) (\log z)^{\frac{1}{2}}, \quad z \rightarrow \infty. \quad (2.17)$$

In addition we need the derivative  $z dI_{-\frac{1}{2}}(z)/dz$ . The integral expression and the series expansion in (2.2) are well defined for  $I_{-\frac{1}{2}}$ , as is the  $\Gamma$ -function. In addition the asymptotic behavior can be deduced from the known asymptotic behavior of  $I_{\frac{1}{2}}(z)$  [3]. Thus, using (2.3),

$$I_{\frac{1}{2}}(z) \asymp \frac{2}{3} (\log z)^{\frac{3}{2}} \quad \text{implies} \quad z \frac{d}{dz} I_{-\frac{1}{2}}(z) \asymp (\log z)^{-\frac{1}{2}}, \quad z \rightarrow \infty \quad (2.18)$$

It turns out that a knowledge of these above mentioned functions will suffice to permit the back substitutions of the solutions of (2.11-12) for  $z$  and  $z_{\text{ion}}$  into (2.10) to give the results for the pressure.

### III. SOLUTION OF THE FUGACITY EQUATIONS

The next step in our program to develop computable expressions of the thermodynamic function through order  $e^4$  is to solve for the fugacities. The following notation will be useful,

$$\zeta = \frac{ZN}{2\Omega} \left( \frac{h^2}{2\pi mkT} \right)^{\frac{3}{2}}, \quad \epsilon = \left( \frac{2\pi me^4}{h^2 kT} \right)^{\frac{1}{4}}, \quad r_b = \left[ \frac{3\Omega}{4\pi N} \right]^{\frac{1}{3}}, \quad x_0 = \frac{r_b}{a_0},$$

$$y^2 = \frac{Ze^2}{r_b kT} = 2 \left( \frac{Z}{9\pi} \right)^{\frac{1}{3}} \zeta^{\frac{2}{3}} x_0, \quad \epsilon = \left( \frac{3}{8\pi Z^2 \zeta} \right)^{\frac{1}{6}} y = \left( \frac{\zeta}{3\pi^2 Z} \right)^{\frac{1}{6}} \sqrt{x_0}, \quad (3.1)$$

where  $a_0 = \hbar^2/m_e^2$  is the Bohr radius. Equations (2.11) and (2.12) become,

$$ZN = 2\Omega \left( \frac{2\pi mkT}{h^2} \right)^{\frac{3}{2}} \left\{ \frac{I_{\frac{1}{2}}(z)}{\Gamma(\frac{3}{2})} + \frac{1}{\pi} \epsilon^2 \left[ I_{-\frac{1}{2}}(z) \right]^2 \right. \\ \left. + \epsilon^3 \left[ Z^2 \left( \frac{h^2 M}{\hbar^2 m} \right)^{\frac{3}{2}} z_{\text{ion}} + \frac{2}{\sqrt{\pi}} I_{-\frac{1}{2}}(z) \right]^{\frac{1}{2}} z \frac{d}{dz} I_{-\frac{1}{2}}(z) \right. \\ \left. - \epsilon^4 \left[ \frac{1}{2} z \frac{d}{dz} \hat{T}(z) + z \frac{d}{dz} \hat{\Theta}(z) \right] + o(e^4) \right\} \quad (3.2)$$

$$N_{\text{ion}} = z_{\text{ion}} \Omega \left( \frac{2\pi MkT}{\hbar^2} \right)^{\frac{3}{2}} \\ \times \left\{ 1 + \sqrt{\pi} \epsilon^3 Z^2 \left[ Z^2 \left( \frac{h^2 M}{\hbar^2 m} \right)^{\frac{3}{2}} z_{\text{ion}} + \frac{2}{\sqrt{\pi}} I_{-\frac{1}{2}}(z) \right]^{\frac{1}{2}} + o(e^4) \right\}, \quad (3.3)$$

where (2.13) has been used. These equations are two, coupled, non-linear equations in the two unknowns,  $z$  and  $z_{\text{ion}}$ . Fortunately, they can be solved through order  $\epsilon^4$  in a fairly straightforward manner. First, given  $z$ , equation (3.3) yields,

$$z_{\text{ion}} = \frac{2\zeta}{Z} \left( \frac{m\tilde{h}^2}{Mh^2} \right)^{\frac{3}{2}} \left\{ 1 - \sqrt{\pi} Z^2 \epsilon^3 \left[ 2Z\zeta + \frac{2}{\sqrt{\pi}} I_{-\frac{1}{2}}(z) \right]^{\frac{1}{2}} + o(\epsilon^4) \right\}, \quad (3.4)$$

where the leading order of  $z$  in powers of  $\epsilon$  is sufficient to the accuracy required here.

As the derivatives of the various functions of the fugacity are more natural in terms of  $d \log z$ , it is most convenient to solve (3.2) by means of the expansion

$$z(\zeta, \epsilon) = \exp(\eta_0(\zeta) + \eta_2(\zeta)\epsilon^2 + \eta_3(\zeta)\epsilon^3 + \eta_4(\zeta)\epsilon^4 + \dots), \quad z_0(\zeta) = \exp(\eta_0(\zeta)). \quad (3.5)$$

To leading order in  $\epsilon$ , *i.e.*,  $\epsilon^0$ , (3.2) yields

$$\zeta = \frac{I_{\frac{1}{2}}(z)}{\Gamma(\frac{3}{2})}. \quad (3.6)$$

Since, (2.2), the right-hand side is a series in  $z$  beginning with  $z + \dots$ , the series may be reverted to give  $z_0(\zeta)$  as its solution. This procedure has been done by Baker and Johnson [5] through order  $\zeta^{35}$ . They carried at least 58 decimal places as the equations are rather ill conditioned. The solutions for the remaining terms are

$$\eta_2(\zeta) = -\frac{1}{\sqrt{\pi}} I_{-\frac{1}{2}}(z_0(\zeta)), \quad (3.7)$$

$$\eta_3(\zeta) = -\sqrt{\pi} \left[ Z^2 \left( \frac{h^2 M}{\tilde{h}^2 m} \right)^{\frac{3}{2}} z_{\text{ion}} + \frac{2}{\sqrt{\pi}} I_{-\frac{1}{2}}(z_0(\zeta)) \right]^{\frac{1}{2}} \frac{z \frac{d}{dz} I_{-\frac{1}{2}}(z_0(\zeta))}{I_{-\frac{1}{2}}(z_0(\zeta))}, \quad (3.8)$$

$$\begin{aligned} \eta_4(\zeta) = & \frac{3}{2\pi} I_{-\frac{1}{2}}(z_0(\zeta)) z \frac{d}{dz} I_{-\frac{1}{2}}(z_0(\zeta)) \\ & + \frac{\sqrt{\pi}}{I_{-\frac{1}{2}}(z_0(\zeta))} \left( \frac{1}{2} z \frac{d}{dz} \hat{T}(z_0(\zeta)) + z \frac{d}{dz} \hat{\Theta}(z_0(\zeta)) \right), \end{aligned} \quad (3.9)$$

where the leading order of  $z_{\text{ion}}$  in powers of  $\epsilon$  is sufficient to the accuracy required here.

When these results are back substituted into (2.4) and expanded in powers of  $y$ , we get,

$$\frac{P\Omega}{NkT} = G_0(\zeta) + G_2(\zeta)y^2 + G_3(\zeta)y^3 + G_4(\zeta)y^4 + o(\epsilon^4). \quad (3.10)$$

The coefficients in this expansion are,

$$G_0(\zeta) = 1 + Z \frac{2I_{\frac{3}{2}}(z_0(\zeta))}{3I_{\frac{1}{2}}(z_0(\zeta))}, \quad (3.11)$$

$$G_2(\zeta) = - \left( \frac{3Z}{8\pi\zeta} \right)^{\frac{1}{3}} \left( \frac{1}{\sqrt{\pi}} I_{-\frac{1}{2}}(z_0(\zeta)) - \frac{1}{\pi\zeta} \hat{X}(z_0(\zeta)) \right), \quad (3.12)$$

$$G_3(\zeta) = - \left( \frac{3}{8\zeta} \right)^{\frac{1}{2}} \left\{ \left( \hat{Z} + \frac{z \frac{d}{dz} I_{-\frac{1}{2}}(z_0(\zeta))}{I_{-\frac{1}{2}}(z_0(\zeta))} \right) \left[ 2\hat{Z}\zeta + \frac{2}{\sqrt{\pi}} I_{-\frac{1}{2}}(z_0(\zeta)) \right]^{\frac{1}{2}} - \frac{1}{3\zeta} \left[ 2\hat{Z}\zeta + \frac{2}{\sqrt{\pi}} I_{-\frac{1}{2}}(z_0(\zeta)) \right]^{\frac{3}{2}} \right\}, \quad (3.13)$$

$$G_4(\zeta) = \frac{1}{4\sqrt[3]{Z}} \left( \frac{3}{\pi\zeta} \right)^{\frac{2}{3}} \left[ \frac{3}{2\pi} I_{-\frac{1}{2}}(z_0(\zeta)) z \frac{d}{dz} I_{-\frac{1}{2}}(z_0(\zeta)) - \frac{1}{2\pi^{\frac{3}{2}}\zeta} \left( I_{-\frac{1}{2}}(z_0(\zeta)) \right)^3 + \frac{\sqrt{\pi}}{I_{-\frac{1}{2}}(z_0(\zeta))} \left( \frac{1}{2} z \frac{d}{dz} \hat{T}(z_0(\zeta)) + z \frac{d}{dz} \hat{\Theta}(z_0(\zeta)) \right) - \frac{1}{\zeta} \left( \frac{1}{2} \hat{T}(z_0(\zeta)) + \hat{\Theta}(z_0(\zeta)) \right) \right], \quad (3.14)$$

where Baker and Johnson [1] report that for a pure element,  $\hat{Z} = Z$ . and in the case of mixtures,

$$Z = \frac{\sum_{\text{species}} N_j Z_j}{\sum_{\text{species}} N_j}, \quad \hat{Z} = \frac{\sum_{\text{species}} N_j Z_j^2}{\sum_{\text{species}} N_j Z_j}, \quad (3.15)$$

where  $N_j$  is the number of ions and  $Z_j$  is the nuclear charge in each species.

#### IV. EVALUATION OF THE COEFFICIENTS OF THE PERTURBATION EXPANSION

The coefficients of the perturbation expansion have been determined as functions of  $\zeta$ . Specifically they have been determined as power series in  $\zeta$ . Here we will give approximations to them in compact form. The most straightforward one follows immediately from (3.6)

$$I_{\frac{1}{2}}(\zeta) \equiv I_{\frac{1}{2}}(z_0(\zeta)) = \sqrt{\pi}\zeta. \quad (4.1)$$

Next, Baker and Johnson [5] have given the representation,

$$\frac{2I_{\frac{3}{2}}(z_0(\zeta))}{3I_{\frac{1}{2}}(z_0(\zeta))} \equiv g_0(\zeta) \approx \left[ \frac{1 + 0.61094880\zeta + 0.12660436\zeta^2 + 0.0091177644\zeta^3}{1 + 0.080618739\zeta} \right]^{\frac{1}{3}}, \quad (4.2)$$

This representation, and all the subsequent ones given in this section are accurate to about 0.1 %. The next ingredient we need was given by Baker and Johnson [6],

$$I_{-\frac{1}{2}}(\zeta) \equiv I_{-\frac{1}{2}}(z_0(\zeta)) = \frac{\sqrt{\pi}\zeta}{g_0(\zeta) + \zeta g_0'(\zeta)} \approx \sqrt{\pi}\zeta \left[ \frac{v_3(\zeta)}{u_5(\zeta)} \right]^{\frac{1}{3}}, \quad (4.3)$$

where

$$\begin{aligned} v_3(\zeta) &= 1 + 0.17549205\zeta + 1.1833437 \times 10^{-2}\zeta^2 + 3.0923597 \times 10^{-4}\zeta^3, \\ u_5(\zeta) &= 1 + 1.2361522\zeta + 0.54327035\zeta^2 + 9.7985998 \times 10^{-2}\zeta^3 \\ &\quad + 6.1912639 \times 10^{-3}\zeta^4 + 1.6191557 \times 10^{-4}\zeta^5. \end{aligned} \quad (4.4)$$

Three further ingredients were given by Baker and Johnson,

$$X(\zeta) \equiv \hat{X}(z_0(\zeta)) \approx \zeta^2 \frac{\pi}{2} \left[ \frac{1 + 0.088412769\zeta}{1 + 0.79551953\zeta + 0.19350034\zeta^2 + 0.013716390\zeta^3} \right]^{\frac{1}{3}}, \quad (4.5)$$

$$\Theta(\zeta) \equiv \hat{\Theta}(z_0(\zeta)) \approx \frac{\mu_6(\zeta)}{\theta_5(\zeta)}, \quad (4.6)$$

where

$$\begin{aligned} \mu_6(\zeta) &= 0.30229989\zeta^3 + 5.0287616 \times 10^{-2}\zeta^4 + 3.6103004 \times 10^{-3}\zeta^5 \\ &\quad + 1.0210313 \times 10^{-4}\zeta^6, \\ \theta_5(\zeta) &= 1 + 1.2478566\zeta + 0.55778521\zeta^2 + 0.10432105\zeta^3 \\ &\quad + 7.2823921 \times 10^{-3}\zeta^4 + 2.1384429 \times 10^{-4}\zeta^5. \end{aligned} \quad (4.7)$$

$$T(\zeta) \equiv \hat{T}(z_0(\zeta)) \approx \frac{\nu_6(\zeta)}{\tau_5(\zeta)}, \quad (4.8)$$

where

$$\begin{aligned} \nu_6(\zeta) &= 1.5397859\zeta^2 + 0.681831\zeta^3 + 0.10939850\zeta^4 \\ &\quad + 8.8741342 \times 10^{-3}\zeta^5 + 2.67165364 \times 10^{-4}\zeta^6, \\ \tau_5(\zeta) &= 1 + 1.3317659\zeta + 0.66394907\zeta^2 + 0.15311424\zeta^3 \\ &\quad + 1.6850905 \times 10^{-2}\zeta^4 + 8.8319130 \times 10^{-4}\zeta^5. \end{aligned} \quad (4.9)$$

In order to complete our set of representations, we need representations for the other three functions. To obtain them we substitute the Baker and Johnson [5] series expansion for  $z_0(\zeta)$  into those three functions to produce series expansions in  $\zeta$ . By combining (2.18) and (3.6), we find the asymptotic result,

$$\zeta \asymp \frac{(\log z)^{\frac{3}{2}}}{\Gamma(\frac{5}{2})}, \quad z \rightarrow \infty, \quad (4.10)$$

which allows us to convert our previously given asymptotic results in  $z$  to results in  $\zeta$ . By use of the Padé approximant method [7], tailored to represent the series about  $\zeta = 0$  and the asymptotic behavior at  $z \rightarrow \infty$ , we have computed the following representations.

$$z \frac{d}{dz} I_{-\frac{1}{2}}(\zeta) \approx \sqrt{\pi}\zeta \left[ \frac{q_9(\zeta)}{r_{13}(\zeta)} \right]^{\frac{1}{3}}, \quad (4.11)$$

where

$$\begin{aligned} q_9(\zeta) &= 1 + 0.37668660\zeta + 9.6301161 \times 10^{-2}\zeta^2 + 1.5693115 \times 10^{-2}\zeta^3 \\ &\quad + 1.9382738 \times 10^{-3}\zeta^4 + 1.7187680 \times 10^{-4}\zeta^5 + 1.1386611 \times 10^{-5}\zeta^6 \\ &\quad + 5.2236572 \times 10^{-7}\zeta^7 + 1.5250645 \times 10^{-8}\zeta^8 + 2.8147079 \times 10^{-10}\zeta^9, \\ r_{13}(\zeta) &= 1 + 3.5586672\zeta + 5.6761084\zeta^2 + 5.3449240\zeta^3 + 3.2936668\zeta^4 \\ &\quad + 1.3912374\zeta^5 + 0.41034013\zeta^6 + 8.4619775 \times 10^{-2}\zeta^7 \\ &\quad + 1.2086067 \times 10^{-2}\zeta^8 + 1.1828498 \times 10^{-3}\zeta^9 + 7.9676618 \times 10^{-5}\zeta^{10} \\ &\quad + 3.7403172 \times 10^{-6}\zeta^{11} + 1.1210162 \times 10^{-7}\zeta^{12} + 2.0835040 \times 10^{-9}\zeta^{13}. \end{aligned} \quad (4.12)$$

$$z \frac{d}{dz} \Theta(\zeta) \approx \zeta^3 \left[ \frac{\sigma_5(\zeta)}{\omega_{13}(\zeta)} \right]^{\frac{1}{3}}, \quad (4.13)$$

where

$$\begin{aligned} \sigma_5(\zeta) = & 0.74589509 + 9.6382201 \times 10^{-2} \zeta + 2.5364237 \times 10^{-2} \zeta^2 \\ & + 1.7998638 \times 10^{-3} \zeta^3 + 1.8272243 \times 10^{-4} \zeta^4 + 6.5777413 \times 10^{-6} \zeta^5, \\ \omega_{13}(\zeta) = & 1 + 5.5159030 \zeta + 14.121520 \zeta^2 + 22.232525 \zeta^3 + 24.033724 \zeta^4 \\ & + 18.855659 \zeta^5 + 11.057783 \zeta^6 + 4.9145985 \zeta^7 + 1.6582118 \zeta^8 \\ & + 0.42040226 \zeta^9 + 7.8062423 \times 10^{-2} \zeta^{10} + 1.0090665 \times 10^{-2} \zeta^{11} \\ & + 8.1802486 \times 10^{-4} \zeta^{12} + 3.1641077 \times 10^{-5} \zeta^{13}. \end{aligned} \quad (4.14)$$

$$z \frac{d}{dz} T(\zeta) \approx \zeta^2 \left[ \frac{s_{11}(\zeta)}{t_{16}(\zeta)} \right]^{\frac{1}{3}}, \quad (4.15)$$

$$\begin{aligned} s_{11}(\zeta) = & 29.205927 + 18.336679 \zeta + 5.7381144 \zeta^2 + 1.2777140 \zeta^3 \\ & + 0.22387177 \zeta^4 + 3.1394202 \times 10^{-2} \zeta^5 + 3.4607956 \times 10^{-3} \zeta^6 \\ & + 3.3616630 \times 10^{-4} \zeta^7 + 2.2772942 \times 10^{-5} \zeta^8 + 1.4387042 \times 10^{-6} \zeta^9 \\ & + 5.0169486 \times 10^{-8} \zeta^{10} + 1.1753523 \times 10^{-9} \zeta^{11}, \\ t_{16}(\zeta) = & 1 + 5.6888442 \zeta + 15.084824 \zeta^2 + 24.728910 \zeta^3 + 28.024183 \zeta^4 \\ & + 23.252756 \zeta^5 + 14.592415 \zeta^6 + 7.0532994 \zeta^7 + 2.6484232 \zeta^8 \\ & + 0.77327943 \zeta^9 + 0.17453022 \zeta^{10} + 3.0057345 \times 10^{-2} \zeta^{11} \\ & + 3.8682590 \times 10^{-3} \zeta^{12} + 3.6101238 \times 10^{-4} \zeta^{13} + 2.3433749 \times 10^{-5} \zeta^{14} \\ & + 9.8914961 \times 10^{-7} \zeta^{15} + 2.2239400 \times 10^{-8} \zeta^{16}. \end{aligned} \quad (4.16)$$

These representations complete the ingredients necessary to compute expansion coefficients  $G_j(\zeta)$  given by equations (3.11-14).

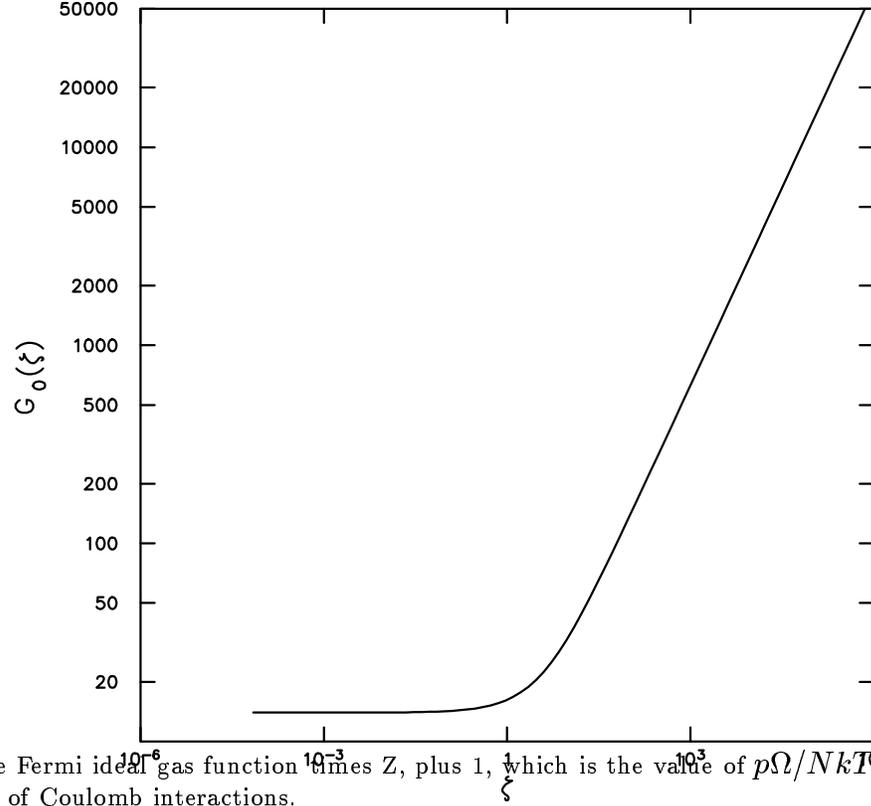
It is worth noting that the information we have obtained so far also allows us to give the leading terms in the expansion in inverse temperature of the first two terms of the low density expansion of the pressure (and, of course, of other thermodynamic quantities as well). For compactness of expression we will use the de Broglie density  $\zeta$ , which is proportional to the ordinary density, and  $\epsilon$  which is an inverse temperature variable (3.1), to express our results.

$$\begin{aligned} \frac{p\Omega}{NkT} = & 1 + Z \left\{ 1 - \zeta^{\frac{1}{2}} \left[ \frac{\sqrt{2\pi}}{3} (\hat{Z} + 1)^{\frac{3}{2}} \epsilon^3 + \dots \right] \right. \\ & \left. + \zeta \left[ \frac{1}{2^{\frac{5}{2}}} - \frac{1}{2} \epsilon^2 + \frac{\pi \ln 2}{2\sqrt{2}} \epsilon^4 + \dots \right] + o(\zeta) \right\}, \end{aligned} \quad (4.17)$$

which conforms well with the result that there is complete ionization in the low density limit [8].

## V. BEHAVIOR OF THE COEFFICIENTS OF THE PERTURBATION EXPANSION

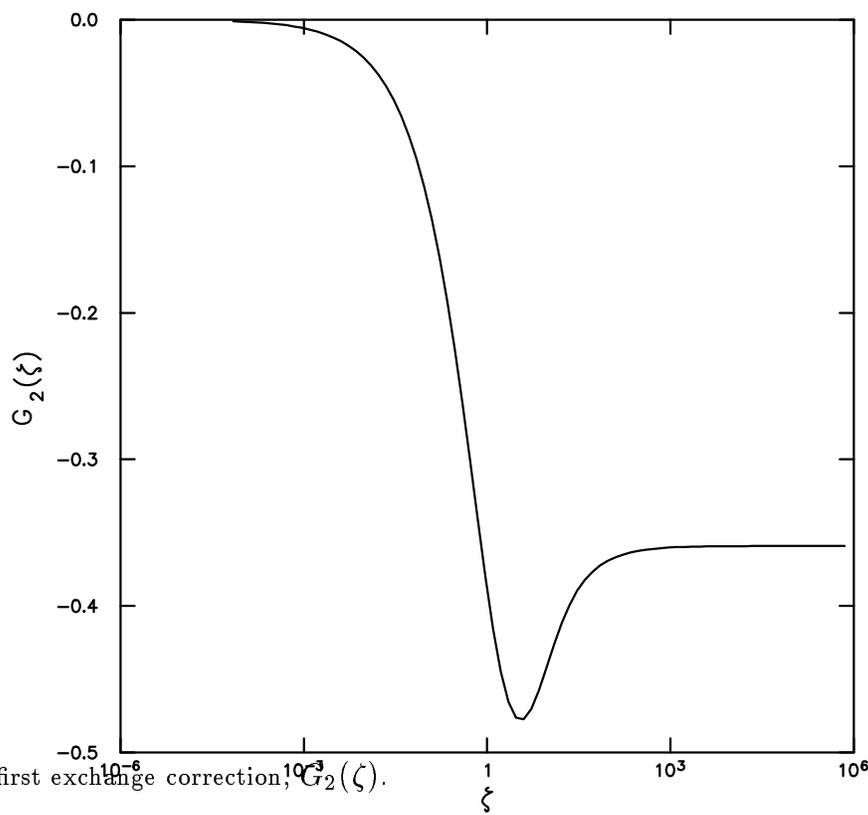
In figures 1 – 4 we plot, as a function of  $\zeta$  the de Broglie density, the values of the coefficients  $G_j$  of (3.11-14) for the sample case of Aluminum ( $Z = 13$ ).



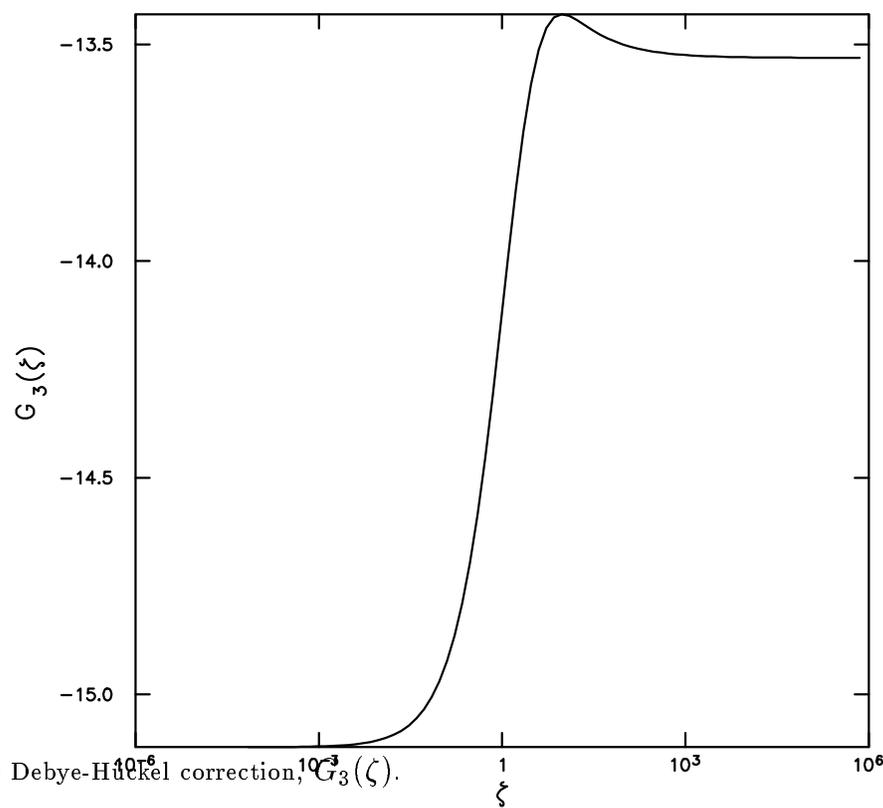
**Fig. 1.** The Fermi ideal gas function  $10^3$  times  $Z$ , plus 1, which is the value of  $p\Omega/NkT$  in the absence of Coulomb interactions.

The structure of the coefficients  $G_j(\zeta)$  shown in the figures reveals three basic regions. The smoothly behaving low density and high density regions, and the somewhat more complex transition region. The function  $G_0(\zeta)$  tends to  $1 + Z$  for small  $\zeta$  and diverges like  $\zeta^{\frac{2}{3}}$  as  $\zeta \rightarrow \infty$ . The function  $G_2(\zeta)$  vanishes like  $\zeta^{\frac{2}{3}}$  when  $\zeta$  vanishes and goes to a constant value for large  $\zeta$ . The function  $G_3(\zeta)$  changes very little over the whole range of  $\zeta$  and is always of order unity. That is to say that this term is basically a classical one with very little dependence on quantum effects, *i.e.*, on  $\zeta$ . The function  $G_4(\zeta)$  vanishes like  $\zeta^{\frac{1}{3}}$  as  $\zeta \rightarrow 0$ . As  $\zeta \rightarrow \infty$ , the leading order terms are of nominal order  $\zeta^{-\frac{2}{3}}$ , however they cancel identically. The next order should be of the order of  $\zeta^{-2}$ , and this probably describes the actual behavior for large  $\zeta$ . Numerically, however it appears to fall off about like  $\zeta^{-\frac{5}{3}}$  because the representations which we use, while good to within a tenth of a percent, will not necessarily adequately represent differences where the dominant terms cancel out. Consequently our numerical difference is smaller than the dominant terms by a factor of  $\zeta^{-1}$  rather than by a factor of  $\zeta^{-\frac{4}{3}}$  as might be expected from the asymptotic behavior [3] of the functions involved. It should, however, be remarked that this cancellation problem only occurs when  $G_4(\zeta)$  is significantly smaller than the other terms.

These remarks concerning the large  $\zeta$  behavior can be summarized in terms of



**Fig. 2.** The first exchange correction,  $G_2(\zeta)$ .



**Fig. 3.** The Debye-Hückel correction,  $G_3(\zeta)$ .

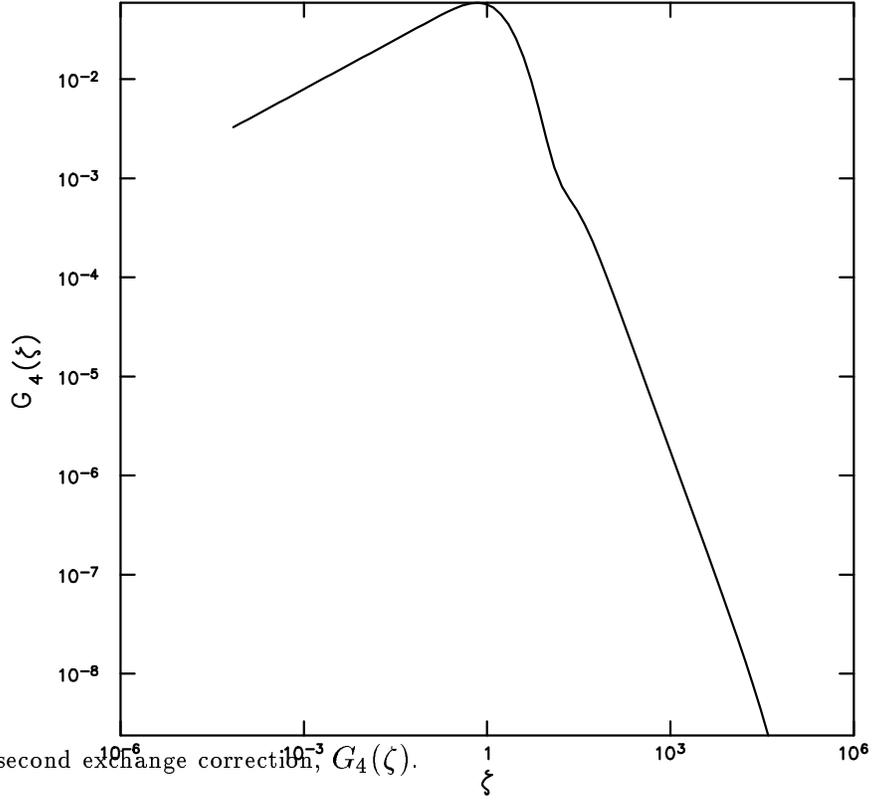


Fig. 4. The second exchange correction,  $G_4(\zeta)$ .

the leading order behavior of the coefficients in the high temperature expansions,

$$\frac{p\Omega}{NkT} \asymp 1 + Z\zeta^{\frac{2}{3}} \left[ \frac{2}{5} \left( \frac{3\sqrt{\pi}}{4} \right)^{\frac{2}{3}} - \frac{1}{2\sqrt{\pi}} \left( \frac{3\sqrt{\pi}}{4} \right)^{\frac{1}{3}} \zeta^{-\frac{1}{3}} \epsilon^2 - \frac{\sqrt{2\pi}}{3} \hat{Z}^{\frac{3}{2}} \zeta^{-\frac{1}{6}} \epsilon^3 + O(\zeta^{-2})\epsilon^4 + o(\epsilon^4) \right]. \quad (5.1)$$

In addition to the inverse-temperature expansions (4.17) and (5.1), there is a high-density version of the electric charge expansion. It is

$$\frac{p\Omega}{NkT} = \hat{G}_0(\zeta) + \hat{G}_2(\zeta)x_0 + \hat{G}_3(\zeta)x_0^{\frac{3}{2}} + \hat{G}_4(\zeta)x_0^2 + o(x_0^2), \quad (5.2)$$

where the coefficients are given by (3.1) and (3.11-14) as

$$\begin{aligned} \hat{G}_0(\zeta) &= G_0(\zeta), & \hat{G}_2(\zeta) &= 2 \left( \frac{Z}{9\pi} \right)^{\frac{1}{3}} \zeta^{\frac{2}{3}} G_2(\zeta), \\ \hat{G}_3(\zeta) &= 2 \left( \frac{2Z}{9\pi} \right)^{\frac{1}{2}} \zeta G_3(\zeta), & \hat{G}_4(\zeta) &= 4 \left( \frac{Z}{9\pi} \right)^{\frac{2}{3}} \zeta^{\frac{4}{3}} G_4(\zeta). \end{aligned} \quad (5.3)$$

The expansion (5.2) is fine for small  $\zeta$  (which actually means very large  $T$ ), but is not a true high-density expansion, because for fixed  $T$ ,  $\zeta$  diverges as  $x_0 \rightarrow 0$  and, as the coefficients diverge with  $\zeta$ , we have a singular expansion. Even when divided by

$\hat{G}_0(\zeta)$ ,  $\hat{G}_3(\zeta)$  still contributes a divergence. This feature is in contrast to Thomas-Fermi theory [6] where the limiting values of the coefficients in (5.2) are all finite. Note that Thomas-Fermi theory also lacks the offending  $\hat{G}_3$  term which spoils this expansion in our case. In addition, it lacks a phase transition as temperature (or density) approach zero along a line of constant  $\zeta$ , as is most likely the case for real substances. A phase transition represents a barrier to the analytic continuation of the series expansion.

There is one more insight that we have noticed from the expansion in the electric charge. Let us consider the limit as  $x_0 \rightarrow 0$  for fixed  $y$ . By (3.1),  $\zeta \rightarrow \infty$  in this limit. One reason that this procedure is of interest is that  $y$  measures the ratio of the interaction energy to the thermal energy. Thus we might expect that for large  $y$  the model will give the ‘‘cold curve.’’ Physically speaking, when this ratio is large enough, we expect that a further reduction in the temperature will make no difference and the pressure will depend on the density alone. If we use the asymptotic behavior that we have previously gotten for this limit, we obtain the expansion terms,

$$p \asymp \frac{2}{5} \left[ \frac{\hbar^2}{2m} \left( \frac{6\pi^2 ZN}{2\Omega} \right)^{\frac{2}{3}} \right] \left( \frac{ZN}{\Omega} \right) \times \left\{ 1 - x_0 \left[ \frac{5}{6\pi} \left( \frac{3}{2\pi Z} \right)^{\frac{1}{3}} + \frac{5\hat{Z}^{\frac{3}{2}}}{9\pi Z^{\frac{2}{3}}} (12\pi^2)^{\frac{1}{6}} y + \dots \right] + o(x_0) \right\}, \quad (5.4)$$

where the first square-bracketed term is the usual Fermi energy. We expect that higher order terms from the repeated scattering of the same two particles will contribute more  $y$  dependence to the  $x_0$  term (the corrections to  $G_0$  contribute to the  $x_0^2$  term). Terms involving the simultaneous interaction between three or more particles should contribute to higher powers of  $x_0$  (except for cases like the ring diagrams which have singularities due to the nature of the Coulomb potential) because at least two particles must be in the same spin-state and so their relative wave function must be anti-symmetric, which puts a zero in the wave function when the positions coincide.

## REFERENCES

1. G. A. Baker, Jr. and J. D. Johnson, ‘‘Many-Body Perturbation Theory for the Pressure of an Electron-Ion System,’’ in *Condensed Matter Theories* **10**, 173, edited by M. Casas, M de Llano, J. Navarro, and A. Polis, Nova Science Pubs., Commack, NY, 1995.
2. T. Matsubara, ‘‘A New Approach to Quantum Statistical Mechanics,’’ *Prog. Theor. Phys.* **14**, 351 (1955).
3. K. Huang, *Statistical Mechanics*, John Wiley & Sons, New York, 1963.
4. A. A. Abrikosov, L. P. Gorkov and I. E. Dzyaloshinski, *Methods of Field Theory in Statistical Physics*, as transl. by R. A. Silverman, Prentice-Hall, Englewood Cliffs, N. J., 1963.
5. G. A. Baker, Jr. and J. D. Johnson, ‘‘Thomas-Fermi Equation of State—The Hot Curve,’’ *Condensed Matter Theories* **5**, 1, edited by V. C. Aguilera-Navarro, Plenum Press, New York, 1990.
6. G. A. Baker, Jr. and J. D. Johnson, ‘‘General structure of the Thomas-Fermi equation of state,’’ *Phys. Rev. A* **44**, 2271 (1991).
7. G. A. Baker, Jr. and P. R. Graves-Morris, *Padé Approximants, second edition, Encyclopedia of Mathematics and Its Applications* **59**, editor G.-C. Rota, Cambridge University Press, London, 1996.
8. J. L. Lebowitz and R. E. Peña, ‘‘Low density form of the free energy for real matter,’’ *J. Chem. Phys.* **59**, 1362 (1973).