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EVALUATION OF SOME INTEGRALS ARISING IN
THE THEORY OF IONIZED GASES

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ABSTRACT

In some recent theories of the equation of state of classical ionized systems, the free energy depends on integrals of the form

$$\int_0^\infty \left[e^{-\beta V_s} - 1 + \beta V_s - \beta^2 V_s^2 / 2 \right] r^2 dr,$$

where V_s is a "screened" potential obtained from the real potential by summing certain infinite series of diagrams.

This integral has been tabulated for V_s appropriate to a potential $\pm(e^2/r)(1 - e^{-\gamma r})$. The equation of state is also given for a one-component electron gas in a uniform background of positive charge (limit $\gamma \rightarrow \infty$).

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In the Meeron-Friedman-Abe¹ theory of ionized systems, the free energy is written in the form

$$\beta F = \bar{N} \sum S_j(\lambda), \quad (1)$$

where each S_j represents the contribution of a certain class of diagrams, and depends on the parameter $\lambda = (4\pi)^{1/2} (e^2 \rho^{1/3} \beta)^{3/2}$, where ρ = density, $\beta = 1/kT$, $\bar{N} = \rho V$. S_1 is the "ring integral" which, in the case of an electron gas in a uniform background of positive charge, is simply the Debye-Hückel result, $-\lambda/3$.

The next term is found to be

$$S_2 = (\rho/2) \int_0^\infty 4\pi r^2 dr \left\{ e^{-\beta V_s} - 1 + \beta V_s - \beta^2 V_s^2/2 \right\}, \quad (2)$$

where V_s is a screened potential function obtained from the real potential $V(r)$ by the operation

$$V_s(r) = F^{-1} \left\{ \frac{FV(r)}{1 + \beta N F V(r)} \right\}; \quad (3)$$

F indicates the Fourier transform. Equation (2) may be considered a modification of the usual second virial coefficient, in which the divergence due to the long range of the Coulomb potential has been eliminated. Expressions similar to Eq. (2) occur in a recent paper by Yukhnovskii.²

In a system with both positive and negative point charges, S_2 is still divergent if $V(r)$ is an attractive Coulomb potential, so some kind of cutoff must be used. We employ here the potential $\pm(e^2/r)(1 - e^{-\gamma r})$, similar to one first used by Kramers³ in considering this problem. The screened potential is then

$$\beta V_s(r) = \pm (\lambda_D/r)(\lambda/y) \left[\exp \left\{ -(r/\lambda_D) [2/(1+y)]^{1/2} \right\} - \exp \left\{ -\gamma \lambda_D (r/\lambda_D) [(1+y)/2]^{1/2} \right\} \right], \quad (4)$$

where

$$\lambda_D = 1/(4\pi\beta e^2 \rho)^{1/2},$$

and

$$y = \left(1 - 4/\lambda_D^2 \gamma^2 \right)^{1/2}, \quad \gamma \lambda_D \geq 2.$$

Substituting $x = r/\lambda_D$ reduces this to

$$\beta V_s(r) = q(x) = (\lambda/xy) \left[\exp \left\{ -x[2/(1+y)] \right\} - \exp \left\{ -x[2/(1-y)] \right\} \right],$$

and Eq. (2) becomes

$$S_2 = (1/2\lambda)I_1(\lambda, y) + I_2. \quad (5)$$

$$I_1 = \int_0^\infty x^2 dx [\exp \{-q(x)\} - 1];$$

$$I_2 = 1/2 + (\lambda/8\sqrt{2} y^3) \{1 - (1 - y^2)^{1/2}\} \{(1 - y)^{1/2} - (1 + y)^{1/2}\}.$$

The integral $I_1(\lambda, y)$ is given in Table 1. The case $y = 1$ (or $\gamma \rightarrow \infty$) is the limit of a pure Coulomb potential. In order to calculate the equation of state, one has to differentiate S_2 with respect to density, and combine the contributions from attractive and repulsive interactions. In some theories it is proposed to let γ vary with density or temperature or both, while in others γ might be constant. We have not yet considered any of these procedures in detail, but we have calculated the correction to the Debye-Hückel equation of state for the one-component system with a pure Coulomb potential. In Table 2 we give values of S' defined by

$$PV/RT = 1 - \lambda/6 + S', \quad (6)$$

$$S' = (\lambda/16) + (1/4\lambda) \int_0^\infty [x^2 \exp \{-\lambda x^{-1} e^{-x}\} + \lambda x \exp \{-x - \lambda x^{-1} e^{-x}\}] dx.$$

Some of these values have previously been published⁴ and compared with results obtained, by a different method, by Bowers and Salpeter.

For small values of λ and y the following expansion is useful;

$$I_1 = \sum_{n=1}^{\infty} \{(-\lambda)^n/n!\} J_n, \quad (7)$$

where

$$J_n = (T/n)^3 R^n \sum_{j=0}^{\infty} \sigma_{n,2j} (Q/n)^{2j},$$

$$T = \sqrt{2} (1 - y^2)^{1/2} / \{ (1 + y)^{1/2} + (1 - y)^{1/2} \},$$

$$R = 2\sqrt{2} / [(1 - y^2)^{1/2} \{ (1 + y)^{1/2} + (1 - y)^{1/2} \}],$$

$$Q = 2y / \{ 1 + (1 - y^2)^{1/2} \},$$

$$\sigma_{n,2j} = \frac{(2j+1)(2j+2)}{2^{2j}} \sum_{k=0}^{2j} (-1)^{2j-k} \binom{2j}{k} n^{2j-k} 2^k B_k^{(-n)},$$

and $B_k^{(-n)}$ is the Bernoulli number of order $(-n)$ and degree k (see Milne-Thompson⁵). The following special cases should be noted:

$$\sigma_{n,0} = 2$$

$$\sigma_{n,2} = n$$

$$\sigma_{n,4} = (n/8)(5n - 2)$$

$$\sigma_{n,6} = (n/72)(35n^2 - 42n + 16)$$

The first few terms in the expansion lead to the expression

$$I_1 = -\lambda + (\lambda^2/8\sqrt{2})(1 + \frac{3}{8}y^2 + \frac{11}{128}y^4 + \dots) - (\lambda^3/81)(1 + \frac{11}{12}y^2 + \dots) \\ + (\lambda^4\sqrt{2}/768)(1 + \frac{3}{2}y^2 + \dots) - (\lambda^5/3750)(1 + \frac{21}{10}y^2 + \dots) + \dots$$

The terms of order λ and λ^2 are cancelled out by I_2 when one calculates S_2 .

The ring integral for the potential $\pm(e^2/r)(1 - e^{-\gamma r})$ is (setting $a = \gamma\lambda_D$)

$$S_1 = (\pi/3) \left(1/4 \pi^2 \rho \lambda_D^3 \right) \left\{ \frac{3}{2} a - a^3 + \left(\frac{1}{2} a^2 - \frac{1}{2} \sqrt{a^4 - 4a^2} \right)^{3/2} + \left(\frac{1}{2} a^2 + \frac{1}{2} \sqrt{a^4 - 4a^2} \right)^{3/2} \right\}. \quad (8)$$

For large a this reduces to the Debye-Hückel result,

$$S_1 = \left(1/12 \pi \rho \lambda_D^3 \right) (1 - 9/8a + 3/2a^2 + \dots).$$

Equation (4) is valid only when y is real, i.e., when $a \geq 2$. If this condition is not satisfied one has instead

$$\beta V_s = (2\lambda/xz) e^{-G_2 x} \sin(G_1 x), \quad (9)$$

where

$$G_1 = \left[\frac{y^2}{(1+z^2) \{ (1+z^2)^{1/2} + 1 \}} \right]^{1/2},$$

$$G_2 = \left\{ \frac{(1+z^2)^{1/2} + 1}{1+z^2} \right\}^{1/2},$$

$$z = \left\{ \left(4/\lambda_D^2 y^2 \right) - 1 \right\}^{1/2}.$$

In Table 3 we present some values of I_1 for this case.

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Table 1. Values of $I_1(\lambda, y)$

$\lambda \backslash y =$	0.0	0.2	0.4	0.6	0.8	1.0
0.2	-0.19656	-0.19651	-0.19634	-0.19600	-0.19528	-0.19218
0.6	-0.57063	-0.57023	-0.56892	-0.56627	-0.56094	-0.54401
1.0	-0.92235	-0.92137	-0.91817	-0.91182	-0.89944	-0.86644
1.4	-1.25476	-1.25305	-1.24751	-1.23662	-1.21605	-1.16746
1.8	-1.57033	-1.56779	-1.55962	-1.54378	-1.51458	-1.45161
2.2	-1.87105	-1.86764	-1.85671	-1.83570	-1.79786	-1.72185
2.6	-2.15861	-2.15430	-2.14053	-2.11433	-2.06804	-1.98028
3.0	-2.43440	-2.42917	-2.41257	-2.38122	-2.32680	-2.22285
3.4	-2.69959	-2.69346	-2.67405	-2.63767	-2.57549	-2.46769
3.8	-2.95518	-2.94816	-2.92600	-2.88475	-2.81521	-2.69889
4.2	-3.20204	-3.19415	-3.16931	-3.12336	-3.04687	-2.92287
4.6	-3.44090	-3.43217	-3.40473	-3.35426	-3.27122	-3.14031
5.0	-3.67241	-3.66286	-3.63291	-3.57812	-3.48891	-3.35177
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-0.2	0.20354	0.20359	0.20377	0.20414	0.20494	
-0.6	0.63182	0.63231	0.63392	0.63727	0.64447	
-1.0	1.08839	1.08974	1.09423	1.10352	1.12353	
-1.4	1.57324	1.57590	1.58468	1.60290	1.64211	
-1.8	2.08638	2.09077	2.10529	2.13541	2.20022	
-2.2	2.62780	2.63436	2.65605	2.70104	2.79787	
-2.6	3.19750	3.20667	3.23697	3.29981	3.43504	
-3.0	3.79549	3.80770	3.84803	3.93169	4.11174	
-3.4	4.42177	4.43745	4.48925	4.59671	4.82796	
-3.8	5.07633	5.09591	5.16062	5.29485	5.58372	
-4.2	5.75917	5.78310	5.86215	6.02612	6.37900	
-4.6	6.47030	6.49900	6.59382	6.79052	7.21382	
-5.0	7.20971	7.24362	7.35565	7.58804	8.08816	

Table 2. Values of S'

λ	S'	λ	S'
0.01	0.00003 08192	1.0	0.04013 175
.02	.00010 30911	1.1	.04536 053
.03	.00020 56772	1.2	.05067 545
.04	.00033 28151	1.3	.05606 562
.05	.00048 09159	1.4	.06152 207
.06	.00064 74687	1.5	.06703 732
.07	.00083 05555	1.6	.07260 500
.08	.00102 86384	1.7	.07821 972
.09	.00124 04469	1.8	.08387 685
.10	.00146 49034	1.9	.08957 236
.20	.00424 764	2.0	.09530 277
.30	.00771 585	2.1	.10106 500
.40	.01163 918	2.2	.10685 637
.50	.01589 373	2.3	.11267 449
.60	.02040 247	2.4	.11851 720
.70	.02511 336	2.5	.12438 264
.80	.02998 923	3.0	.15399 659
0.90	.03500 243	3.5	.18398 237
1.00	0.04013 175	4.0	.21423 829
		4.5	.24469 686
		5.0	0.27531 137

Table 3. Values of $I_1(\lambda, z)$

$\lambda \backslash z =$	0.2	0.6	1.0	2.0	3.0
0.2	-0.19661	-0.19694	-0.19738	-0.19830	-0.19883
0.6	-0.57101	-0.57363	-0.57729	-0.58503	-0.58961
1.0	-0.92330	-0.92981	-0.93909	-0.95927	-0.97154
1.4	-1.25642	-1.26790	-1.28457	-1.32177	-1.34496
1.8	-1.57278	-1.58995	-1.61527	-1.67322	-1.71020
2.2	-1.87436	-1.89767	-1.93254	-2.01427	-2.06759
2.6	-2.16280	-2.19251	-2.23755	-2.34549	-2.41742
3.0	-2.43948	-2.47572	-2.53134	-2.66743	-2.75999
-0.2	0.20348	0.20314	0.20267	0.20172	0.20118
-0.6	0.63135	0.62823	0.62399	0.61546	0.61059
-1.0	1.08709	1.07841	1.06665	1.04295	1.02943
-1.4	1.57070	1.55369	1.53063	1.48418	1.45769
-1.8	2.08218	2.05406	2.01593	1.93915	1.89537
-2.2	2.62152	2.57952	2.52257	2.40786	2.34247
-2.6	3.18874	3.13008	3.05053	2.89031	2.79899
-3.0	3.78382	3.70573	3.59982	3.38651	3.26493

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