Phase Shifts of the Static Screened Coulomb Potential[*]

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Phase shifts and their weighted sums over angular momentum states have been obtained for the static screened Coulomb potential (SSCP). Results are given for both an attractive and a repulsive SSCP. A procedure is given for obtaining the phase shifts which uses direct numerical integration near the origin and the first- and second-order WKB approximation at larger distances. At high energy a simple asymptotic fit to the weighted phase-shift sums is obtained. The results are applied to the calculation of the second virial coefficient of plasmas that have no bound states and of those that do have bound states. Very good agreement with the Wigner-Kirkwood expansion is found for a Boltzmann gas interacting through a repulsive SSCP, except that at high temperature, in agreement with DeWitt, the Wigner-Kirkwood expansion is shown to diverge for the SSCP.

I. INTRODUCTION

A detailed study of the bound states of the static screened Coulomb (Yukawa) potential has recently been carried out by Rogers *et al.*[1] (hereafter referred to as RGH). In this paper the results of a similar study of the phase shifts and their weighted sum over angular momentum states of the static screened Coulomb potential (SSCP) will be given. The purpose of the study is threefold. First, the SSCP is a basic potential and its properties are of general interest. Second, the effective many-body interaction plasma potential reduces to this form at high temperature and low density.[2] Third, the results will give insights, both fundamental and numerical, which can be applied to the study of other potentials.

The theory of the quantum-mechanical partition function of dilute interacting gases was developed by Uhlenbeck and Beth[3] and by Gropper.[4] Its calculation requires a knowledge of bound-state eigenvalues and the phase shifts of scattering states. This theory has been applied primarily to the calculation of the second virial coefficient for hard spheres[5] and for He[3] and He[4]. It has not been applied to a plasma potential such as the SSCP. The results of RGH and the present study will be used to calculate the second virial coefficient over a wide range of temperature and screening length.

II. THEORY

A. Phase-Shift Problem

The problem here is to calculate the phase shifts for the SSCP which is given by

$$V(r) = Ze_a e_b e^{-r/D}/r , \qquad (1)$$

where $Ze_a = \pm Ze$ is the charge on particle a, $e_b = \pm e$ is the charge on particle b, and D is the screening length which in plasma theory is given by

$$D = [(4\pi/kT)\textstyle\sum_j \rho_j e^2 Z_j^2]^{-1/2} , \qquad (2)$$

where ρ_j is the number density of particles of type j, and eZ_j is the charge. The work of Jackson and Klein[2] indicates that for low-lying bound states a constant potential $-e^2/D$ should be added to $V(r)$. This may affect the statistical mechanics of the gas, but the solutions of the Schrödinger equation are equivalent. The results given here also apply to a gas of neutral particles interacting through a Yukawa potential $V(r) = ge^{-r/D}/r$.

The radial Schrödinger equation can be put into dimensionless form with the substitutions

$$\rho = Zr/a_\mu, \qquad \lambda_D = ZD/a_\mu$$
$$q^2 = 2\mu a_\mu^2 E/Z^2 \hbar^2, \quad U(\rho) = 2\mu a_\mu^2 V(r)/Z^2 \hbar^2 , \qquad (3)$$

where

$$a_\mu = \hbar^2/\mu e^2 \quad \text{and} \quad \mu = m_a/(1 + m_a/m_b) ,$$

which results in

$$\frac{d^2 R}{d\rho^2} + \frac{1}{\rho}\frac{dR}{d\rho} + \left(q^2 - \frac{l(l+1)}{\rho^2} - U(\rho)\right) R = 0 . \qquad (4)$$

At large ρ such that $q^2 \gg l(l+1)/\rho^2 + U(\rho)$,

$$R \to (1/\rho) \sin[q\rho - \tfrac{1}{2}\pi l + \delta_l(q)] . \qquad (5)$$

For a particle subject only to the centrifugal potential, $\delta_l(q) = 0$. From Eqs. (4) and (5) it is clear that δ_l is positive for an attractive potential and negative for a repulsive potential. The phase shifts δ_l are normally calculated by numerical integration of Eq. (4) or by an approximation method such as the Born[6] or the WKB approximation. A combination of numerical integration and the WKB method will be used in this study.

B. WKB Approximation for δ_l

Any numerical integration will accumulate errors with increasing distance from the origin, and it is not always practical to numerically integrate the Schrödinger equation out to sufficiently large $\rho = \rho_0$ such that the residual phase shift between ρ_0 and ∞ is sufficiently small. This residual phase shift can be calculated quite accurately with the WKB method since the scattered wave is similar to that of a free particle in this range. The WKB approximation is found to work well even in cases where the residual phase shift is appreciable.

The WKB approximation is an expansion of the Schrödinger equation in powers of $\hbar$. The total phase shift given by the first-order term[7] in this expansion is

$$\delta_l^1(q) = \int_{\rho_1}^{\infty} \left(q^2 - \frac{l(l+1)}{\rho^2} - U(\rho) \right)^{1/2} d\rho$$

$$- \int_{\rho_0}^{\infty} \left(q^2 - \frac{l(l+1)}{\rho^2} \right)^{1/2} d\rho , \quad (6)$$

where ρ_0 is the classical turning point of a free

particle and ρ_1 is the classical turning point of a particle subject to the potential $U(\rho)$. Langer[8] has shown that δ_l^1 is considerably improved if $l(l+1)$ is replaced by $(l+1/2)^2$ in Eq. (6).

The phase shift due to the term in $\hbar^2$ is given by[9]

$$\delta_l^2(q) = -\frac{1}{32} \int_{\rho_1}^{\infty} d\rho \, \frac{4f_1''(q^2 - f_1) + 5f_1'^2}{(q^2 - f_1)^{5/2}}$$

$$+ \frac{1}{32} \int_{\rho_0}^{\infty} d\rho \, \frac{4f_0''(q^2 - f_0) + 5f_0'^2}{(q^2 - f_0)^{5/2}} , \quad (7)$$

where

$$f_1 = \frac{l(l+1)}{\rho^2} + U(\rho), \qquad f_0 = \frac{l(l+1)}{\rho^2} . \quad (8)$$

As it stands Eq. (7) diverges. The correct expression for $\delta_l^2(q)$ is obtained by integrating Eq. (7) by parts, discarding all infinite parts of the integrated terms until a convergent integral is obtained. The result for cases in which f_1' has no singularity in the range of integration is given in several places.[9,10] In the case where f_1' has a singularity the result is

$$\delta_l^2(q) - \frac{\pi}{16[l(l+1)]^{1/2}} = - \left[\frac{-f_1}{8(q^2 - f_1)^{3/2}} + \frac{1}{48} \frac{f_1'}{(q^2 - f_1)^{3/2}} - \frac{1}{24} \frac{f_1''}{f'(q^2 - f_1)^{1/2}} \right]_{\rho_1}^{s^{-\epsilon}}$$

$$- \frac{1}{24} \int_{\rho_1}^{\rho_s^{-\epsilon}} \frac{(f_1'''/f_1 - f_1''/f_1'^2)\,d\rho}{(q^2 - f_1)^{1/2}} \qquad \begin{array}{l} + \text{(identical expressions with limits of} \\ \text{integration between } \rho = \rho_s + \epsilon \text{ and } \rho = \infty). \end{array} \quad (9)$$

It is clear that as $\epsilon \to 0$ the divergence in the integral is canceled by the third term in brackets, so that the phase shift across the singularity can be made arbitrarily small.

If both the first- and second-order terms of the WKB expansion are used to compute the phase shift, then the replacement of $l(l+1)$ by $(l+\frac{1}{2})^2$ is no longer valid. This is easily seen by expanding the first-order term of the free-particle expression

$$\int_{\rho_0}^{\infty} \left(q^2 - \frac{(l+\frac{1}{2})^2}{\rho^2} \right)^{1/2} d\rho$$

$$= \int_{\rho_0}^{\infty} \left(q^2 - \frac{l(l+1)}{\rho^2} - \frac{1}{4\rho^2} \right)^{1/2} d\rho$$

$$= \int_{\rho_0}^{\infty} \left(q^2 - \frac{l(l+1)}{\rho^2} \right)^{1/2} d\rho$$

$$- \frac{1}{8} \int_{\rho_0}^{\infty} \frac{d\rho}{\rho^2 [q^2 - l(l+1)/\rho^2]^{1/2}}$$

$$+ \text{(higher-order terms).} \quad (10)$$

The first two terms in this expansion are exactly those obtained in the first and second WKB approximations using $l(l+1)$. Therefore the replacement $(l+\frac{1}{2})^2$ partly approximates the second-order WKB term. Numerical integration of the WKB expressions for the SSCP and comparison with the numerical solutions of the Schrödinger equation verify this result.

A comparison of the WKB expansion with the numerical solution of the Schrödinger equation is given in Fig. 1 for $e_a = -e_b$, $D = 4.542 a_\mu/Z$, and $l = 1$. The SSCP has one bound state of unit angular momentum for this value of D, and the phase shift should approach π rad as $q \to 0$. It is apparent that the second-order term greatly improves the agree-
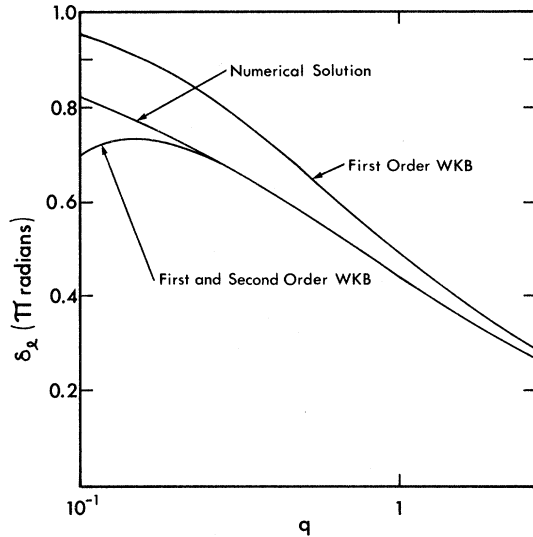
FIG. 1. Comparison of the first- and second-order WKB approximations for the phase shift with the numerical solution of the Schrödinger equation for a particle of unit angular momentum subject to an attractive SSCP with $D = 4.542 a_\mu/Z$.

ment with the numerical solution, and that the first two terms in the WKB expansion are sufficient except at small values of q or if extreme accuracy is desired, as in the present case.

C. Quantum-Mechanical Partition Function and Second Virial Coefficient

The two-body interaction part of the partition function of interacting Boltzmann particles is given by[11]

$$Z_{int} = \sum_l (2l+1) \left(\sum_n e^{-E_{nl}/kT} \right.$$

$$\left. + \frac{1}{\pi} \int_0^\infty dq \, \frac{d\delta_l(q)}{dq} e^{-q^2/T_0} \right) , \quad (11)$$

where $T_0 = 2\mu a_\mu^2 kT/\hbar^2$, and the E_{nl} are the bound-state energies.

In ionization-equilibrium calculations of gases at low temperatures it is usually assumed that only the first term of Eq. (11) is important, and the phase-shift term is ignored. We wish to consider the high-temperature case when the phase-shift term is important, such as in the case of a hydrogen plasma. If one retains only the first term of Eq. (11) for an attractive potential $gu(r)$, as g is decreased the bound states E_{nl} below zero energy move up into the continuum. As each state reaches zero energy, a partition function which includes only the bound-state sum will be discontinuous.

These discontinuities would extend to all the thermal properties, such as pressure and specific heat. However, if we integrate Eq. (11) by parts an interesting fact becomes apparent.[12] From Levinson's theorem we know that the phase shift $\delta_l(q)$ at $q = 0$ is given by $n_l \pi$, where n_l is the number of bound states of angular momentum l. Thus Eq. (11) becomes

$$Z_{int} = \sum_l (2l+1) \sum_n \left(e^{-E_{nl}/kT} - 1 \right)$$

$$+ \frac{2}{\pi T_0} \int_0^\infty q G_B(q) e^{-q^2/T_0} dq , \quad (12)$$

where the double sum in the first term ranges only over bound states, and $G_B(q) = \sum_l (2l+1) \delta_l(q)$.

Equation (12) gives the complete interaction partition function of the system, and can be used to demonstrate two points. First, the zero-energy part of the phase-shift contribution to the partition function exactly cancels the zero-energy part of the bound-state sum, removing the discontinuity, so Z_{int} remains continuous as a function of the interaction strength. Second, there is an additional important contribution from nonzero-energy phase shifts.

This full form of the interacting-particle partition function is essential to a complete and correct calculation of the thermodynamic functions of the system. Obviously, current methods which include only the bound-state sum in Eq. (12) are in error, and introduce discontinuities into the thermodynamic-state function at those points where the bound-state levels pass into the continuum. Accurate thermodynamic results for such a system require that the bound-state levels E_{nl} and the phase shifts δ_l both be calculated in the same manner and to the same degree of accuracy.

For identical particles the exclusion principle modifies the weighting factors depending on whether states have odd or even angular momentum. For Fermi particles the partition function is[13]

$$Z_{int} = (s+1)(2s+1) \left(\sum_{l,odd} (2l+1) \sum_n \left(e^{-E_{nl}/kT} - 1 \right) \right)$$

$$+ s(2s+1) \left(\sum_{l,even} (2l+1) \sum_n \left(e^{-E_{nl}/kT} - 1 \right) \right)$$

$$+ \frac{2(2s+1)}{\pi T_0} \int_0^\infty q G_F(q) e^{-q^2/T_0} dq , \quad (13)$$

where $G_F(q) = (s+1)\sum_{l,odd}(2l+1)\delta_l(q) + s\sum_{l,even}(2l+1) \times \delta_l(q)$. For a Bose gas the spin-weighting factors in G_F are reversed.

The second virial coefficient is composed of the ideal gas exchange virial B_{exch}, and the nonideal

part due to the effective two-body interaction potential B_{int}. It is given by

$$B = B_{exch} + B_{int} = \frac{\pm N\pi^{3/2} a_\mu^3}{2Z^3(2s+1)T_0^{3/2}} - \frac{8N\pi^{3/2} a_\mu^3 Z_{int}}{Z^3(2s+1)^2 T_0^{3/2}} ,$$

(14)

where the minus sign in the first term is for a Bose gas and the plus sign is for a Fermi gas. The second virial coefficient for Boltzmann particles is contained in Eq. (14) in the limit of large quantum numbers $(s \to \infty)$.

The second virial coefficient for a two-component system is given by

$$B = N_a^2 B_{aa} + 2N_a N_b B_{ab} + N_b^2 B_{bb} ,$$

(15)

where N_a and N_b are the mole fractions of components of type a and b, respectively, and B_{aa} and B_{bb} are the second virial coefficients of pure components a and b. B_{ab} is the second cross virial coefficient resulting from ab interactions. The screened second virial coefficient contains a substantial part of the corrections to the Debye-Hückel term for a hydrogen plasma.[14-16] The connection with the known free energy and pressure of a hydrogen plasma and the extension into regions difficult to reach analytically will be made in a later paper.

III. NUMERICAL METHOD

The numerical method used to integrate the Schrödinger equation is the same as that described in RGH, except that in the present problem a single integration is required for each phase shift in contrast with the several integrations (iterations) required to isolate an eigenvalue. This saving in computational requirement is in general more than offset by the large number of states that must be summed over to obtain accurate values of the phase-shift sum. Extensive use of the WKB approximation considerably reduces the amount of computer time required for these calculations, while at the same time providing greater accuracy than can be obtained strictly from numerical integration.

The procedure is to integrate the Schrödinger equation out to $\rho_0/\lambda_D = 4/q^{1/4}$ or to $\rho_0/\lambda_D = 12$, whichever is smallest. The residual phase shift is calculated in the first and second WKB approximations where the integrals now extend from ρ_0 to ∞. At the lowest energies this procedure is used for all values of l. At a given energy the phase shift decreases with increasing l, so that the WKB approximation becomes increasingly accurate and in fact is more accurate than the above procedure at high values of l. At constant l the phase shift decreases with increasing energy, so that the WKB approximation becomes increasingly accurate with increasing energy. At high energy it is found that the WKB approximation can be used exclusively except for a few of the lowest states. At intermediate values of the energy it is found that the combination of numerical integration and the WKB approximation is more accurate up to values of l as high as 50.

At high energy the phase-shift sum for all types of statistics has a simple asymtotic expansion [see below, Eq. (16)], so that it is not necessary
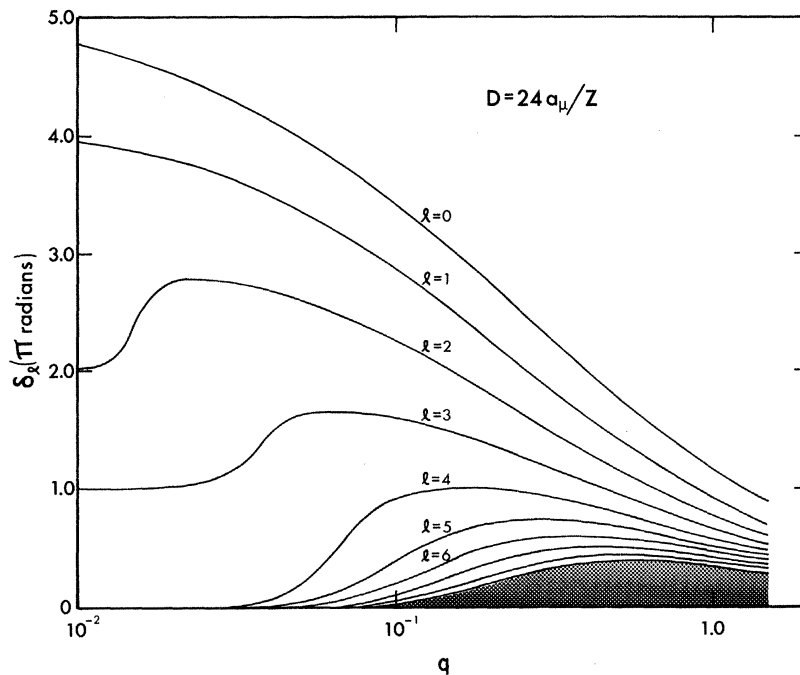

FIG. 2. Phase shift of a particle subject to an attractive SSCP with $D = 24\,a_\mu/Z$, as a function of q for various values of angular momentum.
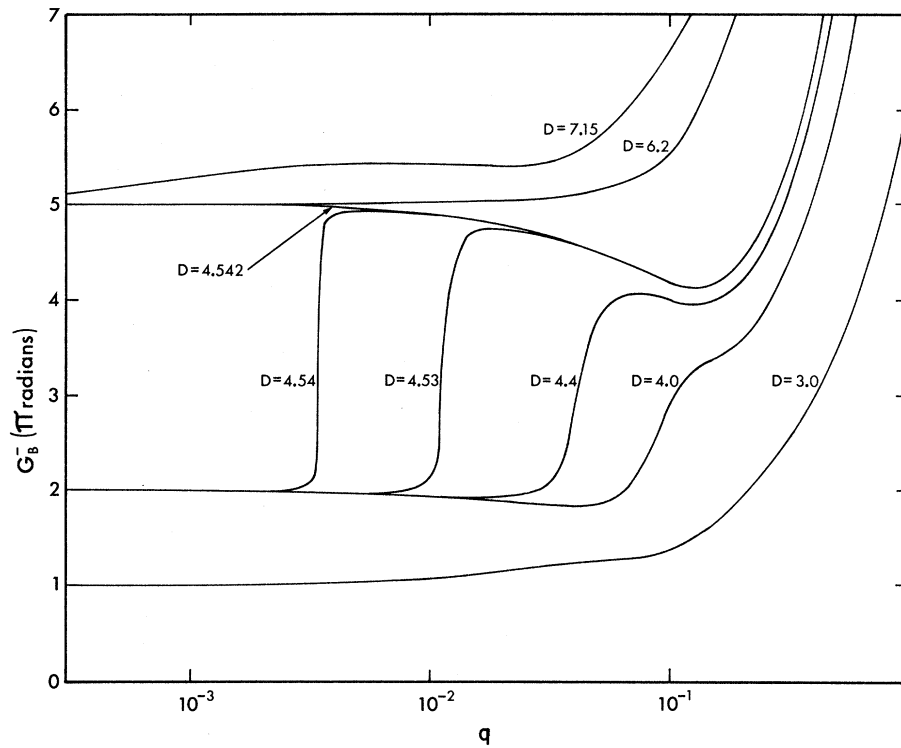
FIG. 3. Phase-shift sum of a Boltzmann particle subject to an attractive SSCP as a function of q for various values of the screening length (in units of a_μ/Z).

to calculate G at very high energies.

These calculations were performed on a CDC 6600 computer which is a 14-place machine. The phase shifts are accurate to a relative error of about 3×10^{-6} and/or to an absolute error of about 1×10^{-11} rad.

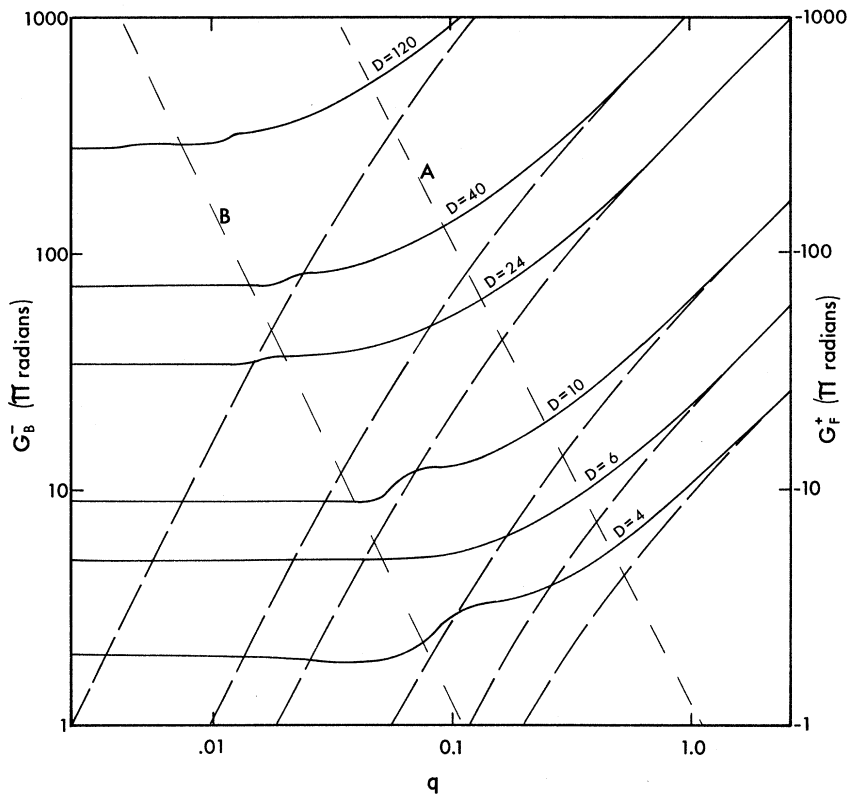

FIG. 4. Phase-shift sum as a function of q for various values of the screening length (in units a_μ/Z). The scale on the right is for Boltzmann particles (solid lines) subject to an attractive SSCP. The scale on the left is for Fermi particles (dashed lines) subject to a repulsive SSCP. The dashed lines labeled A and B delineate regions of special interest.
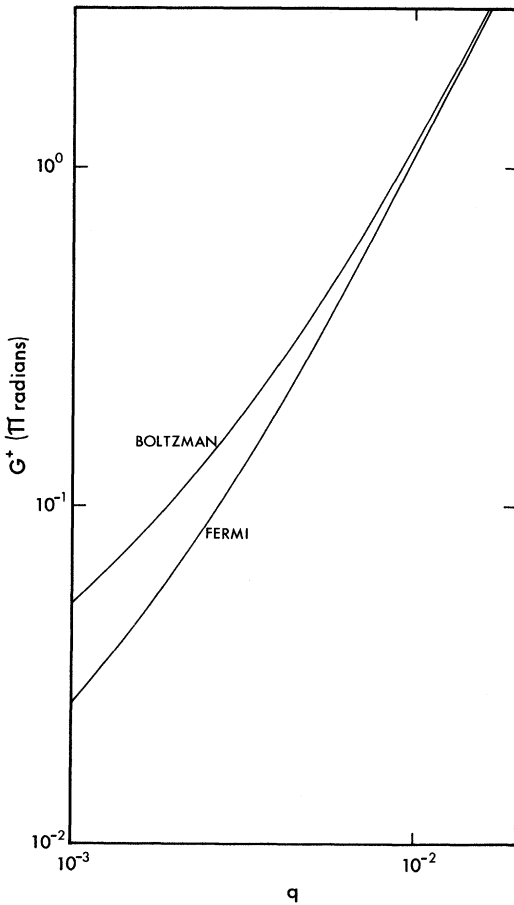
FIG. 5. Comparison of the phase-shift sum for Boltz-mann and Fermi particles interacting through a repulsive SSCP.

IV. RESULTS

A. Phase Shifts and their Weighted Sums

At very small q for the attractive SSCP the phase shift for a given value of l, according to Levinson's theorem, will approach $n_l \pi$, where n_l is the number of bound states of angular momentum l. This is shown in Fig. 2 for $D = 24a_\mu/Z$. The number of bound states for each value of l are the same as the number given in Table III of RGH. For $l = 2$ the phase shift increases with decreasing q, approaching $\delta_l = 3\pi$ rad until at $q = 0.02$ it drops sharply and approaches $\delta_l = 2\pi$ rad. This behavior is typical of potentials which come near to forming a bound state. This is the case here since Table III of RGH indicates that at $D = 25.0 \ a_\mu/Z$ an additional bound state is formed for $l = 2$. Similar behavior is shown by states of higher angular momentum but at increasing values of q, as l increases due to the increasing remoteness of bound states. As l and q increase the phase shifts become more closely

spaced, and the phase-shift sum ranges over larger values of l. For large D and q it was found neces-sary to sum as high as $l = 1500$. When the δ_l be-come closely spaced, the labor involved in the calculations can be reduced by solving for only part of the δ_l's and interpolating for the inter-mediate values.

The sharp behavior of the phase shift at small q for values of D near to where a bound state ap-pears or disappears leads to corresponding rapid changes in the phase-shift sum. This effect is much more pronounced at small D. Figure 3 shows the phase-shift sum at small q for $l = 1$ and for values of D in the range 3–7 a_μ/Z. As D increases from 4 to 4.4 to 4.53 to 4.54 (in units of a_μ/Z), there is an increasing sharp change in G from a value $\approx 2\pi$ to a value $\approx 5\pi$ rad. At $D = 4.542 a_\mu/Z$ the phase-shift sum approaches 5π rad as q ap-proaches zero. This indicates that a bound state is formed between $D = 4.540$ and $D = 4.542 a_\mu/Z$, which agrees with the value 4.541 a_μ/Z given in Table III of RGH. This procedure can be used to isolate to quite high accuracy the values of D at which bound states are formed.

In RGH expressions are given for the total num-ber of bound states n^* and the number of s states g^* in the SSCP as a function of D. Because of the simplicity of the phase-shift method for counting the number of bound states, we have checked these expressions up to $D = 1000 \ a_\mu/Z$, which has 500 bound states. There is exact agreement with the expressions for n^* and g^* given in RGH, if they are rounded to the nearest integer. The phase-shift sums G_B^- and G_F^+ (minus indicates an attractive potential and plus indicates a repulsive potential) are plotted in Fig. 4 for a wide range of screening length. The scale for G_B^- is on the left and the scale for G_F^+ is on the right. We observe that humps in G_B^- tend to move to lower q with increas-ing D. Also, $-G_F^+$ tends to coincide with G_B^- at decreasing q with increasing D. The plot of G_B^- can be considered in three parts. In the part to the right of the line labeled A the phase-shift sum increases rapidly with D and q, and is approxi-mately of the form $f(D) \ g(q)$. The region between the lines B and A is characterized by rapid changes in G_B^-. The region to the left of the line B is char-acterized as a region of very slowly varying values of G_B^-.

The effect of spin on the phase-shift sum is shown in Fig. 5. The difference between G_F^+ and G_B^+ de-creases slowly as q is increased. At high q this difference decreases approximately as $q^{-5/8}$, and is nearly independent of screening length for $D > 4a_\mu/Z$.

The relevant quantities for the calculation of partition functions of a hydrogen plasma are the sums G_B^- and G_F^+. These quantities are given in

TABLE I. G_B^- as a function of screening length and q. (In each entry $A\,n$ means $A \times 10^n$.)

q \ ZD/a_μ	0.5	1	2	4	6	8	10	16	24	40	64	120	300
0.0001		9.9974 −1	9.9995 −1	1.9994 +0	5.0000 +0	5.9983 +0	8.9993 +0	1.7998 +1	3.3998 +1	7.2987 +1	1.5687 +2	3.7798 +2	1.5099 +3
0.0010	3.5121 −4	9.9748 −1	9.9956 −1	1.9942 +0	5.0005 +0	5.9831 +0	8.9931 +0	1.7985 +1	3.3975 +1	7.1875 +1	1.5650 +2	3.7765 +2	1.5222 +3
0.0015	5.2270 −4	9.9622 −1	9.9934 −1	1.9914 +0	5.0007 +0	5.9747 +0	8.9897 +0	1.7977 +1	3.3962 +1	7.1825 +1	1.5646 +2	3.7744 +2	1.5261 +3
0.0022	7.7271 −4	9.9446 −1	9.9903 −1	1.9873 +0	5.0011 +0	5.9631 +0	8.9848 +0	1.7966 +1	3.3944 +1	7.1782 +1	1.5648 +2	3.7809 +2	1.5456 +3
0.0032	1.1239 −3	9.9194 −1	9.9859 −1	1.9816 +0	5.0016 +0	5.9466 +0	8.9778 +0	1.7949 +1	3.3914 +1	7.1808 +1	1.5664 +2	3.7960 +2	1.5469 +3
0.0047	1.6508 −3	9.8817 −1	9.9793 −1	1.9729 +0	5.0023 +0	5.9225 +0	8.9671 +0	1.7922 +1	3.3864 +1	7.2112 +1	1.5690 +2	3.9080 +2	1.5608 +3
0.0069	2.4234 −3	9.8263 −1	9.9695 −1	1.9606 +0	5.0035 +0	5.8892 +0	8.9506 +0	1.7876 +1	3.3780 +1	7.2568 +1	1.5711 +2	3.9187 +2	1.6255 +3
0.0100	3.5119 −3	9.7485 −1	9.9558 −1	1.9435 +0	5.0051 +0	5.8485 +0	8.9256 +0	1.7800 +1	3.3692 +1	7.2793 +1	1.5755 +2	3.9497 +2	1.7109 +3
0.0120	4.2140 −3	9.6984 −1	9.9470 −1	1.9328 +0	5.0063 +0	5.8275 +0	8.9081 +0	1.7746 +1	3.3769 +1	7.3019 +1	1.6466 +2	4.2030 +2	1.7577 +3
0.0150	5.2668 −3	9.6235 −1	9.9345 −1	1.9174 +0	5.0082 +0	5.8063 +0	8.8799 +0	1.7668 +1	3.5259 +1	7.3386 +1	1.6515 +2	4.2812 +2	1.8745 +3
0.0180	6.3198 −3	9.5488 −1	9.9218 −1	1.9029 +0	5.0105 +0	5.8008 +0	8.8497 +0	1.7613 +1	3.6791 +1	7.3830 +1	1.6632 +2	4.3733 +2	1.9868 +3
0.0220	7.7157 −3	9.4498 −1	9.9052 −1	1.8854 +0	5.0141 +0	5.8259 +0	8.8079 +0	1.7646 +1	3.6881 +1	8.2096 +1	1.7181 +2	4.6971 +2	2.1488 +3
0.0260	9.1245 −3	9.3515 −1	9.8890 −1	1.8705 +0	5.0185 +0	5.8985 +0	8.7676 +0	1.8050 +1	3.6859 +1	8.2743 +1	1.7565 +2	4.8872 +2	2.3197 +3
0.0320	1.1225 −2	9.2057 −1	9.8656 −1	1.8545 +0	5.0270 +0	6.1098 +0	8.7225 +0	1.9857 +1	3.7319 +1	8.3886 +1	1.8379 +2	5.2536 +2	2.5896 +3
0.0380	1.3323 −2	9.0629 −1	9.8437 −1	1.8480 +0	5.0384 +0	6.3926 +0	8.7257 +0	2.0485 +1	3.8657 +1	8.7773 +1	1.9348 +2	5.6560 +2	2.8717 +3
0.0470	1.6463 −2	8.8532 −1	9.8141 −1	1.8631 +0	5.0613 +0	6.7191 +0	9.0128 +0	2.0747 +1	4.0501 +1	9.6872 +1	2.1082 +2	6.2905 +2	3.3119 +3
0.0570	1.9940 −2	8.6286 −1	9.7867 −1	1.9302 +0	5.0950 +0	6.9069 +0	1.0784 +1	2.1390 +1	4.2675 +1	1.0268 +2	2.3024 +2	7.0321 +2	3.8181 +3
0.0690	2.4083 −2	8.3718 −1	9.7630 −1	2.1136 +0	5.1461 +0	7.0878 +0	1.2075 +1	2.3191 +1	4.6277 +1	1.1145 +2	2.5478 +2	7.9593 +2	
0.0830	2.8905 −2	8.0914 −1	9.7505 −1	2.4820 +0	5.2223 +0	7.4134 +0	1.2410 +1	2.5318 +1	5.0229 +1	1.2249 +2	2.8474 +2	9.0788 +2	
0.1000	3.4693 −2	7.7794 −1	9.7609 −1	2.9254 +0	5.3478 +0	8.0397 +0	1.2775 +1	2.7299 +1	5.4953 +1	1.3654 +2	3.2252 +2	1.0478 +3	
0.1200	4.1411 −2	7.4516 −1	9.8143 −1	3.2005 +0	5.5572 +0	8.8698 +0	1.3395 +1	2.9678 +1	6.0783 +1	1.5372 +2	3.6841 +2	1.2162 +3	
0.1500	5.1271 −2	7.0342 −1	9.9872 −1	3.3783 +0	5.9957 +0	9.9124 +0	1.4654 +1	3.3535 +1	6.9954 +1	1.8046 +2	4.3930 +2	1.4743 +3	
0.1800	6.0828 −2	6.6948 −1	1.0276 +0	3.5075 +0	6.5237 +0	1.0862 +1	1.6117 +1	3.7602 +1	7.9488 +1	2.0803 +2	5.1189 +2	1.7366 +3	
0.2200	7.3042 −2	6.3430 −1	1.0828 +0	3.7131 +0	7.2672 +0	1.2163 +1	1.8203 +1	4.3235 +1	9.2595 +1	2.4565 +2	6.1044 +2	2.0906 +3	
0.2600	8.4599 −2	6.0847 −1	1.1531 +0	3.9699 +0	8.0235 +0	1.3522 +1	2.0377 +1	4.9040 +1	1.0602 +2	2.8397 +2	7.1033 +2	2.4478 +3	
0.3200	1.0066 −1	5.8348 −1	1.2754 +0	4.4223 +0	9.1859 +0	1.5638 +1	2.3749 +1	5.7972 +1	1.2658 +2	3.4231 +2	8.6184 +2	2.9874 +3	
0.3800	1.1520 −1	5.7140 −1	1.4059 +0	4.9199 +0	1.0384 +1	1.7820 +1	2.7214 +1	6.7093 +1	1.4748 +2	4.0134 +2	1.0146 +3		
0.4700	1.3446 −1	5.7135 −1	1.6042 +0	5.7095 +0	1.2236 +1	2.1179 +1	3.2532 +1	8.1009 +1	1.7924 +2	4.9072 +2			
0.5700	1.5291 −1	5.8950 −1	1.8248 +0	6.6210 +0	1.4348 +1	2.4993 +1	3.8553 +1	9.6689 +1	2.1490 +2	5.9075 +2			
0.6900	1.7216 −1	6.2795 −1	2.0926 +0	7.7439 +0	1.6932 +1	2.9645 +1	4.5881 +1	1.1570 +2	2.5802 +2	7.1140 +2			
0.8300	1.9226 −1	6.8694 −1	2.4112 +0	9.0802 +0	1.9993 +1	3.5141 +1	5.4521 +1	1.3804 +2	3.0861 +2	8.5268 +2			
1.0000	2.1512 −1	7.7030 −1	2.8069 +0	1.0728 +1	2.3754 +1	4.1878 +1	6.5099 +1	1.6533 +2	3.7029 +2	1.0247 +3			
1.2000	2.4157 −1	8.7751 −1	3.2819 +0	1.2691 +1	2.8219 +1	4.9863 +1	7.7620 +1	1.9757 +2	4.4307 +2	1.2274 +3			
1.5000	2.8205 −1	1.0481 +0	4.0080 +0	1.5666 +1	3.4968 +1	6.1911 +1	9.6495 +1	2.4609 +2	5.5250 +2	1.5320 +3			
1.8000	3.2400 −1	1.2252 +0	4.7446 +0	1.8664 +1	4.1754 +1	7.4012 +1	1.1544 +2	2.9472 +2					
2.2000	3.8184 −1	1.4667 +0	5.7369 +0	2.2683 +1	5.0836 +1	9.0194 +1	1.4076 +2	3.5968 +2					
2.6000	4.4121 −1	1.7121 +0	6.7364 +0	2.6718 +1	5.9943 +1	1.0641 +2	1.6612 +2	4.2470 +2					

TABLE II. $G_F^{\ddagger}$ as a function of screening length and q. (In each entry A n means $A \times 10^n$.)

q	0.5	1	2	4	6	8	10	16	24	40	64	120	300
0.0001	-5.4163 -6	-1.6841 -5	-4.8074 -5	-1.2794 -4	-2.2122 -4	-3.2337 -4	-4.3216 -4	-7.8727 -4	-1.3066 -3	-2.4495 -3	-4.3297 -3	-9.2193 -3	-2.8898 -2
0.0010	-5.4196 -5	-1.6843 -4	-4.8074 -4	-1.2797 -3	-2.2140 -3	-3.2387 -3	-4.3333 -3	-7.9406 -3	-1.3373 -2	-2.6384 -2	-5.3116 -2	-1.7122 -1	-1.3334 +0
0.0015	-8.1296 -5	-2.5264 -4	-7.2116 -4	-1.9204 -3	-3.3243 -3	-4.8679 -3	-6.5224 -3	-1.2039 -2	-2.0621 -2	-4.3016 -2	-9.6463 -2	-3.6445 -1	-3.0403 +0
0.0022	-1.1923 -4	-3.7054 -4	-1.0579 -3	-2.8187 -3	-4.8855 -3	-7.1690 -3	-9.6341 -3	-1.8043 -2	-3.1914 -2	-7.2937 -2	-1.8530 -1	-7.6440 -1	-6.8002 +0
0.0032	-1.7343 -4	-5.3903 -4	-1.5392 -3	-4.1063 -3	-7.1362 -3	-1.0516 -2	-1.4218 -2	-2.7395 -2	-5.1292 -2	-1.3274 -1	-3.7284 -1	-1.5911 +0	-1.5040 +1
0.0047	-2.5473 -4	-7.9178 -4	-2.2621 -3	-6.0515 -3	-1.0578 -2	-1.5730 -2	-2.1534 -2	-4.3824 -2	-8.9828 -2	-2.6477 -1	-7.8015 -1	-3.4412 +0	-3.3648 +1
0.0069	-3.7399 -4	-1.1627 -3	-3.3253 -3	-8.9487 -3	-1.5831 -2	-2.3980 -2	-3.3625 -2	-7.4922 -2	-1.7115 -1	-5.4802 -1	-1.6396 +0	-7.5166 +0	-7.3619 +1
0.0100	-5.4208 -4	-1.6859 -3	-4.8323 -3	-1.3160 -2	-2.3828 -2	-3.7308 -2	-5.4421 -2	-1.3620 -1	-3.3827 -1	-1.1122 +0	-3.3990 +0	-1.5877 +1	-1.5240 +2
0.0120	-6.5055 -4	-2.0239 -3	-5.8117 -3	-1.5982 -2	-2.9466 -2	-4.7250 -2	-7.0705 -2	-1.8750 -1	-4.7678 -1	-1.5761 +0	-4.8699 +0	-2.2772 +1	-2.1514 +2
0.0150	-8.1329 -4	-2.5318 -3	-7.2946 -3	-2.0412 -2	-3.8792 -2	-6.4510 -2	-9.9934 -2	-2.8160 -1	-7.2592 -1	-2.4196 +0	-7.5413 +0	-3.5104 +1	-3.2390 +2
0.0180	-9.7612 -4	-3.0409 -3	-8.7972 -3	-2.5122 -2	-4.9322 -2	-8.4903 -2	-1.3529 -1	-3.9512 -1	-1.0222 +0	-3.4354 +0	-1.0733 +1	-4.9578 +1	-4.4736 +2
0.0220	-1.1934 -3	-3.7222 -3	-1.0838 -2	-3.1916 -2	-6.5492 -2	-1.1734 -1	-1.9210 -1	-5.7423 -1	-1.4886 +0	-5.0415 +0	-1.5725 +1	-7.1778 +1	-6.3025 +2
0.0260	-1.4108 -3	-4.4068 -3	-1.2930 -2	-3.9390 -2	-8.4323 -2	-1.5593 -1	-2.5964 -1	-7.8275 -1	-2.0344 +0	-6.9129 +0	-2.1472 +1	-9.6816 +1	-8.2945 +2
0.0320	-1.7875 -3	-5.4412 -3	-1.6181 -2	-5.2052 -2	-1.1786 -1	-2.2516 -1	-3.7961 -1	-1.1474 +0	-2.9940 +0	-1.0167 +1	-3.1319 +1	-1.3874 +2	-1.1506 +3
0.0380	-2.0648 -3	-6.4862 -3	-1.9592 -2	-6.6639 -2	-1.5783 -1	-3.0717 -1	-5.1992 -1	-1.5714 +0	-4.1085 +0	-1.3894 +1	-4.2417 +1	-1.8485 +2	-1.4904 +3
0.0470	-2.5572 -3	-8.0782 -3	-2.5065 -2	-9.2411 -2	-2.2940 -1	-4.5174 -1	-7.6463 -1	-2.3107 +0	-6.0366 +0	-2.0233 +1	-6.0953 +1	-2.5984 +2	-2.0213 +3
0.0570	-3.1070 -3	-9.8882 -3	-3.1727 -2	-1.2668 -1	-3.3291 -1	-6.3928 -1	-1.0803 +0	-3.2626 +0	-8.4485 +0	-2.8138 +1	-8.3604 +1	-3.4489 +2	-2.6272 +3
0.0690	-3.7710 -3	-1.2129 -2	-4.0643 -2	-1.7544 -1	-4.5562 -1	-8.9746 -1	-1.5144 +0	-4.5608 +0	-1.1785 +1	-3.8553 +1	-1.1285 +2	-4.6081 +2	-3.3627 +3
0.0830	-4.5528 -3	-1.4854 -2	-5.2454 -2	-2.4206 -1	-6.3122 -1	-1.2395 +0	-2.0882 +0	-6.2545 +0	-1.6022 +1	-5.1659 +1	-1.4894 +2	-5.9537 +2	-4.2219 +3
0.1000	-5.5146 -3	-1.8353 -2	-6.8971 -2	-3.3533 -1	-8.7207 -1	-1.7067 +0	-2.8682 +0	-8.5198 +0	-2.1597 +1	-6.8542 +1	-1.9452 +2	-7.6146 +2	-5.2593 +3
0.1200	-6.6669 -3	-2.2773 -2	-9.1529 -2	-4.5988 -1	-1.1890 +0	-2.3179 +0	-3.8818 +0	-1.1411 +1	-2.8395 +1	-8.9288 +1	-2.4953 +2	-9.5793 +2	-6.4682 +3
0.1500	-8.4457 -3	-3.0109 -2	-1.3147 -1	-6.7147 -1	-1.7208 +0	-3.3339 +0	-5.5508 +0	-1.6071 +1	-3.9668 +1	-1.2139 +2	-3.3314 +2	-1.2516 +3	-8.2603 +3
0.1800	-1.0296 -2	-3.8378 -2	-1.7802 -1	-9.0733 -1	-2.3062 +0	-4.4394 +0	-7.3492 +0	-2.0988 +1	-5.1143 +1	-1.5401 +2	-4.1691 +2	-1.5426 +3	-1.0033 +4
0.2200	-1.2895 -2	-5.0942 -2	-2.4869 -1	-1.2516 +0	-3.1483 +0	-6.0104 +0	-9.8802 +0	-2.7772 +1	-6.6736 +1	-1.9764 +2	-5.2793 +2	-1.9263 +3	
0.2600	-1.5665 -2	-6.5275 -2	-3.2725 -1	-1.6219 +0	-4.0402 +0	-7.6548 +0	-1.2506 +1	-3.4689 +1	-8.2437 +1	-2.4110 +2	-6.3790 +2	-2.3060 +3	
0.3200	-2.0181 -2	-8.9900 -2	-4.5632 -1	-2.2120 +0	-5.4376 +0	-1.0201 +1	-1.6538 +1	-4.5147 +1	-1.0594 +2	-3.0570 +2	-8.0107 +2	-2.8704 +3	
0.3800	-2.5168 -2	-1.1783 -1	-5.9542 -1	-2.8297 +0	-6.8764 +0	-1.2796 +1	-2.0616 +1	-5.5596 +1	-1.2958 +2	-3.6960 +2	-9.6255 +2		
0.4700	-3.3571 -2	-1.6468 -1	-8.1703 -1	-3.7853 +0	-9.0689 +0	-1.6714 +1	-2.6738 +1	-7.1153 +1	-1.6390 +2	-4.6442 +2	-1.2026 +3		
0.5700	-4.4186 -2	-2.2185 -1	-1.0750 +0	-4.8662 +0	-1.1516 +1	-2.1057 +1	-3.3498 +1	-8.8250 +1	-2.0194 +2	-5.6876 +2	-1.4675 +3		
0.6900	-5.8544 -2	-2.9521 -1	-1.3937 +0	-6.1700 +0	-1.4442 +1	-2.6227 +1	-4.1529 +1	-1.0854 +2	-2.4714 +2	-6.9308 +2	-1.7838 +3		
0.8300	-7.7164 -2	-3.8491 -1	-1.7713 +0	-7.6867 +0	-1.7826 +1	-3.2198 +1	-5.0801 +1	-1.3200 +2	-2.9947 +2	-8.3737 +2			
1.0000	-1.0182 -1	-4.9722 -1	-2.2321 +0	-9.5144 +0	-2.1895 +1	-3.9374 +1	-6.1951 +1	-1.6031 +2	-3.6265 +2	-1.0119 +3			
1.2000	-1.3280 -1	-6.3166 -1	-2.7730 +0	-1.1644 +1	-2.6634 +1	-4.7741 +1	-7.4963 +1	-1.9336 +2	-4.3668 +2	-1.2168 +3			
1.5000	-1.8158 -1	-8.3471 -1	-3.5778 +0	-1.4804 +1	-3.3676 +1	-6.0192 +1	-9.4349 +1	-2.4271 +2	-5.4738 +2	-1.5235 +3			
1.8000	-2.3173 -1	-1.0374 +0	-4.3744 +0	-1.7934 +1	-4.0667 +1	-7.2570 +1	-1.1364 +2	-2.9190 +2	-6.5784 +2	-1.8298 +3			
2.2000	-2.9934 -1	-1.3056 +0	-5.4264 +0	-2.2080 +1	-4.9942 +1	-8.9009 +1	-1.3928 +2						
2.6000	-3.6703 -1	-1.5715 +0	-6.4700 +0	-2.6205 +1	-5.9183 +1	-1.0540 +2	-1.6487 +2						

Tables I and II, for $s = \frac{1}{2}$, over a wide range of screening length and a number of values of q sufficient that the integral over G can be performed accurately. At high q the phase-shift sum is found to be given accurately for all types of statistics by

$$G = \pm \frac{2\lambda_D^2 q}{\pi} + \frac{\lambda_D}{2\pi q} \qquad (16)$$

where the top sign is for an attractive potential and the bottom sign for a repulsive potential. Equation (16) agrees with G_B at decreasing energies with increasing λ_D, the agreement being good almost down to line A of Fig. 4.

The first term on the right of Eq. (16) is easily derivable in the first Born approximation from an expression given by Landau and Lifshiftz.[11] If Eq. (16) is substituted in the Boltzmann form of Eq. (14), the result agrees exactly with the first two terms of the high-temperature virial coefficient given by DeWitt.[14] An additional term in the series at high q is approximately given by

$$\mp \frac{\ln(\lambda_D q^2/4.61)}{3\pi q^3} \; .$$

Note that the integral from $q = 0$ to $q = \infty$ over this term does not diverge if Eq. (12) is integrated by

parts an additional time, and if use is made of Levinson's theorem at $q = 0$. The contribution to the second virial coefficient agrees in its logarithmic dependence on λ_D with the third term given by DeWitt. For the Fermi gas at very low q (less than 10^{-4} for large λ_D) the following relation is seen to be accurate:

$$2G_F^+ = \delta_l(q) = [0.096\lambda_D/(\lambda_D + 1)$$

$$+ \lambda_D(0.246 + 0.264 \; \ln\lambda_D)] q. \qquad (17)$$

B. Partition Function and Virial Coefficient

In the case of Boltzmann particles interacting through a repulsive potential there is a much simpler way than that given above to calculate the second virial coefficient down to low temperatures. This is the Wigner-Kirkwood expansion. The first five terms in this expansion have been worked out by Kihora $et\ al.$[17] The first three terms are

$$B^{cl} = 2\pi N \int_0^\infty (1 - e^{-U/T_0})\rho^2 \, d\rho \; ,$$

$$B^1 = \frac{\pi N}{6T_0^3} \int_0^\infty e^{-U/T_0} U'^2 \rho^2 d\rho \; ,$$

TABLE III. Second virial coefficients[a] for a Boltzmann and a Fermi gas interacting through a repulsive SSCP.

T_0	B_{int}^{Cl}	B_{int}^1	B_{int}^2	$B_{int,WK}$	$B_{int,B}$	$B_{int,F}$
			$D = a_\mu/Z$			
0.002	4.461 51 + 2	7.6975 + 3	− 5.418 + 4	− 4.603 96 + 4	3.347 58 + 3	1.707 99 + 3
0.020	1.499 26 + 2	3.3828 + 2	− 3.128 + 2	1.754 38 + 2	3.524 23 + 2	2.050 86 + 2
0.200	3.539 22 + 1	1.0612 + 1	− 2.604 + 0	4.340 03 + 1	4.352 49 + 1	3.482 32 + 1
0.600	1.525 81 + 1	1.7192 + 0	− 3.482 − 1	1.662 90 + 1	1.660 76 + 1	1.480 94 + 1
2.000	5.443 99 + 0	2.0341 − 1	− 5.071 − 2	5.596 69 + 0	5.596 83 + 0	5.321 79 + 0
6.000	1.969 78 + 0	2.5979 − 2	− 1.155 − 2	1.984 21 + 0	1.987 21 + 0	1.943 47 + 0
20.000	6.148 74 − 1	2.5119 − 3	− 2.877 − 3	6.145 09 − 1	6.162 81 − 1	6.116 34 − 1
			$D = 10a_\mu/Z$			
0.002	1.499 26 + 5	3.3828 + 4	− 3.128 + 3	1.806 27 + 5	1.812 79 + 5	1.661 68 + 5
0.020	3.539 22 + 4	1.0612 + 3	− 2.604 + 1	3.642 74 + 4	3.642 75 + 4	3.593 78 + 4
0.200	5.443 99 + 3	2.0341 + 1	− 5.071 − 1	5.463 82 + 3	5.463 80 + 3	5.448 74 + 3
0.600	1.969 78 + 3	2.5979 + 0	− 1.155 − 1	1.972 26 + 3	1.972 25 + 3	1.969 56 + 3
2.000	6.148 74 + 2	2.5119 − 1	− 2.877 − 2	6.150 97 + 2	6.150 95 + 2	6.147 31 + 2
6.000	2.078 15 + 2	2.8649 − 2	− 9.016 − 3	2.078 34 + 2	2.078 35 + 2	2.077 92 + 2
20.000	6.267 92 + 1	2.6054 − 3	− 2.644 − 3	6.267 92 + 1	6.268 05 + 1	6.267 76 + 1
			$D = 40a_\mu/Z$			
0.002	4.228 73 + 6	7.0887 + 4	− 6.485 − 2	4.298 96 + 6	4.299 02 + 6	4.283 46 + 6
0.020	7.707 44 + 5	1.6734 + 3	− 8.542 + 2	7.724 09 + 5	7.724 10 + 5	7.719 17 + 5
0.200	9.579 38 + 4	2.3929 + 1	− 3.257 + 0	9.581 74 + 4	9.581 71 + 4	9.580 18 + 4
0.600	3.290 18 + 4	2.8082 + 0	− 9.477 − 2	3.290 45 + 4	3.290 44 + 4	3.290 17 + 4
2.000	9.993 79 + 3	2.5878 − 1	− 2.683 − 2	9.994 03 + 3	9.993 99 + 3	9.993 62 + 3
6.000	3.344 22 + 3	2.8972 − 2	− 8.799 − 3	3.344 24 + 3	3.344 24 + 3	3.344 20 + 3
20.000	1.004 69 + 3	2.6148 − 3	− 2.625 − 3	1.004 69 + 3	1.004 69 + 3	1.004 69 + 3

[a]In units $N(a_\mu/Z)^3$.

TABLE IV. Individual terms of the partition function and the second virial coefficient[a] for an attractive SSCP.

T_o	Z_{int}^{BS}	Z_{int}^0	Z_{int}^{cs}	B_{int}^-
		$D = a_\mu/Z$		
0.002	2.929 +4	−1.000 +0	9.041 −1	−7.293 85 + 9
0.020	2.797 +0	−1.000 +0	7.564 −1	−2.010 62 + 4
0.200	1.108 +0	−1.000 +0	6.258 −1	−1.828 02 + 2
0.600	1.035 +0	−1.000 +0	6.856 −1	−3.452 84 + 1
2.000	1.010 +0	−1.000 +0	9.495 −1	−7.558 90 + 0
6.000	1.003 +0	−1.000 +0	1.477 + 0	−2.243 93 + 0
20.000	1.001 +0	−1.000 +0	2.579 + 0	−6.426 03 − 1
		$D = 10a_\mu/Z$		
0.002	9.882 +176	−9.000 +0	9.55840	−2.460 84 +182
0.020	5.006 +17	−9.000 +0	1.379 +1	−3.942 07 +21
0.200	6.935 +1	−9.000 +0	2.860 +1	−2.215 09 +4
0.600	1.259 +1	−9.000 +0	4.607 +1	−2.380 35 +3
2.000	9.703 +0	−9.000 +0	8.131 +1	−6.458 51 +2
6.000	9.211 +0	−9.000 +0	1.392 +2	−2.112 30 +2
20.000	9.061 +0	−9.000 +0	2.529 +2	−6.298 90 +1
		$D = 40a_\mu/Z$		
0.002	3.076 +206	−7.200 +1	9.010 +1	−7.662 12 +211
0.020	4.455 +20	−7.200 +1	1.611 +2	−3.507 93 +24
0.200	2.007 +2	−7.200 +1	4.206 +2	−1.367 73 +5
0.600	7.949 +1	−7.200 +1	7.104 +2	−3.440 52 +4
2.000	7.362 +1	−7.200 +1	1.283 +3	−1.011 93 +4
6.000	7.250 +1	−7.200 +1	2.215 +3	−3.358 11 +3
20.000	7.215 +1	−7.200 +1	4.039 +3	−1.005 94 +3

[a] In units $N/(a_\mu/Z)^3$.

$$B^2 = -\frac{\pi N}{6T_0^3} \int_0^\infty e^{-U/T_0} \left(\frac{1}{10} U''^2 + \frac{1}{5}\frac{U'^2}{\rho^2} + \frac{1}{9T_0}\frac{U'^2}{\rho}\right.$$

$$\left. - \frac{1}{72T_0^2} U'^4\right)\rho^2 d\rho . \quad (18)$$

The first three terms of the Wigner-Kirkwood expansion of the second virial coefficient, their total $B_{int,WK}$, $B_{int,B}$, and $B_{int,F}$ of a repulsive SSCP are given in Table III for several values of screening length. At high temperature B_{int}^1 and B_{int}^2 are practically independent of D, and vary as $1/T^2$ and $1/T$, respectively. This behavior is expected from Eqs. (18) at high temperature, since the screening becomes ineffective and the potential approaches a pure coulomb potential. For $D = 1\ a_\mu/Z$ and $10\ a_\mu/Z$ it is noted that the sum of the first two Wigner-Kirkwood coefficients agrees more closely with $B_{int,B}$ than does the sum

of the first three coefficients. At $D = 40\ a_\mu/Z$ this breaking down of the Wigner-Kirkwood expansion with $B_{int,B}$ is seen to depend strongly on the screening length. The potential varies more slowly with increasing D so that the semiclassical approximation becomes more valid. At $D = 40\ a_\mu/Z$ the agreement is within a few parts in a million over all temperatures above $T_0 = 0.002$.

At very low temperature $B_{int,B} = 2B_{int,F}$, since only the lowest state is important. As the temperature is raised more and more states become important and the phase shifts become more closely spaced, so that the spin-weighting factors become less important and $B_{int,F}$ approaches $B_{int,B}$, as shown in Table III. The difference between Boltzmann and Fermi statistics is nearly independent of screening length except at low temperatures and/or small screening lengths.

For an electrically neutral two-component plasma $(N_a = N_b)$ the second virial coefficient is related to the one-component second virial coefficients and the second cross virial coefficient according to Eq. (15). After integration we see that the contribution to B of the first term of Eq. (16) is identically zero, a result of electrical neutrality. The virial coefficients of the pure components are given in Table III. The second cross virial coefficient[18] $B_{int,B}^-$ is given in Table IV. The cancellation of the λ_D^2 term at high temperatures is apparent.

Table IV also gives the bound-state part of the partition function Z_{int}^{BS}, the part due to the phase shifts at zero energy Z_{int}^0, and the nonzero-energy phase-shift part [last term of Eq. (13)] Z_{int}^{cs}, for several values of screening length. It is clear that Z_{int}^{BS} is the dominant contributor at low temperature, Z_{int}^{cs} is the dominant contributor at high temperature, and that all three terms are necessary at intermediate temperatures. The cancellation of Z_{int}^{BS} by Z_{int}^0 is apparent at higher temperatures.

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[18]$B_{\text{int},B}^{-}$ can be thought of as the virial coefficient of a one-component gas interacting through a potential $V(r) = -g\, e^{-r/D}/r$.

First Quantum-Mechanical Correction to the Classical Viscosity Cross Section of Hard Spheres

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The classical and first quantum correction terms in a high-energy expansion of the viscosity cross section $Q^{(2)}$ for a Boltzmann gas of hard spheres is derived. The first correction is found to be proportional to $(1/k\sigma)^{4/3}$, which is a term nonanalytic in $\hbar$ (i.e., $\hbar^{4/3}$), and results from scattering near the edge of the sphere. A bound is established showing the remainder of the asymptotic series to be of $O[\ln(k\sigma)/(k\sigma)^2]$. This asymptotic formula is compared with calculations based on the exact phase-shift expressions and its range of validity is established. The next correction terms are deduced to be proportional to $(\ln k\sigma)/(k\sigma)^2$ and $1/(k\sigma)^2$ which involve $\hbar^2\ln\hbar$ and $\hbar^2$, respectively.

INTRODUCTION

In both classical and quantum mechanics one can, in a first-order Chapman-Enskog approximation, express the density-independent part of the viscosity in terms of an integral involving a specialized two-body cross section $Q^{(2)}$. While the latter admits of an exact quantum-mechanical formulation in terms of phase shifts, it is by no means trivial to extract from it an asymptotic expansion valid for high energies having the classical result as the leading term. In fact, for the case of a gas subject to Lennard-Jones forces, the quantum-mechanical corrections to the classical answer are still a subject under discussion.[1]

The development of a high-energy expansion is important in that, by providing corrections to the classical expression for the viscosity of light gases, it establishes the domain of validity of the classical term and provides simple formulas valid for a wider range of temperature. It also enables one to check the numerical work involved in evaluating the phase-shift formulas. Finally, by removing the values of these known terms from numerical results, we might expect to find clues to the analytical character of the remaining quantum-mechanical effects.

In this paper we derive the first two terms (classical and first quantum correction) of an expansion, valid at high energies, for the Boltzmann part of the cross section $Q^{(2)}$ of a gas of hard spheres. (Similar analysis should be possible for the other $Q^{(n)}$'s.) For this simple potential we can express phase shifts analytically in terms of Hankel functions and derive our results by using uniform asymptotic expansions for these functions.