

UNCLASSIFIED

AD 92395

Armed Services Technical Information Agency

Reproduced by

DOCUMENT SERVICE CENTER

KNOTT BUILDING, DAYTON, 2, OHIO

This document is the property of the United States Government. It is furnished for the duration of the contract and shall be returned when no longer required, or upon recall by ASTIA to the following address: Armed Services Technical Information Agency, Document Service Center, Knott Building, Dayton 2, Ohio.

NOTICE: WHEN GOVERNMENT OR OTHER DRAWINGS, SPECIFICATIONS OR OTHER DATA ARE USED FOR ANY PURPOSE OTHER THAN IN CONNECTION WITH A DEFINITELY RELATED GOVERNMENT PROCUREMENT OPERATION, THE U. S. GOVERNMENT THEREBY INCURS NO RESPONSIBILITY, NOR ANY OBLIGATION WHATSOEVER; AND THE FACT THAT THE GOVERNMENT MAY HAVE FORMULATED, FURNISHED, OR IN ANY WAY SUPPLIED THE SAID DRAWINGS, SPECIFICATIONS, OR OTHER DATA IS NOT TO BE REGARDED BY IMPLICATION OR OTHERWISE AS IN ANY MANNER LICENSING THE HOLDER OR ANY OTHER PERSON OR CORPORATION, OR CONVEYING ANY RIGHTS OR PERMISSION TO MANUFACTURE, USE OR SELL ANY PATENTED INVENTION THAT MAY IN ANY WAY BE RELATED THERETO.

UNCLASSIFIED

92395
UNIVERSITY OF WISCONSIN
NAVAL RESEARCH LABORATORY
Department of Chemistry

SOME MOLECULAR COLLISION INTEGRALS FOR POINT ATTRACTION
AND REPULSION POTENTIALS

by

M. A. Eliason, D. E. Stogryn, and J. O. Hirschfelder

University of Wisconsin - WIS-ONR-19

5 March 1956

Copy _____

Contract N7-onr-28511

Series 1 and 2

SOME MOLECULAR COLLISION INTEGRALS FOR POINT ATTRACTION AND REPULSION POTENTIALS*

M. A. Eliason,¹ D. E. Stogryn, and J. O. Hirschfelder

ABSTRACT

If the pairs of molecules in a dilute gas interact with an intermolecular energy of the form, $\Phi = d/r^\delta$, the collision integrals which determine the transport properties can be written[†]

$$\Omega^{(1,s)} = A^{(1)}(\delta) \left(\frac{\pi k T}{2 \mu} \right)^{1/2} \left(\frac{\delta d}{k T} \right)^{2/\delta} \Gamma(s + 2 - 2/\delta)$$

Here μ is the reduced mass of the colliding molecules. The following constants are evaluated:

Repulsive Interaction Potential, d positive

$$\begin{array}{ll} A^{(1)}_{(2)} = 0.397601 & A^{(2)}_{(2)} = 0.527843 \\ A^{(1)}_{(3)} = 0.3115 & A^{(2)}_{(3)} = 0.3533 \end{array}$$

Attractive Interaction Potential, d negative

$$\begin{array}{ll} A^{(1)}_{(2)} = 0.806907 & A^{(2)}_{(2)} = 0.710970 \\ A^{(1)}_{(3)} = 0.6750 & A^{(3)}_{(3)} = 0.4641 \end{array}$$

The constants for $\delta = 2$ were readily evaluated in closed form. The constants for the repulsive potential with $\delta = 3$ were evaluated using an expansion development of Mott-Smith. The constants for the attractive potential with $\delta = 3$ were evaluated numerically making use of elliptic integrals for the angles of deflection. For attractive potentials a singular point was encountered corresponding to orbiting.

* This work is being done under the Office of Naval Research Contract N7-onr-28511.

† J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, "Molecular Theory of Gases and Liquids" (John Wiley, 1954), p. 547.

¹ Fellow National Science Foundation.

SOME MOLECULAR COLLISION INTEGRALS FOR POINT ATTRACTION AND REPULSION POTENTIALS

M. A. Eliason, D. E. Stogryn, and J. O. Hirschfelder

University of Wisconsin Naval Research Laboratory
Madison, Wisconsin

The transport coefficients for a dilute gas made up of molecules which have a potential energy of interaction of the form

$$\phi(r) = d r^{-\delta} \tag{1}$$

can be expressed¹ in terms of the constants $A^{(d)}(\delta)$, when d is positive and the molecules repel each other; or in terms of the analogous constants $C^{(d)}(\delta)$, to be defined below, when d is negative and the molecules attract each other. In this paper, the values of $A^{(1)}(\delta)$, $A^{(2)}(\delta)$, $C^{(1)}(\delta)$ and $C^{(2)}(\delta)$ are calculated for $\delta = 2$ and $\delta = 3$.

Although the second virial coefficient would be infinite in each of these cases,² the transport coefficients are finite. The evaluation of the collision integrals is not difficult for either of the repulsive cases. When $\delta = 2$, $A^{(1)}(2)$ and $A^{(2)}(2)$ may be expressed in closed form. When $\delta = 3$, a formulation of Mott-Smith³ may be used to obtain a rapidly converging infinite series for these collision integrals. The integrals resulting from the attractive potentials are somewhat harder to evaluate because of the spiraling of the molecules in collisions where the impact parameter is less than a critical value.

- - - - -

¹ J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird; "Molecular Theory of Gases and Liquids"; (John Wiley, 1954); p. 546.

² We find that for either attractive or repulsive point forces, the $A^{(d)}(1)$ and $C^{(d)}(1)$ are infinite. The second virial coefficients (MTGL, Ref. 1, p. 156) are infinite for either attractive or repulsive potentials if δ is not greater than 3.

³ H. M. Mott-Smith, "A New Approach in the Kinetic Theory of Gases", M. I. T. Lincoln Laboratory, Group Report V-2 (December, 1954).

When $\delta = 2$, this spiraling results in an infinite angle of deflection whenever the impact parameter is less than the critical value, and causes singular behavior in a part of the collision integral. This part of the integral is approximated, and the remainder is obtained in closed form.

For $\delta = 3$, the critical impact parameter corresponds to a singular point in the collision integrals. The asymptotic behavior in the vicinity of the singular point is investigated and the integrals are evaluated numerically. Use is made of the fact that with $\delta = 3$, the angle of deflection is simply expressible in terms of incomplete elliptic integrals of the first kind.

The collision integrals are defined in the following way.⁴ The collision of two molecules is considered as the equivalent one body problem. A particle with reduced mass $\mu = \frac{m_1 m_2}{m_1 + m_2}$ approaches a fixed center of force with initial speed g and impact parameter b . The potential energy of interaction is given by Eq. (1), where d is a constant, and r the distance of the incoming particle from the scattering center. Figure 1 shows the trajectory. The particle is deflected through an angle of deflection χ and the distance of closest approach is r_m .

Now, if we define

$$y = \frac{b}{r} \quad y_m = \frac{b}{r_m} \quad y_0 = \left[\frac{\frac{1}{2} \mu g^2}{\delta d} \right]^{\frac{1}{\delta}} \quad (2)$$

the angle of deflection may be written as a function of y_0 .

$$\chi(y_0) = \pi - 2\theta_m = \pi - 2 \int_0^{y_m(y_0)} \left[1 - y^2 - \frac{1}{\delta} \left(\frac{y}{y_0} \right)^\delta \right]^{-\frac{1}{2}} dy \quad (3)$$

⁴ MTGL, Ref. 1, p. 546. It should be noted that our $A^{(1)}(\delta)$ and that of MTGL are equal to $2^{-\frac{3}{\delta}} A_{\delta}(\delta+1)$ where the $A_{\delta}(\delta+1)$ are the collision integrals of S. Chapman and T. Cowling, "The Mathematical Theory of Non Uniform Gases" (Cambridge Press, 1939), p. 172.

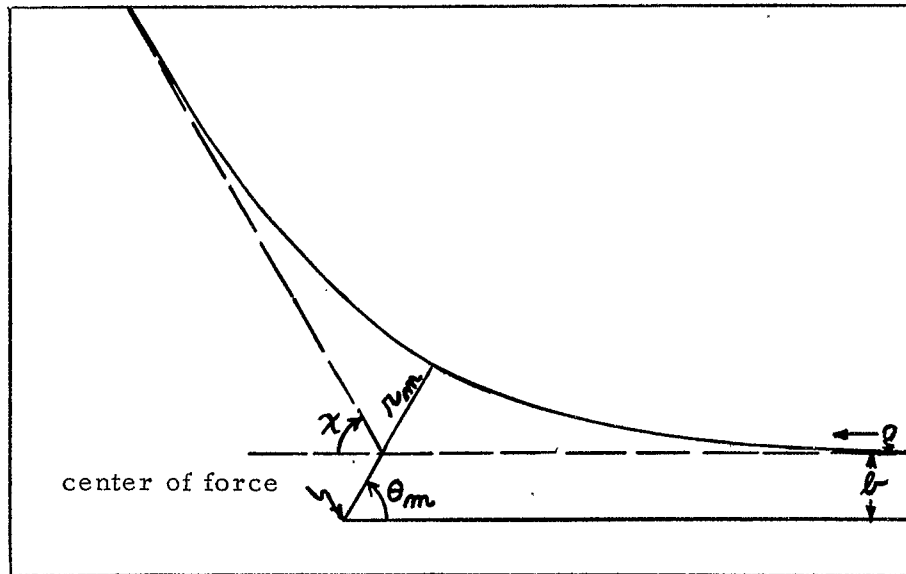


Fig. 1 Trajectory for repulsive potential.

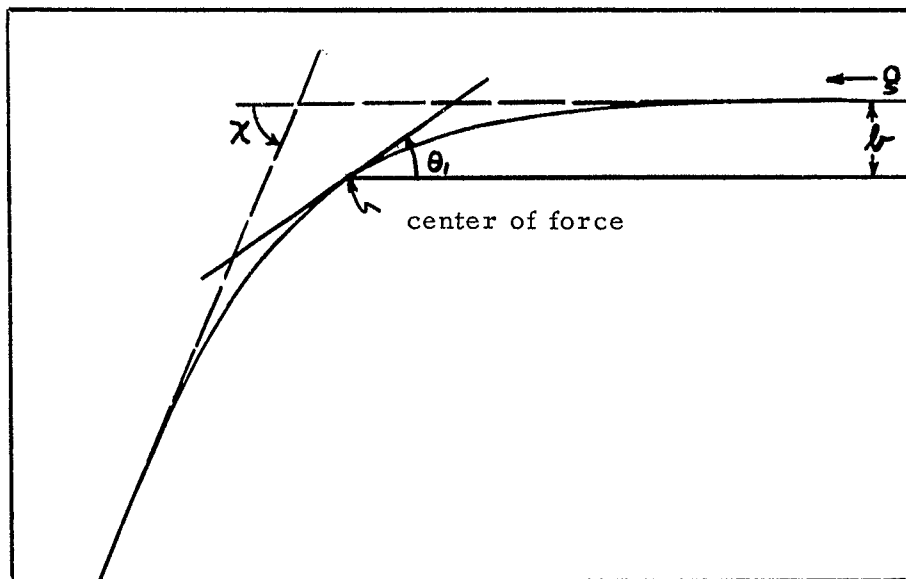


Fig. 2 Trajectory for attractive potential.

Case where particle passes through center of force.

The upper limit on the integral is the first positive root of the polynomial in the denominator of the integrand.

Then the collision cross-sections for the various transport properties are given by

$$Q^{(1)} = 2\pi \left[\frac{\delta d}{\frac{1}{2}\mu g^2} \right]^{2/5} A^{(1)}(\delta) \quad (4)$$

where the molecular collision integral, $A^{(1)}(\delta)$ is given by

$$A^{(1)}(\delta) = \int_0^\infty (1 - \cos^2 \chi) y_0 dy_0 \quad (5)$$

When the potential is attractive, $d = -a$ and the potential has the form

$$\Phi(r) = -a r^{-\delta} \quad (6)$$

Also, let us define

$$\beta = a \left[\frac{\frac{1}{2}\mu g^2}{\delta} \right]^{1/5} \quad (7)$$

It is easily seen that with β , which is a real, positive quantity, Eq. (3) becomes, for an attractive potential

$$\chi(\beta) = \pi - 2\theta_2 = \pi - 2 \int_0^{y_m(\beta)} \left[1 - y^2 + \frac{1}{\delta} \left(\frac{y}{\beta} \right)^\delta \right]^{-1/2} dy \quad (8)$$

If β is greater than β_{crit} , the polynomial in the denominator of the integrand has a first positive root, $y_m(\beta)$. However, if β is less than β_{crit} , $y_m(\beta) = \infty$ corresponding to the fact that the incoming particle actually passes through the center of force, $r_m = 0$, and then goes out again. In this case, the angle of deflection is given by

$$\chi(\beta) = -2\theta_1 = -2 \int_0^\infty \left[1 - y^2 + \frac{1}{\delta} \left(\frac{y}{\beta} \right)^\delta \right]^{-1/2} dy \quad (9)$$

rather than by eq. (8). Such a trajectory is shown in Fig. 2.

For the attractive potentials the various collision cross-sections are given by

$$Q^{(1)} = 2\pi \left(\frac{\delta a}{\frac{1}{2}\mu g^2} \right)^{2/5} C^{(1)}(\delta) \quad (10)$$

where

$$C^{(1)}(\delta) = \int_0^\infty (1 - \cos^2 \chi) \beta d\beta \quad (11)$$

I. Centers of Repulsion

For repulsive potentials, when δ is 2 or greater, the $A^{(1)}(\delta)$ are finite. The case of $\delta = 1$, however, is a potential of sufficiently long range that the integral for $A^{(1)}(1)$ is infinite. In this case, the angle of deflection is

$$\chi(y_0) = 2 \sin^{-1} [(1 + 4y_0^2)^{-1/2}] \quad (12)$$

and the integral in Eq. (5) diverges.

(a) $\delta = 2$.

The repulsive, inverse square potential is of interest because the integrations may be carried out analytically.⁵ First of all, the angle of the deflection from Eq. (3) is

$$\chi(y_0) = \pi - 2 \int_0^{y_m} [1 - (1 + \frac{1}{2y_0^2})y^2]^{-1/2} dy \quad (13)$$

Let $x = 2y_0^2$; then $y_m = (1 + \frac{1}{x})^{-1/2}$

$$\chi(x) = \pi - 2(1 + \frac{1}{x})^{-1/2} \sin^{-1} [y(1 + \frac{1}{x})^{1/2}] \Big|_0^{(1 + \frac{1}{x})^{-1/2}}$$

$$\chi(x) = \pi [1 - (1 + \frac{1}{x})^{-1/2}] \quad (14)$$

⁵ The evaluation of $A^{(1)}(2)$ and $A^{(2)}(2)$ was carried out by John S. Dahler with the help of Donald W. Jepsen.

With this change of variables, Eq. (5) becomes

$$A^{(1)}(2) = \frac{1}{4} \int_0^{\infty} (1 - \cos^2 x) dx \quad (15)$$

Now let $x = z^2 / (1 - z^2)$, then $x = \pi (1 - z)$. Substituting into Eq. (15) and integrating by parts

$$A^{(1)}(2) = -\frac{1}{2} + \frac{\pi}{4} \int_0^1 \frac{\sin \pi z}{1 - z^2} dz \quad (16)$$

$$A^{(2)}(2) = -\frac{\pi}{4} \int_0^1 \frac{\sin 2\pi z}{1 - z^2} dz \quad (17)$$

But it is easy to show that

$$\int_0^1 \frac{\sin m \pi z}{1 - z^2} dz = \frac{1}{2} (-1)^m [Si(2m\pi) - 2Si(m\pi)] \quad (18)$$

where⁶

$$Si(x) = \int_0^x \frac{\sin z}{z} dz \quad (19)$$

Thus we obtain

$$A^{(1)}(2) = 0.397601 \quad (20)$$

$$A^{(2)}(2) = 0.527843 \quad (21)$$

6 "Tables of Sine, Cosine, and Exponential Integrals", Vol. II, WPA (Federal Works Agency, Works Progress Administration for the City of New York.) (1940).

(b) $\delta = 3$.

In the case of the inverse cube repulsive potential, we were able to make use of a method which has been developed by Mott-Smith³ to evaluate the $A^{(0)}(\delta)$. Through the application of Bürmann's Theorem⁷ he has found that Eq. (5) can be written as

$$A^{(0)}(\delta) = 2^{-\frac{2}{\delta}} \int_0^{\pi} (1 - \cos^{\delta} x) F(x) \sin x \, dx \quad (22)$$

where the $F(x) \sin x$ is given by

$$F(x) \sin x = \cos \frac{x}{2} \sum_{\rho=0}^{\infty} D_{\rho} \left(\sin \frac{x}{2} \right)^{\rho-1-\frac{2}{\delta}} \quad (23)$$

The D_{ρ} are constants, depending only on δ .

$$D_{\rho} = \frac{1}{4} \left(\frac{2}{\delta} \right)^{1+\frac{2}{\delta}} \frac{1}{\rho!} \left\{ \frac{d^{\rho}}{dz^{\rho}} (1+z)^{\frac{2}{\delta}-2} \left(1 + \frac{\delta}{2} z \right) \left(\frac{z}{\sin \frac{1}{2} H(z)} \right)^{\rho-\frac{2}{\delta}} \right\}_{z=0} \quad (24)$$

with the $H(z)$ given by

$$H(z) = - \sum_{s=1}^{\infty} \binom{-\frac{1}{2}}{s} z^s \sum_{t=0}^s (-1)^t \binom{s}{t} \frac{\Gamma(\frac{1}{2}\delta t + \frac{1}{2}) \Gamma(-s + \frac{1}{2})}{\Gamma(\frac{1}{2}\delta t - s + 1)} \quad (25)$$

For $\delta = 3$, we obtain the results given in Table I.

Table I

The Mott-Smith Coefficients D_{ρ} for $\delta = 3$

ρ	D_{ρ}
0	0.25438
1	0.12487
2	0.01019
3	-0.00282
4	0.00317

7

E. T. Whittaker and G. N. Watson: "A Course of Modern Analysis"; 4th Ed. (Cambridge University Press) (1952) p. 128.

Substitution of Eq. (23) into Eq. (22), and integration gives the general expression

$$A^{(l)}(\delta) = -2^{-\frac{2}{\delta}} \sum_{\rho=0}^{\infty} D_{\rho} \sum_{m=1}^l (-1)^m 2^{m+1} \binom{l}{m} \left(\frac{\delta}{\delta \rho + 2 \delta m - 2} \right) \quad (26)$$

The two cases which are of interest are then

$$A^{(1)}(3) = 2^{\frac{4}{3}} \sum_{\rho=0}^{\infty} D_{\rho} \left[\frac{1}{\rho + \frac{4}{3}} \right] \quad (27)$$

$$A^{(2)}(3) = 2^{\frac{7}{3}} \sum_{\rho=0}^{\infty} D_{\rho} \left[\frac{1}{\rho + \frac{4}{3}} - \frac{1}{\rho + \frac{10}{3}} \right] \quad (28)$$

Thus we obtain

$$A^{(1)}(3) = 0.3115 \quad (29)$$

$$A^{(2)}(3) = 0.3533 \quad (30)$$

II. Centers of Attraction

When the potential is attractive there is a singularity in the expression for the angle of deflection. The Mott-Smith formulation is no longer applicable so we proceed as follows.

There exists a critical value of $b = b_{\text{crit}}$ for any relative kinetic energy $\frac{1}{2} \mu g^2$ such that for b less than b_{crit} there are no positive roots to the equation

$$f(y) = 1 - y^2 + c y^{\delta} = 0 \quad (31)$$

where

$$c = \frac{1}{\delta \beta^{\delta}} = \frac{a}{(\frac{1}{2} \mu g^2) b^{\delta}} \quad (32)$$

and for $b = b_{\text{crit}}$, $c = c_{\text{crit}}$. This critical value may be obtained by noting that Eq. (31) has a double root at the critical value. Therefore, both $f(y)$ and $f'(y)$ vanish for the same positive root, y_{crit} .

$$f'(y) = y^{-1} [-2y^2 + c \delta y^\delta] = 0 \quad (33)$$

One may combine Eqs. (31) and (33), to solve for this root

$$y_{\text{crit}} = \left[\frac{\delta}{\delta-2} \right]^{\frac{1}{2}} \quad (34)$$

and then go back and obtain the critical value of c

$$c_{\text{crit}} = 2 \delta^{-\frac{\delta}{2}} [\delta-2]^{\frac{\delta}{2}-1} \quad (35)$$

Thus

$$\beta_{\text{crit}} = 2^{-\frac{1}{\delta}} \left(\frac{\delta}{\delta-2} \right)^{(\frac{1}{2}) - (\frac{1}{\delta})} \quad (36)$$

(a) $\delta = 2$.

For the attractive case, with $\delta = 2$, the angle of deflection is, from Eq. (8) and (9)

$$\chi(\beta) = \pi - 2 \int_0^{[1-\frac{1}{2\beta^2}]^{-\frac{1}{2}}} [1 - (1 - \frac{1}{2\beta^2}) y^2]^{-\frac{1}{2}} dy \quad ; \quad \beta^2 > \frac{1}{2} \quad (37)$$

and

$$\chi(\beta) = -2 \int_0^\infty [1 - (1 - \frac{1}{2\beta^2}) y^2]^{-\frac{1}{2}} dy \quad ; \quad \beta^2 < \frac{1}{2} \quad (38)$$

Thus,

$$\chi(\beta) = \pi \left[1 - \left(1 - \frac{1}{2\beta^2} \right)^{-\frac{1}{2}} \right] \quad ; \quad \beta^2 > \frac{1}{2} \quad (39)$$

$$\begin{aligned} \chi(\beta) &= -2 \left(\frac{1}{2\beta^2} - 1 \right)^{-\frac{1}{2}} \ln \left\{ \left(\frac{1}{2\beta^2} - 1 \right)^{\frac{1}{2}} y + \left[1 + \left(\frac{1}{2\beta^2} - 1 \right) y^2 \right]^{\frac{1}{2}} \right\} \Big|_0^\infty \\ &= -\infty \quad ; \quad \beta^2 < \frac{1}{2} \end{aligned} \quad (40)$$

In spite of the infinite value of the angle of deflection for all values of β^2 less than $\frac{1}{2}$, one may still obtain the collision integrals. Eq. (11) is split into two parts

$$\begin{aligned} C^{(0)}(2) &= \int_0^{2^{-\frac{1}{2}}} (1 - \cos^2 \chi) \beta d\beta + \int_{2^{-\frac{1}{2}}}^\infty (1 - \cos^2 \chi) \beta d\beta \\ &= G^{(0)} + H^{(0)} \end{aligned} \quad (41)$$

The second of these, the $H^{(0)}$, are obtained in closed form. Taking the expression for χ from Eq. (39), and letting $x = \left(1 - \frac{1}{2\beta^2} \right)$, it is found that

$$H^{(1)} = \frac{1}{2} \int_0^\infty \cos^2 \frac{\pi x}{2} x d\left(\frac{1}{x^2-1}\right) \quad (42)$$

$$H^{(2)} = \frac{1}{4} \int_0^\infty \sin^2 \pi x d\left(\frac{1}{x^2-1}\right) \quad (43)$$

These expressions may be integrated by parts to give

$$H^{(1)} = \frac{\pi}{4} \int_1^\infty \frac{\sin \pi x}{1-x^2} dx \quad (44)$$

$$H^{(2)} = -\frac{\pi}{4} \int_1^\infty \frac{\sin 2\pi x}{1-x^2} dx \quad (45)$$

These may be rewritten as

$$H^{(1)} = \frac{\pi}{4} \left\{ \int_0^\infty \frac{\sin \pi x}{1-x^2} dx - \int_0^1 \frac{\sin \pi x}{1-x^2} dx \right\} \quad (46)$$

$$H^{(2)} = \frac{\pi}{4} \left\{ - \int_0^\infty \frac{\sin 2\pi x}{1-x^2} dx + \int_0^1 \frac{\sin 2\pi x}{1-x^2} dx \right\} \quad (47)$$

The first integral in each case is found in Bierens de Haan⁸, and second we found in the evaluation of $A^{(1)}(2)$ and $A^{(2)}(2)$. Thus

$$H^{(1)} = \frac{\pi}{4} \left\{ [Ci(\pi) \sin \pi - Si(\pi) \cos \pi] + \frac{1}{2} Si(2\pi) - Si(\pi) \right\} \quad (48)$$

$$H^{(2)} = \frac{\pi}{4} \left\{ - [Ci(2\pi) \sin 2\pi - Si(2\pi) \cos 2\pi] + \frac{1}{2} Si(4\pi) - Si(2\pi) \right\} \quad (49)$$

Therefore,

$$H^{(1)} = \frac{\pi}{2} Si(2\pi) = 0.556907 \quad (50)$$

$$H^{(2)} = \frac{\pi}{8} Si(4\pi) = 0.585970 \quad (51)$$

The values of the integrals $G^{(l)}$ may be approximated in the following way.

$$G^{(l)} = \frac{1}{2} \int_0^{\frac{1}{2}} (1 - \cos^l x) d\beta^2 \quad (52)$$

⁸ D. Bierens de Haan, "Nouvelles Tables D'Integrales Definies", (G. E. Stechert and Co., 1939), Table 161, 3.

$$\int_0^\infty \frac{\sin px}{q^2 - p^2} dx = \frac{1}{q} \{ Ci(pq) \sin pq - Si(pq) \cos pq \}$$

With

$$Ci(pq) = \int_\infty^{pq} \frac{\cos x}{x} dx$$

If the upper limit on the integral for the angle of deflection is taken to be an arbitrarily large, but finite number Z ,

$$\chi = -2 \left(\frac{1}{2\beta^2} - 1 \right)^{-1/2} \ln \left\{ \left(\frac{1}{2\beta^2} - 1 \right)^{1/2} Z + [1 + \left(\frac{1}{2\beta^2} - 1 \right) Z^2]^{1/2} \right\} \quad (53)$$

With this expression for the angle of deflection, the integrand of Eq. (52) is a very rapidly oscillating function of β^2 ; oscillating between 0 and 2 for $G^{(1)}$, and between 0 and 1 for $G^{(2)}$. As Z becomes very large, the peaks become very close, and the average value of the integrand becomes very close to 1 for the $G^{(1)}$ and to $\frac{1}{2}$ for the $G^{(2)}$. Thus, in the limit that Z becomes infinite, corresponding to the actual kinetic theory problem,

$$G^{(1)} = 0.25 \quad (54)$$

$$G^{(2)} = 0.125 \quad (55)$$

Thus we obtain

$$C^{(1)}(2) = G^{(1)} + H^{(1)} = 0.806907 \quad (56)$$

$$C^{(2)}(2) = G^{(2)} + H^{(2)} = 0.710970 \quad (57)$$

(b) $\delta = 3$

In the case of the inverse cube attractive potential, $\beta_{\text{crit.}} = \left(\frac{3}{4}\right)^{1/6}$ and $y_m(\beta)$ varies from unity for $\beta = \infty$ to $y_m(\beta_{\text{crit.}}) = 3^{1/2}$. Because of the singular point it is convenient to divide the integration of $C^{(1)}(3)$ into two parts

$$C^{(1)}(3) = C_1^{(1)}(3) + C_2^{(1)}(3) \quad (58)$$

where

$$C_1^{(0)}(3) = \frac{1}{2} \int_0^{(\frac{3}{4})^{1/3}} [1 - \cos^2(2\theta_1)] d\beta^2 \quad (59)$$

$$C_2^{(0)}(3) = \frac{1}{2} \int_{(\frac{3}{4})^{1/3}}^{\infty} [1 - (-1)^l \cos^l(2\theta_2)] d\beta^2 \quad (60)$$

Here θ_1 and θ_2 are given in Eqs. (9) and (8) respectively.

In evaluating $C_1^{(l)}(3)$ it is convenient to change the variable of integration from β^2 to q^2 to y^2 where q is minus the (only) real root of the polynomial in the denominator of Eq. (9)

$$\beta^2 = q^2 [3(1 - q^2)]^{-2/3} \quad (61)$$

Since the real root is negative in the range $0 < \beta^2 < (\frac{3}{4})^{1/3}$, q is positive.

Making the change of variables,

$$\theta_1 = \left(\frac{q^3}{1 - q^2}\right)^{1/2} \int_0^{\infty} \left[\frac{q^3}{1 - q^2} - \frac{q^3}{1 - q^2} y^2 + y^3 \right]^{-1/2} dy \quad (62)$$

which is an incomplete elliptic integral of the first kind⁹.

Thus,

$$\theta_1 = \left(\frac{q^3}{1 - q^2}\right)^{1/2} g F(\varphi, k) \quad (63)$$

where

$$g = \left[\frac{1 - q^2}{q^2(3 - q^2)} \right]^{1/4} \quad (64)$$

$$k^2 = \frac{1}{2} + \frac{1}{4}(3 - 2q^2) [(1 - q^2)(3 - q^2)]^{-1/2} \quad (65)$$

$$\varphi = \cos^{-1} \left[q^2 - 2 + \{ (1 - q^2)(3 - q^2) \}^{1/2} \right] \quad (66)$$

⁹ P. F. Byrd and M. D. Friedman, "Handbook of Elliptic Integrals for Engineers and Physicists", (Springer, 1954), p. 88, Eq. 241.00.

Since $\frac{d(\beta^2)}{d(q^2)} = 3^{-5/3} \frac{(3-q^2)}{(1-q^2)^{5/3}}$, the first integral, $C_1^{(l)}(3)$ is now given by

$$C_1^{(l)}(3) = \frac{1}{2 \cdot 3^{5/3}} \int_0^{3/4} [1 - \cos^l(2\theta_1)] \frac{(3-q^2)}{(1-q^2)^{5/3}} dq^2 \quad (67)$$

Figs. 3 and 4 show the integrands for $l = 1$ and for $l = 2$ respectively as functions of q^2 .

It is seen that the integrands oscillate wildly as q^2 approaches 0.75. The integrals are subdivided into four ranges of q^2 . For the smaller values of q^2 numerical integration is satisfactory making use of the elliptical functions. However, for the larger values of q^2 it is convenient to use $2\theta_1$ as the integration variable and develop approximate expressions for $\frac{d(\beta^2)}{d(2\theta_1)}$ which will allow analytic evaluation of the required integrals. Thus, $C_1^{(l)}(3)$ is divided into the ranges $0 \leq q^2 \leq .52$, $.52 \leq q^2 \leq .68$, $.68 \leq q^2 \leq .748$, and $.748 \leq q^2 \leq .75$.

$$C_1^{(l)}(3) = I_1^{(l)} + I_2^{(l)} + I_3^{(l)} + I_4^{(l)} \quad (68)$$

where

$$I_1^{(l)} = \frac{1}{2 \cdot 3^{5/3}} \int_0^{.52} [1 - \cos^l(2\theta_1)] \frac{(3-q^2)}{(1-q^2)^{5/3}} dq^2 \quad (69)$$

$$I_2^{(l)} = \frac{1}{2} \int_{5.87292}^{9.10288} [1 - \cos^l(2\theta_1)] \frac{d(\beta^2)}{d(2\theta_1)} d(2\theta_1) \quad (70)$$

$$I_3^{(l)} = \frac{1}{2} \int_{9.10288}^{16.91616} [1 - \cos^l(2\theta_1)] \frac{d(\beta^2)}{d(2\theta_1)} d(2\theta_1) \quad (71)$$

$$I_4^{(l)} = \frac{1}{2} \int_{16.91616}^{\infty} [1 - \cos^l(2\theta_1)] \frac{d(\beta^2)}{d(2\theta_1)} d(2\theta_1) \quad (72)$$

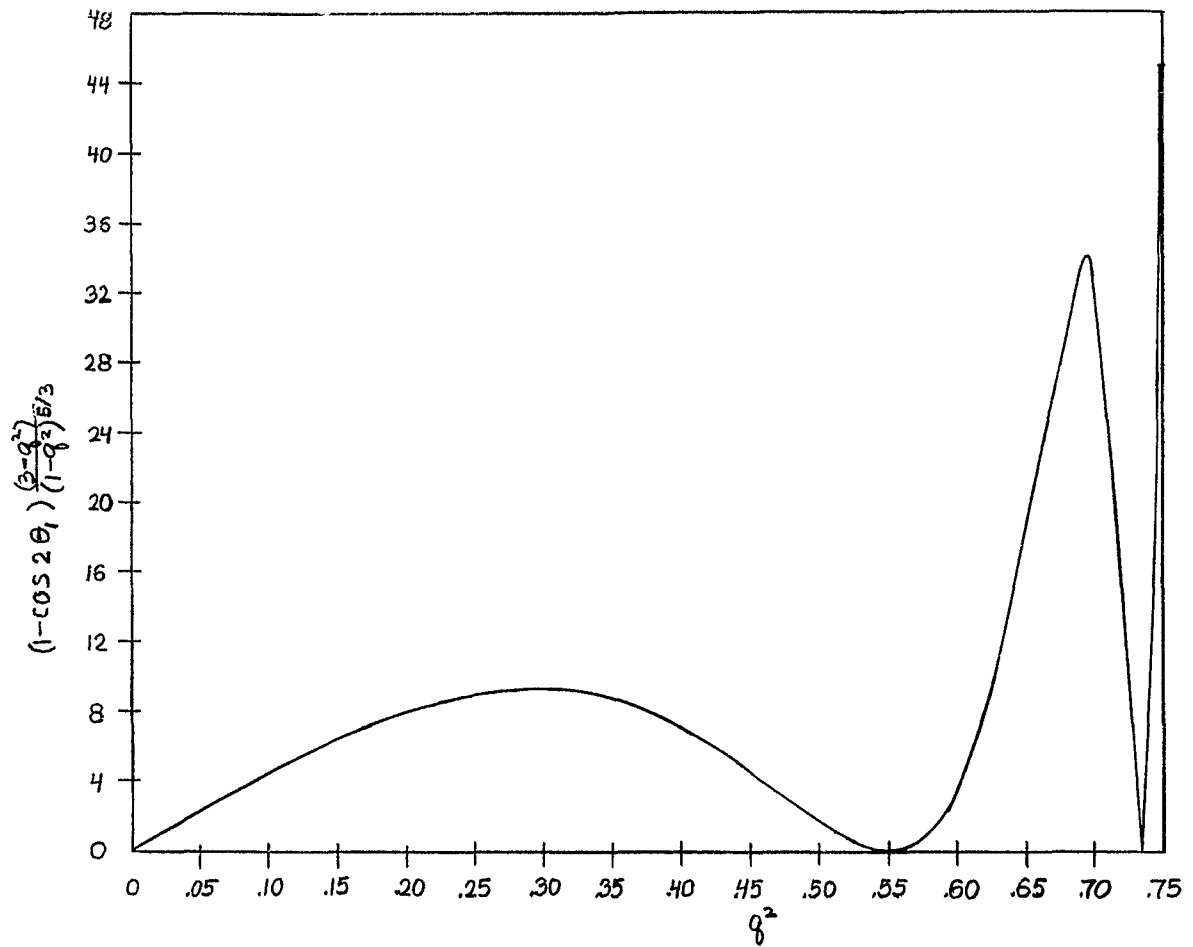


Fig. 3 Integrand of $C_1^{(1)}(3)$ from Eq. (67).

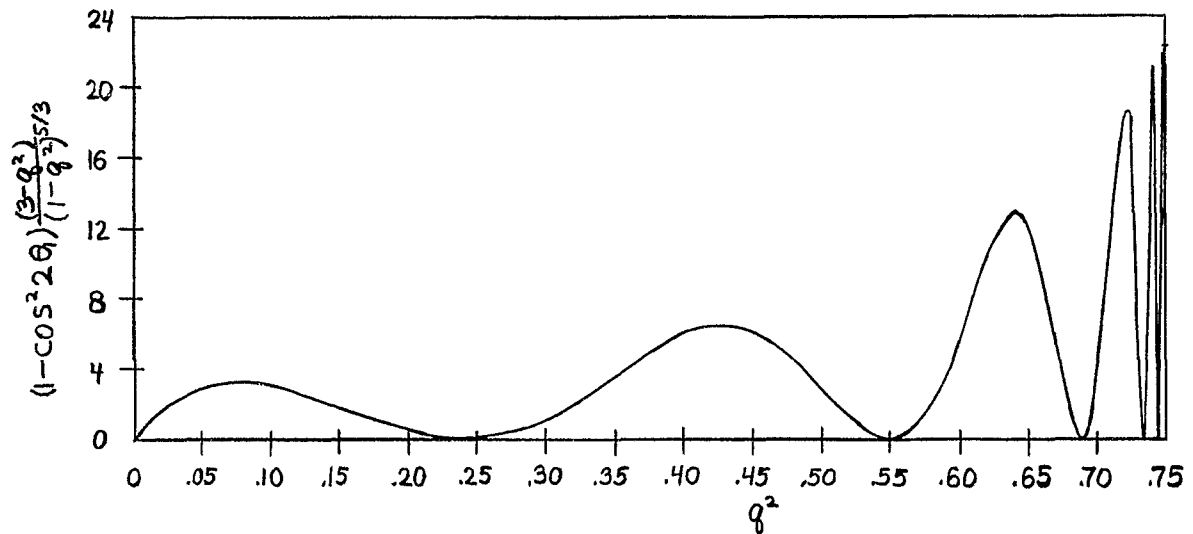


Fig. 4 Integrand of $C_1^{(2)}(3)$ from Eq. (67).

The integrals $I_1^{(1)}$ and $I_1^{(2)}$ were evaluated numerically using Simpson's Rule with interval sizes of .04 in q^2 from $0 \leq q^2 \leq .40$ and intervals of .02 for larger values of q^2 . The integrands were evaluated at these values of q^2 by making use of Eqs. (63) and (67) together with interpolated values of the elliptical integral. Four point Lagrangian interpolation coefficients were used to interpolate along both the rows and the columns in the table of Byrd and Friedman.¹⁰ Thus we obtained

$$I_1^{(1)} = .2449 \quad (73)$$

$$I_1^{(2)} = .1136 \quad (74)$$

An expression for $\frac{d(\beta^2)}{d(2\theta_1)}$, sufficiently accurate in the interval $5.87292 \leq 2\theta_1 \leq 9.10288$ is obtained by fitting the curve of $\beta_{crit}^2 - \beta^2$ vs. $2\theta_1$, with a cubic equation. (See Fig. 5 for a plot of $\beta_{crit}^2 - \beta^2$ vs. $2\theta_1$)

$$\beta_{crit}^2 - \beta^2 = D + E(2\theta_1) + F(2\theta_1)^2 + G(2\theta_1)^3 \quad (75)$$

The points

$2\theta_1$	5.87292	6.74996	7.94016	9.10288
$\beta_{crit}^2 - \beta^2$	.500778	.411380	.300569	.209800
q^2	.52	.58	.64	.68

are used to evaluate the constants in Eq. (75). The constants are $D = 1.062129$, $E = -.0640403$, $F = -.0092255$, and $G = .0006563$. With these constants, Eq. (75) fits the actual curve better than .05% in the region of interest.

¹⁰ Ref. 9, pp. 324.

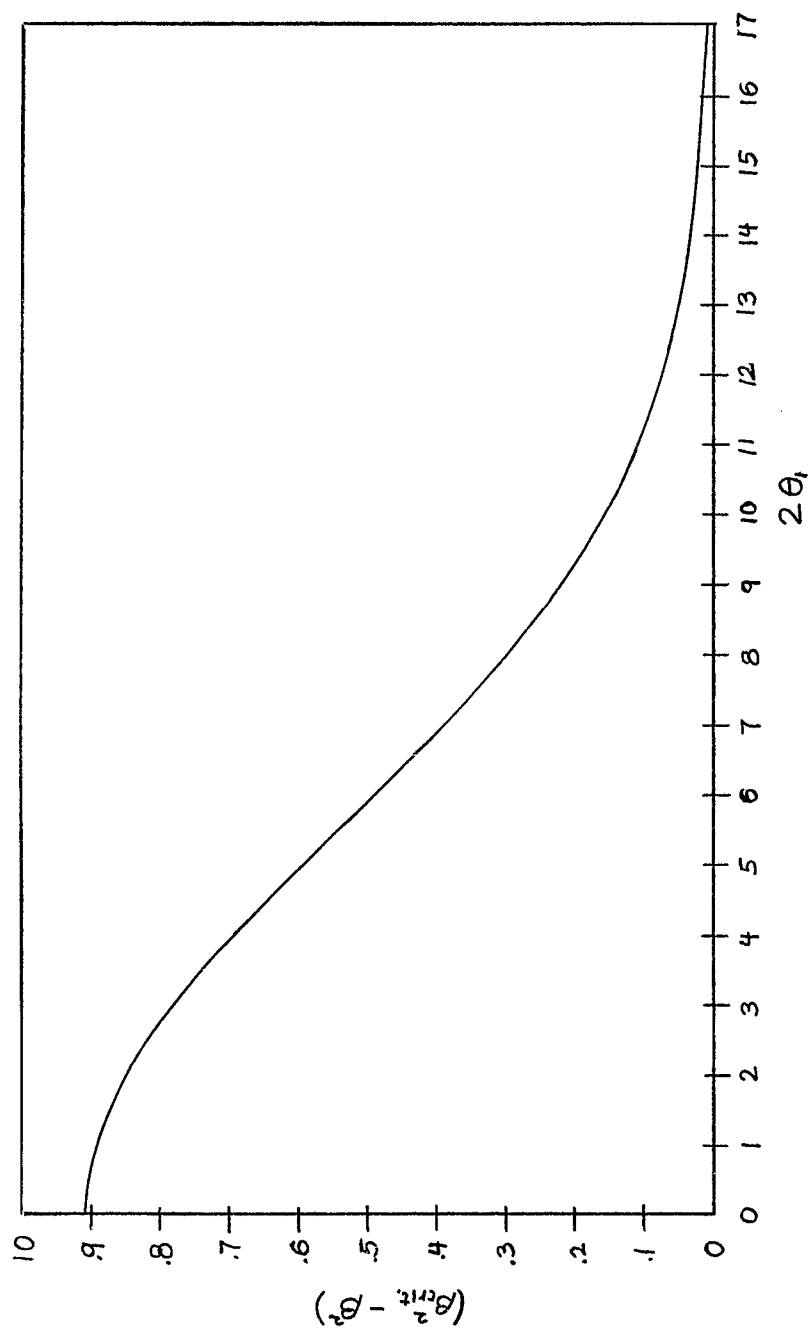


Fig. 5. $(\beta_{crit}^2 - \beta^2)$ vs. $2\theta_1$ when $\beta \leq \beta_{crit}$.

Integration of Eq. (70) gives

$$I_2^{(1)} = -\frac{1}{2} \left[E(2\theta_1) + F(2\theta_1)^2 + G(2\theta_1)^3 \right. \\ \left. - \{E + 2F(2\theta_1) + 3G(2\theta_1)^2 \cdot 6G\} \sin(2\theta_1) \right. \\ \left. - \{2F + 6G(2\theta_1)\} \cos(2\theta_1) \right]_{2\theta_1=5.87292}^{2\theta_1=9.10288} \quad (76)$$

$$I_2^{(2)} = \frac{1}{2} \left[-\frac{1}{2} \{E(2\theta_1) + F(2\theta_1)^2 + G(2\theta_1)^3\} \right. \\ \left. + \frac{1}{4} \{E + 2F(2\theta_1) + 3G(2\theta_1)^2 - \frac{3}{2}G\} \sin(4\theta_1) \right. \\ \left. + \frac{1}{4} \{F + 3G(2\theta_1)\} \cos(4\theta_1) \right]_{2\theta_1=5.87292}^{2\theta_1=9.10288} \quad (77)$$

We obtained

$$I_2^{(1)} = .1020 \quad (78)$$

$$I_2^{(2)} = .0690 \quad (79)$$

The integrals $I_3^{(1)}$ and $I_4^{(1)}$ are evaluated with the aid of an asymptotic expression for $d(\beta^2)/d(2\theta_1)$ accurate near β_{crit} . The asymptotic form for θ_1 as q^2 approaches .75 may be obtained as follows:

From Eqs. (63) and (64),

$$\theta_1 = g[(1-g^2)(3-g^2)]^{-1/4} F(\varphi, k) \quad (80)$$

As $q^2 \rightarrow .75$, $k \rightarrow 1$ and $\varphi \rightarrow 120^\circ$. Since ¹¹

$$F(\varphi, k) = 2K(k) - F(\pi - \varphi, k), \quad (81)$$

$$F(\varphi, k) \approx 2K(k) - F(60^\circ, 1). \quad (82)$$

¹¹ Ref. 9, p. 12, Eq. 113.02

If $k' = (1 - k^2)^{1/2}$, the expansion for $K(k)$ is¹²

$$K(k) = \left(\ln \frac{4}{k'} \right) \left[1 + \frac{1}{4} k'^2 \right] - \frac{1}{4} k'^2 + \dots \quad (83)$$

Since $k \cong 1$,

$$2K \cong 2 \ln \frac{4}{k'} = \ln \frac{16}{1 - k^2} \quad (84)$$

$$F(\varphi, k) \cong \ln \frac{16}{1 - k^2} - F(60^\circ, 1) \quad (85)$$

If the substitution $q^2 = \frac{3}{4} - z^2$ is made,

$$q[(1 - q^2)(3 - q^2)]^{-1/4} = 1 - \frac{16}{9} z^2 + \dots \quad (86)$$

and

$$\frac{16}{1 - k^2} = \frac{36}{z^2} [1 + 4z^2 + \dots] \quad (87)$$

Therefore,

$$\theta_1 \cong \ln \frac{36}{z^2} - F(60^\circ, k) \quad (88)$$

Since

$$-F(60^\circ, 1) = -\ln(\tan 60^\circ + \sec 60^\circ) = \ln(2 - 3^{1/2}) \quad (89)$$

$$z^2 = 36(2 - 3^{1/2}) e^{-\theta_1} \quad (90)$$

¹² Ref. 9, p. 298, Eq. 900.05

*. See Appendix A for an alternate derivation of this equation.

$$\frac{d(\beta^2)}{d(2\theta_1)} = \frac{d(\beta^2)}{d(z^2)} \cdot \frac{d(z^2)}{d(2\theta_1)} \quad (91)$$

From Eq. (61), it is found that asymptotically

$$\beta^3 \cong \frac{3^{1/2}}{2} [1 - 6z^2] \quad (92)$$

Therefore,

$$\frac{d(\beta^2)}{d(2\theta_1)} \cong 36(48)^{1/2} (2 - 3^{1/2}) e^{-\theta_1} = 17.5283 e^{-\theta_1} = k e^{-\theta_1} \quad (93)$$

$$\int_{\beta^2}^{\beta_{crit}^2} d(\beta^2) = 2k \int_{\theta_1}^{\infty} e^{-\theta_1} d\theta_1 \quad (94)$$

$$\beta_{crit}^2 - \beta^2 = 2k e^{-\theta_1} \quad (95)$$

This suggests approximating β^2 by an equation of the form

$$\beta_{crit}^2 - \beta^2 = e^{-\theta_1} [A + B(2\theta_1) + C(2\theta_1)^2] \quad (96)$$

over the range $9.10288 \leq 2\theta_1 \leq 16.91616$. The points

$2\theta_1$	9.10288	11.74086	16.91616
$\beta_{crit}^2 - \beta^2$	.209800	.0780498	.0072236
q^2	.68	.727	.748

are used to evaluate the constants in Eq. (96). The constants are $A = -30.419284$, $B = 7.524143$, and $C = -.219515$. Eq. (96) fits the actual curve better than .5% in the region of interest. Eq. (71) may now be integrated analytically; the results

are:

$$I_3^{(1)} = -e^{-\theta_1} \left[\begin{aligned} &0.5 \{ A + B(2\theta_1) + C(2\theta_1)^2 \} \\ &- \{ (0.1A - 0.32B + 0.128C) \\ &\quad + (0.1B - 0.64C)(2\theta_1) + 0.1C(2\theta_1)^2 \} \cos(2\theta_1) \\ &+ \{ (0.2A - 0.24B - 0.704C) \\ &\quad + (0.2B - 0.48C)(2\theta_1) + 0.2C(2\theta_1)^2 \} \sin(2\theta_1) \end{aligned} \right] \Bigg|_{2\theta_1=16.91616}^{2\theta_1=9.10288} \quad (94)$$

$$I_3^{(2)} = -e^{-\theta_1} \left[\begin{aligned} &(0.264706A - 0.055364B + 0.084674C) \\ &+ (0.264706B - 0.110726C)(2\theta_1) + 0.264706C(2\theta_1)^2 \\ &+ \{ (0.058824A - 0.103806B - 0.076532C) \\ &\quad + (0.058824B - 0.207612C)(2\theta_1) + (0.058824C)(2\theta_1)^2 \} \sin(4\theta_1) \\ &- \{ (0.029412A - 0.110727B + 0.169346C) \\ &\quad + (0.029412B - 0.221454C)(2\theta_1) + 0.029412C(2\theta_1)^2 \} \cos^2(2\theta_1) \end{aligned} \right] \Bigg|_{2\theta_1=16.91616}^{2\theta_1=9.10288} \quad (95)$$

Thus we obtained

$$I_3^{(1)} = .1217 \quad (96)$$

$$I_3^{(2)} = .0444 \quad (97)$$

The integrals $I_4^{(1)}$ and $I_4^{(2)}$ are evaluated with the help of Eq. (93).

$$I_4^{(1)} = -k e^{-\theta_1} \left[1 + 0.4 \left(\sin(2\theta_1) - \frac{1}{2} \cos(2\theta_1) \right) \right] \Bigg|_{2\theta_1=16.91616}^{2\theta_1=\infty} \quad (98)$$

$$I_4^{(2)} = -k e^{-\theta_1} \left[1 - 0.117647 \left(\frac{1}{2} \cos^2(2\theta_1) - \sin(4\theta_1) + 4 \right) \right] \Bigg|_{2\theta_1=16.91616}^{2\theta_1=\infty} \quad (99)$$

Thus we obtained

$$I_4^{(1)} = .0026 \quad (100)$$

$$I_4^{(2)} = .0022 \quad (101)$$

From Eqs. (68), (73), (78), and (100) and Eqs. (68), (74), (79), and (101) respectively, we obtained

$$C_1^{(1)}(3) = .4712 \quad (102)$$

$$C_1^{(2)}(3) = .2292 \quad (103)$$

To evaluate the $C_2^{(0)}(3)$, as defined in Eq. (60), it is convenient to change the variable of integration from β^2 to p^2 , where p is the first positive root of the denominator in equation (8),

$$\beta^2 = p^2 [3(p^2 - 1)]^{-2/3} \quad (104)$$

Since $y_m(\beta) = p$, it follows that

$$\theta_2 = \left(\frac{p^3}{p^2-1}\right)^{1/2} \int_0^p \left[\frac{p^3}{p^2-1} - \frac{p^3}{p^2-1} y^2 + y^3\right]^{-1/2} dy \quad (105)$$

which is another elliptic integral of the first kind.¹³

Thus

$$\theta_2 = \left(\frac{p^3}{p^2-1}\right)^{1/2} g' F(\varphi', k') \quad (106)$$

where

$$g' = 2 \left[p(p^2-1)^{-1} (4p^2-3)^{1/2} \right]^{-1/2} \quad (107)$$

¹³ Ref. 9, p. 74, eq. 234.00.

$$k'^2 = \frac{1}{2} + \frac{1}{2} (2p^2 - 3)(4p^2 - 3)^{-1/2} \quad (108)$$

$$\varphi' = \sin^{-1} \left[\frac{3(4p^2 - 3)^{1/2} - 4p^2 + 3}{2(3 - p^2)} \right]^{1/2} \quad (109)$$

Eq. (60) for the $C_2^{(\ell)}(3)$ becomes

$$C_2^{(\ell)}(3) = \frac{1}{2 \cdot 3^{5/3}} \int_1^3 \left[1 - (-1)^\ell \cos^\ell(2\theta_2) \right] \frac{(3 - p^2)}{(p^2 - 1)^{5/3}} dp^2 \quad (110)$$

Figures 6 and 7 show the integrands for $\ell = 1$ and $\ell = 2$ respectively, as functions of p^2 .

Here again, the integrations were carried out in several parts, with the method chosen to fit the behavior of the integrand in the various ranges of p^2 . $C_2^{(\ell)}(3)$ is divided into the ranges $1 \leq p^2 \leq 1.025$; $1.025 \leq p^2 \leq 1.050$; $1.050 \leq p^2 \leq 2.90$; and $2.90 \leq p^2 \leq 3.00$. Thus,

$$C_2^{(\ell)}(3) = J_1^{(\ell)} + J_2^{(\ell)} + J_3^{(\ell)} + J_4^{(\ell)} \quad (111)$$

where

$$J_1^{(\ell)} = \frac{1}{2 \cdot 3^{5/3}} \int_1^{1.025} \left[1 - (-1)^\ell \cos^\ell(2\theta_2) \right] \frac{(3 - p^2)}{(p^2 - 1)^{5/3}} dp^2 \quad (112)$$

$$J_2^{(\ell)} = \frac{1}{2 \cdot 3^{5/3}} \int_{1.025}^{1.050} \left[1 - (-1)^\ell \cos^\ell(2\theta_2) \right] \frac{(3 - p^2)}{(p^2 - 1)^{5/3}} dp^2 \quad (113)$$

$$J_3^{(\ell)} = \frac{1}{2 \cdot 3^{5/3}} \int_{1.05}^{2.9} \left[1 - (-1)^\ell \cos^\ell(2\theta_2) \right] \frac{(3 - p^2)}{(p^2 - 1)^{5/3}} dp^2 \quad (114)$$

$$J_4^{(\ell)} = \frac{1}{2 \cdot 3^{5/3}} \int_{2.9}^3 \left[1 - (-1)^\ell \cos^\ell(2\theta_2) \right] \frac{(3 - p^2)}{(p^2 - 1)^{5/3}} dp^2 \quad (115)$$

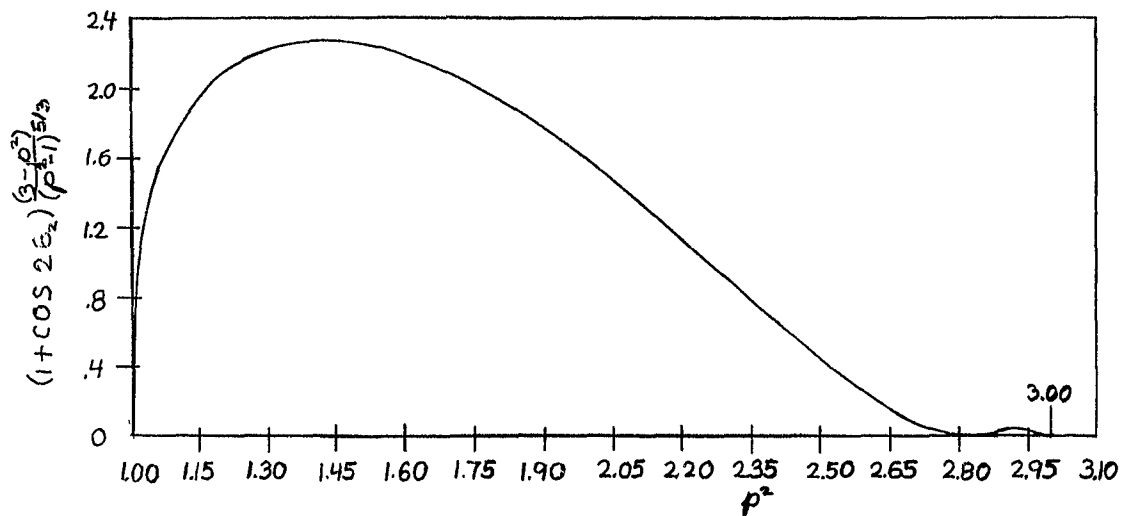


Fig. 6 Integrand of $C_2^{(1)}(3)$ from Eq. (110).

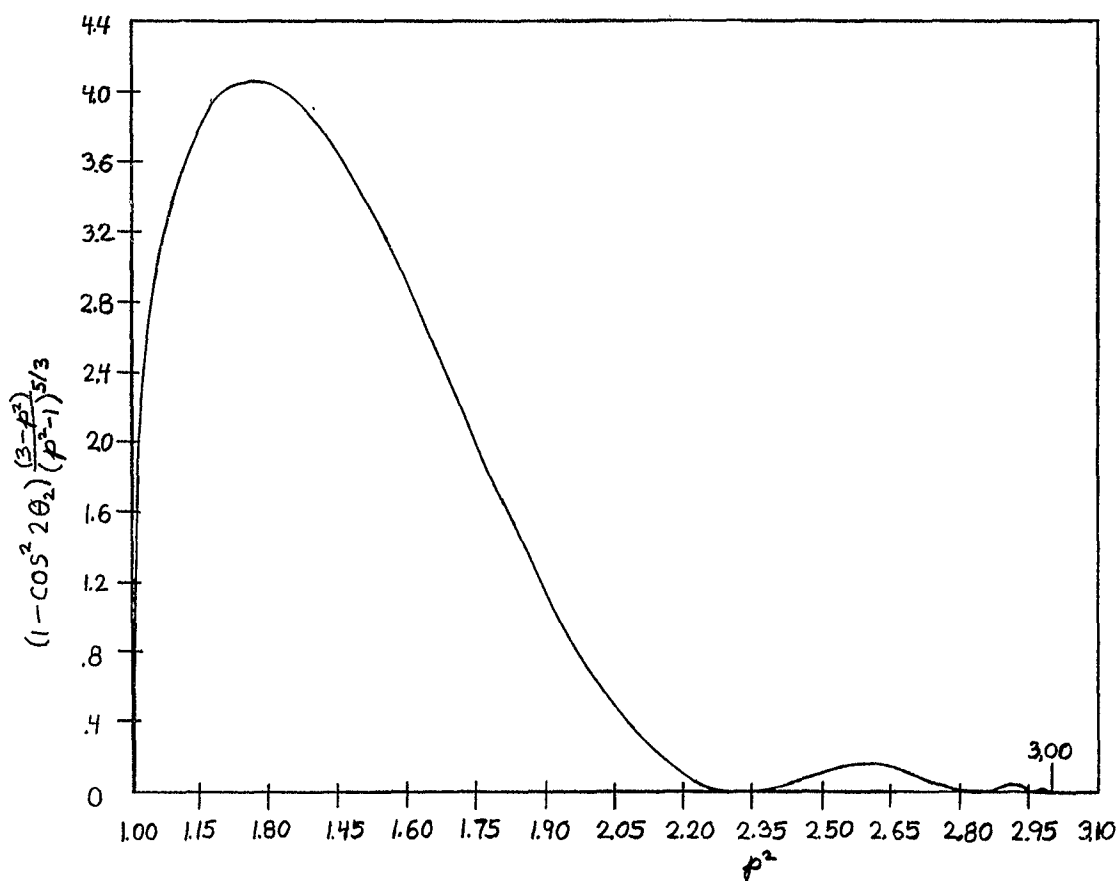


Fig. 7 Integrand of $C_2^{(2)}(3)$ from Eq. (110).

To obtain $J_1^{(1)}$, write Eq. (105) as

$$\theta_2 = \int_0^p \left[\left(1 - \frac{y}{p}\right) \left(1 + \frac{y}{p} - (p^2 - 1) \left(\frac{y}{p}\right)^2\right) \right]^{-\frac{1}{2}} dy \quad (116)$$

Since $p^2 \cong 1$, the term $(p^2 - 1) \left(\frac{y}{p}\right)^2$ can be neglected, and

$$\theta_2 \cong \int_0^p \left[1 - \left(\frac{y}{p}\right)^2 \right]^{-\frac{1}{2}} dy = \frac{\pi}{2} p \quad (117)$$

Using the fact that $[1 - (-1)^l \cos^l(2\theta_2)] = (1 - \cos^l \chi)$ and Eq. (112),

$$J_1^{(1)} = \frac{1}{2 \cdot 3^{5/3}} \int_1^{1.025} (1 - \cos^3 \chi) \frac{(3 - p^2)}{(p^2 - 1)^{5/3}} dp^2 \quad (118)$$

Since p is almost 1, Eq. (118) may be written as

$$J_1^{(1)} \cong \frac{1}{2 \cdot 3^{5/3}} \int_1^{1.025} (1 - \cos^3 \chi) 2^{-3/3} (p-1)^{-5/3} dp^2 \quad (119)$$

From Eqs. (8), (117), and a power series expansion of $\cos \chi$, one finds that

$$1 - \cos^3 \chi = \frac{\pi^2}{2} (p-1)^2 + \alpha (p-1)^3 + \dots \quad (120)$$

Powers of $(p-1)$ higher than three are neglected in Eq. (120) and α is chosen so that the integrand of Eq. (119) is equal to 1.15406, the value of the integrand of Eq. (110) when $p^2 = p_1^2 = 1.025$. α equals 239.49. From Eq. (119),

$$\begin{aligned} J_1^{(1)} &= 6^{-5/3} \int_1^{1.025} \left[\frac{\pi^2}{2} (p-1)^2 + \alpha (p-1)^3 \right] (p-1)^{-5/3} dp^2 \\ &= 6^{-5/3} \left[\frac{3}{4} \pi^2 (p_1 - 1)^{4/3} + \frac{3}{7} (\pi^2 + 2\alpha) (p_1 - 1)^{7/3} + \frac{3}{5} \alpha (p_1 - 1)^{10/3} \right] \end{aligned} \quad (121)$$

and

$$\begin{aligned} J_1^{(2)} &= 6^{-5/3} \int_1^{1.025} \left[\pi^2 (p-1)^2 + 2\alpha (p-1)^3 - \frac{\pi^4}{4} (p-1)^4 - \pi^2 \alpha (p-1)^5 - \alpha^2 (p-1)^6 \right] (p-1)^{-5/3} dp^2 \\ &= 3 \cdot 6^{-5/3} \left[\frac{\pi^2}{2} (p_1 - 1)^{4/3} + \frac{2}{7} (\pi^2 + 2\alpha) (p_1 - 1)^{7/3} + \frac{1}{10} (4\alpha - \frac{\pi^2}{2}) (p_1 - 1)^{10/3} \right. \\ &\quad \left. - \frac{\pi^2}{13} \left(\frac{1}{2} + 2\alpha \right) (p_1 - 1)^{13/3} - \frac{2}{17} (\pi^2 \alpha + \alpha^2) (p_1 - 1)^{16/3} - \frac{2}{19} \alpha^2 (p_1 - 1)^{19/3} \right] \end{aligned} \quad (122)$$

Thus we obtained

$$J_1^{(1)} = 0.0015 \quad (123)$$

$$J_1^{(2)} = 0.0029 \quad (124)$$

Four point Lagrangian integration coefficients are used to get the $J_2^{(1)}$

$$J_2^{(1)} = 0.0026 \quad (125)$$

$$J_2^{(2)} = 0.0081 \quad (126)$$

$J_3^{(1)}$ is obtained by using Simpson's rule with interval sizes of 0.025 in p^2 from 1.05 to 1.20, 0.05 in p^2 from 1.20 to 1.30, and .10 in p^2 from 1.30 to 2.90

$$J_3^{(1)} = .1996 \quad (127)$$

$$J_3^{(2)} = .2267 \quad (128)$$

$J_4^{(1)}$ is found by noting that an upper limit to the value of Eq. (115) is obtained by setting $\cos 2\theta_2 = 1$. Thus,

$$J_4^{(1)} < J_{max}^{(1)} = 3^{-5/3} \int_{2.9}^3 (3-p^2)(p^2-1)^{-5/3} dp^2 \cong 0.00026 \quad (129)$$

Since the cosine term of Eq. (115) has infinitely many oscillations in this region, to a sufficient degree of accuracy, the factor $(1 + \cos 2\theta_2)$ can be replaced by its mean value of unity in the integral for $J_4^{(1)}$. Thus, a good estimate of $J_4^{(1)}$ is $\frac{1}{2} J_{max}^{(1)}$ and

$$J_4^{(1)} = .0013 \quad (130)$$

The best estimate of $J_4^{(2)}$ is obtained in a similar fashion. Here, the maximum value of $(1 - \cos^2 2\theta_2)$ is unity so that the maximum value of $J_4^{(2)} = \frac{1}{2} J_{\text{Max}}^{(1)}$. The average value of $(1 - \cos^2 2\theta_2)$ is one-half, so that our best estimate of $J_4^{(2)}$ is $\frac{1}{4} J_{\text{Max}}^{(1)}$ or

$$J_4^{(2)} = .0007 \quad (131)$$

Eq. (111) gives

$$C_2^{(1)}(3) = .2038 \quad (132)$$

$$C_2^{(2)}(3) = .2349 \quad (133)$$

From Eq. (58), the collision integrals are found to be

$$C^{(1)}(3) = .6750 \quad (134)$$

$$C^{(2)}(3) = .4641 \quad (135)$$

SUMMARY

The collision integrals we evaluated are:

Repulsive Potential

$$A^{(1)}_{(2)} = .397601$$

$$A^{(2)}_{(2)} = .527843$$

$$A^{(1)}_{(3)} = .3115$$

$$A^{(2)}_{(3)} = .3533$$

Attractive Potential

$$C^{(1)}_{(2)} = .806907$$

$$C^{(2)}_{(2)} = .710970$$

$$C^{(1)}_{(3)} = .6750$$

$$C^{(2)}_{(3)} = .4641$$

APPENDIX A

In this appendix, an alternate derivation of the asymptotic equation, Eq. (90), is given. Write

$$\Theta_1 = \Theta_{11} + \Theta_{12} = \int_0^{3^{1/2}} [1 - y^2 + \frac{1}{3}(\frac{y}{\beta})^3]^{-1/2} dy + \int_{3^{1/2}}^{\infty} [1 - y^2 + \frac{1}{3}(\frac{y}{\beta})^3]^{-1/2} dy \quad (A-1)$$

and make the substitution $x = 1 - 3^{-1/2}y$ in Θ_{11} and $z = 3^{-1/2}y - 1$ in Θ_{12} . Then,

$$\Theta_{11} = \int_0^1 [x^2(1 - \frac{2}{3}x) + c^2(1-x)^3]^{-1/2} dx \quad (A-2)$$

$$\Theta_{12} = \int_0^{\infty} [z^2(1 + \frac{2}{3}z) + c^2(1+z)^3]^{-1/2} dz \quad (A-3)$$

$$c^2 = 3^{1/2} \left[\frac{1}{3\beta^3} - \frac{1}{3\beta_{crit}^3} \right]; \quad (\beta_{crit} = (\frac{2}{3})^{1/2}) \quad (A-4)$$

Let x_0 be a small positive number and take β close to β_{crit} so that c^2 is much smaller than x_0 . Then

$$\begin{aligned} \Theta_{11} &\cong \int_0^{x_0} (x^2 + c^2)^{-1/2} dx + \int_{x_0}^1 x^{-1} (1 - \frac{2}{3}x)^{-1/2} dx \\ &\cong \ln \left\{ \frac{1}{c} [x_0 + (x_0^2 + c^2)^{1/2}] \left(\frac{1 - 3^{1/2}}{1 + 3^{1/2}} \right) \left(\frac{(1 - \frac{2}{3}x_0)^{1/2} + 1}{(1 - \frac{2}{3}x_0)^{1/2} - 1} \right) \right\} \end{aligned} \quad (A-5)$$

$$\Theta_{11} \cong \ln \left[\frac{12(2 - 3^{1/2})}{c} \right] \quad (A-6)$$

In order to evaluate Θ_{12} , take z_0 small and choose c^2 much less than z_0 . Then,

$$\begin{aligned}\Theta_{12} &\cong \int_0^{z_0} [Z^2 + 3c^2Z + c^2]^{-1/2} dZ + \int_{z_0}^{\infty} Z^{-1} (1 + \frac{2}{3}Z)^{-1/2} dZ \\ &\cong \ln \left\{ \frac{2(Z_0^2 + 3c^2Z_0 + c^2)^{1/2} + 2Z_0 + 3c^2}{2c + 3c^2} \right\} \\ &\quad + \ln \left\{ \frac{(1 + \frac{2}{3}Z_0)^{1/2} - 1}{(1 + \frac{2}{3}Z_0)^{1/2} + 1} \right\} \\ &\cong \ln \frac{2Z_0}{c} + \ln \frac{6}{Z_0}\end{aligned}\tag{A-7}$$

$$\Theta_{12} \cong \ln \frac{12}{c}\tag{A-8}$$

Therefore,

$$\Theta_1 \cong \ln \left[\frac{144(2 - 3^{1/2})}{c^2} \right]\tag{A-9}$$

By using the equation $q^2 = \frac{3}{4} - z^2$, we obtain

$$c^2 \cong \frac{4z^2}{1 - 2z^2}\tag{A-10}$$

$$\therefore \Theta_1 \cong \ln \left[\frac{144(2 - 3^{1/2})(1 - z^2)}{4z^2} \right] \cong \ln \left[\frac{36(2 - 3^{1/2})}{z^2} \right]\tag{A-11}$$

Eq.(90) follows immediately.

APPENDIX B

In this appendix, values for the angle of deflection χ are given together with a graph of χ vs. β^2 .

The angle χ is evaluated for values of q^2 listed in Table a by using Eqs. (9) and (63). Since in this case $\varphi > 90^\circ$, Eq. (81) is also used. Four point Lagrangian interpolation coefficients are used to interpolate along both the rows and columns in the table for $F(\varphi, k)$ found in Byrd and Friedman¹⁴ for all q^2 . For all values of q^2 except $q^2 = .734, .741, \text{ and } .748$, the four point Lagrangian interpolation coefficients are used to interpolate along the column of the table for $K(k)$. For the three values of q^2 just given, it is more accurate to use the equation¹⁵

$$K = \Lambda + \frac{\Lambda - 1}{4} k'^2 + \frac{9}{64} (\Lambda - \frac{7}{6}) k'^4 + \dots \quad (\text{B-1})$$

where

$$\Lambda = \ln \frac{4}{k'} \quad (\text{B-2})$$

$$k' = (1 - k^2)^{1/2} \quad (\text{B-3})$$

For values of p^2 listed in Table b, Eqs. (8) and (106) are used to evaluate χ . Four point Lagrangian interpolation coefficients are used as explained above to evaluate the elliptic function.

¹⁴ Ref. 10.

¹⁵ E. Jahnke and F. Emde, "Tables of Functions", (Dover, 1945), p. 73.

Table a

$$(\beta^2 \leq \beta_{\text{crit}}^2)$$

β^2	q^2	$-\chi$	β^2	q^2	$-\chi$
0	0	0	0.40778224	0.52	5.87292
0.01976052	0.04	1.14281	0.43565336	0.54	6.14246
0.04065843	0.08	1.64778	0.46537752	0.56	6.43332
0.06282202	0.02	2.06022	0.4971807	0.58	6.74996
0.08640116	0.16	2.43106	0.5313292	0.60	7.09994
0.11157215	0.20	2.78204	0.5681396	0.62	7.49232
0.13854409	0.24	3.12378	0.6079917	0.64	7.94016
0.16756714	0.28	3.46410	0.6513440	0.66	8.46456
0.19894356	0.32	3.81040	0.6987600	0.68	9.10288
0.23304244	0.36	4.16814	0.7509361	0.70	9.93132
0.27032007	0.40	4.54440	0.8087475	0.72	11.13542
0.29032412	0.42	4.74186	0.8305105	0.727	11.74086
0.31134829	0.44	4.94660	0.8531540	0.734	12.55009
0.33348871	0.46	5.16038	0.87674009	0.741	13.79346
0.35685478	0.48	5.38462	0.90133673	0.748	16.91616
0.38186008	0.50	5.62188	0.90856029	0.750	∞

Table b

$$(\beta^2 \geq \beta_{\text{crit}}^2)$$

β^2	p^2	$-\chi$	β^2	p^2	$-\chi$
0.908561	3.000	∞	1.08128	1.600	1.22953
0.908832	2.900	7.33231	1.14471	1.500	1.01080
0.909693	2.800	5.88405	1.23977	1.400	0.80593
0.911285	2.700	5.01853	1.39459	1.300	0.60135
0.913713	2.600	4.38617	1.51426	1.250	0.50003
0.917210	2.500	3.88115	1.68686	1.200	0.39967
0.921956	2.400	3.45659	1.80551	1.175	0.34957
0.928299	2.300	3.08831	1.95835	1.150	0.29959
0.936595	2.200	2.75875	2.16338	1.125	0.24961
0.947424	2.100	2.46005	2.45458	1.100	0.19967
0.961500	2.000	2.18679	2.90595	1.075	0.14979
0.979892	1.900	1.92637	3.71930	1.050	0.09981
1.00415	1.800	1.68321	5.76345	1.025	0.04995
1.03666	1.700	1.45191	∞	1.000	0

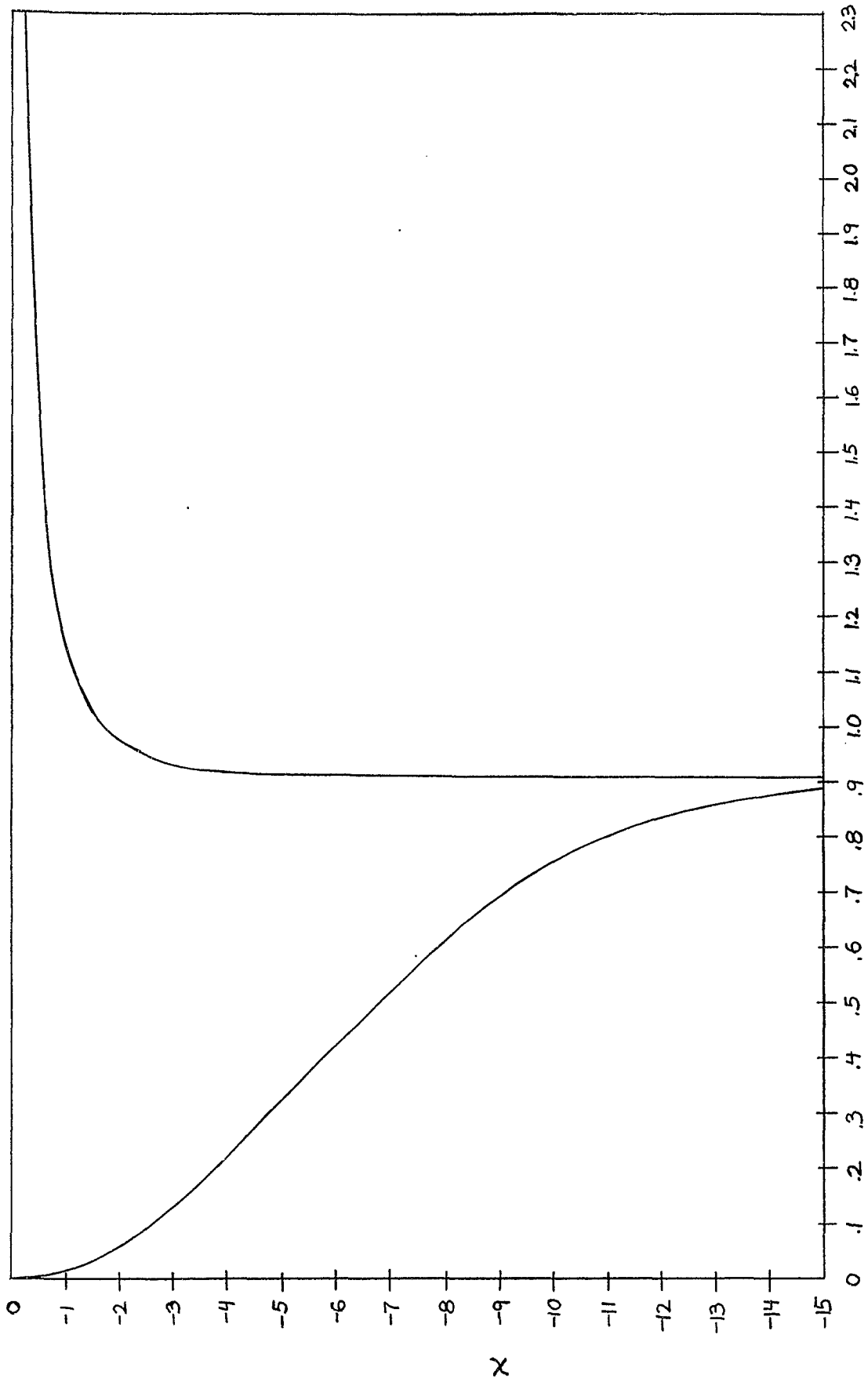


Fig. 8. Angle of deflection χ vs. β^2 for attractive potential with $\delta = 3$.
 $\beta^2 = k^2 \left[\frac{1}{8} \frac{U^2}{a^2} \right]^{2/3}$