

If $0 < g < g_c$ then, as is shown in Appendix C, when $\mathcal{J}C \rightarrow 0$ it follows that $z \rightarrow z_m > 3$ and $\mathfrak{M} \rightarrow 0$. Hence $d^2 f_3(z)/dz^2 \rightarrow d^2 f_3(z_m)/dz^2 \neq 0$. Upon substitution into (D.2) of the limits attained by z , \mathfrak{M} , and $d^2 f_3(z)/dz^2$ as $\mathcal{J}C \rightarrow 0$ we obtain (43). If $g > g_c$ then from Appendix C we find that as $\mathcal{J}C \rightarrow 0$, $z \rightarrow 3$ and $\mathfrak{M}^2 \rightarrow (1 - g_c/g) > 0$.

Hence from (D.3), $d^2 f_3/dz^2 \rightarrow -[2^{3/2}\pi(z-3)^{1/2}]^{-1}$. Substitution of these limiting values of z , \mathfrak{M} , and $d^2 f_3(z)/dz^2$ into (D.2) yields (44).

Equation (53) then follows upon substitution of (41d) and (43) into (D.1), and (54) follows upon substitution of (41c) and (44) into (D.1).

Approximate Analytic Approach to the Classical Scattering Problem*

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An approximate analytic approach to the problem of determining differential scattering cross sections for classical central-field repulsive forces is described. It is shown that the impact parameter, b , can be approximated by $b = R \cos(\theta/2)$, where R is approximately the distance of closest approach and θ is the scattering angle in the center-of-mass system. A simple approximation gives the potential energy of interaction between two atoms as $V(R) = 2E \sin(\theta/2)$, where E is the energy in the center-of-mass system. Simple analytic expressions for the differential scattering cross section, σ , are derived from the above two relationships for three special cases of a two-parameter screened

Coulomb potential energy,

$$V(R) = Z_1 Z_2 e^2 A \exp(-pAR) [1 - \exp(-AR)]^{-1},$$

where $Z_i e$ is the charge on the i th atom, A^{-1} is a screening radius, and p is an adjustable parameter which is restricted to $\frac{1}{2}$, 1, and 2 in this paper.

A new and improved method for calculating σ exactly is also discussed and is used to compute the exact behavior of σ for $p=1$. A table is presented which allows one to compare the exact and approximate σ 's for $p=1$ over a wide range of energy and scattering angles. The agreement is particularly good for large energy transfer.

I. INTRODUCTION

THE purpose of this paper is to present a method for obtaining approximate analytic representations for classical differential scattering cross sections suitable for studying slowing down processes in radiation damage theory.¹ Briefly, this approximation will be shown to interpolate remarkably well between the impulse and hard-sphere approximations valid, respectively, for small and large angle scattering.

In Sec. II, the problem of determining an approximate relationship between the impact parameter, b , and the angle, θ , associated with an arbitrary central repulsive force scattering of an incident atom by a target atom will be discussed.

Approximate analytic expressions for the impact parameter and differential scattering cross section will be derived in Sec. III for three types of screened Coulomb potential energy functions suggested by Brinkman and Meehan.² Exact solutions for the impact parameter and differential scattering cross section have been worked out for a special case of the aforementioned potential energy and a comparison between

these results and those derived from the analytic approximations will be given in Sec. IV.

II. DERIVATION OF APPROXIMATE SCATTERING EQUATIONS

Figure 1 shows the path described by an incident atom being scattered by a repulsive central force through an angle, θ , by a fixed target atom. In this figure, the impact parameter is denoted by b and the coordinates (r, ϕ) define the path of the incident atom relative to the target atom as the origin. The differential equation for the (r, ϕ) trajectory is given by the well-known expression³

$$(u')^2 + u^2 = b^{-2}(1 - E^{-1}V), \quad (1)$$

where $u = 1/r$, V is the potential energy of interaction, and E is the energy of the incident atom measured in the center-of-mass system. The prime on u denotes differentiation with respect to ϕ . The exact relationship between θ and b is easily derived from Eq. (1) and is well known to be³

$$\theta = \pi - 2 \int_0^{u_0} du [b^{-2}(1 - E^{-1}V) - u^2]^{-1/2}, \quad (2)$$

where u_0 is the zero of the integrand and physically

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¹ For a recent review article concerning the status of slowing down processes in radiation damage theory, see G. J. Dienes and G. H. Vineyard, *Radiation Effects in Solids* (Interscience Publishers, New York, 1957).

² J. A. Brinkman and C. J. Meehan (to be published).

³ H. Goldstein, *Classical Mechanics* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1950).

equal to the reciprocal of the distance of closest approach.

Equation (2) must be numerically integrated for V 's appropriate to radiation damage theory. For example, Everhart, Stone, and Carbone,⁴ have solved this equation for the case of the Bohr screened Coulomb potential.

A. Integral Equation for Trajectory

Approximate relations between θ and b for arbitrary V can be obtained from Eq. (1) by converting this equation into the following equivalent integral equation, derived in Appendix A.

$$u = b^{-1} \sin \phi - \int_0^\phi d\phi' \sin(\phi - \phi') g(u(\phi')), \quad (3)$$

where

$$g(u) = \frac{1}{2} b^{-2} E^{-1} (\partial V / \partial u). \quad (4)$$

The first term in Eq. (3) represents the initial straight line trajectory of the incident particle. The second term accounts for the deflection in the trajectory associated with the repulsive potential energy, V .

Figure 1 shows that ϕ_m defines the angle at which the radial momentum or $(du/d\phi)$ vanishes. This figure also shows that the scattering angle, θ , is related to ϕ_m by $\theta = \pi - 2\phi_m$. Consequently, one readily finds by differentiation of Eq. (3) with respect to ϕ and subsequent appropriate change of variable of integration that

$$\sin(\theta/2) = b \int_{\theta/2}^{\pi/2} d\phi'' \cos(\phi'' - \pi/2) g(u(\pi/2 - \phi'')). \quad (5)$$

This expression is exact and can be evaluated after Eq. (3) has been solved for $u(\phi)$.

B. Approximate Relationship Between Scattering Angle and Impact Parameter

A simple approximate relationship between θ and b can now be established by substituting $u = b^{-1} \sin \phi$, the straight line trajectory of the incident particle, into Eq. (5). Using this approximation, one can transform Eq. (5) into the following expression.

$$V(R) + \frac{b}{[R^2 - b^2]^{3/2}} H(R) = 2E, \quad (6)$$

where

$$H(R) = - \int_R^\infty dr \frac{b}{[r^2 - b^2]^{3/2}} \frac{d}{dr} V(r). \quad (7)$$

The distance R appearing in these expressions is related to θ by

$$R = b \sec(\theta/2). \quad (8)$$

⁴E. Everhart, G. Stone, and R. G. Carbone, Phys. Rev. **99**, 1287 (1955).

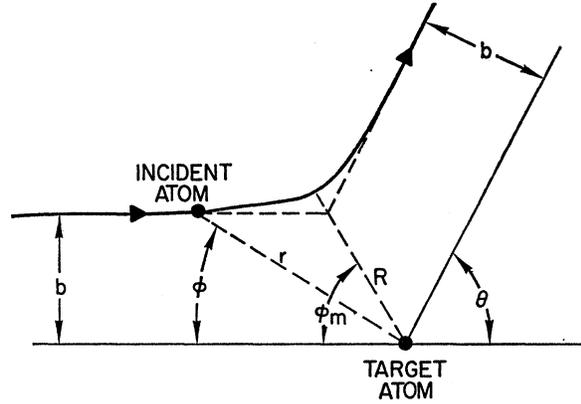


FIG. 1. Trajectory of an incident atom colliding with a fixed target atom. In this figure, r denotes the distance between the atoms.

Figure 1 shows that R is approximately equal to the distance of closest approach.

For small angle scattering, R is nearly equal to b and the second term in Eq. (6) dominates. One can also show that Eq. (6) reduces to the impulse approximation for small θ and behaves like a hard sphere approximation for large scattering angles. Finally, one should note that Eq. (6) is *exact* for Coulomb scattering, i.e., for $V(r)$ varying as $1/r$, since $g(u)$ in Eq. (5) is a constant [see Eq. (4)].

C. Approximate Evaluation of H for Arbitrary V

It has been possible to approximate H for arbitrary V by a procedure described in Appendix B. It is shown in this appendix that the simplest approximation which appears physically significant leads to

$$H(R) = V(R) [\sec(\theta/2) - \tan(\theta/2)]. \quad (9)$$

When this expression is substituted into Eq. (6), one finds that

$$\sin(\theta/2) = V(R)/2E, \quad (10)$$

with $b = R \cos(\theta/2)$, [see Eq. (8)] forms the basis for deriving analytic expressions for b in terms of θ . Again, Eq. (10) is exact for the Coulomb potential.

We stress the fact that Eq. (10) is equivalent to Eq. (6) for large angles, but is only an approximation for small angles excepting, of course, the singular case of the Coulomb potential. A more accurate expression for $H(R)$, given in Appendix B, can be used for numerical integration but leads to unwieldy analytic expressions for b in terms of θ and will not be used in this paper.

III. ANALYTIC APPROXIMATIONS FOR DIFFERENTIAL SCATTERING CROSS SECTIONS

Brinkman and Meehan² point out that the potential energy given by

$$V(r) = Z_1 Z_2 A e^2 \exp(-Br) [1 - \exp(-Ar)]^{-1} \quad (11)$$

TABLE I. Analytic approximations for distance of closest approach, R_p , impact parameter, b_p , and differential scattering cross section, σ_p , for the Brinkman-Meechan potential, $V = \exp(-pR)[1 - \exp(-R)]^{-1}$. In this table, $t = (T/T_m)^{1/2}$, $Q = (1-t^2)^{1/2}$, $F = (2Et)^{-1}$, and $L_p = b_p^{-1}Q^2Ft^{-2}$.

p	$b_p Q^{-1} = R_p$	$(T_m R_p^{-2}/\pi)\sigma_p$
$\frac{1}{2}$	$2 \ln\{[1 + (F^2/4)]^{1/2} + (F/2)\}$	$1 + L_1[1 + (F^2/4)]^{-1/2}$
1	$\ln(1+F)$	$1 + L_1[1+F]^{-1}$
2	$\ln[1 + (1+4F)^{1/2}] - \ln 2$	$1 + 2L_2[1+4F + (1+4F)^{1/2}]^{-1}$

is well-suited for studying the interaction between two atoms of charge Z_1e and Z_2e . This potential energy behaves like $Z_1Z_2e^2/r$ for small r and has a Born-Mayer or Huntington exponential character for large r . The choice of A and B is discussed elsewhere since we consider only three special cases $B=A/2$, A , and $2A$ for arbitrary A . However, these three cases cover a considerable range of interest and still allow us to determine R in terms of E and $\sin(\theta/2)$ using Eq. (10).

The unit of length used in the remainder of this paper will be $1/A$ while the unit of energy (measured in the center-of-mass system) will be taken as $Z_1Z_2e^2A$. With these conventions, one notes that

$$V(R) = \exp(-pR)[1 - \exp(-R)]^{-1}, \quad (12)$$

where $p = B/A$.

The differential scattering cross section per unit energy transferred to the struck atom, $\sigma(T)$, is given by

$$(T_m/2)\sigma(T) = d(\pi b^2)/d(\cos\theta), \quad (13)$$

where T_m is the maximum possible energy transferred. The energy transferred to the struck atom, T , is related to θ by

$$T = T_m[\sin(\theta/2)]^2. \quad (14)$$

A. Approximate Differential Scattering Cross Section for Brinkman-Meechan Potential

The Brinkman-Meechan potential energy, in the units previously described, is characterized by a single parameter, $p = B/A$. Consequently, b_p and σ_p will be used to denote the impact parameter and differential scattering cross section appropriate to $p = B/A$.

When $p = \frac{1}{2}$, 1, or 2, one can obtain R in terms of θ from Eqs. (10) and (12). The impact parameter, b_p , is now obtained from Eq. (8) and σ_p is found by a differentiation with respect to θ [see Eq. (13)]. These results are presented in Table I, where σ has been derived from an expression, equivalent to Eq. (13), given by

$$(2T_m/\pi)\sigma = - (db^2/dt), \quad (15)$$

where $t = (T/T_m)^{1/2} = \sin(\theta/2)$.

IV. COMPARISON OF EXACT AND APPROXIMATE RESULTS FOR $p=1$ SCATTERING

In order to test the validity of the analytic approximations presented in Table I, we have evaluated the differential scattering cross section exactly for the special case of the Brinkman-Meechan potential with $p=1$. Since V is a rapidly varying function of r or u , it appeared undesirable to us to follow the usual procedure of solving Eq. (2) numerically to obtain θ as a function of b . Furthermore, as Everhart, Stone, and Carbone⁴ have pointed out, the integrand of Eq. (2) has a singularity which requires special attention.

A. Transformation of Scattering Integral to a New Representation

Fortunately, our search for an improved method for determining θ as a function of b has been successful. Our approach is new but is based upon the work of Keller, Kay, and Shmoys⁵ who have solved the inverse problem of determining the potential energy function from scattering data. It is shown in Appendix C that Eq. (2) can be transformed into

$$\theta = 2 \int_0^w dY \sin(Y) [(\mathcal{R}\mathcal{R}_0^{-1})^2 - (\cos Y)^2]^{-1/2}, \quad (16)$$

where

$$V(\mathcal{R}) = E[1 - (\cos(w) \sec Y)^2]$$

and

$$V(\mathcal{R}_0) = E[1 - (\cos w)^2]$$

define the distances \mathcal{R} and \mathcal{R}_0 in terms of the potential energy, V . The impact parameter is now found to be

$$b = \cos w \mathcal{R}_0. \quad (17)$$

The parameter w varies from 0 to $\pi/2$ while θ varies from 0 to π . The integrand of Eq. (16) is bounded and varies slowly with Y in contrast to the previously described behavior of the integrand of Eq. (2).

In order to determine the differential scattering cross section, it is necessary to compute $(db/d\theta) = (db/dw) \times (dw/d\theta)^{-1}$. The derivative, (db/dw) , can be obtained analytically from Eq. (17) but $(d\theta/dw)$ must be evaluated from Eq. (16). A simple calculation shows that the latter derivative can be obtained directly as

$$(d\theta/dw) = E \sin(2w) \mathcal{R}_0^{-2} \times \int_0^w dY \sin(Y) \mathcal{R} [(\mathcal{R}\mathcal{R}_0^{-1})^2 - (\cos Y)^2]^{-3/2} J \quad (18)$$

where

$$J = -F(\mathcal{R}) \sec^2 Y + \mathcal{R}\mathcal{R}_0^{-1}F(\mathcal{R}_0), \quad (19)$$

with

$$F(\mathcal{R}) = [dV(\mathcal{R})/d\mathcal{R}]^{-1}. \quad (20)$$

⁵ J. B. Keller, I. Kay, and J. Shmoys, Phys. Rev. **102**, 557 (1956).

A careful inspection of the integrand of Eq. (18) shows that it is also slowly varying and bounded and enables one to compute $(d\theta/dw)$ directly.

B. Numerical Comparison of Exact and Approximate Impact Parameters and Differential Scattering Cross Sections for $p=1$

Numerical results obtained from the analytic approximations for σ , given in Table I, have been compared with the exact solutions for the case $p=1$ in order to establish the usefulness of the analytic approximations. Equations (16) and (18) were evaluated numerically for a set of E 's and w 's by using Gauss's mechanical quadrature.⁶ Our numerical procedures were checked out for $V(R)=R^{-2}$ for which b and σ are known exactly.³

Table II shows exact and approximate results obtained for $p=1$ scattering. It is to be recalled that the units of length and energy are $1/A$ and $Z_1Z_2e^2A$, respectively. This table shows that the simple analytic approximation for σ_1 , which is given in Table I, compares quite favorably with the exact differential scattering cross section for $p=1$ scattering over the entire range of energies involved. The agreement is very good for large energy transfer.

V. SUMMARY AND DISCUSSION

An approach has been presented for obtaining analytic approximations for the differential scattering cross section for an arbitrary potential energy function, $V(R)$, which can be solved explicitly for R as a function of V . It was found that the impact parameter, b , is related to the scattering angle, θ , by $b=R \cos(\theta/2)$, where $V(R)=2E \sin(\theta/2)$ defines R which is the approximate distance of closest approach in terms of θ . The differential scattering cross section per unit energy transferred to the struck atom, σ , is then given by $(T_m/2)\sigma = [d\pi b^2/d(\cos\theta)]$, where T_m is the maximum energy transferred in a collision.

Analytic approximations for σ were presented in Table I for three special cases of the potential energy function proposed by Brinkman and Meehan [see Eq. (12)].

A new approach for computing σ exactly was described in Sec. IV by using a parametric representation which eliminates the usual singularity in the integrand of the scattering integral. Briefly, this new approach allows one to compute θ in terms of a slowly varying function of a parameter w . A direct method of computing $(d\theta/dw)$ was also presented. The impact parameter was given by $b=\cos w \mathcal{R}_0$, where $V(\mathcal{R}_0)=E[1-(\cos w)^2]$ defines the distance \mathcal{R}_0 in terms of w . The energy dependence of σ is primarily accounted for by the variation of \mathcal{R}_0 with E which can be expressed analytically for the Brinkman-Meehan potential energy.

⁶ W. E. Milne, *Numerical Calculus* (Princeton University Press, Princeton, New Jersey, 1949), p. 285.

TABLE II. Comparison of approximate and exact differential scattering cross sections for $p=1$ as a function of incident atom energy, E , and fractional energy transferred to struck atom, T/T_m . Units of energy and length are defined in text.

T/T_m	$(T_m/4\pi)\sigma_1$	$E=10$	$E=10^{-1}$	$E=10^{-3}$	$E=10^{-5}$
1	Exact	5.3×10^{-4}	7.1×10^{-1}	8.3	26.3
	Approx.	6.0×10^{-4}	8.0×10^{-1}	9.7	29.3
10^{-1}	Exact	5.9×10^{-2}	11.2	43.7	85.1
	Approx.	5.1×10^{-2}	8.0	30.2	62.8
10^{-2}	Exact	5.0	1.5×10^2	3.3×10^2	5.3×10^2
	Approx.	3.4	1.0×10^2	2.3×10^2	3.7×10^2
10^{-3}	Exact	2.5×10^2	1.8×10^3	2.9×10^3	4.5×10^3
	Approx.	1.5×10^2	1.3×10^3	2.4×10^3	3.6×10^3
10^{-4}	Exact	6.0×10^3	2.1×10^4	3.2×10^4	5.0×10^4
	Approx.	3.7×10^3	1.6×10^4	2.7×10^4	3.8×10^4

A comparison of the exact and approximate differential scattering cross sections was made in Table II for the $p=1$ potential energy, $V(R)=[\exp(R)-1]^{-1}$. The agreement appears to be good and in fact shows that the simple analytic approximations for σ given in Table I are suitable for characterizing collisions between atoms in radiation damage calculations.

APPENDIX A. DERIVATION OF INTEGRAL EQUATION FOR TRAJECTORY

Equation (3) of the text was derived from Eq. (1) by converting the latter to a second order differential equation. If Eq. (1) is differentiated with respect to u one obtains

$$u'' + u = -g, \quad (\text{A-1})$$

since $d(u^2)/du = 2u'$ and g is defined by Eq. (4). This differential equation is easily converted to an integral equation by considering g to be a known function of ϕ . A particular solution, u_p , of Eq. (A-1) is

$$u_p = - \int_0^\phi d\phi' \sin(\phi - \phi') g(u(\phi')),$$

since $u_p'' + u_p = -g(u)$. Similarly, the general solution of the homogeneous equation, $u'' + u = 0$, is $u = C \cos\phi + D \sin\phi$. Hence, the general solution of Eq. (A-1) is $u = u_p + C \cos\phi + D \sin\phi$. Now, from Fig. 1, $u \rightarrow b^{-1} \sin\phi$ as $\phi \rightarrow 0$; however, u_p tends to zero much faster than ϕ for potentials which fall off more rapidly than $1/r$ as $r \rightarrow \infty$. Consequently, $C=0$ and $D=b^{-1}$ which proves our assertion that Eq. (3) of the text is the proper solution of Eq. (A-1).

APPENDIX B. EVALUATION OF $H(R)$ FOR ARBITRARY $V(R)$

The integral, $H(R)$, of the text will be evaluated here for arbitrary $V(R)$. An integration of Eq. (7) by parts yields

$$H(R) = R^2 V'(R) \cot(\theta/2) + b^{-1} \int_R^\infty dr [1 - (b/r)^2]^{\frac{1}{2}} [r^2 V'(r)], \quad (\text{B-1})$$

where the prime denotes differentiation with respect to r or R as the case may be. It should be noted that the integral in Eq. (B-1) must be evaluated numerically for potential energies of interest in this paper. Note that $b=R \cos(\theta/2)$ by Eq. (8) so that

$$\psi(x,\theta)=[1-(b/r)^2]^{\frac{1}{2}}=[1-\cos^2(\theta/2)x^{-2}]^{\frac{1}{2}}, \quad (\text{B-2})$$

where $x=r/R$ varies from unity to infinity. Our somewhat devious procedure is to approximate $\psi(x,\theta)$ by $\alpha_n+x^{-1}\beta_n$ for $x_n \leq x \leq x_{n+1}$, where α_n and β_n are functions of θ only. Our motivation comes from the fact that this approximation allows us to evaluate Eq. (B-1) in closed form. The parameters α_n and β_n are chosen so that

$$\begin{aligned} \psi(x_n,\theta) &= \alpha_n + x_n^{-1}\beta_n, \\ \psi(x_{n+1},\theta) &= \alpha_n + x_{n+1}^{-1}\beta_n, \end{aligned} \quad (\text{B-3})$$

where $x_1=1$ and $x_N=\infty$ with N being the maximum number of points used. With these conventions, one can show that

$$H(R) = \sec(\theta/2) \sum_{n=1}^{N-1} \beta_n(\theta)(V_{n+1}-V_n), \quad (\text{B-4})$$

where

$$\alpha_n = \frac{x_n + x_{n+1}}{G_n + G_{n+1}}, \quad (\text{B-5})$$

and

$$\beta_n = G_n - x_n \alpha_n, \quad n=1, 2, \dots, N-1. \quad (\text{B-6})$$

Here, $G_n = \{x_n^2 - [\cos(\theta/2)]^2\}^{\frac{1}{2}}$, $V_n = V(Rx_n)$, and $\alpha_{N-1}=1$.

The simplest approximation to $H(R)$ is obtained by choosing $N=2$, i.e., $x_1=1$ and $x_2=\infty$. For this case, only $\beta_1=G_1-1$ or $\sin(\theta/2)-1$ is needed to evaluate $H(R)$ approximately. Since $V_1=V(R)$, one finds that Eq. (9) of the text represents the simplest possible approximation to $H(R)$.

We have also investigated a more exact approximation by taking $x_1=1$, $x_2=1.1$, $x_3=2$, and $x_4=\infty$. The β_n 's derived for this case have been approximated analytically and it is found that

$$H(R) = [\sec(\theta/2) - \tan(\theta/2)] [(4.58V_1 - 3.48V_2 - 0.83V_3) + t(5.24V_2 - 4.58V_1 - 0.39V_3)], \quad (\text{B-7})$$

where $t = \sin(\theta/2)$, $V_1 = V(R)$, $V_2 = V(1.1R)$, and $V_3 = V(2R)$. Preliminary investigations indicate that

this approximation is in error by less than 10% for the Brinkman-Meehan potential.

APPENDIX C. DERIVATION OF TRANSFORMED SCATTERING INTEGRAL

Equation (16) of the text will be derived in this appendix. Our starting point is Eq. (5) of Keller, Kay, and Shmoys⁵ who show that

$$\theta = \pi - 2 \int_0^x dy h(y) [x-y]^{-\frac{1}{2}}, \quad (\text{C-1})$$

where $x=b^{-2}$ and

$$h(y) = (2y^{\frac{1}{2}})^{-1} + y^{\frac{1}{2}}(dv/dy)(2v)^{-1}. \quad (\text{C-2})$$

This formulation is satisfactory for monotonically decreasing potential energies. In these equations,

$$v = 1 - E^{-1}V(\mathcal{R}); \quad y = \mathcal{R}^{-2}v^{-1}. \quad (\text{C-3})$$

An inspection of Eqs. (C-1) and (C-2) shows that the integration associated with the first term of Eq. (C-2) can be carried out so that

$$\theta = - \int_0^x dy \left[\frac{dv}{dy} \right] v^{-1} [xy^{-1} - 1]^{-\frac{1}{2}}. \quad (\text{C-4})$$

Now, introduce v as the new variable of integration; the limits of integration are fixed by

$$v = 1 \quad \text{for} \quad y = 0, \quad (\text{C-5})$$

and

$$v = v_0 = 1 - E^{-1}V(\mathcal{R}_0) \quad \text{for} \quad y = x = \mathcal{R}_0^{-2}v_0^{-1}. \quad (\text{C-6})$$

Hence, using Eqs. (C-3), (C-5), and (C-6), one finds that Eq. (C-4) becomes

$$\theta = \int_{v_0}^1 dv v^{-\frac{1}{2}} v_0^{\frac{1}{2}} [(\mathcal{R}\mathcal{R}_0^{-1})^2 - (v_0/v)]^{-\frac{1}{2}}. \quad (\text{C-7})$$

Equation (16) of the text follows by introducing the new variables Y and w given by $v = v_0(\sec Y)^2$, $v_0 = (\cos w)^2$ and making the appropriate transformations.

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