

Energy Loss to a Cold Background Gas. I. Higher Order Corrections to the Fokker-Planck Operator for a Lorentz Gas

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The relaxation of an isotropic distribution of test particles in a homogeneous background gas is considered when the mass ratio is not necessarily very small. For the most part, the temperature of the background gas molecules is assumed to be zero, although a method is presented for including nonzero-temperature effects. The Boltzmann collision integral is represented by an infinite-series differential operator which, for all force laws, reduces to the usual Fokker-Planck equation when terms of second order in the mass ratio are discarded. For the case of Coulomb interactions, the usual Fokker-Planck equation is obtained if either the second-order mass-ratio terms or the terms of order $1/\ln\Lambda$ are discarded. A random-walk analysis is used to obtain a differential operator which agrees with the infinite-series differential operator when third-order terms in the mass ratio are discarded. When the background-gas temperature approaches zero, the usual Fokker-Planck equation predicts that an initial delta-function distribution will always remain a delta function during the relaxation process; whereas it is shown that both the random-walk analysis and the infinite-series differential operator give exact values for the dispersion of the initial delta function.

I. INTRODUCTION

THIS paper is concerned with the slowing down of light test particles in a homogeneous background gas of heavy molecules when the kinetic energy of the test particles is much greater than the average thermal energy of the background molecules. In particular, we will usually consider the limit as the background-gas temperature approaches zero. This simplification allows us to obtain more complete solutions which provide some insight into the approximations which are involved when the Boltzmann collision integral is represented by a differential operator. It will be demonstrated in Sec. II that, in the limit as the background-gas temperature approaches zero, the usual Fokker-Planck equation^{1,2} for a Lorentz gas predicts that the distribution function will always remain a delta function if it is initially a delta function. A similar result has recently been shown by May³ for the case of a fast test particle losing energy by Coulomb collisions to a homogeneous plasma of ions and electrons.

The preservation of an initial delta function would imply that every particle of a given initial energy behaves exactly the same during the slowing-down process. However, even when the background-gas temperature approaches zero, it is apparent that the energy lost in a collision is a statistical quantity, as is the time between successive collisions. One of the purposes of this paper will be to show that the lack of dispersion predicted by the usual Fokker-Planck equation for a cold background gas can be corrected by including higher-order terms in the mass ratio.

A random-walk analysis of the energy loss is employed in Sec. III to take into account the stochastic properties of the collisions. Some results for the case of constant collision frequency are given in Sec. IV and a partial differential equation of the Fokker-Planck type is obtained in Sec. V for an arbitrary velocity dependence of the collision frequency. The problem of defining the collision frequency for inverse-power molecular forces within the framework of the random-walk analysis is considered in an Appendix.

In Sec. VI we formally obtain a differential operator from the Boltzmann collision integral by extending the method of Allis² *without making the assumption that the mass ratio is small*. The differential operator has the form of an infinite series where the n th term involves the n th order partial derivative of the distribution function and an explicit form is given for the coefficients. If we omit the partial derivatives of third order and higher in the mass ratio, the resulting Fokker-Planck equation is identical with the equation obtained in Sec. V from the random-walk analysis. For Coulomb forces, the differential operator reduces to the usual Fokker-Planck operator for any value of the mass ratio, if terms of order $1/\ln\Lambda$ are discarded.

The problem of deriving a partial differential operator from the Boltzmann equation has been considered by several authors.¹⁻⁶ In particular, Siegel⁷ obtained second-order terms in the mass ratio for the linear Boltzmann equation satisfied by a gas of infinitely thin disks constrained to move in one direction with a non-zero background-gas temperature. Although the Boltzmann equation and its approximation by the usual Fokker-Planck equation have nonpositive eigenvalues,

¹ S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases* (Cambridge University Press, New York, 1960).

² W. P. Allis, *Handbuch der Physik* edited by S. Flügge (Springer-Verlag, Berlin, 1956), Vol. 21, pp. 383-444.

³ R. M. May, *Phys. Rev.* **135**, A1009 (1964).

⁴ J. Kielson and J. E. Storer, *Quart. Appl. Math.* **10**, 248 (1952).

⁵ N. G. van Kampen, *Can. J. Phys.* **39**, 551 (1961).

⁶ K. Andersen and K. E. Shuler, *J. Chem. Phys.* **40**, 633 (1964).

⁷ A. Siegel, *J. Math. Phys.* **1**, 378 (1960).

Siegel demonstrated that, when the second-order terms were obtained in a straightforward manner, the second-order operator possessed *positive* eigenvalues which raised the possibility of runaway solutions which grow indefinitely in amplitude.⁸ This important result obviously raises serious questions concerning the validity of differential operators which are obtained by including powers of the mass ratio greater than unity. However, the simplifications introduced by the zero-temperature background gas allow us to obtain an exact analytic solution for the second-order operator and show explicitly that the solutions do not grow in amplitude as $t \rightarrow \infty$. We remark here that our second-order operator formally includes *positive* eigenvalues in the same sense as Siegel's operator but we reserve a discussion of the eigenvalue spectrum and the resolution of the apparent paradox for a second paper on this topic. The analytic solution for the test-particle distribution function approaches the appropriate equilibrium distribution as $t \rightarrow \infty$, namely a delta function centered at the origin corresponding to the zero-temperature background gas.

In Sec. VII, we discuss the criterion for the effect of a nonzero background-gas temperature to be less than the effect of the second-order terms in the mass ratio. For constant collision frequency, exact solutions are obtained for certain moments when the initial distribution function is a delta function; the average energy and the dispersion of the average energy for the zero-temperature background gas are shown to be given exactly by the random-walk analysis when second-order terms in the mass ratio are included.

II. BEHAVIOR OF THE FOKKER-PLANCK SOLUTION FOR A COLD LORENTZ GAS

For small mass ratios, the usual Fokker-Planck approximation to the Boltzmann equation for an isotropic, spatially homogeneous distribution function in a Lorentz gas is

$$\frac{\partial f}{\partial t} = \frac{1}{2} \epsilon v^{-2} \frac{\partial}{\partial v} \left[v^3 \nu \left(1 + \frac{kT_0}{mv} \frac{\partial}{\partial v} \right) f \right], \quad (1)$$

where f is the test-particle distribution function defined so that $4\pi f v^2 dv$ is the expected number of particles with speeds between v and $v+dv$. The background-gas temperature is T_0 and $\epsilon = 2mM(m+M)^{-2}$, where m is the light test particle and M is the mass of a heavy background molecule. The collision frequency $\nu(v)$ is in general a function of velocity. Equation (1) can be obtained by expanding the Boltzmann integral in powers of ϵ and retaining only the first term.

⁸ Siegel describes a technique for revising the second-order operator by including third-order terms which render the eigenvalue spectrum nonpositive; however, the revised operator involves an arbitrary constant.

Let the temperature $T_0 \rightarrow 0$, so that Eq. (1) becomes

$$\frac{\partial f}{\partial t} = \frac{1}{2} \epsilon v^{-2} \frac{\partial}{\partial v} (v^3 \nu f). \quad (2)$$

The solution of Eq. (2) which vanishes as $v \rightarrow \infty$ is

$$f(v, t) = [\nu(v_1) v_1^3 / \nu(v) v^3] f_0(v_1), \quad (3)$$

where $v_1(v, t)$ is defined by the equation

$$\int_v^{v_1} \frac{dx}{x\nu(|x|)} = \frac{1}{2} \epsilon t \quad (4)$$

and the function f_0 is the initial distribution function.

By substituting back into Eq. (2), Eq. (3) can be verified, and it can also be shown that the number density

$$\int_0^\infty v^2 f(v, t) dv,$$

as calculated from Eq. (3), is a constant provided that $\lim_{v \rightarrow +0} v_1(v, t) = v^*(t) = 0$. The last condition will be obeyed only if $\lim_{v \rightarrow 0} \nu(v)$ is less than some constant M . The physical meaning of this is that "soft" molecules, whose collision frequencies increase as $v \rightarrow 0$, reach the origin of v -space within a finite time. In this case, Eq. (3) must be augmented by the term

$$v^{-2} \delta(v) \int_0^{v^*(t)} f_0(x) x^2 dx,$$

which represents the "pool" of test particles with zero energy.

When the collision frequency is independent of velocity, Eq. (3) becomes simply

$$f(v, t) = e^{(3/2)\epsilon v t} f_0(v e^{(1/2)\epsilon v t}). \quad (5)$$

If the initial distribution is the delta function

$$f_0 = (4\pi v^2)^{-1} \delta(v - v_0),$$

Eq. (5) yields

$$f(v, t) = (4\pi v^2)^{-1} \delta(v - v_0 e^{\epsilon v t/2}). \quad (6)$$

Coulomb forces provide an example of "soft" molecules since $\nu = \alpha v^{-3}$. Then the delta-function solution becomes

$$f(v, t) = (4\pi v^2)^{-1} \delta \left[v - (v_0^3 - \frac{3}{2} \alpha \epsilon t)^{1/3} \right], \quad t < t^* \\ = (4\pi v^2)^{-1} \delta(v), \quad t > t^*, \quad (7)$$

where $t^* = 2v_0^3/3\alpha\epsilon$ is the time required for a particle of velocity v to slow to the origin.

The results of this section show that, when we consider the limit of zero background temperature in the usual Fokker-Planck equation, an initial delta function will be maintained with no dispersion during the slowing-down process. Thus, it is clear that the dispersion pre-

dicted by the Fokker-Planck equation is due only to the random velocities of the *background* gas molecules.

III. RANDOM-WALK ANALYSIS

In order to obtain a Fokker-Planck equation correct through terms of ϵ^2 , we consider a random-walk analysis of the slowing-down process. Let $G_k(x)dx$ be the probability that a particle which has undergone k collisions retains a *fraction* between x and $x+dx$ of its original energy.

If δ_i is the fractional energy loss during the i th collision, the fraction of the original energy remaining after k collisions is

$$x = \prod_{i=1}^k (1 - \delta_i) = \exp\left[\sum_{i=1}^k \ln(1 - \delta_i)\right]. \quad (8)$$

For inverse-power molecular force laws, the discussion in the Appendix shows that μ and σ are independent of particle velocity, where μ and σ are, respectively, the mean and variance of $\ln(1 - \delta_i)$. Since the δ_i are uncorrelated for these force laws, the central limit theorem,⁹ which holds for sufficiently large values of k , can be invoked to show that the probability density function for $y = \sum \ln(1 - \delta_i)$ is the Gaussian distribution

$$p(y) = (2\pi k\sigma^2)^{-1/2} e^{-(y - k\mu)^2 / 2k\sigma^2}, \quad (9)$$

and we note that μ is negative since $\ln(1 - \delta_i)$ is always negative in a collision between the test particle and a stationary background molecule.

The probability density $G_k(x)$, which may be found from Eqs. (8) and (9), is

$$G_k(x) = (2\pi k\sigma^2)^{-1/2} x^{-1} \exp[-(\ln x - k\mu)^2 / 2k\sigma^2]. \quad (10)$$

The probability density $G(x, t)$ that a test particle retains a fraction x of its original energy at time t is

$$G(x, t) = \sum_{k=0}^{\infty} h_k(t) G_k(x), \quad (11)$$

where $h_k(t)$ is the probability that k collisions occur in a time t . If the collision frequency ν is independent of velocity, $h_k(t)$ is the Poisson distribution

$$h_k(t) = [(\nu t)^k / k!] e^{-\nu t}, \quad (12)$$

which, for sufficiently large k , can be approximated in the usual way⁹ by the continuous Gaussian density

$$h(k, t) = (2\pi\nu t)^{-1/2} \exp[-(k - \nu t)^2 / 2\nu t]. \quad (13)$$

Thus, when $\nu t \gg 1$, the summation in Eq. (11) can be

replaced by an integration and, using Eq. (10), we obtain

$$G(x, t) = (4\pi^2\sigma^2\nu t x^2)^{-1/2} \int_{-\infty}^{\infty} k^{-1/2} \times \exp\left\{-\frac{1}{2}[(\ln x - k\mu)^2 / k\sigma^2 + (k - \nu t)^2 / \nu t]\right\} dk. \quad (14)$$

The time development of the distribution function $f(v, t)$ can be obtained in the form of an integral equation by noting that the probability that a test particle which has a speed v' at time zero will have a speed between v and $v+dv$ at time t is $G(x, t)2v dv/v'^2$, where $x = v^2/v'^2$. Then

$$f(v, t) = \frac{2}{v} \int_0^{\infty} f(v', 0) G(v^2/v'^2, t) dv'. \quad (15)$$

In particular, if $f(v, 0) = (4\pi v^2)^{-1} \delta(v - v_0)$, we have

$$f(v, t) = (2\pi v v_0^2)^{-1} G(v^2/v_0^2, t). \quad (16)$$

The equations following Eq. (12) depend on the collision frequency being independent of velocity. However, if the initial velocity is v_0 , it is easily seen that for short times Δt the change in test-particle velocity is of the order of $\frac{1}{2}\epsilon v_0 \nu(v_0)\Delta t$. Thus, an effective collision frequency exists whose magnitude is equal to $\nu(v_0)(1 + \Delta)$ where the correction term Δ is of order $\frac{1}{2}\epsilon v_0 [\partial \nu(v_0) / \partial v_0] \Delta t$. The correction term may be ignored for short times, and Eq. (14) holds, provided that

$$\nu^{-1} \ll \Delta t \ll (\frac{1}{2}\epsilon v_0 \partial \nu / \partial v_0)^{-1}. \quad (17)$$

The collision frequency in Eq. (14) must now be evaluated at v_0 , so that $G(x, t)$ must be written as $G(x, \Delta t; v_0)$.

IV. RESULTS FOR CONSTANT COLLISION FREQUENCY

A. Moments of the Distribution Function

The moments of the distribution function are defined as

$$M_n(t) = 4\pi \int_0^{\infty} f(v, t) v^{2(n+1)} dv. \quad (18)$$

Assuming an initial delta function

$$f(v, 0) = (4\pi v^2)^{-1} \delta(v - v_0),$$

we obtain from Eq. (16)

$$\begin{aligned} M_n(t) &= \frac{2}{v_0^2} \int_0^{\infty} G\left(\frac{v^2}{v_0^2}, t\right) v^{2n+1} dv \\ &= v_0^{2n} \int_0^{\infty} x^n G(x, t) dx \\ &= v_0^{2n} \langle x^n \rangle. \end{aligned} \quad (19)$$

⁹ W. Feller, *Probability Theory and Its Applications, I* (John Wiley & Sons, Inc., New York, 1950).

From Eq. (14) we have

$$\langle x^n \rangle = (4\pi^2\sigma^2\nu t)^{-1/2} \int_0^\infty x^{n-1} dx \int_{-\infty}^\infty k^{-1/2} \times \exp\left\{-\frac{1}{2}\left[\frac{\ln x - k\mu}{k\sigma^2} + \frac{(k-\nu t)^2}{\nu t}\right]\right\} dk, \quad (20)$$

which can be integrated by completing the squares, giving

$$\langle x^n \rangle = \exp\nu t \left\{ n\mu + \frac{1}{2}n^2(\sigma^2 + \mu^2) + \frac{1}{2}n^3\mu\sigma^2 + \frac{1}{4}n^4\sigma^4 \right\}. \quad (21)$$

The average energy $\langle u \rangle$, which is given by $\frac{1}{2}m$ times the first moment, is just

$$\langle u \rangle = u_0 \langle x \rangle = u_0 \exp\nu t \left\{ \mu + \frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\mu\sigma^2 + \frac{1}{4}\sigma^4 \right\}, \quad (22)$$

where $u_0 = \frac{1}{2}mv_0^2$. A second quantity of interest is the variance or dispersion of u , defined as

$$\langle u^2 \rangle - \langle u \rangle^2 = u_0^2 \left\{ \langle x^2 \rangle - \langle x \rangle^2 \right\} = u_0^2 e^{2\nu t} \mu \left\{ \exp 2\nu t \left[\sigma^2 + (\mu + \sigma^2)^2 \right] - \exp\nu t \left[\sigma^2 + (\mu + \frac{1}{2}\sigma^2)^2 \right] \right\}. \quad (23)$$

B. Typical Values of the Energy Decay and Dispersion

The fractional energy loss in a collision is

$$\delta_i = \epsilon(1 - \cos\chi), \quad (24)$$

where χ is the scattering angle in the reference frame of the center mass.

In order to estimate the values for μ and σ^2 , we will assume that the scattering is isotropic in the center-of-mass system. This assumption is exact for rigid sphere molecules, and is a good approximation for other laws of force.¹⁰ Then the probability for scattering through an angle χ is just $\frac{1}{2}\sin\chi$, and the probability that $y = \ln(1 - \delta_i)$ lies between y and $y + dy$ is therefore

$$p(y)dy = (2\epsilon)^{-1}e^{y}dy, \quad 0 \geq y \geq \ln(1 - 2\epsilon) \\ = 0, \quad y < \ln(1 - 2\epsilon). \quad (25)$$

It follows that

$$\mu = (1 - 1/2\epsilon) \ln(1 - 2\epsilon) - 1, \quad (26)$$

and

$$\sigma^2 = 1 + (1/2\epsilon)(1 - 1/2\epsilon)[\ln(1 - 2\epsilon)]^2. \quad (27)$$

When the masses of the test particle and the gas molecules differ greatly, Eqs. (26) and (27) reduce to

$$\mu = -\epsilon(1 + \frac{2}{3}\epsilon) \quad (28)$$

and

$$\sigma^2 = \frac{1}{3}\epsilon^2, \quad (29)$$

with an error of order ϵ^3 .

If terms of order ϵ^3 are neglected in Eq. (22), the

average energy¹¹ is

$$\langle u \rangle = u_0 \exp\nu t \left[\mu + \frac{1}{2}(\mu^2 + \sigma^2) \right] = u_0 e^{-\epsilon\nu t}. \quad (30)$$

The last result is identical with the average energy obtained from the usual Fokker-Planck equation [Eq. (2)]. This is fortuitous since the usual derivations^{1,2} of the Fokker-Planck equation are not accurate to order ϵ^2 . In fact, the coefficient $\frac{1}{2}\epsilon$ in Eq. (1) is often taken to be either^{1,2} m/M or $m/(m+M)$, which of course does not give the correct second-order results.

In contrast to the usual Fokker-Planck equation which gives a zero value for the variance, the variance given by Eq. (23) is

$$\langle (u - \langle u \rangle)^2 \rangle = \langle u \rangle^2 [e^{3\epsilon\nu t} - 1], \quad (31)$$

where we have neglected terms of order ϵ^3 . Thus the dispersion becomes large compared with $\langle u^2 \rangle$ for times greater than $(\frac{1}{3}\nu\epsilon^2)^{-1}$.

The time behavior of an arbitrary moment $M_n(t)$, as given by Eqs. (19) and (21), is

$$M_n(t) = v_0^{2n} e^{-\nu t [n\epsilon + \frac{1}{3}\epsilon^2(n-n^2)]}, \quad (32)$$

where terms of order ϵ^3 are neglected. Equation (32) predicts an exponential relaxation to zero when $n \ll \epsilon^{-1}$. However, for extremely large values of n , both Eq. (32) and the full Eq. (21) predict exponentially increasing moments. This result is physically impossible since a test particle always loses energy in a collision with a stationary molecule. It is obvious that this error was introduced into our calculations when we made use of the central limit theorem to obtain Eq. (9). This assigned a finite probability for a particle to have an energy greater than its initial energy after k collisions, and even though this probability is extremely small, it gives an anomalous result when multiplied by a high enough power of velocity. It is easily shown that if $G(x,t)$ were set equal to zero for $x > 1$ to agree with the physical facts, only a negligible change would result in the lower order moments, but the higher order moments would approach zero for large t , as they should.

C. Saddle-Point Approximation to the Distribution Function

The distribution function given by Eq. (16) can be written in the form

$$f(v,t) = \frac{1}{4\pi^2\sigma v^3(\nu t)^{1/2}} \int_{-\infty}^\infty e^{J(k)} dk, \quad (33)$$

where

$$J(k) = -\frac{1}{2} \left\{ \frac{[\ln(v^2/v_0^2) - k\mu]^2}{k\sigma^2} + \frac{(k-\nu t)^2}{\nu t} + \ln k \right\}. \quad (34)$$

¹⁰ The exact values for μ and $\mu^2 + \sigma^2$ for inverse-power molecules are derived in the Appendix. It is shown that the isotropic scattering approximation is reasonable for "hard" molecules.

¹¹ Equation (30) is unchanged if the isotropic scattering values for μ and $\mu^2 + \sigma^2$ are replaced by the exact values for Maxwell molecules given in the Appendix; the argument of the exponential in Eq. (31) is changed to $0.966 \epsilon^2 \nu t$.

¹² S. L. Kahalas and H. C. Kashian, Phys. Fluids 2, 100 (1959).

The form of the last expression suggests that the integration can be approximated by a saddle-point integration. The saddle point occurs at the value $k=k_0$ which is the solution of

$$J'(k) = -\frac{1}{2} \left\{ \frac{k^2 \mu^2 - [\ln(v^2/v_0^2)]^2}{k^2 \sigma^2} + \frac{2(k-\nu t)}{\nu t} + \frac{1}{k} \right\} = 0, \quad (35)$$

which leads to a cubic equation for k_0 .

By the usual arguments, the saddle-point integration gives

$$f(v, t) \cong [4\pi^2 \sigma v^3]^{-1} (-2\pi/\nu t J''(k_0))^{1/2} e^{J(k_0)}, \quad (36)$$

where $J''(k_0)$ is the second derivative of $J(k)$.

An approximate solution for k_0 can be obtained by noting that value of the distribution function is small except near $v=v_0 e^{-\mu\nu t/2}$. Thus we can write $[\ln(v^2/v_0^2)]^2 = (1+\delta)(\mu\nu t)^2$ and consider that $\delta(\nu) \ll 1$ in the region of interest. Substituting this form into Eq. (35), we obtain

$$k_0 = \nu t \left\{ 1 + \frac{1}{2} [\mu^2/(\mu^2 + \sigma^2)] \delta \right\} + O(\delta^2), \quad (37)$$

where we have assumed $\nu t \gg 1$.

Substituting Eq. (37) into Eq. (34), we obtain

$$J(k_0) = -\frac{1}{2} \left\{ \ln k_0 + \frac{[\ln(v^2/v_0^2) - \nu t \mu]^2}{\nu t (\mu^2 + \sigma^2)} \right\}, \quad (38)$$

where the error is of order δ^2 . Similarly, we find

$$J''(k_0) = -(\nu t)^{-1} [(\mu^2 + \sigma^2)/\sigma^2] + (2\nu^2 t^2)^{-1}, \quad (39)$$

where the final term can be neglected for $\nu t \gg 1$. Equations (36), (38), and (39) yield the distribution function

$$f(v, t) = \frac{1}{2\pi v^3} \left(\frac{1}{2\pi \nu t (\mu^2 + \sigma^2)} \right)^{1/2} \times \exp \left\{ -\frac{[\ln(v^2/v_0^2) - \mu\nu t]^2}{2\nu t (\mu^2 + \sigma^2)} \right\}. \quad (40)$$

It is easily verified that all of the moments of the distribution function in Eq. (40) are in agreement with Eq. (32).

V. PASSAGE TO A PARTIAL DIFFERENTIAL EQUATION

It was remarked at the end of Sec. III that Eq. (15) is valid for an arbitrary velocity dependence of ν , provided we considered only short times Δt satisfying Eq. (17). This allows a differential equation to be derived from Eq. (15) by a method which is similar in concept to that of Chandrasekhar,¹³ although different

in detail. From Eq. (15),

$$f(v, t + \Delta t) = \frac{2}{v} \int_0^\infty f(v', t) G\left(\frac{v^2}{v'^2}, \Delta t; v'\right) dv' = \int_0^\infty f(vx^{-1/2}, t) G(x, \Delta t; vx^{-1/2}) x^{-3/2} dx. \quad (41)$$

For short times, the major contribution to the integral comes from the neighborhood of $x=1$, so we expand $f(vx^{-1/2}, t)$ and $G(x, \Delta t; vx^{-1/2})$ in Taylor's series in powers of $(x^{-1/2}-1)$. Thus,

$$f(v, t) + \Delta t \frac{\partial f}{\partial t} = \int_0^\infty x^{-3/2} \left\{ \sum_{k=1}^\infty \frac{v^k}{k!} (x^{-1/2}-1)^k \left(\frac{\partial}{\partial v} \right)^k f(v, t) \right\} \times \left\{ \sum_{j=0}^\infty \frac{v^j}{j!} (x^{-1/2}-1)^j \left(\frac{\partial}{\partial v} \right)^j G(x, \Delta t; v) \right\} dx = \sum_{n=0}^\infty \frac{v^n}{n!} \left(\frac{\partial}{\partial v} \right)^n [\langle x^{-3/2} (x^{-1/2}-1)^n \rangle f(v, t)], \quad (42)$$

where

$$\langle x^{-3/2} (x^{-1/2}-1)^n \rangle = \int_0^\infty x^{-3/2} (x^{-1/2}-1)^n G(x, \Delta t; v) dx. \quad (43)$$

Omitting terms of order $(\Delta t)^2$, we obtain from Eq. (21)

$$\langle x^{-n/2} \rangle = 1 - \frac{1}{2} \nu \Delta t [n\mu - \frac{1}{4} n^2 (\sigma^2 + \mu^2)], \quad (44)$$

where we have omitted the terms in Eq. (21) which are of order ϵ^3 or smaller. Substituting Eq. (44) into Eq. (43) yields

$$\langle x^{-3/2} (x^{-1/2}-1)^n \rangle = (-1)^n \sum_{j=0}^n \binom{n}{j} (-1)^j \{ a_0 + a_1 j + \frac{1}{2} a_2 j(j-1) \}, \quad (45)$$

where

$$a_0 = 1 - \frac{3}{4} (\mu - \frac{3}{4} (\mu^2 + \sigma^2)) \nu \Delta t, \\ a_1 = -\frac{1}{2} (\mu - (7/4) (\mu^2 + \sigma^2)) \nu \Delta t, \\ a_2 = \frac{1}{4} (\mu^2 + \sigma^2) \nu \Delta t.$$

It follows from the combinatorial relation

$$\sum_{j=0}^n (-1)^j \binom{n}{j} \frac{j!}{(j-k)!} = (-1)^k k! \quad \text{if } k=n \\ = 0 \quad \text{if } k \neq n$$

¹³ S. Chandrasekhar, Rev. Mod. Phys. 15, 1 (1943).

that

$$\begin{aligned} \langle x^{-3/2}(x^{-1/2}-1)^n \rangle &= a_n \quad \text{for } n \leq 2 \\ &= 0 \quad \text{for } n > 2. \end{aligned} \quad (46)$$

The summation in Eq. (42) is therefore terminated at the term $n=2$. (If terms of order ϵ^3 and greater had not been omitted in going from Eq. (21) to Eq. (44), the summation would be cut off at $n=4$.)

Substituting Eq. (46) into Eq. (42) and rearranging terms, yields

$$\frac{\partial f}{\partial t} = -\frac{\mu}{2} \frac{1}{v^2} \frac{\partial}{\partial v} (v^3 \nu f) + \frac{1}{8} (\mu^2 + \sigma^2) \frac{1}{v^2} \frac{\partial}{\partial v} \left[v \frac{\partial}{\partial v} (v^3 \nu f) \right], \quad (47)$$

which gives the second-order correction term for the Fokker-Planck equation. In the case of constant collision frequency, it can be verified by direct substitution that the distribution function of Eq. (40) is an *exact* solution of Eq. (47). Thus the passage to a differential equation leads to the same result as the saddle-point approximation to the integral equation.

VI. DERIVATION OF THE DIFFERENTIAL OPERATOR FROM THE BOLTZMANN EQUATION

In this section we derive an infinite-order differential operator from the Boltzmann equation and obtain explicit expressions for the coefficients in terms of an expansion in powers of ϵ . Our method is similar to that used by Allis² to obtain the first-order terms.

The Boltzmann equation for a spatially homogeneous problem with no external fields has the form

$$\frac{\partial f}{\partial t} = \int \{F(\mathbf{w}')f(\mathbf{v}') - F(\mathbf{w})f(\mathbf{v})\} g\sigma(g, \Omega) d\Omega d\mathbf{w}'. \quad (48)$$

Here we consider only a zero-temperature background gas for which $F(\mathbf{w}) = N_0 \delta(\mathbf{w})$, where $\delta(\mathbf{w})$ is a three-dimensional delta function. For the *first* term of the Boltzmann operator, it is then convenient, following Allis,² to change the integration variable to $d\mathbf{w}'$ where

$$d\mathbf{w}' = (|\mathbf{v}' - \mathbf{w}'| / |\mathbf{v} - \mathbf{w}'|)^3 d\mathbf{w}'$$

and, carrying out the integrations over the delta function, we obtain

$$\begin{aligned} \frac{\partial f}{\partial t} &= N_0 \left[\int \left(\frac{v'}{v} \right)^3 f(\mathbf{v}') v' \sigma(v', \Omega) d\Omega, \right. \\ &\quad \left. - \int f(\mathbf{v}) v \sigma(v, \Omega) d\Omega \right], \end{aligned} \quad (49)$$

where v and v' are the *magnitudes* of \mathbf{v} and \mathbf{v}' .

We now consider inverse-power molecular forces for which $F = K/r^s$. It can then be shown¹ that

$$v' \sigma(v', \Omega) = (v'/v)^{(s-5)/(s-1)} v \sigma(v, \Omega),$$

so that Eq. (49) becomes

$$\begin{aligned} \frac{\partial f}{\partial t} &= N_0 \int \left[\left(\frac{v'}{v} \right)^L f(\mathbf{v}') - f(\mathbf{v}) \right] v \sigma(v, \Omega) d\Omega \\ &= \frac{2\pi N_0}{v^L} \int_0^\infty [v'^L f(\mathbf{v}') - v^L f(\mathbf{v})] v b db, \end{aligned} \quad (50)$$

where the last integration is over the impact parameter and $L = 3 + (s-5)/(s-1)$.

It proves convenient to expand $v'^L f(\mathbf{v}')$ in a Taylor expansion in the variable $\ln(v)$. Thus, we write

$$v'^L f(\mathbf{v}') = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\ln \frac{v'}{v} \right)^n \left(\frac{\partial}{\partial v} \right)^n [v^L f(\mathbf{v})], \quad (51)$$

where, for the first time, we have introduced the assumption that $f(\mathbf{v})$ depends only on the magnitude of \mathbf{v} . However, our subsequent derivation will still be valid for a general $f(\mathbf{v})$ if we interpret $f(v)$ to be $(4\pi)^{-1} \int f(\mathbf{v}) d\Omega$, where the integration is over all possible directions of the velocity.

From Eqs. (50) and (51) we have

$$\frac{\partial f}{\partial t} = \frac{2\pi N_0}{v^L} \sum_{n=1}^{\infty} \frac{1}{n!} B_n(v) \left(\frac{\partial}{\partial v} \right)^n [v^L f(v)], \quad (52)$$

where

$$B_n(v) = \int_0^\infty \left(\ln \frac{v'}{v} \right)^n v b db. \quad (53)$$

From the collision laws, it is easily shown² that, when $\mathbf{w}' = 0$,

$$v'/v = [1 - \epsilon(1 - \cos\chi)]^{-1/2},$$

where χ is the angle between the relative velocity vector before and after collision. Thus, we obtain

$$B_n(v) = \frac{1}{2^n} \int_0^\infty \{ \ln[1 - \epsilon(1 - \cos\chi)]^{-1} \}^n v b db. \quad (54)$$

Expanding the logarithm in powers of ϵ , we obtain

$$\begin{aligned} &\{ \ln[1 - \epsilon(1 - \cos\chi)]^{-1} \}^n \\ &= \sum_{j_1=1}^{\infty} \cdots \sum_{j_n=1}^{\infty} \frac{\epsilon^{j_T} (1 - \cos\chi)^{j_T}}{j_1 j_2 \cdots j_n}, \end{aligned} \quad (55)$$

where $j_T = j_1 + j_2 + \cdots + j_n$.

The last factor in Eq. (55) can be written

$$(1 - \cos\chi)^{j_T} = \sum_{k=1}^{j_T} \frac{j_T!}{(j_T - k)! k!} (-1)^{k+1} (1 - \cos^k \chi). \quad (56)$$

Following Chapman and Cowling's¹ notation, let

$$\phi^{(k)} = \int_0^\infty (1 - \cos^k \chi) v b db, \quad (57)$$

and, from Eqs. (54) to (57), we obtain

$$B_n(v) = \frac{1}{2^n} \sum_{j_1=1}^{\infty} \cdots \sum_{j_{n-1}=1}^{\infty} \frac{e^{j_T}}{j_1 j_2 \cdots j_n} \\ \times \sum_{k=1}^{j_T} \frac{j_T!}{(j_T-k)! k!} (-1)^{k+1} \phi^{(k)} \\ = \frac{1}{2^n} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k!} \phi^{(k)} \sum_{j_1=1}^{\infty} \cdots \sum_{j_{n-1}=1}^{\infty} \frac{e^{j_1+\cdots+j_{n-1}}}{j_1 \cdots j_{n-1}} G, \quad (58)$$

where

$$G = \sum_{j_n=k-(j_1+\cdots+j_{n-1})}^{\infty} \frac{j_T!}{(j_T-k)! j_n} \frac{e^{j_n}}{j_n},$$

and the lower limit of the last sum is to be taken as 1 whenever $j_1+\cdots+j_{n-1}$ is greater than $k-1$.

From the identity

$$\ln(1-\epsilon) = - \sum_{j_n=1}^{\infty} \frac{\epsilon^{j_n}}{j_n}$$

it is easily verified that

$$G = - \epsilon^{k-(j_1+\cdots+j_{n-1})} \left(\frac{d}{d\epsilon}\right)^k [\epsilon^{j_1+\cdots+j_{n-1}} \ln(1-\epsilon)]. \quad (59)$$

After substituting the last result into Eq. (58), the sums over the remaining j_n can be carried out, yielding

$$B_n(v) = \frac{(-1)^n}{2^n} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k!} \phi^{(k)} \epsilon^k \left(\frac{d}{d\epsilon}\right)^k [\ln(1-\epsilon)]^n. \quad (60)$$

The quantity $\phi^{(k)}$ has been shown by Chapman and Cowling¹ to have the form

$$\phi^{(k)} = \{[(m+M)/mM]K\}^{2/s-1} v^{(s-5)/(s-1)} A_k(s), \quad (61)$$

where $A_k(s)$ is a numerical constant of order unity which has been evaluated for many force laws. The collision frequency for momentum transfer, as defined by Allis,² is

$$\nu = 2\pi N_0 \phi^{(1)},$$

so that we can write

$$\phi^{(k)} = (\nu/2\pi N_0) [A_k(s)/A_1(s)]. \quad (62)$$

Then Eq. (52) can be written in the form

$$\frac{\partial f}{\partial t} = \sum_{n=1}^{\infty} \frac{1}{n!} -C_n \frac{1}{v^3} \left(\frac{\partial}{\partial v}\right)^n (v^3 \nu f), \quad (63)$$

where

$$C_n = \frac{(-1)^n}{2^n} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k!} \frac{A_k}{A_1} \epsilon^k \left(\frac{d}{d\epsilon}\right)^k [\ln(1-\epsilon)]^n. \quad (64)$$

So far no assumption has been made that ϵ is small. For small ϵ , it is easily seen that C_n is of order ϵ^n and

the operator of Eq. (63) may be approximated by the first few terms.

By referring to Eqs. (A10) and (A12) which define μ and $\mu^2+\sigma^2$ for the random-walk analysis, it can be seen that

$$C_1 = -\frac{1}{2}\mu, \quad (65)$$

$$C_2 = \frac{1}{4}(\mu^2+\sigma^2), \quad (66)$$

and thus, if we truncate Eq. (63) at $n=2$, the differential operator will be *identical* with Eq. (47) which was obtained from the random-walk analysis. Neglecting terms of order ϵ^3 , we obtain

$$C_1 = \frac{1}{2}[\epsilon/(1-\epsilon)] \{1 - \frac{1}{2}(A_2/A_1)[\epsilon/(1-\epsilon)]\} \quad (67)$$

and

$$C_2 = \frac{1}{2}\epsilon^2(1 - \frac{1}{2}A_2/A_1). \quad (68)$$

For some purposes it may be preferable to write Eq. (63) in the equivalent form

$$\frac{\partial f}{\partial t} = \nu(v) \sum_{n=0}^{\infty} \frac{D_n}{n!} \frac{\partial^n f}{\partial v^n}, \quad (69)$$

where

$$D_n = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k!} \frac{A_k}{A_1} \epsilon^k \left(\frac{d}{d\epsilon}\right)^k \left\{ \frac{[(1-\epsilon)^{-1/2}-1]^n}{(1-\epsilon)^2} \right\}. \quad (70)$$

For the Coulomb force law, it can be shown that¹

$$A_k = 2k \ln \Lambda + \frac{1}{2} \sum_{j=2}^k \frac{(-2)^j}{(j-1) j!(k-j)!} (\Lambda^{-2(j-1)} - 1), \quad (71)$$

where $\Lambda = (\sin \frac{1}{2}\theta_0)^{-1}$ and θ_0 is the minimum angle of scattering which is related to the Debye length. Terms of order $1/\ln \Lambda$ are neglected in all calculations of the Fokker-Planck equation for Coulomb scattering³; if we discard these terms, then $A_k = kA_1$. Substituting this result into Eq. (64), it can be shown that all $C_n = 0$ except $C_1 = \frac{1}{2}\epsilon$. [This result is most easily obtained by returning to Eq. (58) and carrying out the summation over k .] Thus, for Coulomb forces, the usual Fokker-Planck equation is obtained if we neglect *either* terms of order ϵ^2 or terms of order $1/\ln \Lambda$. However, the value of $\ln \Lambda$ is not extremely large (between 10 and 20 in most cases of interest), and the discarded terms will control the dispersion of an initial delta function when T_0 is small. For example, the coefficient C_2 , which introduces the dispersion, is equal to $\epsilon^2/4 \ln \Lambda$ when terms of order ϵ^3 and ϵ^2/Λ^2 are neglected.

VII. FINITE BACKGROUND TEMPERATURE EFFECTS

A. Differential Operator

In the approximation to first order in the mass ratio, the usual Fokker-Planck equation for finite background gas temperature can be obtained² from the zero-tem-

perature Fokker-Planck equation simply by replacing $f(v,t)$ on the right-hand side of Eq. (2) by $\mathfrak{D}f(v,t)$ where

$$\mathfrak{D} = 1 + (kT_0/mv)(\partial/\partial v)$$

and \mathfrak{D} acts as a destruction operator which annihilates the equilibrium Maxwellian distribution. Applying the same procedure to Eq. (63), we obtain

$$\frac{\partial f}{\partial t} = \sum_{n=1}^{\infty} \frac{1}{n!} C_n \left(\frac{\partial}{\partial v} \right)^n (v^3 \nu \mathfrak{D} f), \quad (72)$$

where, unless the collision frequency is independent of velocity, $\nu(v)$ no longer has the simple zero-temperature form given by Eq. (61) but depends upon T_0 . For example, the collision frequency for Coulomb forces should be taken as

$$\nu = \frac{8\pi e^4 \ln \Lambda N_0}{emMv^3} \left[\operatorname{erf} \left(\frac{Mv^2}{2kT_0} \right)^{1/2} - \left(\frac{2Mv^2}{\pi kT_0} \right)^{1/2} \exp \left(-\frac{Mv^2}{2kT_0} \right) \right],$$

which gives agreement with the results of Rosenbluth *et al.*¹⁴ For $M \gg m$ and v^2 on the order of the equilibrium thermal speed, the quantities in parentheses are approximately unity and we recover the zero-temperature collision frequency. On the other hand, for $M \ll m$ and v^2 on the order of the equilibrium thermal speed, the parenthesis is approximately $(4v^3/3\sqrt{\pi})(M/2kT_0)^{3/2}$ and ν becomes a constant in agreement with the Rayleigh gas results,⁶ which have been used to treat the thermalization of a fast ion in a plasma by Ree and Kidder.¹⁵

The correct finite temperature equation is actually more complicated than Eq. (72) since it would also involve higher powers of the operator \mathfrak{D} . Nevertheless, Eq. (72) is certainly a good approximation to the correct equation since: (1) its solution relaxes to the equilibrium Maxwellian distribution as $t \rightarrow \infty$; (2) it reduces to the correct equation when $T_0 \rightarrow 0$; and (3) it reduces to the correct equation when terms of order ϵ^2 are neglected.

For constant collision frequency, Eq. (72) has the form

$$\frac{\partial f}{\partial t} = \epsilon \nu \sum_{j=0}^3 a_j \left(\frac{\partial}{\partial v} \right)^j f(v,t) \quad (73)$$

when terms of order ϵ^3 are neglected. For simplicity we will assume $A_2 = A_1$ although, for constant collision frequency (Maxwell molecules), the exact relationship¹ is $A_2 = 1.033A_1$. Then

$$\begin{aligned} a_0 &= \frac{3}{2} [1 + (5/4)\epsilon], \\ a_1 &= \frac{1}{2} [1 + (9/4)\epsilon] \nu + (1 + \epsilon)(kT_0/mv), \\ a_2 &= \frac{1}{2} [1 + (7/4)\epsilon] (kT_0/m) + \frac{1}{8} \epsilon v^2, \end{aligned}$$

¹⁴ M. N. Rosenbluth, W. M. MacDonald, and D. L. Judd, *Phys. Rev.* **107**, 1 (1957).

¹⁵ F. H. Ree and R. E. Kidder, *Phys. Fluids* **6**, 857 (1963).

and

$$a_3 = \frac{1}{8} \epsilon (kT_0/m)v. \quad (74)$$

The dispersion which occurs when the initial distribution is a delta function is due to the coefficient of the second derivative a_2 . The correction term to a_2 which has been derived in this paper is $\frac{1}{8} \epsilon v^2$ and is larger than the term due to the nonzero background-gas temperature whenever $v^2 > 4kT_0/em$; that is, whenever the test-particle energy exceeds $\frac{4}{3}$ of the average background molecule energy divided by ϵ .

B. Exact Moment Solutions

Multiplying Eq. (72) by $4\pi v^{2(j+1)}$ and integrating the resulting equation yields

$$\frac{\partial M_j}{\partial t} = \sum_{n=1}^{\infty} \frac{1}{n!} C_n Q_{nj}, \quad (75)$$

where the moment M_j is defined by Eq. (18) and

$$Q_{nj} = 4\pi \int_0^{\infty} v^{2j-1} \left(\frac{\partial}{\partial v} \right)^n (v^3 \nu \mathfrak{D} f).$$

The result of integrating Q_{nj} by parts n times is

$$\frac{\partial M_j}{\partial t} = -4\pi \alpha_j \left[\int_0^{\infty} v^{2(j+1)} \nu f dv - \frac{kT}{m} \int_0^{\infty} f \frac{\partial}{\partial v} (\nu v^{2j+1}) dv \right], \quad (76)$$

where

$$\alpha_j = - \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} (2j)^n C_n. \quad (77)$$

From the definition of C_n in Eq. (64),

$$\begin{aligned} \alpha_j &= \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \frac{A_k}{A_1} \left(\frac{d}{d\epsilon} \right)^k \sum_{n=1}^{\infty} \frac{1}{n!} [j \ln(1-\epsilon)]^n \\ &= \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \frac{A_k}{A_1} \left(\frac{d}{d\epsilon} \right)^k [(1-\epsilon)^j - 1]. \end{aligned} \quad (78)$$

The first two α_j are *exactly*

$$\alpha_1 = \epsilon \quad (79)$$

and

$$\alpha_2 = 2\epsilon - 2\epsilon^2 (1 - \frac{1}{2} A_2/A_1). \quad (80)$$

For the case of constant collision frequency, Eq. (76) becomes

$$\partial M_j / \partial t = -\nu \alpha_j [M_j(t) - (2j+1)(kT_0/m)M_{j-1}(t)] \quad (81)$$

which can be solved for successive values of j . Thus, the zeroth equation yields $M_0(t) = M_0(0)$ showing the conservation of number density. The first moment, normalized to give the average energy, is

$$\langle u \rangle = \frac{3}{2} kT_0 + (\langle u \rangle_0 - \frac{3}{2} kT_0) e^{-\nu t}, \quad (82)$$

where $\langle u \rangle_0$ is the initial value of $\langle u \rangle$. From the equation for the second moment, the mean square energy is

$$\langle u^2 \rangle = (15/4)(kT_0)^2 + B_2 e^{-\alpha_2 \nu t} + B_3 e^{-\epsilon \nu t}, \quad (83)$$

where

$$B_3 = [5kT_0 \alpha_2 / 2(\alpha_2 - \epsilon)] (\langle u \rangle_0 - \frac{3}{2} kT_0)$$

and

$$B_2 = \langle u^2 \rangle_0 - B_3 - (15/4)(kT_0)^2.$$

As we have mentioned, a correct finite temperature equation would contain higher powers of the destruction operator \mathfrak{D} than appear in Eq. (72). However, for constant collision frequency with the background gas molecules in a Maxwellian distribution at temperature T_0 , it can be shown directly from the Boltzmann equation that Eq. (82) is an exact result for the energy relaxation, while Eq. (83) is modified only by multiplying the constant B_3 by a correction factor $(1 - \epsilon^2(2 - A_2/A_1)/\alpha_2)$, where the fractional increase is of order ϵ .

Recently Osipov^{16,17} has shown that, if the initial distribution function is Maxwellian, the solution of the Fokker-Planck equation [either Eq. (1) or Eq. (2)] for constant collision frequency, will retain the Maxwellian form during the relaxation process. A necessary condition for Osipov's result is that the relationship $\langle u^2 \rangle = (5/3)\langle u \rangle^2$ be satisfied throughout the slowing-down process whenever it is satisfied initially. From Eqs. (82) and (83), it can be shown that this condition will be satisfied only if second-order powers of ϵ are discarded, and α_2 is taken to be 2ϵ . Thus, Osipov's result is an approximation which is valid only to first order in the mass ratio.

Returning to the limit $T_0 \rightarrow 0$ and considering the case where the initial distribution is a delta function, Eq. (82) yields the *exact* solution for the average energy:

$$\langle u \rangle = u_0 e^{-\epsilon \nu t} \quad (84)$$

and Eq. (83) yields the exact solution for the dispersion:

$$\langle u^2 \rangle - \langle u \rangle^2 = \langle u \rangle^2 (\exp[2\epsilon^2(1 - \frac{1}{2}A_2/A_1)\nu t] - 1). \quad (85)$$

These results agree exactly with the results of the random-walk analysis in Eqs. (30) and (31) provided we make the same rigid-sphere approximation, $A_2 = \frac{2}{3}A_1$, as was done in Eq. (31). Using the correct value, $A_2 = 1.033A_1$, for Maxwell molecules changes the argument of the exponential in Eq. (85) to $0.966\epsilon^2\nu t$.

VIII. DISCUSSION

For a cold background gas, the results of Sec. V show that the random-walk analysis and Chandrasekhar's techniques for passing to a differential equation¹³ can be extended to give results which are correct through second order in the mass ratio. Moreover, in the limit of zero background-gas temperature, a delta-function

distribution remains a delta function throughout the slowing-down process if the second-order terms are neglected. For constant collision frequency, the dispersion due to the second-order terms is greater than the dispersion due to finite temperature terms whenever the test-particle velocity is greater than $2(kT_0/\epsilon m)^{1/2}$.

In order to compare the random-walk analysis with the Boltzmann-equation approach, the distribution function inside the collision integral was expanded in a Taylor series without assuming that the mass ratio is necessarily small. An infinite-series differential operator was thereby obtained in which the coefficient of the n th derivative was proportional to ϵ^n . Here ϵ proves to be a convenient parameter rather than m/M , since ϵ approaches zero when m/M approaches either zero or infinity and has a maximum value of $\frac{1}{2}$ when $m=M$. This differential form of the Boltzmann equation is shown to be identical with the random-walk results if terms of order ϵ^3 are neglected. For a constant collision frequency, we have shown from the infinite-series differential operator that the exact values for the relaxation of both the average energy and its dispersion are obtained when terms of order ϵ^3 are neglected. It is also shown that Osipov's¹⁶ result indicating that a distribution function which is originally Maxwellian will remain Maxwellian during the slowing-down process is an approximation which is not valid when terms of order ϵ^2 are included.

For Coulomb forces, it is shown that every term of order ϵ^2 or higher is divided by $\ln\Lambda$. Thus if *either* terms of order ϵ^2 or terms of order $1/\ln\Lambda$ are neglected, Eq. (72) reduces to the usual Fokker-Planck equation, in agreement with the results of Rosenbluth *et al.*¹⁴ However, the dispersion due to the ϵ^2 terms will exceed the dispersion due to a nonzero background-gas temperature whenever the test-particle velocity is greater than $2(kT_0 \ln\Lambda/m\epsilon)^{1/2}$.

For constant collision frequency and zero background-gas temperature, the distribution function $f(v,t)$ given in Eq. (40), which was obtained by a saddlepoint approximation of the random-walk integral equation, is also an exact solution of the second-order operator obtained by neglecting terms of order ϵ^2 in the infinite-series operator obtained from the Boltzmann equation. In the limit $t \rightarrow \infty$, $f(v,t)$ can be shown to approach the equilibrium distribution $(4\pi v^2)^{-1}\delta(v)$, where the delta function is to be interpreted according to Lighthill's theory of generalized functions.¹⁸ Here, it is important to recall that the definition of a generalized delta function requires that $\int_0^\infty \delta(v)F(v)dv = F(0)$ only if F is a "good" function,¹⁸ that is, a function which decreases sufficiently rapidly as $v \rightarrow \infty$. The very high order moments $M_n(t)$, for $n > \frac{3}{2}\epsilon^{-1}$, do not approach zero as $t \rightarrow \infty$, as shown by Eq. (32), but this involves no contradiction since v^n is not a "good" function. How-

¹⁶ D. I. Osipov, AIAA J. 1, 261 (1963).

¹⁷ C. F. Eaton, AIAA J. 2, 2033 (1964).

¹⁸ M. J. Lighthill, *Fourier Analysis and Generalized Functions* (Cambridge University Press, London, 1960).

ever, the moments $M_n(t)$ are accurately given for $n \ll \epsilon^{-1}$ and the average energy and its dispersion are, in fact, given exactly.

For the zero-temperature gas, it is physically apparent that, when the initial distribution function is $(4\pi v^2)^{-1} \delta(v-v_0)$, $f(v,t)$ should always be identically zero for $v > v_0$. However, the second-order solution is not identically zero for $v > v_0$ although it is always very small in magnitude. The same defect is incurred either by truncating the infinite-series Boltzmann differential operator after the second derivative term or by the random-walk analysis; in the latter case it is clear that the problem arises from the application of the central limit theorem which gives a finite though small probability for test particles to lie in the tail of the Gaussian distribution corresponding to energies greater than the initial energy. An analogous defect occurs when the telegrapher's equation which has a finite speed of propagation is replaced by the diffusion equation which has an infinite speed of propagation.

APPENDIX: COLLISION FREQUENCIES FOR THE RANDOM-WALK ANALYSIS

If the random-walk analysis is to be considered as an independent method, the collision frequencies must be obtained without reference to the Boltzmann collision integral. In fact, for a central-force law, the force field extends to infinity and the collision frequency is not uniquely defined. However, only the products $\nu\mu$ and $\nu(\mu^2 + \sigma^2)$ appear in the final results of the random-walk analysis.

Consider a series of cutoff angles $\chi_0, \chi_1, \dots, \chi_n, \dots$, where $\chi_{n+1} < \chi_n$. Each of the χ_n is to be considered small, and each formally defines a random-walk problem in which we ignore deflections in the center-of-mass system less than χ_n .

Corresponding to each χ_n is a maximum impact parameter b_n and a collision frequency $\nu_n = N_0 \pi b_n^2 v$. We shall show that as $n \rightarrow \infty$, $\nu_n \mu_n$ approaches a limit $\nu\mu$.

From Sec. 10.3 of Ref. 1 it can be shown that

$$\chi = 2 \int_0^{\pi/2} \left(\beta^2 \left(\frac{\alpha}{\beta \sin \theta} \right)^{s-1} + 1 \right)^{-1} d\theta, \quad (A1)$$

where $\alpha = b \{ m M v^2 / K (m + M) \}^{1/(s-1)}$ when the force law is $F = K/r^2$. (The relative velocity is equal to the particle velocity for stationary background molecules.) The quantity β is implicitly defined by $\beta^2 = 1 - [2/(s-1)] \times (\beta \sin \theta / \alpha)^{s-1}$. For small deflection angles χ , $\alpha \gg 1$ and $\beta \cong 1$, so that

$$\chi = a v^{-2} b^{1-s}, \quad (A2)$$

where

$$a = \frac{2(m+M)K}{mM} \int_0^{\pi/2} (\sin \theta)^{s-1} d\theta.$$

Given a small cutoff parameter χ_n , the probability of an impact parameter occurring in the range db about b

is $p_n(b)db$ where $p_n(b)$ equals $2b/b_n^2$ for $b < b_n$ and equals zero for $b > b_n$, where b_n is given in terms of χ_n by Eq. (A2). The probability $P_n(\chi)d\chi$ that χ lies in the interval $d\chi$ about χ is

$$P_n(\chi) = p_n(b) |\partial b / \partial \chi| = (2/b_n^2) b |\partial b / \partial \chi|, \quad (\chi > \chi_n) \quad (A3)$$

and P_n equals zero for χ less than χ_n . It follows that, if $m < n$,

$$P_n(\chi) = (b_m^2/b_n^2) P_m(\chi) \quad \text{for } \chi > \chi_m. \quad (A4)$$

By choosing χ_m small enough, Eq. (A2) will hold for $\chi < \chi_m$ and Eq. (A3) becomes

$$P_n(\chi) = \frac{2}{b_n^{2(s-1)}} \left(\frac{a}{v^2} \right)^{2/(s-1)} \chi^{-(s+1)/(s-1)}, \quad (\chi_m > \chi > \chi_n). \quad (A5)$$

We desire the mean logarithmic energy decrement in a single collision for a cutoff angle χ_n , i.e., $\mu_n = \int P_n(\chi) y d\chi$, where $y = \ln[1 - \epsilon(1 - \cos \chi)]$ from Eq. (24). For angles less than χ_m , y can be expanded in a Taylor series with leading term $\epsilon \chi^2/2$. From Eqs. (A3) to (A5), it follows that

$$\nu_n \mu_n - \nu_m \mu_m = [N_0 \pi \epsilon / 2 (s-2)] a^{2/(s-1)} v^{(s-3)/(s-1)} \times (\chi_m^{2(s-2)/(s-1)} - \chi_n^{2(s-2)/(s-1)}). \quad (A6)$$

Thus, in the limit, as $n \rightarrow \infty$, $\nu_n \mu_n$ approaches a limiting value $\nu\mu$, if $s > 2$. For the Coulomb law, a particular value of the cutoff angle must be chosen by appealing to the usual arguments involving the Debye length.

The limiting value $\nu\mu$ can be found in terms of numbers tabulated in Ref. 1. From Eq. (A3) we have

$$\mu_n = \int_0^{b_n} y p_n(b) db = 2b_n^{-2} \int_0^{b_n} y b db. \quad (A7)$$

By methods similar to those in Sec. VI, y can be expanded in the form

$$y = \sum_{m=1}^{\infty} \frac{(-1)^m}{m} \left(\frac{\epsilon}{1-\epsilon} \right)^m (1 - \cos^m \chi), \quad (A8)$$

and, in the limit $b_n \rightarrow \infty$, Eq. (A7) yields

$$\nu\mu = 2N_0 \pi \sum_{m=1}^{\infty} \frac{(-1)^m}{m} \left(\frac{\epsilon}{1-\epsilon} \right)^m \phi^{(m)}, \quad (A9)$$

where $\phi^{(m)}$ is defined by Eq. (57). Only the product $\nu\mu$ affects the final results of the random-walk analysis, and it is convenient to arbitrarily choose $\nu = 2\pi N_0 \phi^{(1)}$. Then, from Eqs. (62) and (A9), we have

$$\mu = \sum_{m=1}^{\infty} \frac{(-1)^m}{m} \left(\frac{\epsilon}{1-\epsilon} \right)^m \frac{A_m(s)}{A_1(s)}. \quad (A10)$$

By similar arguments, it can be shown that $\nu_n(\mu_n^2 + \sigma_n^2)$

approaches a limit $\nu(\mu^2 + \sigma^2)$ as $n \rightarrow \infty$. Here

$$\nu_n(\mu_n^2 + \sigma_n^2) = 2N_0\pi \int_0^{b_n} y^2 v b db, \quad (\text{A11})$$

and using the expansion

$$y^2 = -\sum_{j=1}^{\infty} \frac{(1 - \cos^j \chi)}{j!} (-1)^j \epsilon^j \left(\frac{d}{d\epsilon}\right)^j [\ln(1 - \epsilon)]^2,$$

we obtain

$$\mu^2 + \sigma^2 = -\sum_{j=1}^{\infty} \frac{A_j(s)}{A_1(s)} \frac{(-1)^j \epsilon^j}{j!} \left(\frac{d}{d\epsilon}\right)^j [\ln(1 - \epsilon)]^2. \quad (\text{A12})$$

Although the choice of ν we have made is somewhat

arbitrary, since only the products $\nu\mu$ and $\nu(\mu^2 + \sigma^2)$ are determined, it has the advantage of making μ rather insensitive to the particular force law so that the values of μ determined in Sec. IV by assuming isotropic scattering are reasonable approximations for "hard" molecules ($s > 5$). For example, $A_1(\infty)$ (rigid spheres) is greater than $A_1(5)$ (Maxwell molecules) by about 16%. For rigid spheres,

$$A_m(\infty) = \frac{1}{4} \left\{ 2 - \frac{1 + (-1)^m}{m+1} \right\},$$

and it can be verified that Eqs. (A10) and (A12) sum to give the results obtained in Eqs. (26) and (27), as should be expected since rigid-sphere scattering is isotropic in the center-of-mass system.

Path-Integral Calculation of the Two-Particle Slater Sum for He⁴†

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The Wiener integral formulation combined with Monte Carlo sampling has been used to compute the two-particle Slater sum for He⁴ for temperatures ranging from 273°K down to 2°K, the lower practical limit for this computational method. This is equivalent to a calculation of the density-independent part of the pair distribution function. A Lennard-Jones 6-12 potential has been used to describe the interaction. Contributions from exchange were found negligible at 5°K and above. Comparisons with the Wigner-Kirkwood expansion are made. The second virial coefficients derived from these results are within two or three percent of the results obtained from the usual phase-shift calculation.

1. INTRODUCTION

FOR a system of N identical particles of mass m enclosed in a volume Ω , with Hamiltonian H_N , the Slater sum¹ is

$$W_N = N! \lambda^{3N} \sum_i \Psi_i^*(\mathbf{1}, \mathbf{2}, \dots, \mathbf{N}) e^{-\beta H_N} \times \Psi_i(\mathbf{1}, \mathbf{2}, \dots, \mathbf{N}), \quad (\text{1.1})$$

where $\Psi_i(\mathbf{1}, \dots, \mathbf{N})$ is the wave function of the system in the state i ; $\mathbf{1}$ is the position coordinate of particle 1, $\mathbf{2}$ is the position coordinate of particle 2, etc.; λ is the thermal wavelength

$$\lambda = (2\pi\hbar^2\beta/m)^{1/2}; \quad (\text{1.2})$$

and

$$\beta = 1/kT. \quad (\text{1.3})$$

The wave functions are normalized to 1 in the volume Ω ,

$$\int_{\Omega} \Psi_i^*(\mathbf{1}, \mathbf{2}, \dots, \mathbf{N}) \Psi_i(\mathbf{1}, \mathbf{2}, \dots, \mathbf{N}) d\mathbf{1} d\mathbf{2} \dots d\mathbf{N} = 1, \quad (\text{1.4})$$

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¹ Contrary to custom we include the multiplying factor $N! \lambda^{3N}$ in this definition.

and the summation in Eq. (1.1) extends over all states appropriate to the statistics of the system. A superscript is used on W_N to explicitly denote Bose-Einstein (W_N^B) or Fermi-Dirac (W_N^F) statistics.

We present here the results of computing W_2^B for ten temperatures extending from 273°K down to 2°K. The potential describing the interaction is the Lennard-Jones 6-12 potential

$$V = 4\alpha((\sigma/r)^{12} - (\sigma/r)^6), \quad (\text{1.5})$$

where α and σ are the deBoer, Michels² values appropriate to He⁴:

$$\begin{aligned} \alpha &= 14.04 \times 10^{-16} \text{ erg}, \\ \sigma &= 2.56 \times 10^{-8} \text{ cm}. \end{aligned} \quad (\text{1.6})$$

A central feature of this calculation is the use of the Wiener integral formulation of the Slater sum,³ described in the following section. The Wiener integrals have been evaluated by a Monte Carlo sampling scheme on the ILLIAC II computer.

² J. deBoer and A. Michels, *Physica* **6**, 409 (1939).

³ M. Kac, *Lectures in Applied Mathematics, Volume 1, Proceedings of the Summer Seminar, Boulder, Colorado, 1957* (Interscience Publishers, Inc., New York, 1958).