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Kinetic equation for a weakly-coupled test particle*

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This paper is concerned with the generalized kinetic equation for the motion of a test particle in a weakly-coupled classical fluid. The distribution function for the test particle satisfies a generalized Fokker-Planck equation in velocity. The equation has "memory" and a diffusion tensor that is time and velocity dependent. We study the case of the relaxation of a spatially uniform distribution in considerable detail. In particular, we find that the coupling of interaction, velocity, time, and mass ratio make questionable the traditional methods of solution by expansion in a small parameter.

I. INTRODUCTION

The generalized kinetic equation has come to play an important role in modern statistical mechanics. Such an equation, free of the limitations of low density, low frequency, and long wavelength that characterize Boltzmann's equation, is an ideal starting point for the analysis of fluctuation and relaxation in many-body systems. Generalized equations have been particularly useful in the study of classical fluids, and their language has begun to appear in studies of magnetic systems, and of plasmas near equilibrium.[1-5]

The generalized equation is extremely complicated, and approximation is needed before much that is interesting can be extracted. Systematic approximation has been based upon expansion in coupling strength, in density, and in terms of clusters of interacting particles, while "model" theories have been based upon the assignment of simple functional forms to key quantities. This paper is concerned with the former approach. It is a study of the equation for the relaxation of a distribution of marked particles (test particles) in a classical system that is weakly coupled. In this first paper, we study a homogeneous system ($k=0$). Two time scales appear naturally. They are characterized by t_1, the duration of a collision, and t_2, the mean-free time between collisions. Their ratio is $n_0\pi a^3$, where a is the range of force. When this quantity is set equal to zero, we obtain a Markoffian equation that has been known and studied for three decades. However, it is the general case to which we turn our attention. Although the assumption of weak coupling makes the model a poor choice for describing a real fluid, it portrays, nevertheless, some interesting physics. One finds speed, time, mass, and coupling strength combined so that uniformly good approximations are difficult to obtain. One finds that quantitative details of the approach to equilibrium depend upon the shape of the two-body potential. And, finally, one finds that the approach is different, for any $n_0\pi a^2\neq 0$, than that predicted by the Markoffian model. If these results are not all due to the weak-coupling approximation, they add something to our understanding of kinetic theory.

The kinetic equation we study has the form of a diffusion equation (Fokker-Planck equation) in velocity. It is complicated by the fact that it has memory. The first part of this paper is concerned with the derivation of the equation and the study of its key ingredient, the diffusion tensor. We use this knowledge in the second part, to analyze the equation itself. Since it remains too complicated for solution in terms of elementary functions it must, alas, be mutilated to obtain further insight. The additional approximations are discussed in the final technical section, where we take the mutilated kinetic equation as far as we can. Though many mathematical questions remain unanswered, the results we have obtained are being published at this time, in the hope of stimulating further research into this important subject.

II. ANALYSIS

A. Derivation of the kinetic equation

We consider a classical system of N point masses, interacting through a common two-body force. Positions will be denoted by $\vec{q}_i$, momenta by $\vec{p}_i$. All particles but one, the test particle, have the same mass m_2. The test-particle mass is m_1. Thus, the Hamiltonian is

$$H=\sum_{i=1}^{N}\frac{1}{2m_i}\vec{p}_i^{\,2}+\sum_{\text{pairs}}V(\vec{q}_i-\vec{q}_j), \tag{1}$$

$$m_2=m_3=\cdots=m_N .$$

We consider a Gibbs ensemble of such systems. The ensemble develops through Liouville's equation, which we write

$$\frac{\partial}{\partial t}\rho(Q,P,t) = -iL\rho(Q,P,t)\,,$$

$$iL = \sum_{i=1}^{N}\frac{1}{m_i}\vec{p}_i\cdot\frac{\partial}{\partial\vec{q}_i} + \vec{F}_i\cdot\frac{\partial}{\partial\vec{p}_i}\,, \qquad (2)$$

$$\int dQ\,dP\,\rho(Q,P,t) = 1\,.$$

Here, $\rho(Q,P,t)$ is the phase-space density, (Q,P) denotes $(\vec{q}_1\cdots\vec{p}_N)$, and (Q,P') will denote $(\vec{q}_1\cdots\vec{q}_N, \vec{p}_2\cdots\vec{p}_N)$. $\vec{F}_i$ is the force experienced by the ith particle. The initial value of the ensemble describes the subject of this paper. It is

$$\rho(Q,P,0) = \frac{f(\vec{p}_1)}{M_1(\vec{p}_1)}\left[(e^{-\beta H'})\Big/\left(\int dQ\,dP\,e^{-\beta H'}\right)\right]$$

$$= \frac{f(\vec{p}_1)}{M_1(\vec{p}_1)}\rho_0(H')$$

$$= f(\vec{p}_1)\prod_{i=2}^{N}M_2(\vec{p}_i)\rho_0(Q)\,, \qquad (3)$$

with

$$\int d^3p_1 f(\vec{p}_1) = 1, \quad \int d^3p\, M_i(\vec{p}) = 1\,,$$

$$\int dQ\,\rho_0(Q) = 1\,.$$

In Eq. (3), we have $\beta = 1/kT$, and $\rho_0(H')$ is the canonical distribution; $f(\vec{p}_1)$ is the (arbitrary) initial distribution of test-particle momenta, and $M_i(\vec{p}_i)$ are appropriate normalized Maxwellians. The Hamiltonian H' is the Hamiltonian of Eq. (1) augmented by "external forces" that constrain the system to lie in a volume Ω, and thereby ensure convergence of the integrals in Eqs. (2) and (3). (We distinguish between H' and H only when necessary.) Note that $\rho(Q,P,0)$ need not be close to equilibrium.

We are particularly concerned with the evolution of

$$f(\vec{p}_1,t) = \int dQ\,dP'\,\rho(Q,P,t)\,.$$

To obtain an equation for $f(\vec{p}_1,t)$ we follow Zwanzig[1] and introduce an appropriate projection operator. Thus, the projector

$$P\rho \equiv [f(\vec{p}_1,t)/M_1(\vec{p}_1)]\,\rho_0(H') = \rho_\parallel \qquad (4)$$

is idempotent and particularly useful since $(1-P)\rho(Q,P,0) = 0$. The equation for $\rho_\parallel$,

$$\frac{\partial}{\partial t}\rho_\parallel + P(iL)\rho_\parallel = \int_0^t d\tau\,P(iL)e^{-i\tau(1-P)L} \times(1-P)(iL)\rho_\parallel(t-\tau) \qquad (5)$$

is then closed. Next, we need some obvious properties of P,

$$P(iL)\rho = P\vec{F}_1\cdot\frac{\partial}{\partial\vec{p}_1}\rho\,,$$

$$iLP\rho = \vec{F}_1\cdot\left(\frac{\partial}{\partial\vec{p}_1} + \frac{\beta}{m_1}\vec{p}_1\right)P\rho, \qquad (6)$$

and

$$P(iL)P\rho = 0\,.$$

Thus, Eq. (5) becomes

$$\frac{\partial}{\partial t}f(\vec{p},t) = \frac{\partial}{\partial\vec{p}}\cdot\int_0^t d\tau\,\{\cdots\}\cdot\left(\frac{\partial}{\partial\vec{p}} + \frac{\beta}{m_1}\vec{p}\right)f(\vec{p},t-\tau)\,,$$

$$\{\cdots\} = \int dQ\,dP'\,\vec{F}_1 e^{-i\tau(1-P)L}\vec{F}_1\frac{\rho_0}{M_1(\vec{p})}\,. \qquad (7)$$

Equation (7) is exact. It has the form of a "generalized Fokker-Planck" equation, but since the quantity in curly brackets is a very complicated operator, the similarity is superficial, at best. We cannot proceed further without approximation. In this paper, we explore an approximation which might be called "weak coupling" or "linear trajectory." It consists in writing

$$\exp[-it(1-P)L] \to \exp(-itL) \to \exp(-itL_0)\,, \qquad (8)$$

and causes the operator in curly brackets in Eq. (7) to become a simple function. In physical terms, the deflection of the test particle in a collision is based not upon the true paths of test and target particles, but upon modified paths—linear trajectories. Though the test particle is deflected by the collision, the target particles do not recoil, but remain in equilibrium. The scheme resembles the "impulse approximation" of collision theory. It is a severe approximation, particularly for dense systems. Yet, the system relaxes to equilibrium, and it is possible to develop a consistent hydrodynamics, based on weak coupling.[6,26] We wish to examine the model more closely. This, our first paper, deals with a particularly simple class of phenomena. We hope that it yields some insight. In any case, it has the appeal of treating an (almost) solvable model in statistical mechanics.

Before beginning the analysis, we note that a true weak-coupling theory would replace $\rho_0(Q)$ by Ω^{-N}. This is a second, and less-serious approximation, suggesting that the aggregate potential energy is small compared with the kinetic. We shall defer making it, and thereby retain some static correlations. Thus, our model extends the "linear-trajectory approximation" (LTA) of Kirkwood and Helfand,[7] who were interested primarily in its time-averaged version.

After approximation, Eq. (7) contains the diffusion tensor

$$D_{\alpha\beta}(\vec{p}_1, t) = \int dQ\, dP'\, F_{1\alpha} e^{-itL_0} F_{1\beta} \frac{\rho_0(Q,P)}{M_1(\vec{p}_1)} \quad (9a)$$

$$= \int dQ\, dP' \frac{\rho_0}{M_1(p_1)} F_{1\beta} e^{itL_0} F_{1\alpha}, \quad (9b)$$

with

$$iL_0 = \sum_{i=1}^{N} \frac{1}{m_i} \vec{p}_i \cdot \frac{\partial}{\partial \vec{q}_i}.$$

Note that

$$\int d^3p_1 M_1(\vec{p}_1) D_{\alpha\beta}(\vec{p}_1, t) = \int dQ\, dP\, \rho_0 F_{1\beta} e^{itL_0} F_{1\alpha} = \langle F_{1\beta} F_{1\alpha}(t) \rangle_0$$

is, in the linear trajectory approximation, the autocorrelation function for the force experienced by the test particle. The diffusion tensor is a real isotropic tensor function of the vector $\vec{p}_1$. It is also symmetric in its indices, and symmetric in time. The first two properties are established upon inspection; the latter two will appear as we evaluate the tensor.

Since $\rho_0 \vec{F}_1 = kT(\partial/\partial\vec{q}_1)\rho_0$, we may also write

$$M_1(\vec{p}_1) D_{\alpha\beta}(\vec{p}_1, t) = -kT \int dQ\, dP'\, \rho_0 \frac{\partial}{\partial q_{1\beta}} e^{itL_0} F_{1\alpha}. \quad (11)$$

Since

$$\exp(itL_0) f(\vec{q}_1 \cdots \vec{q}_N) = f\left(\vec{q}_1 + \frac{1}{m_1}\vec{p}_1 t, \ldots, \vec{q}_N + \frac{1}{m_N}\vec{p}_N t\right),$$

the $q_{1\beta}$ derivative may be exchanged for $p_{1\beta}$, and we have $D_{\alpha\beta}$ in the form

$$D_{\alpha\beta}(\vec{p}, t) = \frac{\partial}{\partial p_\beta} \phi_\alpha,$$

where ϕ_α is an isotropic vector function of p_α. Thus, we must have

$$D_{\alpha\beta}(\vec{p}, t) = (\partial/\partial p_\beta)[p_\alpha \phi(p, t)], \quad (12)$$

and $D_{\alpha\beta}$ is symmetric. A general representation of such a tensor is

$$D_{\alpha\beta}(\vec{p}, t) = \frac{p_\alpha p_\beta}{p^2} D_\parallel(p, t) + \left(\delta_{\alpha\beta} - \frac{p_\alpha p_\beta}{p^2}\right) D_\perp(p, t). \quad (13)$$

The invariants $D_\parallel$ and $D_\perp$ are the diagonal elements of $D_{\alpha\beta}$ in the (diagonal) representation in which $\vec{p}$ lies along a coordinate axis. We also have

$$D_\parallel = \frac{p_\alpha D_{\alpha\beta} p_\beta}{p^2}, \quad D_\perp = \frac{1}{2}\left(\delta_{\alpha\beta} - \frac{p_\alpha p_\beta}{p^2}\right) D_{\alpha\beta}. \quad (14)$$

If we compare (13) with (12) we find

$$D_{\alpha\beta}(\vec{p}, t) = \frac{\partial}{\partial p_\alpha}(p_\beta D_\perp) = \frac{\partial}{\partial p_\beta}(p_\alpha D_\perp), \qquad D_\parallel = \frac{\partial}{\partial p}(p D_\perp). \quad (15)$$

The fact that $D_\parallel$ and $D_\perp$ are related simply, does not seem to have been noted before.

Equations (9) and (11) may be reduced by the assumption of pair forces

$$\vec{F}_1 = \sum_{k=2}^{N} \vec{F}(\vec{q}_1 - \vec{q}_k).$$

Then, Eq. (11) becomes

$$D_{\alpha\beta}(\vec{p}_1, t) = -(N-1)kT \int d^3q_1 d^3q_2 d^3p_2\, \rho_2(\vec{q}_1, \vec{q}_2) M_2(p_2) \times e^{itL_{12}^0} \frac{\partial}{\partial q_{1\beta}} F_\alpha(\vec{q}_1 - \vec{q}_2), \quad (16)$$

where ρ_2 is the two-particle distribution function (test particle + bath particle) and

$$iL_{12}^0 = \frac{1}{m_1}\vec{p}_1 \cdot \frac{\partial}{\partial \vec{q}_1} + \frac{1}{m_2}\vec{p}_2 \cdot \frac{\partial}{\partial \vec{q}_2}.$$

With the introduction of $\vec{q} = \vec{q}_1 - \vec{q}_2$, and the replacement of momentum by velocity, Eq. (16) becomes

$$D_{\alpha\beta}(\vec{v}, t) = -n_0 kT \int d^3v_2 M_2(\vec{v}_2) \times \int d^3q\, g_2(\vec{q}) \frac{\partial}{\partial q_\beta} F_\alpha(\vec{q} + (\vec{v} - \vec{v}_2)t), \quad (17)$$

where $g_2(\vec{q})$ is the static, pair correlation function (test-particle–bath-particle) and we have gone to the limit $N, \Omega \to \infty, N/\Omega \to n_0$. $M(\vec{v})$ now denotes the normalized Maxwellian for velocities. We may reduce Eq. (9b) instead, to obtain

$$D_{\alpha\beta} = n_0 \int d^3v_2 M_2(\vec{v}_2)\left(\int d^3q\, g_2(\vec{q}) F_\alpha(\vec{q}) + n_0 \int d^3q \int d^3q'\, g_3(\vec{q}, \vec{q}') F_\alpha(\vec{q}')\right) F_\beta(\vec{q} + (\vec{v} - \vec{v}_2)t). \quad (18)$$

The partial integration which converts Eq. (17) to Eq. (18) is an expression of the first equation in the Bogoliubov-Born-Green-Kirkwood-Yvon "hierarchy." In the weak-coupling approximation, the second term of Eq. (18) vanishes. In either case,

$$D_{\alpha\beta} = \int d^3v_2 M_2(\vec{v} - \vec{v}_2) \mathfrak{D}_{\alpha\beta}(\vec{v}_2 t), \quad (19)$$

where $\mathfrak{D}_{\alpha\beta}$, as well as $D_{\alpha\beta}$, is of the form

$$\mathfrak{D}_{\alpha\beta}=(\partial/\partial v_\alpha)(v_\beta\mathfrak{D}_\perp) \tag{20}$$

and

$$D_{\alpha\beta}\to\mathfrak{D}_{\alpha\beta} \text{ as } m_1/m_2\to 0\,.$$

At this point we introduce dimensionless variables. The two-body potential will have strength λ, and range a. Thus, $V=\lambda\phi(\vec{r})$, $\vec{q}=a\vec{r}$. The velocity is $\vec{v}=\vec{u}v_B$ where $\frac{1}{2}m_1v_B^2=kT$. Then,

$$\frac{\partial}{\partial t}f(\vec{u},t)=\epsilon\frac{\partial}{\partial\vec{u}}\cdot\int_0^t d\tau\,\overleftrightarrow{D}(\vec{u},\tau)\cdot\left(\frac{\partial}{\partial\vec{u}}+2\vec{u}\right)f(\vec{u},t-\tau)\ , \tag{21}$$

$$D_{\alpha\beta}(\vec{u},t)=\int d^3w\,M_*(\vec{u}-\vec{w})\mathfrak{D}_{\alpha\beta}(\vec{w}t)\,, \tag{22}$$

$$\epsilon=\tfrac{1}{4}n_0a^3\left(\frac{\lambda}{kT}\right)^2,$$

$$M_*(\vec{u})=\frac{e^{-(u^2/\theta^2)}}{(\theta\sqrt{\pi})^3}\ ,$$

$$\theta^2=(m_1/m_2)\,, \tag{23}$$

$$\mathfrak{D}_{\alpha\beta}(\mathrm{w}t)=\int d^3r\,\bar{g}_2(\vec{r})\frac{\partial}{\partial r_\alpha}F_\beta(\vec{r}+\vec{w}t)\,,$$

and

$$\bar{g}_2(\vec{r})=\frac{kT}{\lambda}\left[1-g_2(\vec{r})\right]\,.$$

[In the weak-coupling limit, $\bar{g}_2(\vec{r})\to\phi(\vec{r})$.] These are the equations we propose to study.

There are two natural units for time, $t_1=a/v_B$ and $t_2=(\pi a^2n_0v_B)^{-1}$. The first is a collision time for a thermal test particle, the second is a mean free time between collisions. Their ratio, $t_1/t_2=\delta=n_0\pi a^3$, is familiar enough. It will be small for dilute and moderately dense gases. In Eqs. (21)–(23) we scale with t_1. If we prefer t_2 as the unit of time, we obtain a kinetic equation in which

$$\epsilon=\tfrac{1}{4}n_0a^3\left(\frac{\lambda}{kT}\right)^2=\frac{1}{4\pi}\delta\left(\frac{\lambda}{kT}\right)^2$$

is replaced by $(1/4\pi)(\lambda/kT)^2$ and $D(u,\tau)$ by $D(u,\tau/\delta)$. The Laplace time transform of the kinetic equation, which produces $\overleftrightarrow{D}(\vec{u},s)$ in the first case, produces $\overleftrightarrow{D}(\vec{u},\delta s)$ in the second. The limiting case, $\delta\to 0$ suggests that we replace $\overleftrightarrow{D}(\vec{u},\delta s)$ by $\overleftrightarrow{D}(\vec{u},0)$. Thus, we arrive at the Markoffian approximation, to be discussed later. Finally, note that after "scaling," both the exact and the approximate kinetic equations depend upon the three dimensionless parameters θ, $n_0\pi a^3$, and $(\lambda/kT)^2$. It is the selective suppression of these in the operator kernel of Eq. 7 that produces the weak-coupling model.

B. Diffusion tensor

The most important representation of $D_{\alpha\beta}$ is given by Eq. (22). Yet, other representations must be explored, for they aid in getting the various expansion needed in the analysis of the kinetic equation. The reader who is bored easily may wish to proceed at once to Sec. III.

We begin by noting that Eq. (20) and partial integration give

$$D_{\alpha\beta}=\frac{2}{\theta^2}\int d^3w\,(w_\alpha-u_\alpha)w_\beta M_*(\vec{u}-\vec{w})\mathfrak{D}_\perp(wt)\,, \tag{24}$$

whence

$$u^2D_\perp=\frac{1}{\theta^2}\int d^3w\,(\vec{u}\times\vec{w})^2M_*(\vec{u}-\vec{w})\mathfrak{D}_\perp(wt)\,,$$

$$u^2D_\parallel=\frac{2}{\theta^2}\int d^3w\,(\vec{u}\cdot\vec{w}-u^2)(\vec{u}\cdot\vec{w})M_*(\vec{u}-\vec{w})\mathfrak{D}_\perp(wt)\,. \tag{25}$$

On the other hand, partial integration also gives

$$u^2D_\perp=\int d^3w\,M_*(\vec{u}-\vec{w})(\vec{u}\cdot\vec{w})\mathfrak{D}_\perp(wt)\ . \tag{26}$$

In both instances, $D_\parallel=(d/du)(uD_\perp)$.

If the potential has a Fourier transform

$$\phi(\vec{r})=\int\frac{d^3k}{(2\pi)^3}\,e^{i\vec{k}\cdot\vec{r}}\,\phi(\vec{k})\,,$$

we find

$$\mathfrak{D}_{\alpha\beta}(\vec{w}t)=\int\frac{d^3k}{(2\pi)^3}\,k_\alpha k_\beta\psi(k)\,e^{i\vec{k}\cdot\vec{w}t}\,, \tag{27}$$

where $\psi(\vec{k})=\phi(\vec{k})\bar{g}_2(\vec{k})$. Since these functions depend upon the magnitude of $\vec{k}$ only, we may do the angle integration in Eq. (27). The identity

$$\int\frac{d\hat{\Omega}}{4\pi}\hat{\Omega}_\alpha\hat{\Omega}_\beta e^{i\hat{\Omega}\cdot\vec{a}}=\frac{1}{2}\left(\delta_{\alpha\beta}-\frac{a_\alpha a_\beta}{a^2}\right)\left(1+\frac{\partial^2}{\partial a^2}\right)\frac{\sin a}{a}-\frac{a_\alpha a_\beta}{a^2}\,\frac{\partial^2}{\partial a^2}\,\frac{\sin a}{a}$$

enables us to deduce

$$\begin{pmatrix}\mathfrak{D}_\parallel(wt)\\ \mathfrak{D}_\perp(wt)\end{pmatrix}=\frac{1}{2\pi^2}\int_0^\infty dz\,\psi(z)z^4\begin{pmatrix}f_\parallel(zwt)\\ f_\perp(zwt)\end{pmatrix}\ , \tag{27a}$$

with

$$f_\parallel(z)=\left(\frac{\sin z}{-z}\right)_{zz}\ ,\quad f_\perp(z)=\frac{1}{2}\left(1+\frac{\partial^2}{\partial z^2}\right)\frac{\sin z}{z}\,. \tag{27b}$$

We also need the Laplace transforms

$$\mathfrak{D}_{\alpha\beta}(\vec{w},s)=\int_0^\infty dt\,e^{-st}\mathfrak{D}_{\alpha\beta}(\vec{w}t)$$

$$=\int\frac{d^3\vec{k}}{(2\pi)^3}\,k_\alpha k_\beta\,\frac{\psi(k)}{s-i\vec{k}\cdot\vec{w}} \tag{28}$$

and

$$D_{\alpha\beta}(\vec{u}, s) = \int d^3w\, M_*(\vec{u} - \vec{w})\mathfrak{D}_{\alpha\beta}(\vec{w}, s) . \qquad (29)$$

The Fourier transforms of $\mathfrak{D}_\parallel$ and $\mathfrak{D}_\perp$ also play a role in our analysis. One finds

$$\begin{pmatrix} \mathfrak{D}_\perp(wt) \\ \mathfrak{D}_\parallel(wt) \end{pmatrix} = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \begin{pmatrix} \psi_\perp(k) \\ \psi_\parallel(k) \end{pmatrix} e^{ikwt} , \qquad (30)$$

where

$$\psi_\perp = \int_k^\infty dk\, k\phi_1(k) = \tfrac{1}{2}[\phi_3(k) - k^2\phi_1(k)] ,$$

$$\psi_\parallel = k^2\phi_1(k) ,$$

and we have introduced

$$\phi_n(k) = \int_k^\infty \frac{dk}{2\pi} k^n \psi(k) .$$

[ϕ_n will be used to denote $\phi_n(k=0)$ occasionally.] The requirement that ϕ_1 and ϕ_3 exist limits the Fourier-transformable potentials for which much of our analysis holds. We shall also require that a few terms in the expansion of ϕ_1 and ϕ_3 about $k=0$ exist. The constraints at large and small k would exclude Coulomb behavior at large and small r.

Returning to $D_{\alpha\beta}$, we note that

$$D_{\alpha\beta}(\vec{u}, t) = \int \frac{d^3k}{(2\pi)^3} k_\alpha k_\beta \psi(k) \exp[i\vec{k}\cdot\vec{u}t - \tfrac{1}{4}k^2(\theta t)^2] , \qquad (31)$$

courtesy of Eqs. (22) and (27). By analogy with Eqs. (27a) and (27b) we have

$$\begin{pmatrix} D_\parallel(u,t) \\ D_\perp(u,t) \end{pmatrix} = \frac{1}{2\pi^2} \int_0^\infty dz\, \psi(z) z^4\, e^{-(\theta^2 t^2/4)z^2} \begin{pmatrix} f_\parallel(zut) \\ f_\perp(zut) \end{pmatrix} , \qquad (32)$$

and, by analogy with Eq. (30),

$$D_\perp(ut, \theta t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \psi_\perp(k, \theta t) e^{ikut} ,$$

$$\Psi_\perp(k, \theta t) = \tfrac{1}{2}[\Phi_3(k, \theta t) - k^2\Phi_1(k, \theta t)] , \qquad (33)$$

$$\Phi_n(k, \theta t) = \int_k^\infty \frac{dk}{2\pi} k^n e^{-(k^2/4)(\theta t)^2} \psi(k) .$$

A similar expression holds for $D_\parallel(ut, \theta t)$. Finally we have the Laplace transform of Eq. (31) which introduces the function $w(z) = \exp(-z^2)\,\mathrm{erfc}(-iz)$. One finds

$$D_{\alpha\beta}(\vec{u}, s) = \int \frac{d^3k}{(2\pi)^3} k_\alpha k_\beta \psi(k) \frac{\sqrt{\pi}}{k\theta} w(z) ,$$
$$z = i(s - i\vec{k}\cdot\vec{u})/k\theta . \qquad (34)$$

Similar mathematical expressions occur in the literature of plasma physics.

Since the diffusion tensor is a complicated function of its arguments and the law of force, it is useful to have a special example to contemplate. We select the Gaussian potential $\phi(r) = \exp(-r^2)$, $\phi(k) = \pi^{3/2}\exp(-\tfrac{1}{4}k^2)$. Then, we have, in the weak-coupling case:

$$\mathfrak{D}_\perp(ut) = \left(\frac{\pi}{2}\right)^{3/2} e^{-(ut)^2/2} ,$$

$$\mathfrak{D}_\parallel(ut) = \left(\frac{\pi}{2}\right)^{3/2} [1 - (ut)^2]\, e^{-(ut)^2/2} , \qquad (35)$$

$$\mathfrak{D}_\perp(ut, \theta t) = \left(\frac{\pi}{2}\right)^{3/2} \frac{\exp\{-\tfrac{1}{2}(ut)^2/[1 + \tfrac{1}{2}(\theta t)^2]\}}{[1 + \tfrac{1}{2}(\theta t)^2]^{5/2}} ,$$

$$D_\parallel(ut, \theta t) = \frac{\partial}{\partial u}(uD_\perp) .$$

For the $\mathfrak{D}$ tensor, the Laplace transforms are

$$u\mathfrak{D}_\perp(u, s) = \tfrac{1}{4}\pi^2 w(i\sigma) ,$$
$$u\mathfrak{D}_\parallel(u, s) = \tfrac{1}{2}\pi^{3/2}\sigma[1 - \sqrt{\pi}\,\sigma w(i\sigma)] , \qquad (36)$$

where $\sigma = s/(2u)^{1/2}$. The coefficients $\phi_{n+1} = \pi^2 2^{n/2-1}\Gamma(n/2+1)$. Reference to Eq. (32) shows that the t^{-5} behavior is characteristic of the weak-coupling case, holding for any potential that is finite at $r=0$.

[It has been remarked that it is possible to mimic an attractive potential by combining Gaussians. It would be interesting to see what ensues. Of course, one is not limited to Gaussian potentials. For example, the Lorentzian, $(r^2+a^2)^{-1}$ has an easy transform, and one might use it to illustrate the effects of long-ranged interactions. These questions belong to a later paper.]

C. Autocorrelation function for force

Before descending into a detailed study of the diffusion tensor, we consider Eq. (10), the expression for the autocorrelation of force, in the approximate theory. Thus,

$$\langle F_{1\beta} F_{1\alpha}(t)\rangle_0 = \int d^3p_1 M_1(\vec{p}_1) D_{\alpha\beta}(\vec{p}_1, t)$$
$$= \int d^3v_1 \int d^3v_2 M_1(\vec{v}_1) M_2(\vec{v}_1 - \vec{v}_2)\mathfrak{D}_{\alpha\beta}(\vec{v}_2 t)$$
$$= \int d^3v_3 M_3(\vec{v}_3)\mathfrak{D}_{\alpha\beta}(\vec{v}_3 t) , \qquad (37)$$

where we have reverted to "dimensional" variables. The Maxwellian $M_3(\vec{v}_3)$ is characterized by the reduced mass $m_3 = m_1 m_2/(m_1 + m_2)$. In terms of dimensionless variables,

$$\langle F_{1\beta}F_{1\alpha}(t)\rangle_0 = n_0 a\lambda^2 \int d^3w\, M_4(\vec{w})\mathfrak{D}_{\alpha\beta}(\vec{w}t)$$

$$\langle \vec{F}_1\cdot\vec{F}_1(t)\rangle_0 = n_0 a\lambda^2 8\pi\eta \int_0^\infty dw\, w^4 M_4(\vec{w})\mathfrak{D}_\perp(wt) \tag{38}$$

$$= \frac{4n_0 a\lambda^2}{\pi}\eta^{5/2}\frac{\partial^2}{\partial\eta^2}\frac{1}{\sqrt{\eta}} \times \int_0^\infty dk\,\psi_\perp(k)\,e^{-(k^2t^2/4\eta)}\,,$$

where

$$M_4(\vec{w}) = \frac{e^{-(w^2/\theta_1^2)}}{(\theta_1\sqrt{\pi})^3}\,,\quad \theta_1^2 = \frac{1}{\eta} = \frac{m_1+m_2}{m_2}\,,$$

and we have used trace $\mathfrak{D}_{\alpha\beta} = \operatorname{div}(\vec{w}\mathfrak{D}_\perp)$ to aid the calculation. The form of the last integral suggests that the long-time behavior is power law. It is easy to see that the relaxation is t^{-5}. The particular case of the Gaussian potential gives

$$\langle \vec{F}_1\cdot\vec{F}_1(t)\rangle_0 = 3\left(\frac{\pi}{2}\right)^{3/2} n_0 a\lambda^2 \frac{1}{[1+\frac{1}{2}(\theta_1 t)^2]^{5/2}}\,, \tag{39}$$

with t measured in collision times $t_1 = a/v_B$.[8] Thus, the weak-coupling approximation is not a uniform approximation. Very likely the expansion in density has the same defect.

Another aspect of Eq. (39) is that it can be integrated to obtain an approximate coefficient of self-diffusion. A Kubo-Zwanzig relation gives

$$\frac{1}{D} = \lim_{s\to 0}\frac{1}{3(k_BT)^2}\langle \vec{F}_1\cdot\vec{F}_1(s)\rangle$$

$$= \frac{4}{3\sqrt{\pi}}\frac{\epsilon}{\theta_1}\frac{\phi_3}{v_B a}$$

$$= \frac{1}{3a}\frac{(n_0a^3)(\lambda^2\phi_3)}{(k_BT)^{5/2}}\left(\frac{m_3}{2\pi}\right)^{1/2}\,. \tag{40}$$

If we compare this result with that arising from the classical analysis of the Boltzmann equation,[9] we note that the dependence upon density and mass are alike, but that the $\frac{5}{2}$ power of T suggests a potential that is inverse-square repulsive. Though the comparison ought not to be taken too seriously, it is nice to see that the "corresponding" force is weak, and Fourier transformable. Of course, the weak-coupling analysis gives $T^{5/2}$ independent of potential.

D. Diffusion tensor (details)

1. Positivity

Both tensors $D_{\alpha\beta}(\vec{u},t)$ and $\mathfrak{D}_{\alpha\beta}(\vec{w}t)$ are real isotropic tensor functions of velocity. In the case of weak coupling $[\psi(k)\to\phi^2(k)]$ the longitudinal and transverse components of the Laplace-transformed tensor are positive for positive s. This is not necessarily so in the LTA. Positivity enables us to rule out solutions to the kinetic equation which grow exponentially at large time (see Appendix A). Thus, the LTA "lies under a cloud." Situations of this sort have been remarked upon before, under the notion of stability of the approximation.[6]

2. Analyticity

We shall be interested in $D_\perp(u,s)$ as a function of complex u^2, for s real and positive. The general case is difficult, but the Gaussian case is easy. There, one expands the exponential and observes that $D_\perp$ is entire in u^2.

3. Dependence upon mass-ratio

The dependence of $\vec{\mathfrak{D}}$ upon velocity and time is particularly simple. $\vec{\mathfrak{D}} = \vec{\mathfrak{D}}(\vec{u}t)$. The tensor $\vec{D}$ is a function of velocity, time, and mass ratio [as well as parameters appearing in $g(\vec{r})$]. Inspection of Eqs. (22) and (24) shows that $\vec{D} = \vec{D}(\vec{u}t,\theta t)$, or $D_1[(u/\theta),\theta t]$. Thus, expansion in terms of θ, the mass ratio, cannot lead to solutions which are accurate for all values of time. The expansion is nonuniform. Mindful of this caveat, we nevertheless single out two limiting cases. In the first $\theta\to 0$ and $\vec{D}(\vec{u}t,\theta t)\to\vec{D}(\vec{u}t)$. We call this the Lorentz, or L limit. Here, the host, or background particles are infinitely massive. No "thermalization" takes place. The second limit is $\theta\to\infty$. Then $\vec{D}$ assumes a form which is independent of $\vec{u}$, and is coupled to the long-time behavior. We denote this the Brownian limit, for it gives (yet another) model for Brownian motion. Specifically, the L limit—and higher terms—are generated by expanding Eq. (22):

$$D_{\alpha\beta} = \int d^3w\, M_*(\vec{u}-\vec{w})\left(\mathfrak{D}_{\alpha\beta}(\vec{u}t) + \frac{1}{2}\sum_{i,j}(u_i-w_i)(u_j-w_j)\frac{\partial^2}{\partial u_i\partial u_j}\mathfrak{D}_{\alpha\beta}+\cdots\right) = \mathfrak{D}_{\alpha\beta}(\vec{u}t) + \tfrac{1}{4}(\theta t)^2[\nabla_x^2\mathfrak{D}_{\alpha\beta}(\vec{x})]_{\vec{x}=\vec{u}t}+\cdots\,, \tag{41}$$

or, through Eq. (31),

$$D_{\alpha\beta} = \mathfrak{D}_{\alpha\beta}(\vec{u}t) - \tfrac{1}{4}(\theta t)^2\int\frac{d^3k}{(2\pi)^3}k_\alpha k_\beta\, k^2\psi(k)\,e^{i\vec{k}\cdot\vec{u}t}+\cdots\,. \tag{42}$$

The function $D_\perp$ is represented compactly through Eq. (33). We find the mass expansion

$$\Psi_\perp(k,\theta t) = \psi_\perp(k) = -\tfrac{1}{8}(\theta t)^2[\phi_5(k) - k^2\phi_3(k)]+\cdots\,. \tag{43}$$

Since all ϕ_n exist only for special potentials, we infer that the expansion will produce singular terms when extended to sufficiently high order. Note that the small-θ approximation is in fact, $\theta t \to 0$, $ut=$ const, as one expects. For the Gaussian potential we have

$$D_\perp(ut,\theta t)=(\tfrac{1}{2}\pi)^{3/2}e^{-(ut)^2/2}\{1-\tfrac{5}{4}(\theta t)^2[1-\tfrac{2}{5}(ut)^2]+\cdots .$$

The Brownian limit may be obtained from an expansion which gives the long-time ($\theta t \gg 1$) behavior as well. We write Eq. (26) as

$$xD_\perp(x,\theta t)=\frac{2}{\sqrt{\pi}}e^{-x^2}\int_0^\infty dy\, y^3\mathfrak{D}_\perp(y\theta t)\times\int_{-1}^{1}d\eta\,\eta\exp[-y^2+2xy\eta]\,, \qquad (44)$$

with $x=u/\theta$, and note that the exponential generates the Hermite polynomials. Then, the heavy-mass expansion is

$$xD_\perp(x,\theta t)\sim\frac{1}{\sqrt{\pi}}e^{-x^2}\sum_{n=\text{odd}}\mathfrak{D}_\perp^{(n+3)}\frac{a_n(x)}{(\theta t)^{n+4}}\,, \qquad (45)$$

with

$$a_n(x)=\frac{1}{(n+2)!}\frac{d}{dx}\frac{H_{n+2}(x)}{x}$$

and

$$\mathfrak{D}_\perp^{(n)}=\int_0^\infty dy\, y^n\mathfrak{D}_\perp(y)\,.$$

The moments of $\mathfrak{D}_\perp(y)$ may be expressed in terms of derivative of $\psi_\perp$ or ψ, and one finds that the dominant terms at long times are affected by the potential at large distances. The first term gives $D_\perp$ independent of x, so that the diffusion tensor is isotropic, and independent of velocity. This limiting form has been used by several investigators in studies of Brownian motion.[10,11] The particular behavior, $(\theta t)^{-5}$, is characteristic of the weak-coupling model. For the Gaussian potential, the expression is

$$D_\perp(x,\theta t)=\left(\frac{\pi}{2}\right)^{3/2}\frac{e^{-x^2}}{(\theta t)^5}\left[1+\frac{1}{(\theta t)^2}\left(x^2-\frac{5}{2}\right)+\cdots\right]. \qquad (46)$$

4. *Large and small speeds and times*

Expansions for small speeds may be generated by considering ut small, and t fixed. For $ut \ll 1$, the easiest expansion is via Eq. (33). Thus,

$$D_\perp(ut,\theta t)=\int_0^\infty\frac{dk}{\pi}\Psi_\perp(k,\theta t)[1-\tfrac{1}{2}(kut)^2+\cdots]=\frac{1}{3\pi}\left(\Phi_4(0,\theta t)-\frac{1}{10}\Phi_6(0,\theta t)(ut)^2+\cdots\right), \qquad (47)$$

$$D_\parallel(ut,\theta t)=\frac{1}{3\pi}\left(\Phi_4(0,\theta t)-\frac{3}{10}\Phi_6(0,\theta t)(ut)^2+\cdots\right),$$

with

$$\Phi_n(0,\theta t)=\int_0^\infty\frac{dk}{2\pi}k^n\psi(k)e^{-k^2(\theta t)^2/4}\,.$$

Note that the tensor is isotropic as $ut\to 0$ (the test particle becomes stationary) and that the expansion appears well behaved as long as $\theta t\neq 0$. The behavior at large speeds is not easy to extract. Since we do not need the information—we need it for the Laplace transformed tensor—we eschew its calculation here.

The time dependence of $D_{\alpha\beta}$ lies close at hand. For short times ($ut\ll 1, \theta t \ll 1$) we expand Eq. (47) to get

$$D_\perp\left(\frac{u}{\theta},\theta t\right)=\phi_4-\frac{1}{4}\phi_6\left[1+\frac{2}{5}\left(\frac{u}{\theta}\right)^2\right](\theta t)^2+\cdots,$$
$$D_\parallel\left(\frac{u}{\theta},\theta t\right)=\frac{1}{3\pi}\left\{\phi_4-\frac{1}{4}\phi_6\left[1+\frac{6}{5}\left(\frac{u}{\theta}\right)^2\right](\theta t)^2+\cdots\right\}. \qquad (48)$$

For long times, and u fixed, we simply refer to expansion (45).

5. *Laplace transformed tensor*

Since we shall study the kinetic equation in its Laplace-transformed version, $D_{\alpha\beta}(\vec{u},s)$ is particularly important. It is no surprise that $D_\perp(u,s)$ and $D_\parallel(u,s)$ are analytic in the half-plane. $\mathrm{Re}s>0$, when $0\le u<\infty$. The tensor components have a weak singularity at $s=0$. Inspection of Eq. (32) or Eq. (45) or the specific example of Eq. (35) shows t^{-5} behavior before transformation. Thus we expect a singularity $\sim s^4\ln s$. An Abelian theorem, applied to Eq. (45) gives

$$uD_\perp(u,s)\sim\frac{1}{\sqrt{\pi}}e^{-(u/\theta)^2}\times\left[\sum_{\text{odd}}\frac{\mathfrak{D}_\perp^{(n+3)}}{(n+3)!}a_n\left(\frac{u}{\theta}\right)\left(-\frac{s}{\theta}\right)^{n+3}\right]\ln s \qquad (49)$$

for the *singular* part of $uD_\perp(u,s)$. A similar expression holds for $D_\parallel(u,s)$.

One would not expect this singularity to give the behavior of the distribution function at long times. It gives the t^{-5} relaxation, characteristic of the short time scale. The relaxation at longer times is provided by the structure of the kinetic equation itself. We shall find that the *regular* part of $D_{\alpha\beta}(\vec{u},s)$ near $s=0$ is important then. To get at this portion, recall Eq. (32). The Laplace transform of $D_\parallel$ may be written

$$uD_\parallel(u,s)=\int_0^\infty\frac{dk}{2\pi}k^3\psi(k)F_\parallel\left(\frac{s}{ku},\frac{\theta}{2u}\right), \qquad (50)$$

$$F_\parallel(\sigma,\alpha)=\frac{1}{\pi}\left(\sigma+\int_0^\infty dt\, e^{-\phi(t)}[\phi_{tt}-(\phi_t)^2]\frac{\sin t}{t}\right),$$

where $\phi(t) = \sigma t + \alpha^2 t^2$. The function $F_\parallel(\sigma, \alpha)$ is analytic in a neighborhood of $\sigma = 0$, and the coefficients of σ^n may be computed by expanding the exponential, as long as $\alpha^2 > 0$. The nonanalyticity of $D_\parallel$ arises from the subsequent integration over k. One can go to $n = 3$ for the smooth potentials we are considering, before encountering the singularity $s^4 \ln s$. In any case, the coefficients may be expressed in terms of the integrals

$$f_n(\alpha) = \int_0^\infty dt\, e^{-\alpha^2 t^2} t^n \sin t, \quad (n = -1, 0, 1, \ldots),$$

which belong to the family of error functions $[f_{-1}(\alpha) = \frac{1}{2}\pi \operatorname{erf}(1/2\alpha)]$, for example. But the functions themselves are too complicated to afford insight. It is their large u (small α) limits that are particularly important.

We may use standard techniques in getting expansions of the f_n ($n \geq 0$) for large u. In particular, the f_n for n odd are purely exponential and are dominated by those for n even, which are 0(1) as $u/\theta \to \infty$, and are expressible as a series of powers of $1/u$. When the algebra is completed we find

$$D_\parallel \sim \frac{1}{4}\phi_3 \frac{\theta^2}{u^3} + s\phi_2 \frac{1}{\pi u^2}\left(1 - \frac{3}{2}\frac{\theta^2}{u^2} + \cdots\right) - s^2\phi_1 \frac{1}{2u^3} + s^3\phi_0 \frac{1}{\pi u^4}\left(1 - \frac{2}{3}\frac{\theta^2}{u^2} + \cdots\right) \quad (51)$$

plus singular parts. In another grouping, according to powers of $1/u$,

$$\begin{aligned} uD_\perp(u, s) &= \frac{1}{4}\phi_3 - \frac{1}{\pi}\phi_2 \frac{s}{u} + \frac{1}{4}\left[\phi_1 - \frac{1}{2}\phi_3\left(\frac{\theta}{s}\right)^2\right]\frac{s^2}{u^2} - \frac{1}{2\pi}\left[\frac{2}{3}\phi_0 - \phi_2\left(\frac{\theta}{s}\right)^2\right]\frac{s^3}{u^3} + \cdots, \\ uD_\parallel(u, s) &= \frac{1}{\pi}\phi_2 \frac{s}{u} - \frac{1}{2}\left[\phi_1 - \frac{1}{2}\phi_3\left(\frac{\theta}{s}\right)^2\right]\frac{s^2}{u^2} + \frac{1}{\pi}\left[\phi_0 - \frac{3}{2}\phi_2\left(\frac{\theta}{s}\right)^2\right]\frac{s^3}{u^3} - \cdots. \end{aligned} \quad (52)$$

We also need the behavior of $D_\parallel$ and $D_\perp$ near $u = 0$, for arbitrary s. The calculation is straightforward. We may expand $f_\parallel$ and $f_\perp$ to get a series in u^2. For example,

$$D_\parallel(u, s) = \sum_{n=0,2,\ldots} C_n u^n \int_0^\infty \frac{dk}{2\pi}\psi(k)k^3 \times \int_0^\infty dt\, e^{-\sigma t} t^n e^{-\theta^2 t^2/4}, \quad (53)$$

with $\sigma = s/k$. The inner integrals are entire functions of σ, related, again, to error functions. For $\psi(k)$ positive—as it is in the weakly-coupled Gaussian case—the coefficients of u^n do not vanish for s real and ≥ 0, and have the same signs as the C_n, which oscillate. It is apparent that each of the coefficients has the $s^4 \ln s$ singularity.

6. *Markoffian limit*

This limit is reached when $\delta = t_1/t_2 \to 0$ [see the discussion following Eq. (21)]. If we replace $D_{\alpha\beta}(\vec{u}, s)$ by $D_{\alpha\beta}(\vec{u}, 0)$ in the kinetic equation, we are treating the equation "in the Markoffian limit." Memory has been suppressed, and correlations in the diffusion tensor relax instantaneously when compared with the relaxation of the distribution function. This is the traditional form of the kinetic equation. [Note that $\mathfrak{D}_\parallel \equiv D_\parallel(\theta = 0)$ vanishes as $s \to 0$. This reflects the fact that in the Lorentz model, the energy of the test particle is conserved in a collision.]

$D_\parallel(u, 0)$ and $D_\perp(u, 0)$ may be obtained from equations like Eq. (50) at $s = 0$. For variety, we give another approach, based on Eq. (22). Thus,

$$D_{\alpha\beta}(\vec{u}, s) \to D_{\alpha\beta}(\vec{u}, 0) = \int d^3w\, M_*(\vec{u} - \vec{w}) \times \left(\delta_{\alpha\beta} - \frac{w_\alpha w_\beta}{w^2}\right)\frac{1}{4w}\phi_3, \quad (54)$$

$$\begin{aligned} uD_\perp(u, 0) &= \tfrac{1}{4}\phi_3 \int d^3w\, M_*(\vec{u} - \vec{w})\frac{\vec{u}\cdot\vec{w}}{uw} \\ &= \tfrac{1}{4}\phi_3\left(\frac{d}{dx} + 2x\right)\frac{1}{2x}\operatorname{erf} x \quad \left(x = \frac{u}{\theta}\right), \\ D_\parallel(u, 0) &= \frac{1}{4\theta}\phi_3 \frac{d}{dx}\left(\frac{d}{dx} + 2x\right)\frac{1}{2x}\operatorname{erf} x. \end{aligned} \quad (55)$$

Equation (54), with $\frac{1}{4}\phi_3$ replaced by $2\pi(e^2/m)^2 \ln\Lambda$, is well known in plasma physics.

The Markoffian expression is equivalent to that given originally by Chandrasekhar[12] and then by others. Our form is more compact. If the exponentially small portions are neglected, we have

$$\begin{aligned} D_\parallel(u, 0) &\sim \tfrac{1}{4}\phi_3\theta^2/u^3, \\ uD_\perp(u, 0) &\sim \tfrac{1}{4}\phi_3(1 - \theta^2/2u^2). \end{aligned} \quad (56)$$

These expressions were used by Mazo and Resibois[13] (MR) in a study of the Markoffian kinetic equation for small mass ratio. Since the mass ratio occurs in combination with the velocity, the approximation, θ small, is not uniform in u and fails in a region of width θ, near $u = 0$. However, the gain in analytical simplicity is considerable. We shall return to the "MR" model.

One can proceed to a "post-Markoffian approximation" by including the term proportional to s in the expansion of Eq. (50). We must evaluate the integrals f_0 and f_2, whence we find

$$\begin{aligned} D_\parallel(u, s) &\sim D_\parallel(u, 0) + s\frac{\phi_2}{\pi u^2}\left[1 - \frac{1}{2x^2}\left(3 - x\frac{\partial}{\partial x}\right)f_0\right], \\ f_0 &= -\sqrt{\pi}\, i x e^{-x^2} \operatorname{erf}(ix). \end{aligned} \quad (57)$$

The expansion in s, which is at best, asymptotic, does not give a sequence of approximations uniform in u. One sees this from Eq. (52) for $uD_{\parallel}$. The Markoffian approximation gives $uD_{\parallel} \sim \frac{1}{4}\phi_3\theta^2 u^{-2}$ at large speeds, while the post-Markoffian gives $(1/\pi)\phi_2 s u^{-1}$, which dominates when $s \neq 0$. Thus, one anticipates that the Markoffian kinetic equation does not give accurate information about the distribution of high-speed particles at long times. One also notes the distinction between $\theta \neq 0$ and the Lorentz model, $\theta = 0$. For that reason, the latter case will be treated separately.[14]

Figures 1–3 display $D_{\perp}(u, s)$ and $D_{\parallel}(u, s)$ for the Gaussian potential. The Markoffian components depend only upon u/θ. The non-Markoffians are computed for $\theta = 1$.

III. KINETIC EQUATION

We shall analyze the kinetic equation in two stages. First, we discuss general properties of the equation and its solutions, as far as we can. Then, since the solutions are not expressible in terms of elementary functions, and do not lend themselves to numerical computation, we shall discuss simpler equations, which retain the important features of the weak-coupled equation.

The kinetic equation, Eq. (21), is best analyzed through Laplace transformation. Thus,

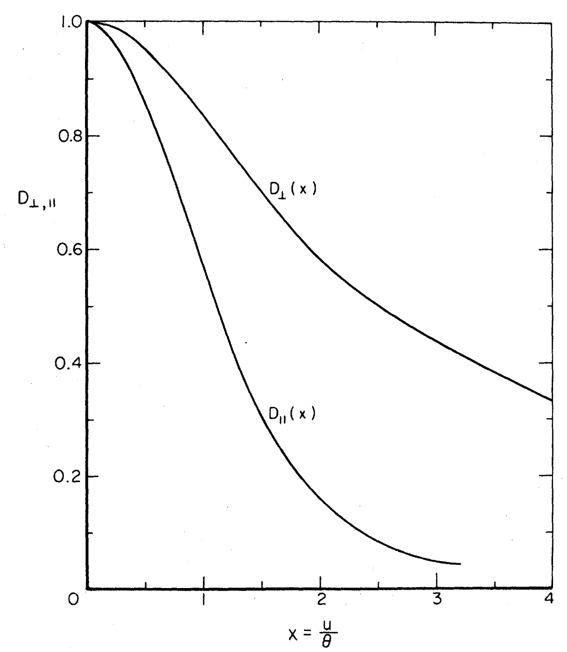

FIG. 1. Components of the Markoffian D tensor, $D_{\alpha\beta}(u, s=0)$. $D_{\perp}$ and $D_{\parallel}$ depend only upon $x = u/\theta$. They have been reduced in scale for ease of presentation. The corresponding functions of Figs. 2 and 3 are $\frac{1}{3}\pi^{3/2}$ times larger. In all cases, the Gaussian potential is used.

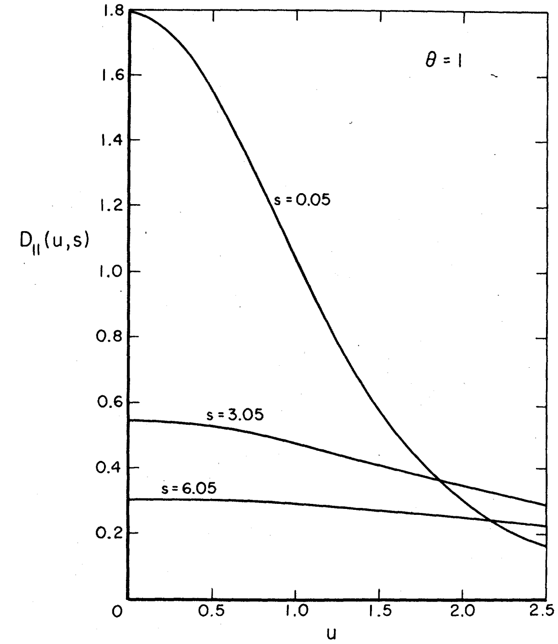

FIG. 2. Laplace transform of the time dependent $D_{\parallel}$. s may be thought of as inverse time; the scale is in terms of the collision time, t_1.

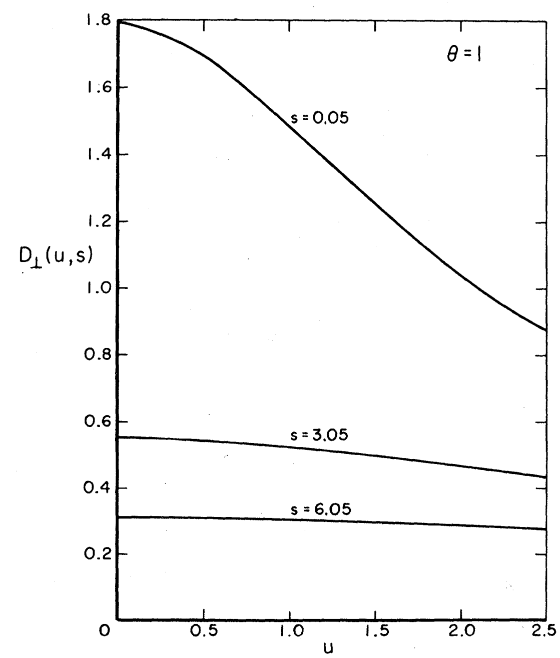

FIG. 3. Laplace transform of the time dependent $D_{\perp}$.

$$\epsilon \frac{\partial}{\partial \vec{u}} \cdot \vec{D}(\vec{u}, s) \cdot \left(\frac{\partial}{\partial \vec{u}} + 2\vec{u}\right) f(\vec{u}, s) - s f(\vec{u}, s) = -f(\vec{u}, t=0) \tag{58}$$

or

$$\frac{\epsilon}{u^2} \frac{\partial}{\partial u} u^2 D_{\parallel}(u, s)\left(\frac{\partial}{\partial u} + 2u\right) f(\vec{u}, s) + \frac{\epsilon}{u^2} D_{\perp}(u, s) \nabla_{\perp}^2 f(\vec{u}, s) = s f(\vec{u}, s) - f(\vec{u}, t=0),$$

where

$$\nabla_{\perp}^2 = \frac{1}{\sin\vartheta} \frac{\partial}{\partial\vartheta} \sin\vartheta \frac{\partial}{\partial\vartheta} + \frac{1}{\sin^2\vartheta} \frac{\partial^2}{\partial\varphi^2},$$

and $\vec{u} = (u, \vartheta, \varphi)$. An expansion of $f(\vec{u}, s)$ in spherical harmonics

$$f(\vec{u}, s) = \sum_{l,m} f_{lm}(u, s) Y_l^m(\vartheta, \varphi)$$

produces

$$\epsilon \frac{d}{du} u^2 D_{\parallel}\left(\frac{d}{du} + 2u\right) f_{lm}(u, s) - [s u^2 + \epsilon l(l+1) D_{\perp}] f_{lm}(u, s) = -u^2 f_{lm}(u, t=0). \tag{59}$$

In the particular case of the Green's function $u^2 f(\vec{u}, t=0) = \delta^2(\hat{\Omega} - \hat{\Omega}_0)\delta(u - u_0)$ and the right-hand side of Eq. (59) becomes $-\delta(u - u_0) Y_l^m(\vartheta_0, \varphi_0)$. In the future, we neglect m dependence, and denote $f_{lm}(u, t=0)$ by $f_l^0(u)$.

We get another useful form of Eq. (58) by writing $f_l = \exp(-u^2) g_l$. Then

$$\epsilon \frac{d}{du} u^2 e^{-u^2} D_{\parallel} \frac{d}{du} g_l - [s u^2 + \epsilon l(l+1) D_{\perp}] e^{-u^2} g_l = -u^2 f_l^0(u). \tag{60}$$

Often, we denote the function $u^2 e^{-u^2} D_{\parallel}$ by $\Delta(u, s)$. Δ is positive for $u > 0$ and s real and positive. Another useful equation is generated through $g_l = \Delta^{-1/2} h_l(u, s)$. We have

$$\frac{d^2}{du^2} h_l(u, s) - v_l(u, s, \epsilon) h_l(u, s) = \frac{-u^2 f_l^0(u)}{\epsilon\sqrt{\Delta}}, \tag{61}$$

with

$$v_l = \frac{s}{\epsilon D_{\parallel}} + \frac{l(l+1)}{u^2} \frac{D_{\perp}}{D_{\parallel}} + \frac{1}{\sqrt{\Delta}} (\sqrt{\Delta})_{uu}. \tag{62}$$

We may bring the equation to a more familiar form if we make the Schwarz transformation

$$h_l(u, s) = \frac{1}{(\xi_u)^{1/2}} H_l(\xi, s),$$

with

$$\xi_u \equiv \frac{d\xi}{du} = \frac{1}{[D_{\parallel}(u, s)]^{1/2}}.$$

Then,

$$\frac{d^2}{d\xi^2} H_l(\xi, s) + [\lambda - \omega_l(\xi, s)] H_l(\xi, s) = -\frac{1}{\epsilon} u^2 f_l^0(u) \left(\frac{D_{\parallel}}{\Delta_1}\right)^{1/2}, \tag{63}$$

with

$$\lambda = -s/\epsilon, \quad \Delta_1 = \Delta/(D_{\parallel})^{1/2} = u^2 e^{-u^2} (D_{\parallel})^{1/2},$$

and

$$\omega_l(\xi, s) = \frac{l(l+1)}{u^2} D_{\perp} + \frac{1}{\sqrt{\Delta_1}} (\sqrt{\Delta_1})_{\xi\xi}. \tag{64}$$

The homogeneous form of Eq. (63) is an equation of the Schrödinger type, with eigenvalue λ, and effective potential $\omega_l(\xi, s)$. Both forms of the equation will be used ahead. Effective potentials are displayed in Figs. 4–6.

A. "Potentials" v_l and ω_l

We consider these complicated expressions for s real and non-negative. Since $D_{\perp}$ and $D_{\parallel}$ are regular functions of u, free of zeros for finite u, the potentials are also regular functions. We begin with v_l. Expansion in u gives

$$v_l(u, s) = \frac{l(l+1)}{u^2} + v_l^{(0)}(s) + v_l^{(2)}(s) u^2 + \cdots \tag{65}$$

for small u. The coefficients are, for example,

$$c_0(s) v_l^{(0)}(u, s) = -3c_0(s) + s/\epsilon + [3 - \tfrac{2}{3} l(l+1)] c_2(s),$$

where

$$D_{\parallel}(u, s) = c_0(s) + c_2(s) u^2 + \cdots$$

[see Eq. (53)]. The coefficients $c_n(s)$ have branch

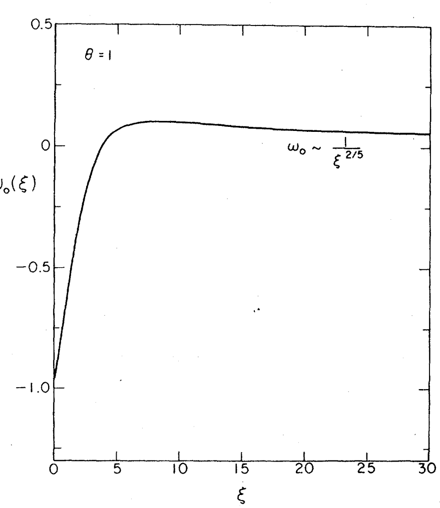

FIG. 4. Markoffian "potential" for $l=0$, $\omega_0(\xi)$. Note the possibility of a "bound state of zero energy"—the Maxwellian. The slow decrease of ω_0 with increasing ξ indicates a singular potential with continuous spectrum.

points at $s=0$. The weak, logarithmic singularity has been described earlier. This representation for $v_l(u,s)$ is continuous as $s\to 0$, the Markoffian limit being obtained by replacing $c_m(s)$ by $c_m(0)$.

The situation is different when u is large, for the expansion is not so well behaved. We have

$$v_l(u,s)=\left(1+\frac{1}{\epsilon_1}\right)u^2+\frac{\pi}{2\phi_2}\left[\phi_1-\frac{1}{2}\,\phi_3\left(\frac{\theta}{s}\right)^2\right]\frac{s}{\epsilon_1}\,u+\cdots\,, \tag{66}$$

with $\epsilon_1=(\epsilon/\pi)\phi_2$. The terms involving ϵ come from $s/\epsilon D_{11}$, which is the important term in this region. Note that the coefficients diverge as $s\to 0$, so that Eq. (66) does not give the correct form, which is

$$v_l(u,0)=u^2+\frac{3}{4u^2}+\frac{l(l+1)}{\theta^2}\left(1-\frac{\theta^2}{2u^2}\right)+\cdots\,,$$

where the remaining terms $(\cdots)$ are exponentially small. On the other hand, the Markoffian kinetic equation produces

$$v_l^M(u,s)=(s/\epsilon\delta_2)u^3+v_l(u,0),\quad \delta_2=\tfrac{1}{4}\phi_3\theta^2\,, \tag{67}$$

whose leading term is quite different from that of Eq. (66). The potentials are illustrated in Figs. 4–6. Note that the $l=0$ potential has a negative portion near $u=0$. In fact, $v_0^M(0,0)=-3(1+3/5\theta^2)$.

If we make further approximation, and take Eq. (56a) seriously for *all* u, we find

$$v_0^{\rm MR}(u,0)=\frac{s}{\epsilon\delta_2}\,u^3+u^2+\frac{3}{4u^2}\,,$$
$$v_l^{\rm MR}(u,0)=v_0^{\rm MR}+\frac{l(l+1)}{\theta^2}\left(1-\frac{\theta^2}{2u^2}\right)\,, \tag{67'}$$

characterized by pathologic behavior as $u\to 0$. Turning to $\omega_l(\xi,s)$, we note that since $D_{\parallel}(0,s)$ does not vanish, ξ is proportional to u when u is small, and $\omega_l(\xi,s)$ resembles $v_l(u,s)$ in that region. Thus, $\omega_l\sim A_l(s)/\xi^2$ for $l>0$, $\omega_l\to -B(s)$ for $l=0$. When u is large, ξ is large, but the relationship is singular at $s=0$. Details may be extracted from the alternate form

$$\omega_l(\xi,s)=\frac{1}{\xi_u^2}\left[\frac{1}{\sqrt{\Delta}}(\sqrt{\Delta})_{uu}-\sqrt{\xi_u}\left(\frac{1}{\sqrt{\xi_u}}\right)_{uu}+\frac{l(l+1)}{u^2}\,\frac{D_\perp}{D_\parallel}\right]$$
$$=\frac{(\sqrt{\Delta\xi_u})_{\xi\xi}}{\sqrt{\Delta\xi_u}}+\frac{l(l+1)}{u^2\xi_u^2}\,\frac{D_\perp}{D_\parallel}\,. \tag{68a}$$

We note that when u is large, the first term domin-

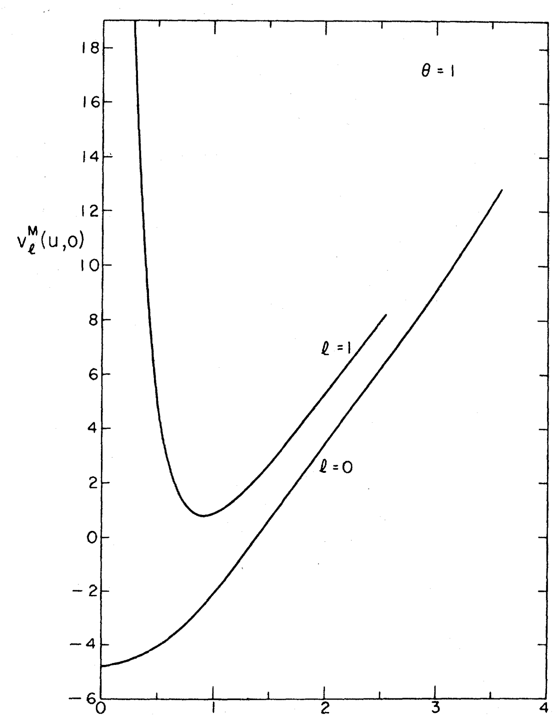

FIG. 5. Function $v_l^M(u,s)$, another Markoffian "potential," in the limit $s\to 0$. The $l=0$ potential shows the possibility of a state of zero energy—the Maxwellian—as $t\to\infty$. The $l=0$ potential has the characteristic "centrifugal barrier," and admits no zero-energy states.

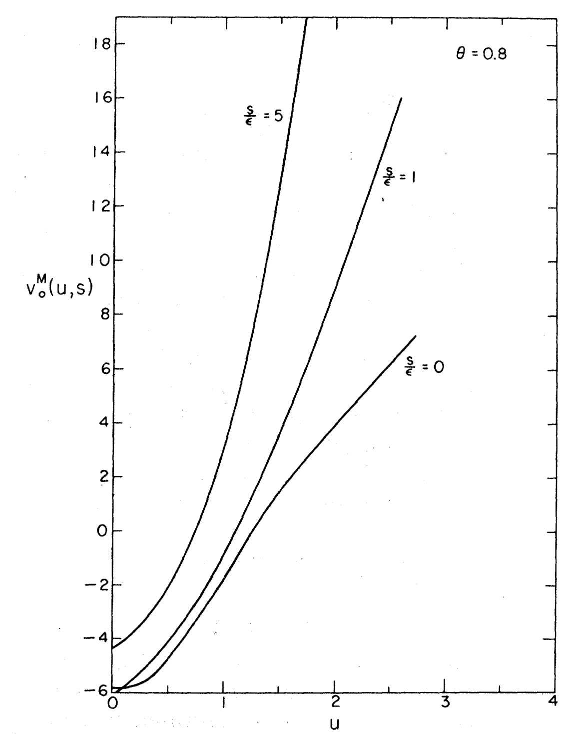

FIG. 6. Function $v_0^M(u,s)$ for various s. Note that this "potential" whose time dependence governs the relaxation of the distribution function at long time, relaxes according to the long (slow) time scale, whose unit is ϵt_1.

ates. Then,

$$\omega_l(\xi, s) = a_2 s + \frac{a_3}{(4a_2 s)^{1/4}} \frac{1}{\sqrt{\xi}} - 2\frac{[a_3^2 + 2(a_2 s)^2]}{(4a_2 s)^{3/2}} \frac{1}{\xi} + \cdots \tag{68b}$$

with $a_2 = (1/\pi)\phi_2$; $a_3 = \frac{1}{4}\phi_3\theta^2 - \frac{1}{2}\phi_1 s^2$. The singularity at $s = 0$ is apparent. Otherwise, the function has simple behavior. The Markoffian version is

$$\omega_l^M(\xi) = \frac{1}{4}\phi_3\theta^2\left(\frac{1}{(b\xi)^{2/5}} - \frac{1}{(b\xi)^{6/5}} + \cdots\right), \tag{69}$$

with $b = \frac{5}{4}\theta(\phi_3)^{1/2}$. We are reminded of the Schrödinger equation for a particle in a potential that is of extremely long range.

B. Boundary conditions

The boundary conditions come from the requirement that $f(\vec{v}, t)$ be positive and integrable in any region of $\vec{v}$ space. Further, $\int d^3v\, f(\vec{v}, t)$ is independent of time. When applied to Eq. (58) the latter gives

$$\left[u^2 D_\parallel(u, s)\left(\frac{\partial}{\partial u} + 2u\right) f_0(u, s)\right]_0^\infty = 0 \tag{70}$$

or

$$\left[\Delta(u, s)\frac{\partial}{\partial u} g_0\right]_0^\infty = 0$$

for the particular case, $l = 0$. Since the solutions to the homogeneous equation behave as $g_0 \sim u^{-1}\exp(\pm u)$ for small u, Eq. (70) enables one to reject one solution. In the case of $l > 0$, one finds $g_l \sim u^l, u^{-(l+1)}$, and we reject the singular solution. In both cases, the solution retained behaves properly as $u \to \infty$.

Finally, it is interesting to note that the kinetic equation based upon Eq. (56) yields solutions $(l = 0) g_1 = 1 + au^3 + \cdots$, $g_2 = u^2(1 + bu^3 + \cdots)$ which respond to Eq. (70). Thus, one may speak of particle conservation in that case. When $l > 0$, one must face the approximate $D_\perp(u, 0)$ which has the wrong sign at $u = 0$, in addition to being singular. There is not much point pursuing the model further.

1. Aspects of the solution

As usual, the Maxwellian distribution plays a special role in the solution of the kinetic equation. The equation for the angle-integrated density is

$$\frac{\partial}{\partial t} f_0(u, t) = \frac{\epsilon}{u^2}\frac{\partial}{\partial u}\int_0^t d\tau\, D_\parallel(u, t - \tau)\left(\frac{\partial}{\partial u} + 2u\right) f_0(u, \tau),$$

and it is clear that if $f_0(u, t)$ is proportional to $\exp(-u^2)$, then $f_0(u, t) = f_0(u, t = 0)$ is a (time-independent) solution. There is also a strong indication that $f_0(u, t)$ approaches a Maxwellian as $t \to \infty$, independent of initial condition, as long as $m_1/m_2 \neq 0$. Consider $f_0(u, t)$ for t large. Then, *if* $[(\partial/\partial u) + 2u] f_0(u, t)$ approaches some $\phi(u)$, we have, for sufficiently long time

$$\frac{\partial}{\partial t} f_0(u, t) \cong \frac{\epsilon}{u^2}\frac{\partial}{\partial u} u^2\left(\int_0^\infty dt\, D_\parallel(u, t)\right)\phi(u).$$

The left-hand side will vanish if either $\phi(u) = 0$ or $\int_0^\infty dt\, D_\parallel = 0$. In the first case, the final distribution is Maxwellian. The second case occurs in the L model. There, since no moderation occurs, the final distribution—if it exists—is not necessarily Maxwellian. We give its precise form in a subsequent paper.

The distribution functions $f_l(u, t)$ evolve in a complicated manner. At first glance, three distinct time scales are involved; the averaged diffusion tensor relaxes in a time $t_1 = a/v_B$, characteristic of the duration of a collision, the higher spherical harmonics ($l \neq 0$) relax after a few collisions, with characteristic time $t_2 = (\pi a^2 n_0 v_B)^{-1}$, while the isotropic mode ($l = 0$), in its approach to the Maxwellian, depends upon the mass ratio as well. Inspection of $D_\parallel$ in the Markoffian limit shows that this last time is $\sim[(m_2/m_1)\pi a^2 n_0 v_B]^{-1}$ for $m_2/m_1 \gg 1$. These estimates, which suggest a neat separation of epochs, are too simple. They are blurred when the diffusive particles have a wide range of speeds. Thus a very slow particle will take a long time to complete a collision; a very fast particle will undergo small deflections upon collision (unless the potential has a hard core) and the relaxation of higher harmonics will be inhibited. We are led to suspect a continuous distribution of relaxation times. The following examples illustrate the point.

Consider the case of no velocity dependence at all:

$$\frac{df(t)}{dt} = \epsilon\int_0^t dt\, D(\tau) f(t - \tau),$$

with $D(\tau) = \exp(-\tau)$. This equation, which is a differential equation in disguise, has two exponential solutions. They are, approximately $\exp(-t)$ and $\exp(-\epsilon t)$. However, if we consider velocity dependence, through, say

$$\frac{\partial f(u, t)}{\partial t} = \epsilon\int_0^t d\tau\, D(\tau) L_u f(u, t - \tau),$$

with L_u an operator having eigenfunctions $\psi_n(u)$ and real nonpositive eigenvalues $-\lambda_n$, $(\lambda_0 = 0)$ we have two groups of exponential solutions. Their decay constants are, approximately $-1 + \epsilon\lambda_n$ and $-\epsilon\lambda_n$, when $\epsilon\lambda_n$ is small. The "blurring" is manifest. We expect to find our distribution functions relaxing (to the Maxwellian for $l = 0$, to zero for $l \neq 0$)

in a nonexponential manner, controlled by the continuous spectrum of an operator upon the velocity variable.

A final general remark about perturbation theory: In the first example of the previous paragraph, an expansion in ϵ will lead to a regular perturbation series (with "secular" terms). The second example—with L_u a differential operator of second order—leads to approximate solutions which are not uniformly good in u (and t). Straightforward attempts to get approximate solutions to our kinetic equation are plagued by nonuniformity. Such approximations lead to results which neglect "boundary-layer effects." We shall return to this point later.

A more precise discussion of the initial value problem for our kinetic equation rests upon the eigenfunction expansions associated with Eqs. (61) or (63). Thus we consider the spectral theory of the corresponding differential operators in the appropriate Hilbert space of functions.[15-17] The Markoffian operators are easier to treat, and we begin with them.

One sees immediately that the spectral problem is singular, because of the infinite domain of the independent variable, and because of the behavior of the coefficients at $u=0$. Further inspection shows that the singularity at $u\to\infty$ is of limit-point type, and the singularity at $u=0$ is limit point for $l\neq 0$ and limit circle for $l=0$, the latter case becoming regular upon transformation Eq. (60) to Eqn. (61). The equation in ξ is essentially a radial Schrödinger equation, one whose spectral theory is well established. The slow decrease of the potential to zero ensures that a continuous spectrum fills the negative half-axis $s<0$. The point $s=0$ is also present, and points $s>0$ are excluded by stability arguments. Mazo[18] has analyzed the equation in the case $\theta=1$. He shows, moreover, that the point spectrum is restricted to $s=0$. McLeod and Ong[19] and Su,[20] have considered a closely related equation. McLeod and Ong show that the relaxation of smooth, initial distributions is uniform, and $O(1/t)$, but not as fast as $O(e^{-\alpha t})$.

The full, non-Markoffian equations are complex. As we noted earlier, their coefficients feature nonuniformities as $u\to\infty$, and $s\to 0$. We can obtain an inkling of the nature of the spectrum, by considering $v_l(u,s)$. In the Markoffian case, this smooth function diverged as $su^3 (u\to\infty)$. Thus for s real and negative, the associated operator has a continuous spectrum in $(-\infty, 0)$. Since zero is in the spectrum for all real, negative s, we expect a continuous spectrum in $s<0$. In the full case, $v_l(u,s) \sim Au^2 - B(u/s)+\cdots$ [Eq. (66)] with $A, B>0$. Then, the operator appears to have a discrete spectrum, implying that the spectrum in s is very "thin"—possibly discrete! At this stage these remarks are little more than conjectures.

IV. FURTHER APPROXIMATION

Although $v_l(u,s)$ is a smooth and relatively featureless function, its analytical form is too complicated to permit solution to Eq. (61). We must seek useful approximations. It is natural to consider solutions for short time, and long time.

When we refer to short time (s large) we may mean $t<t_1<t_2$, or $t_1<t<t_2$. The latter case leads to the Markoffian approximation. The former suggests several possibilities: one might write Eq. (58) as

$$f(\vec{u},s)=\frac{1}{s}f(u,t=0)+\frac{\epsilon}{s}\frac{\partial}{\partial\vec{u}}\cdot\vec{D}(\vec{u},s)\cdot\left(\frac{\partial}{\partial\vec{u}}+2\vec{u}\right)f(\vec{u},s)$$

and iterate, to obtain a series good for a few collisions. The result is not terribly interesting. Or, one can replace $\vec{D}(u,t)$ by $\vec{D}(\vec{u},t=0)$, which is also independent of $\vec{u}$, in the *time*-dependent equation (21). Then we have a paradox. The equation should be good only for the very short interval during which the $\vec{D}$ tensor is unchanged. Yet, since the approximate equation admits Maxwellian solutions, and is relatively easy to solve, one wants to study it in the full domain $0<t<\infty$.[21,22] It turns out that the relaxation to equilibrium is much too simple.

We focus, therefore, upon the long-time behavior of $f_l(u,t)$, and upon $l=0$ in particular. In terms of Laplace transformed functions, we seek their behavior in the neighborhood of $s=0$. We have noted a weak singularity there, associated with the t^{-5} relaxation of the diffusion tensor. That singularity—associated with the short time scale—is *not* dominant. Rather, it is the singular behavior of the large-u expansions of v_l (or ω_l) as $s\to 0$ that produces the dominant singularity, and the characteristic behavior at long times. We shall try to retain it in whatever further modeling we use.

We shall be seeking the Green's function for the kinetic equation in every case. It will be constructed for s real and positive and continued analytically. In our modeling, we neglect the weak singularity in v_l. Then, in cases where v_l turns out to be analytic in s in a neighborhood of $s=0$, the Laplace inversion becomes a little simpler.

A. Markoffian equation

Consider the Markoffian model first, and the response to an initial pulse, $f(\vec{u},t=0)=\delta^3(\vec{u}-\vec{u}_0)$. If we focus upon the case $l=0$, and replace $D_\parallel$ by its dominant part at large u, $D_\parallel \sim \delta_2/u^3$, the kinetic equation becomes

$$\frac{d^2}{du^2}h(u,\sigma)-\left(\sigma u^3+u^2+\frac{3}{4u^2}\right)h(u,\sigma)=-\frac{1}{\epsilon(4\pi\delta_2)^{1/2}}\sqrt{u}\,e^{u^2/2}\,\delta(u-u_0)\,, \tag{71a}$$

with $\sigma=s/\epsilon\delta_2$. We are tempted to analyze the equation for all u, $0\leq u<\infty$; unfortunately, it has no simple solutions. The Schwarz transformation, $u^2=2\xi, h=(1/\sqrt{u})y(\xi)$ changes Eq. (71a) to

$$\frac{d^2}{d\xi^2}y(\xi,\sigma)-[1+\sigma(2\xi)^{1/2}]\,y(\xi,\sigma)=-\frac{1}{\epsilon(4\pi\delta_2)^{1/2}}\,e^{\xi}\delta(\xi-\xi_0)\,, \tag{71b}$$

an equation noted first by Mazo and Resibois,[13] who sought an approximate solution by replacing $\sqrt{\xi}$ by a constant. The equation one obtains is again too simple. Note, that extending Eq. (71a) to the full domain of u introduces a spurious singularity at $u=0$. The Markoffian version of the correct $v_0(u,s)=s/\epsilon D_{\parallel}+(1/\sqrt{\Delta})(\sqrt{\Delta})_{uu}$ is analytic at $u=0$, and in a neighborhood of $s=0$.

We are forced to mutilate the kinetic equation further. The choice is of approximate solutions to Eqs. (71), or exact solutions to a less-accurate equation. The first approach seems promising, for the coefficients seem to have the smooth form that recommends the Wentzel-Kramers-Brillouin (WKB) approach. However, we have been unable to progress in that manner, for the WKB solutions are not accurate in the full 2π domain of $\arg\sigma$. We need behavior on the negative real axis of σ for the Laplace inversion, and there, the equation features a turning point. We must make another alteration.

The approximation should be in terms of $D_{\parallel}$, so that we may transform back to $f_0(u,t)$ sensibly. Further, since the boundary condition(s) become

$$\left[\xi_u\Delta\,\frac{d}{d\xi}\left(\frac{y(\xi)}{(\xi_u\Delta)^{1/2}}\right)\right]_0^{\infty}=0$$

under transformation, we might wish to keep them simple. [The transformation leading to Eq. (71b) requires $dy/d\xi+y=0$ at $\xi=0$.] Thus, consider the transformation $h_0(u,s)=1/(\xi_u)^{1/2}y(\xi,s)$ which converts Eqs. (61) and (62) to

$$\frac{d^2y}{d\xi^2}-\left[\frac{s}{\epsilon}\,\frac{1}{\xi_u^2D_{\parallel}}+\frac{1}{\sqrt{\Delta\xi_u}}\,(\sqrt{\Delta\xi_u})_{\xi\xi}\right]y=-\frac{1}{\epsilon(4\pi)^{1/2}}\,\frac{\delta(\xi-\xi_0)}{\sqrt{\Delta\xi_u}}\,. \tag{72a}$$

The choice $\Delta\xi_u=e^{-2\xi}$ simplifies the second term in square brackets. ξ_u is positive and single-valued, so that the transformation is not crazy. We are particularly interested in u and ξ large, when

$$2\xi=u^2-\ln(u^3D_{\parallel})-\ln[1-\tfrac{1}{2}u[\ln(u^3D_{\parallel})]_u]+\cdots$$

and the quantity in large square brackets in Eq. (72a) is

$$1+\frac{s}{\epsilon}\,\frac{1}{u^2D_{\parallel}}\,\frac{1}{\left\{1-\dfrac{1}{2u}\,[\ln(u^3D_{\parallel})]_u\right\}^2}\cdots\,. \tag{72b}$$

We can aim for a tractable model by setting $D_{\parallel}\sim\delta/u^k(k>0)$. Then, the leading terms in Eq. (72b) are $1+s/\epsilon\delta(2\xi)^{(k-2)/2}$. Thus, $k=3$ (reality) produces the $\sqrt{\xi}$ of Eq. (71b) while $k=4,6$ lead to equations solvable in terms of known functions. We shall study

$$\frac{d^2y}{d\xi^2}-(1+\sigma\xi)y=-\frac{1}{\epsilon(4\pi)^{1/2}}\,e^{\xi}\delta(\xi-\xi_0)\,, \tag{73}$$

$\sigma=(2/\delta)s/\epsilon$, which is the large $-u$ form of $k=4$, extended now to all ξ, $0\leq\xi<\infty$. We shall retain our boundary conditions, requiring that $e^{-2\xi}(d/d\xi)(e^{\xi}y)$ vanishes at $\xi=0$ and $\xi\to\infty$.[23]

The function $y(\xi_1\xi_0;\sigma)$ of Eq. (73) is proportional to the Green's function, $y=[\epsilon(4\pi)^{1/2}]^{-1}e^{\xi_0}\mathcal{G}$, and we consider the latter. It may be constructed from the two solutions to the homogeneous equation, $y_0(\xi)$ and $y_1(\xi)$, defined through $y_0=0$, $dy_0/d\xi=1$; $y_1=1$, $dy_1/d\xi=0$, at $\xi=0$. Note that both solutions must be entire functions of s. Then, the Green's function is

$$\mathcal{G}(\xi_1\xi_0,\sigma)=-\frac{y_2(\xi_<)y_3(\xi_>)}{W(2,3;\sigma)} \tag{74a}$$

$$=\frac{y_2(\xi)y_2(\xi_0)}{W(2,3;\sigma)}-y_2(\xi_<)y_1(\xi_>)\,, \tag{74b}$$

where $y_2=y_1-y_0$ satisfies the boundary condition at $\xi=0$ and $y_3=y_0+m(\sigma)y_1$ is the decreasing solution, which satisfies the condition at infinity. The Wronskian, $W(2,3)$ is equal to $1+m(\sigma)$. When $\sigma=0$, y_0 is $\sinh\xi$, y_1 is $\cosh\xi$ and $y_2=e^{-\xi}$. The singularities of $\mathcal{G}(\xi_1\xi_0;\sigma)$ in the finite σ plane enter only through $W(\sigma)$. One notes, however, that the two parts of Eq. (74b) are not separately Laplace invertible.

The $y(\xi)$ are to be expressed in terms of known functions; these are Airy functions of argument $z=\sigma^{1/3}\xi+1/\sigma^{2/3}$. Thus,

$$\begin{aligned}y_0&=\pi\sigma^{-1/3}[A_i(p)B_i(z)-B_i(p)A_i(z)]\,,\\ y_1&=\pi[B_i'(p)A_i(\xi)-A_i'(p)B_i(z)]\,,\\ y_2&=y_1-y_0\\ &=\pi[(LB_i)(p)A_i(\xi)-(LA_i)(p)B_i(\xi)]\,,\end{aligned} \tag{75}$$

with $p=\sigma^{-2/3}$ and $(Lf)(p)=f'(p)+\sqrt{p}\,f(p)$. The primes denote differentiation with respect to argument, and A_i and B_i are the conventional designations for the decreasing and increasing Airy functions, respectively. Thus, inspection of Eq. (75)

leads to

$$W(\sigma) = 1 + \sqrt{p}\, A_i(p)/A_i'(p)\ . \quad (76)$$

We are concerned only with the long-time behavior of $\mathcal{G}(\xi_1\xi_0, t)$; thus we deform the Laplace inversion contour in the usual way and restrict our analysis to the portion enclosing the origin of the σ plane. Since y_1 and y_2 are analytic in σ, we need consider only the singularities and zeros of $W(\sigma)$. Consider first the possibility of zeros, accumulating at $\sigma = 0 (p \to \infty)$. For $|p|$ large, and $|\arg p| = |\arg \sigma^{-2/3}| < \pi$ we may use the asymptotic expansion

$$\ln A_i(p) = \text{const} - \tfrac{2}{3} p^{3/2} - \tfrac{1}{4} \ln p + \ln \sum_0^\infty (-)^k \bar{C}_k p^{-3k/2},$$

$$W(\sigma) = 1 - \sqrt{p}\left(\sqrt{p} + \frac{1}{4p} - \frac{\partial}{\partial p} \ln \sum_0^\infty \cdots\right)^{-1} = \frac{\sigma}{4}\left[1 + \sigma W_1(\sigma)\right],$$

where $W_1(\sigma)$ is a (formal) power series in σ. Thus, there is no evidence of accumulation.[24] Integration around the circle gives $2\delta\epsilon e^{-(\xi+\xi_0)}$ for $\mathcal{G}_1$, the $t \to \infty$ portion of $\mathcal{G}(\xi_1\xi_0; t)$, or $(\delta/\sqrt{\pi})e^{-u^2}$ for $f_0(u, t)$. (The dependence upon δ is a flaw in the model. One might patch it by taking $\delta = 2/\sqrt{\pi}$.)

In getting $\mathcal{G}_2$, the contribution from the branch cut, we note again that the second term in Eq. (74b) is analytic. Thus

$$\mathcal{G}_2(\xi_1\xi_0; t) = \int_{\leftarrow} \frac{ds}{2\pi i} e^{st} y_2(\xi, \sigma) y_2(\xi_0, \sigma) \times \left(\frac{1}{W_+(\sigma)} - \frac{1}{W_-(\sigma)}\right),$$

with $W_\pm = W_1 \pm i W_2$ being the values of $W(\sigma)$ on the upper and lower edges, respectively. The quantity in large parentheses is $2i(W_2/|W|^2)$ and we express it in terms of A_i and B_i. The key is provided by the connection formula

$$A_i(p e^{2\pi i/3}) = \tfrac{1}{2} e^{\pi i/3}[A_i(p) - i B_i(p)]\ ,$$

which we use for p real. Then, noting that $B_i(p)$ is exponentially large for $p \to \infty$, we find

$$\frac{W_2}{|W|^2} \to \frac{1}{\pi\sqrt{p} B_i^2(p)} \sim e^{-4/3\sigma}, \quad \arg\sigma = 0$$

for p large (σ small). We have arrived at the simple result that the approach to equilibrium, as expressed by $\mathcal{G}_2(\xi_1\xi_0; t)$ is

$$\mathcal{G}_2(\xi_1\xi_0; t) \sim e^{-(\xi+\xi_0)} \int_0^{\epsilon_1} ds\, e^{-(st + 4/3\sigma)} \sim e^{-(\xi+\xi_0)} a\sqrt{\pi}\, \frac{e^{-2(at)^{1/2}}}{(at)^{3/4}}, \quad a = \tfrac{8}{3}\delta\epsilon\ . \quad (77)$$

The relaxation is *faster* than t^{-5} and, therefore a little puzzling. It may be due to our modeling of $D_\parallel$, or to a fundamental inconsistency in the Markoffian approximation. The relaxation proceeds according to a "slow time," ϵt, and is independent of ξ. This feature may be traced to the simple, analytic form of the coefficients in the kinetic equation.

B. Non-Markoffian models

One wants to consider the non-Markoffian version of Eq. (72a) to understand matters more clearly. Again, we claim that the large $-u$ behavior is crucial. The nonuniformity is expressed through the asymptotic piece

$$D_\parallel(u, s) \sim \frac{1}{4}\phi_3 \frac{\theta^2}{u^3} + \frac{1}{\pi}\phi_2 \frac{s}{u^2} = \frac{\delta}{u^3}\left(1 + \frac{\alpha}{2} su\right),$$

and we might wish to use it in factor $(u^2 D_\parallel)^{-1}$ of Eq. (72b), ignoring all else. Unfortunately, the $[(2\xi)^{1/2}]$'s of Eq. (71b) reappear and we must fall back onto a modified $D_\parallel$, $D_\parallel = (\delta/u^4)[1 + (\alpha/2)su^2]$. Then we get a kinetic equation ($\beta = \frac{1}{2}\alpha\delta\epsilon$),

$$\frac{d^2y}{d\xi^2} - \left(1 + \frac{\sigma\xi}{1 + \beta\sigma\xi}\right)y = -\frac{1}{\epsilon(4\pi)^{1/2}} e^{\xi}\delta(\xi - \xi_0)\ , \quad (78)$$

whose solutions can be expressed in terms of known functions. The equation displays nonuniformity clearly enough. When $\beta = 0$, the coefficient of y increases as ξ, while for any $\beta \neq 0$, the coefficient is constant at large ξ. The transformation $\beta\sigma x = \gamma^{-1}(1 + \beta\sigma\xi)$, with $2\gamma = [\beta/(1+\beta)]^{1/2}$ converts the equation to

$$\frac{d^2y}{dx^2} + \left(-\frac{1}{4} + \frac{\kappa}{x}\right)y = -\frac{\gamma}{\epsilon(4\pi)^{1/2}} e^{\xi}\delta(x - x_0)\ , \quad (79)$$

with $\kappa = \gamma/\beta^2\sigma$. β, the key physical parameter, gives the ratio of short to long time scales. Equation (79) is a special case of Whittaker's equation.[25]

Note the complexity introduced by nonzero β. First, the coefficient of y in Eq. (78) is not an entire function of σ, so that we can not construct the Green's function from entire basis functions, as we did earlier. The singularities in the Green's function will be much more complicated; as a consequence, the temporal relaxation will be ξ dependent. Second, the solutions of the homogeneous version of Eq. (78) will be expressed in terms of Whittaker functions of argument $x = (1/\gamma)(\xi + 1/\beta\sigma)$. The argument is singular at $\sigma = 0$; so was the corresponding argument in the Markoffian case. However, here, κ, the index of the Whittaker function, is also singular at $\sigma = 0$. This makes the asymptotic analysis extremely difficult.

One can proceed a bit farther, by remarking that the Green's function associated with Eq. (78) may be written

$$\bar{\mathcal{G}}(\xi_1\xi_0;\sigma) = -\bar{y}_2(\xi_<,\sigma)\bar{y}_3(\xi_>,\sigma)/\bar{W}(2,3;\sigma)\,,$$

as before. $\bar{y}_3$ is the solution decreasing, as $\exp(-\xi/2\gamma)$, at infinity, and $\bar{y}_2$ satisfies the boundary condition at $\xi=0$. However, $\bar{y}_2$ and $\bar{y}_3$ are singular at $\sigma=0$ and, possibly, at other points in the left half-plane. They are linear combinations of the Whittaker functions $M(\gamma/\beta^2\sigma;\frac{1}{2};\gamma^{-1}(\xi+1/\beta\sigma))$ and $W(\kappa;\frac{1}{2};x)$. The behavior at $\sigma=0$, which yields the relaxation rate, rests on the asymptotics of M and W when $|\kappa|, |x|\to\infty, |\kappa/x|\to$ const. This difficult analysis has yet to be done.

V. CONCLUSION

We have examined the kinetic equation for a test particle weakly coupled to the rest of an N-particle system. One can learn quite a bit about the structure of the generalized Fokker-Planck equation that governs the relaxation, through a study of the associated diffusion tensor. The two time scales which are present, are, strictly speaking, inseparable. Although we have not had much success in solving the equation, there are strong indications that the Markoffian approximation is inconsistent.

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APPENDIX A

A simple way to show the connection between the sign of $D_\perp$ and $D_\parallel$ and the possibility of "runaway" solutions is to assume that for $t\to\infty$, Eq. (22) may be written

$$\frac{\partial f}{\partial \tau} = \epsilon\,\frac{\partial}{\partial \vec{u}}\cdot\int_{-\infty}^{t} d\tau\,\vec{D}(\vec{u},t-\tau)\cdot\left(\frac{\partial}{\partial\vec{u}}+2\vec{u}\right)f(\vec{u},\tau) \tag{A1}$$

or

$$=\epsilon\,\frac{\partial}{\partial \vec{u}}\cdot\int_{0}^{\infty} d\tau\,\vec{D}(\vec{u},\tau)\cdot\left(\frac{\partial}{\partial\vec{u}}+2\vec{u}\right)f(\vec{u},t-\tau)\,. \tag{A2}$$

With this form, there is the possibility of a real exponential solution $f_\lambda(\vec{u},t)=\psi_\lambda(\vec{u})e^{\lambda t}$, where

$$\epsilon\,\frac{\partial}{\partial\vec{u}}\cdot\vec{D}^0(\vec{u})\cdot\left(\frac{\partial}{\partial\vec{u}}+2\vec{u}\right)\psi_\lambda(\vec{u})=\lambda\psi_\lambda(\vec{u})\,, \tag{A3}$$

$$\vec{D}^0(\vec{u})=\int_0^\infty dt\,\vec{D}(\vec{u},t)=\vec{D}(\vec{u},s=0)\,. \tag{A4}$$

Now, introduce $\bar{\psi}_\lambda$ through $\psi_\lambda(\vec{u})=e^{-u^2}\bar{\psi}_\lambda(\vec{u})$. Multiply Eq. (A3) by $\bar{\psi}_\lambda$ and integrate. After a partial integration, we have

$$\lambda\int d^3u\,\bar{\psi}_\lambda\psi_\lambda = -\epsilon\int d^3u\,\frac{\partial\bar{\psi}_\lambda}{\partial u_\alpha}D^0_{\alpha\beta}e^{-u^2}\frac{\partial\bar{\psi}_\lambda}{\partial u_\beta} \tag{A5}$$

$$=-\epsilon\int d^3u\,\frac{e^{-u^2}}{u^2}\times\{(\vec{u}\times\nabla\bar{\psi}_\lambda)^2D^0_\perp+[(u\cdot\nabla)\bar{\psi}_\lambda]^2D^0_\parallel\}\,, \tag{A6}$$

provided the integrals exist. Thus, the property $D^0_\perp$, $D^0_\parallel\geq 0$ ensures against "runaway" solutions

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[1]One can interpret "generalized kinetic equation" in many ways, going back, if one wishes, to Enskog. Here, I use it to mean the concise, abstract forms introduced by R. W. Zwanzig in his *Boulder Lectures*, edited by W. E. Brittin, W. B. Downs, J. Downs (Wiley, New York, 1961), and developed by H. Mori [Prog. Theor. Phys. 33, 423 (1965)] and A. Z. Akcasu and J. J. Duderstadt [Phys. Rev. 188, 479 (1969)].

[2]Closely related, but expressed in a different language, is the important work of the Brussels school, described in part, in I. Prigogine, *Non-Equilibrium Statistical Mechanics* (Wiley, New York, 1962).

[3]For application to fluids, the reader is invited to consult the rich literature, composed for the most part of papers in Phys. Rev. A, 1970 onwards, and associated with A. Z. Akcasu, C. Boley, R. Desai, D. Forster, E. Gross, G. Mazenko, S. Yip, and their colleagues. See, for example, Phys. Rev. A 7, 1700 (1973); 7, 2192 (1973); 9, 360 (1974); 9, 943 (1974); 12, 1653 (1975); Ann. Phys. (N.Y.) 69, 42 (1972), and references cited therein.

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