TEST PARTICLE MOTION
IN A
LORENTZ GAS

Thesis by

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In Partial Fulfillment of the Requirements
For the Degree of
Doctor of Philosophy

California Institute of Technology
Pasadena, California

1975

(Submitted July 26, 1974)

ACKNOWLEDGMENTS

I wish to express my gratitude to Professor Corngold for the many ways in which he made this research possible and shaped its development. I also wish to thank Jeff Smith and Charles Boley for their patience and many helpful suggestions, Mrs. Carol Timkovich for her friendliness and professional typing, and Mrs. Janice Scott for her excellent illustrations.

This research was made possible by financial aid from the AEC, NSF, and the Institute itself. I also wish to thank Professor Donald Burnett for his appreciated summer jobs which not only helped financially, but provided truly stimulating challenges as well.

Finally, I wish to thank my wife, Sara, for her constant support, as well as my parents for theirs.

ABSTRACT

This is a two-part thesis concerning the motion of a test particle in a bath. In part one we use an expansion of the operator $PLe^{it(1-P)L}LP$ to shape the Zwanzig equation into a generalized Fokker-Planck equation which involves a diffusion tensor depending on the test particle's momentum and the time.

In part two the resultant equation is studied in some detail for the case of test particle motion in a weakly coupled Lorentz Gas. The diffusion tensor for this system is considered. Some of its properties are calculated; it is computed explicitly for the case of a Gaussian potential of interaction.

The equation for the test particle distribution function can be put into the form of an inhomogeneous Schroedinger equation. The term corresponding to the potential energy in the Schroedinger equation is considered. Its structure is studied, and some of its simplest features are used to find the Green's function in the limiting situations of low density and long time.

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I. INTRODUCTION

The N-body problem is one of the oldest and most challenging problems in science. Consider N particles in a volume Ω. Let these particles interact with one another by means of a specified potential energy. Given an initial condition, find the resulting motion.

In this thesis we concern ourselves with some of the modern techniques that have been developed to deal with such a system. We consider a system governed by Newtonian mechanics. All forces are central. All speeds are non-relativistic. In particular, we are concerned with following the motion of a single particle in this N-body system.

Up until quite recently we have had to rely on the Boltzmann equation to furnish us with this kind of information. Now, important new work has been done which may enable us to probe deeper than the Boltzmann equation has allowed. This is, then, our general area of investigation.

A. General Background

We begin with Hamilton's formulation of Newtonian mechanics.(1) Denote the set of all coordinates in an N-particle system by $\underline{Q} = \{\underline{q}_1, \underline{q}_2, \ldots, \underline{q}_N\}$, the set of momenta by $\underline{P} = \{\underline{p}_1, \ldots, \underline{p}_N\}$ and $\underline{\Gamma} = \{\underline{q}_1, \ldots, \underline{q}_N, \underline{p}_1, \ldots, \underline{p}_N\}$. If the Hamiltonian is $H(\underline{P}, \underline{Q})$, the equations of motion can be expressed as

$$\frac{d\underline{Q}}{dt} = \frac{\partial H}{\partial \underline{P}} \quad \text{and} \quad \frac{d\underline{P}}{dt} = -\frac{\partial H}{\partial \underline{Q}} .$$

Any function of the $\underline{q}_i^{(t)}$'s and $\underline{p}_i^{(t)}$'s in this system is called a dynamical variable. Examples are the momentum $\underline{p}_i$, the kinetic energy $p_i^2/2m_i$, and the one-particle density $\sum_{i=1}^{N} \delta^3(\underline{r}-\underline{q}_i)\delta^3(\underline{p}-\underline{p}_i)$. If A and B are dynamical variables, the Poisson bracket of A and B is

$$[A, B] = \sum_{i=1}^{N} \left(\frac{\partial A}{\partial \underline{q}_i} \cdot \frac{\partial B}{\partial \underline{p}_i} - \frac{\partial B}{\partial \underline{q}_i} \cdot \frac{\partial A}{\partial \underline{p}_i} \right) .$$

Hamilton's equations can be expressed as

$$\frac{d\underline{Q}}{dt} = [\underline{Q}, H] \qquad \frac{d\underline{P}}{dt} = [\underline{P}, H] .$$

From the chain rule for differentiation one can see that

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + [A, H] .$$

The Poisson bracket formulation of classical mechanics is also useful in describing the evolution of distribution functions. An ensemble of N-particle systems is a set of identical N particle systems, prepared in a prescribed way. For an ensemble of systems define $\rho(\underline{q}_1, \ldots, \underline{q}_N, \underline{p}_1, \ldots, \underline{p}_N, t)d^3\underline{q}_1 \ldots d^3\underline{q}_N d^3\underline{p}_1 \ldots d^3\underline{p}_N$ to be the number of systems in the ensemble which at time t, have positions and momenta in a differential volume element of phase space about $\underline{\Gamma}$.

Liouville's Theorem[1] states that

$$\frac{d\rho(\underline{Q}, \underline{P})}{dt} = 0 \ .$$

That is,

$$\frac{\partial\rho(\underline{Q}, \underline{P})}{\partial t} = -[\rho, H] \ .$$

The N-particle distribution function, $\rho(\underline{Q}, \underline{P}, t)$, often contains more information than we need to understand a particular system. An especially useful function in this regard is the one particle distribution function $f(\underline{q}_1, \underline{p}_1, t)$ defined as $\int d^3\underline{q}_2 \ldots d^3\underline{q}_N d^3\underline{p}_2 \ldots d^3\underline{p}_N \rho(\underline{Q}, \underline{P}, t)$. Note that f may also be given in terms of a dynamical variable: $f(\underline{q}_1, \underline{p}_1, t) = \int d^3\underline{q}_1' \ldots d^3\underline{p}_N' \, \rho(\underline{Q}', \underline{P}', 0)\delta^3(\underline{q}_1(t) - \underline{q}_1')\delta^3(\underline{p}_1(t) - \underline{p}_1')$.

The Poisson bracket can be regarded as a linear operator in a vector space of dynamical variables A. We can define the Liouville (or Poisson bracket) operator L by

$$LA = -i[A, H] \ .$$

Then

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

The formulation of classical mechanics in a Hilbert space, with dynamical variables as vectors and the Liouville operator as a self adjoint linear transformation was accomplished by B. Koopman[2] and J. von Neumann[3]. For our purposes, let it suffice to say that this formulation is extensive and complete. There are several possible inner products that one can use. All operations which one normally performs in a Hilbert space are justified in this space, the proofs are contained in the works of these two authors. With the equation

$$\frac{\partial \rho(\underline{q}_1, \ldots, \underline{p}_N, t)}{\partial t} = -iL\rho(\underline{q}_1, \ldots, \underline{p}_N, t)$$

and the initial condition

$$\rho(\underline{q}_1, \ldots, \underline{p}_N, 0) = \rho(\underline{q}_1, \ldots, \underline{p}_N, t=0) \quad ,$$

we have

$$\rho(\underline{q}_1, \ldots, \underline{p}_N, t) = e^{-itL}\rho(\underline{q}_1, \ldots, \underline{p}_N, 0) \quad .$$

The mean value of a dynamical variable A at time t is

$$\langle A(t) \rangle = \int A(\Gamma, t)\rho(\Gamma, t=0)d^3\underline{q}_1 \ldots d^3\underline{p}_N$$

Since $A(t) = e^{itL} A(0)$, and L is self adjoint

$$\langle A(t) \rangle = \int A(\Gamma, t=0)\rho(\Gamma, t)d^3\underline{q}_1 \ldots d^3\underline{p}_N \quad .$$

This formula is useful in connection with autocorrelation functions. The autocorrelation of variable A is simply $\langle A(0)A(t) \rangle$. All autocorrelation functions can be computed by using the definition given above. Some special autocorrelation functions can also be computed by finding a distribution function subject to particular initial conditions.

In the work that follows we will assume that all distribution functions vanish as any argument becomes extremely large. We also confine ourselves to time-independent Hamiltonians so that the Liouville operator becomes

$$iL = \sum_i \frac{\underline{p}_i}{m_i} \cdot \frac{\partial}{\partial \underline{q}_i} + \sum_{i<j} \underline{F}_{ij} \cdot \left(\frac{\partial}{\partial \underline{p}_i} - \frac{\partial}{\partial \underline{p}_j}\right) .$$

B. The Zwanzig Equation

In the early 60's Robert Zwanzig[4] extended Koopman's work by utilizing still other Hilbert space ideas. A projection operator P is one which satisfies the property that

$$P^2 = P \, .$$

Zwanzig noticed that starting with the Liouville equation for a yet unspecified projection operator, a new equation may be obtained by projecting the old one

$$i\frac{\partial}{\partial t}\rho(\underline{\Gamma}, t) = L\rho(\underline{\Gamma}, t) \, .$$

Thus,

$$i\frac{\partial}{\partial t}P\rho(\underline{\Gamma}, t) = PL\rho(\underline{\Gamma}, t) \, .$$

Similarly,

$$i\frac{\partial}{\partial t}(1-P)\rho(\underline{\Gamma}, t) = (1-P)L\rho(\underline{\Gamma}, t) \, .$$

Now,

$$PL\rho(\underline{\Gamma}, t) = PLP\rho(\underline{\Gamma}, t) + PL(1-P)\rho(\underline{\Gamma}, t)$$

and

$$(1-P)L\rho(\underline{\Gamma}, t) = (1-P)LP\rho(\underline{\Gamma}, t) + (1-P)L(1-P)\rho(\underline{\Gamma}, t) \, .$$

Designating $P\rho(\underline{\Gamma}, t)$ as $\rho_{\parallel}(\underline{\Gamma}, t)$, and $(1-P)\rho(\underline{\Gamma}, t)$ as $\rho_{\perp}(\underline{\Gamma}, t)$. We can rewrite our two equations as

$$i\frac{\partial}{\partial t}\rho_{\parallel}(\underline{\Gamma}, t) = PL\rho_{\parallel}(\underline{\Gamma}, t) + PL\rho_{\perp}(\underline{\Gamma}, t)$$

$$i\frac{\partial}{\partial t}\rho_{\perp}(\underline{\Gamma}, t) = (1-P)L\rho_{\parallel}(\underline{\Gamma}, t) + (1-P)L\rho_{\perp}(\underline{\Gamma}, t) \, .$$

Introducing the Laplace Transform in t

$$\tilde{f}(s) = \int_0^\infty dt\, e^{-st} f(t)$$

$$i\left[s\tilde{\rho}_{\parallel}(\underline{\Gamma}, s) - \rho_{\parallel}(\underline{\Gamma}, t=0)\right] = PL\tilde{\rho}_{\parallel}(\underline{\Gamma}, s) + PL\tilde{\rho}_{\perp}(\underline{\Gamma}, s)$$

and

$$i\left[s\tilde{\rho}_{\perp}(\underline{\Gamma}, s) - \rho_{\perp}(\underline{\Gamma}, t=0)\right] = (1-P)L\tilde{\rho}_{\parallel}(\underline{\Gamma}, s) + (1-P)L\tilde{\rho}_{\perp}(\underline{\Gamma}, s) .$$

From the second equation we see that

$$[s+i(1-P)L]\tilde{\rho}_{\perp}(\underline{\Gamma}, s) = -i(1-P)L\tilde{\rho}_{\parallel}(\underline{\Gamma}, s) + (1-P)\rho(\underline{\Gamma}, t=0) .$$

This gives us $\tilde{\rho}_{\perp}(\underline{\Gamma}, s)$ in terms of $\tilde{\rho}_{\parallel}(\underline{\Gamma}, s)$ and the initial condition, $\rho(\underline{\Gamma}, t=0)$. Substituting this into the first equation

$$i\left[s\tilde{\rho}_{\parallel}(\underline{\Gamma}, s) - \rho_{\parallel}(\underline{\Gamma}, t=0)\right]$$

$$= PL\tilde{\rho}_{\parallel}(\underline{\Gamma}, s) + PL\frac{1}{s+i(1-P)L}\left[(1-P)\rho(\underline{\Gamma}, t=0) - i(1-P)\tilde{\rho}_{\parallel}(\underline{\Gamma}, s)\right]$$

$$= PL\left[1-\frac{i}{s+i(1-P)L}(1-P)L\right]\tilde{\rho}_{\parallel}(\underline{\Gamma}, s) + PL\frac{1}{s+i(1-P)L}(1-P)\rho(\underline{\Gamma}, t=0)$$

Simplifying and Laplace transforming back into t

$$\frac{\partial\rho_{\parallel}(\underline{\Gamma}, t)}{\partial t} = -iPLP\rho(\underline{\Gamma}, t) + \int_0^t d\tau\, iPL\, e^{-i\tau(1-P)L} i(1-P)LP\rho(\underline{\Gamma}, t-\tau)$$

$$-PiL\, e^{-it(1-P)L}(1-P)\rho(\underline{\Gamma}, t=0) .$$

Known as the Zwanzig equation, this equation has some surprising and interesting features. It is exact. That is, it is nothing more than the Liouville equation for a portion of ρ projected into a particular subspace. It tells us that the time behavior of the projected portion of the N-particle distribution function is governed by a system with memory. The term

$$\int_0^t d\tau\, K(\underline{\Gamma}, \tau)\rho(\underline{\Gamma}, t-\tau)$$

clearly demonstrates that the present behavior of the system is subject to the integrated evolution.

The equation is nearly closed

$$\frac{\partial}{\partial t}\rho_{\parallel}(\underline{\Gamma}, t) = 0_1\rho_{\parallel}(\underline{\Gamma}, t) + 0_2\rho_{\perp}(\underline{\Gamma}, t=0)$$

However, the innocent-looking term involving $\rho_{\perp}(\underline{\Gamma}, t=0)$ is difficult. Prigogine[(5)] called this term the "destruction fragment". Most investigators assume at one point or other that it is small, or rapidly becomes small compared to the other terms[(6)].

In both the destruction fragment term and the "0_1" term there appears the operator $e^{-it(1-P)L}$. The physical meaning of this important factor appears somewhat obscure. We do understand e^{-itL}. This operator is that which describes the time evolution of the N-particle system. But $e^{-it(1-P)L}$? We shall investigate this in the course of our work.

An example of an application of the Zwanzig equation uses the particular projection operator

$$P\rho(\underline{\Gamma}) \equiv \rho_0(\underline{q}_2, \ldots, \underline{q}_N, \underline{p}_2, \ldots, \underline{p}_N)\int d^3\underline{q}_2 \ldots d^3\underline{q}_N d^3\underline{p}_2 \ldots d^3\underline{p}_N \rho(\underline{\Gamma}) \,. \tag{c}$$

If we single out particle number one to be a test-particle, and consider particles 2 through N as a kind of "bath" we can rewrite the projection operator as

$$Pf = \rho_B(\underline{\Gamma}_B)\int d\,\underline{\Gamma}_B f \quad \text{and} \quad \langle f\rangle_B = \int d\underline{\Gamma}_B \rho_B f \,.$$

In the late 1960's Corngold[7] showed that the use of this particular projection operator shapes the Zwanzig equation into a Generalized Fokker-Planck equation. The Zwanzig equation becomes

$$\left(\frac{\partial}{\partial t} + \frac{1}{m_1}\underline{p}_1 \cdot \frac{\partial}{\partial \underline{q}_1}\right) f(q_1, p_1, t) = \int_0^t d\tau \left(\frac{\partial}{\partial p_1} \cdot \underline{\underline{\mathfrak{D}}} \cdot \frac{\partial}{\partial \underline{p}_1} \cdot + \frac{\partial}{\partial \underline{p}_1} \cdot \underline{E}\right) f(q_1, p_1, t-\tau)$$

$$+ \int d\Gamma_B \underline{F}_1 \cdot \frac{\partial}{\partial p_1} e^{-it(1-P)L}(1-P)\rho(\underline{\Gamma}, t=0)$$

where

$$\underline{\underline{\mathfrak{D}}} = \langle \underline{F}_1(\underline{\Gamma}) e^{-it(1-P)L} \underline{F}_1(\underline{\Gamma}) \rangle_B$$

$$\underline{E} = \langle \underline{F}_1(\underline{\Gamma}) e^{-it(1-P)L} \sum_{j=2} F_{1j}(\underline{\Gamma}) \cdot \frac{\beta \underline{p}_j}{m_j} \rangle_B$$

and

$$\beta = \frac{1}{k_B T} .$$

This is nearly in the form of the classic Fokker-Planck equation[8]. The appearance of the destruction fragment adds an additional term not found in the usual theory. There are other differences. Unlike the ordinary Fokker-Planck equation this is exact. Note that the $\underline{\underline{\mathfrak{D}}}$ and $\underline{E}$ coefficients which are merely numbers in the ordinary Fokker-Planck equation are now operators in q_1, p_1 and t. We return to this equation later in our study.

Another application of the Zwanzig equation is an expression for autocorrelation functions. Consider the autocorrelation function $\langle A(0)A(t)\rangle = \psi(t)$ with $\psi(0) = 1$. Using his own projection operator techniques, Zwanzig[4][9] was able to show that

$$\frac{d\psi(t)}{dt} = -\int_0^t d\tau\, K(\tau)\psi(t-\tau) \qquad [\text{I-A}]$$

where

$$K(\tau) = \frac{\langle \frac{dA}{dt}(t=0) e^{i\tau(1-P)L} \frac{dA}{dt}(t=0) \rangle}{\langle A(0)A(0) \rangle} .$$

We will make use of this formula in the course of our investigation.

Just as projection operator techniques can lead to Generalized Fokker-Planck equations, they lead to Generalized Langevin equations as well. The most important of these is associated with the work of H. Mori(10).

Mori studied equations formed by the projection operator

$$P\underline{B} = \frac{\langle \underline{A} \cdot \underline{B} \rangle}{\langle \underline{A} \cdot \underline{A} \rangle} \underline{A} \qquad \underline{A} = \underline{A}(t=0) .$$

This is a particularly interesting projection operator for, $P\underline{A}(t)$ is the autocorrelation function of $\underline{A}$.

Using this projection operator Mori was able to derive an exact equation of motion for $\underline{A}(t)$. We consider the case $\underline{A}(t)$ being real

$$\frac{d\underline{A}(t)}{dt} = i\Omega\underline{A}(t) - \int_0^t d\tau\, K(\tau)\underline{A}(t-\tau) + \underline{F}(t) .$$

$$\Omega = \frac{\langle \underline{A} L \cdot \underline{A} \rangle}{\langle \underline{A} \cdot \underline{A} \rangle} = 0 \quad \text{for } \underline{A} \text{ real.}$$

$$K(\tau) = \frac{\langle \underline{F}(o) \cdot e^{i\tau(1-P)L} \underline{F}(t) \rangle}{\langle \underline{A} \cdot \underline{A} \rangle}$$

$\underline{F}(t)$ is called the fluctuating force and is defined by

$$\underline{F}(t) = e^{it(1-P)L}(1-P)iL\underline{A} .$$

Mori showed that the Generalized Langevin equation simplified under certain conditions. By projecting P onto the equation of motion for $\underline{A}(t)$, we obtain an equation for the autocorrelation function of $\underline{A}$. The autocorrelation function equation obtained in this manner is the same as the Zwanzig equation for autocorrelation functions. Just as in Zwanzig's autocorrelation function equation, the destruction fragment term vanishes.

Our investigation is concerned with still another projection operator. The projection operator we study here is of interest in that it leads to a Generalized Fokker-Planck Equation in which the destruction fragment vanishes independent of assumptions about whether the solution to the equation is or is not an autocorrelation function. We make contact with two important kinetic equations derived recently and described below. The solution is then studied in detail for the case of a Lorentz Gas.

C. Important Special Cases

Recent work by Forster and Martin[11], Mazenko[12] ~~and~~ Boley and Desai[13] has been concerned with generalized kinetic equations for autocorrelation functions. These are limiting cases of the general forms presented above. In the thermodynamic limit[14], the distribution function itself as well as the other terms we study all depend parametrically on the density of the system and the strength of the interaction between particles. Forster and Martin systematically expanded all pertinent quantities in the interaction strengths and arrived at a tractable result by considering only terms of second and lower orders. Mazenko and Boley did the same for density. In classical systems it turns out that the weakly coupled system is a special case of the low density system.

All of the equations discussed so far are quite general. For example, there are no constraints as to the mass that each particle must have. The problem we will be considering in Parts II-IV is the test particle problem. One particle is distinguished in some way from all of the other particles and is referred to as the test particle. All of the other particles are taken to be the same as each other. These are the "bath" particles. When the mass of the test particle is much larger than the mass of a bath particle we have a Brownian system. When the mass of the test particle is much smaller than the mass of a bath particle we have a Lorentz Gas.[15]

A particularly interesting description of Brownian motion has been developed by Lebowitz[16][17] and his co-workers. They have demonstrated that the distribution function for the test particle obeys the Fokker-Planck like-equation

$$\frac{\partial f(\underline{u}, t)}{\partial t} = \int_0^t d\tau \, \frac{\partial}{\partial \underline{u}} G(t-\tau) \cdot \left(\frac{\partial}{\partial \underline{u}} + \underline{u}\right) f(\underline{u}, \tau) \, .$$

Mazo[18] has investigated some of the properties of the solution to this equation.

It is most important to note that the kernel G(t) depends only on time, not on momentum or space. We hope to show in the course of our investigation that this is a severely restrictive model, physically unreasonable except in the case of a Brownian particle. In Mazo's work G(t) is "modelled" in order to arrive at analytical results.

The Lorentz Gas limit has received much less attention. However, J. Van Leeuwen and A. Weijland, have published some interesting work on this problem. Their paper, Non Analytic Behavior of the Diffusion Coefficient of a Lorentz Gas[19] is concerned with the Lorentz Gas with $m_{light}/m_{heavy} = 0$, and the interaction between particles being that of hard spheres. Their final goal is to derive from first principles a density expansion for the mutual diffusion coefficient. Since the terms in this expansion begin to diverge logarithmically after the n^2 term, they are addressing themselves to a difficult problem.

Our work is concerned with a different aspect of Lorentz Gas motion. As far as our investigation of the literature has taken us, we are unable to findmuch further new work on Lorentz Gas motion.

II. A NEW FORM OF THE ZWANZIG EQUATION

A. Introduction

In this section we shall work with a particularly simple form of the Zwanzig equation. We achieve this form by choosing a projection operator which causes the destruction fragment to vanish. The resulting equation is of the form

$$\frac{\partial f(\underline{p}_1, t)}{\partial t} = \int_0^t d\tau \int d^3\underline{p}'\, 0_1(\underline{p}_1, \underline{p}', \tau) f(\underline{p}', t-\tau)$$

0_1 is then studied in detail. Its low density limit is shown to be entirely equivalent to the self-correlation part of the Mazenko kernel for solutions uniform in the spatial variable, while its weak coupling limit is equivalent to the self-correlation part of the Forster-Martin kernel uniform in space.

B. A Judicious Choice of P

Consider a spatially uniform system such as a liquid or gas. Let

$$M(p_j) = \left(\frac{\beta}{2\pi m_j}\right)^{\frac{3}{2}} e^{-\beta p_j^2/2m_j}$$

where j refers to particle j and $\beta = 1/k_B T$. This is the famous Maxwell-Boltzmann distribution. Let $U(\underline{Q})$ be the potential energy of interaction for the system, taken to be pairwise additive. We will denote by $d^N\underline{Q} = d^3\underline{q}_1 \ldots d^3\underline{q}_N$ and $d^{N-1}\underline{P} = d^3\underline{p}_2 \ldots d^3\underline{p}_N$. $\rho_0(\underline{Q})$ is defined to be $e^{-\beta U(\underline{Q})} / \int d^N\underline{Q}\, e^{-\beta U(\underline{Q})}$. $\rho_0(\underline{\Gamma})$ will be defined as

$\prod_{j=1}^{N} M(p_j)\, e^{-\beta U(\underline{Q})} \Big/ \int d^N\underline{Q}\, e^{-\beta U(\underline{Q})}$. This is the canonical distribution function.

Choose P to be

$$P = \prod_{j=2}^{N} M(p_j)\rho_0(\underline{Q}) \int d^N\underline{Q} d^{N-1}\underline{P} \, .$$

Then

$$P\rho(\underline{\Gamma}) = \prod_{j=2}^{N} M(p_j)\rho_0(\underline{Q}) f(\underline{p}_1) = \rho_0(\underline{\Gamma}) \frac{f(\underline{p}_1)}{M(p_1)} \, .$$

The Zwanzig equation is

$$\frac{\partial[P\rho(\underline{\Gamma}, t)]}{\partial t} = -iPLP\rho(\underline{\Gamma}, t) + \int_0^t d\tau\, PiL\, e^{-i\tau(1-P)L} iLP\rho(\underline{\Gamma}, t-\tau)$$

$$-iPL e^{-it(1-P)L}(1-P)\rho(\underline{\Gamma}, t=0) \, .$$

Consider

$$PiLP = P\left(\sum_{j=1}^{N} \frac{\underline{p}_j}{m_j} \cdot \frac{\partial}{\partial \underline{q}_j} + \underline{F}_j \cdot \frac{\partial}{\partial \underline{p}_j}\right) P$$

Then since

$$\int d^{N-1}\underline{P}\, d^N\underline{Q} \frac{\partial}{\partial \underline{q}_j} \psi = 0$$

PiLP becomes

$$\prod_{j=2}^{N} M(p_j)\rho_0(\underline{Q}) \int d^N\underline{Q} d^{N-1}\underline{P} \sum_k \underline{F}_k \cdot \frac{\partial}{\partial \underline{p}_k} \prod_{\ell=2}^{N} M(p_\ell)\rho_0(\underline{Q}) \int d^N\underline{Q} d^{N-1}\underline{P}$$

Which leaves upon integrating over $d^{N-1}\underline{P}$

$$PiLP = \prod_{j=2}^{N} M(p_j)\rho_0(\underline{Q}) \int d^N\underline{Q}\, \underline{F}_1 \rho_0(\underline{Q}) \cdot \frac{\partial}{\partial \underline{p}_1} \int d^N\underline{Q} d^{N-1}\underline{P} \, .$$

$$\underline{F}_1\rho_0(\underline{Q}) = -\frac{\partial U(\underline{Q})}{\partial \underline{q}_1}\frac{e^{-\beta U(\underline{Q})}}{\int d^N\underline{Q}e^{-\beta U(\underline{Q})}} = \frac{1}{\beta}\frac{\partial}{\partial \underline{q}_1}\rho_0(Q) .$$

Hence, since

$$\frac{1}{\beta}\int d^N\underline{Q}\,\frac{\partial}{\partial \underline{q}_1}\rho_0(\underline{Q}) = 0 ,$$

PiLP vanishes.

With PiLP = 0 our original equation becomes

$$\frac{\partial[P\rho(\Gamma, t)]}{\partial t} = \int_0^t d\tau PiLe^{-i\tau(1-P)L}iLP\,\rho(\underline{\Gamma}, t-\tau)$$

$$-PiL\,e^{-it(1-P)L}(1-P)\rho(\underline{\Gamma}, t=0).$$

Furthermore, for the destruction fragment

$$(1-P)\rho(\underline{\Gamma}, t=0) = \rho(\underline{\Gamma}, t=0) - \prod_{j=2}^{N} M(p_j)\rho_0(\underline{Q})\int d^N\underline{Q}d^{N-1}\underline{P}\rho(\underline{\Gamma}, t=0)$$

$$= \rho(\underline{\Gamma}, t=0) - \prod_{j=2}^{N} M(p_j)\rho_0(\underline{Q})\int d^{N-1}\underline{P}\,f[\underline{p}_1, t=0]\prod_{j=2}^{N} M(p_j)$$

$$= \rho(\underline{\Gamma}, t=0) - f(\underline{p}_1, t=0)\prod_{j=2}^{N} M(p_j)\rho_0(\underline{Q}) .$$

For a test particle problem, we take the initial ensemble to be $f(\underline{p}_1)\prod_{j=2}^{N} M(p_j)\rho_0(\underline{Q})$ which causes the destruction fragment to vanish.

The Zwanzig equation becomes

$$\frac{\partial[P\rho(\Gamma, t)]}{\partial t} = \int_0^t d\tau\, PiL\,e^{-i\tau(1-P)L}iLP\rho(\underline{\Gamma}, t-\tau) .$$

The left hand side is proportional to $f(\underline{p}_1, t)$. We now consider properties of the kernel $PL\,e^{-i\tau(1-P)L}LP$ in some detail.

C. A Study of the Operator $PLe^{it(1-P)L}LP$

We begin by Laplace transforming the operator into s space. That is, we study

$$PL\frac{1}{s-i(1-P)L}LP$$

Recalling the operator identity

$$\frac{1}{A+B} = \frac{1}{A} - \frac{1}{A}B\frac{1}{A+B}$$

$$PL\frac{1}{s-i(1-P)L}LP$$

$$= PL\frac{1}{s-iL+iPL}LP$$

$$= PL\left[\frac{1}{s-iL} - \frac{1}{s-iL}iPL\frac{1}{s-iL+iPL}\right]LP\,.$$

Continuing in this manner

$$= PL\left[\frac{1}{s-iL} - \frac{1}{s-iL}iPL\frac{1}{s-iL} + \frac{1}{s-iL}iPL\frac{1}{s-iL}iPL\frac{1}{s-iL} - +\dots\right]LP$$

$$= PL\frac{1}{s-iL}LP - PL\frac{1}{s-iL}iPL\frac{1}{s-iL}LP + PL\frac{1}{s-iL}iPL\frac{1}{s-iL}iPL\frac{1}{s-iL}LP - \dots \tag{II-A}$$

Note that

$$PLe^{itL}LP = \frac{1}{i}\frac{d}{dt}PLe^{itL}P$$

which implies (since $PLP = 0$) that

$$PL\frac{1}{s-iL}LP = \frac{1}{i}s\,PL\frac{1}{s-iL}P = -s\,iPL\frac{1}{s-iL}P$$

Putting this back into equation [II-A] we get

$$PL\frac{1}{s-i(1-P)L}LP = PL\frac{1}{s-iL}LP + \frac{1}{s}PL\frac{1}{s-iL}LP\,PL\frac{1}{s-iL}LP$$

$$+\frac{1}{s}PL\frac{1}{s-iL}LP\frac{1}{s}PL\frac{1}{s-iL}LP\,PL\frac{1}{s-iL}LP + \dots$$

Now consider $PL\frac{1}{s-iL}LP$ in t space; $PLe^{itL}LP$.

$$PLe^{itL}LP = PL\left[1+itL-\frac{t^2L^2}{2!}+i^3\frac{t^3L^3}{3!}+\frac{t^4L^4}{4!}-\ldots\right]LP$$

$$= PL^2P+it\,PL^3P-\frac{t^2}{2!}PL^4P+\ldots \quad .$$

But for a homogeneous isotropic medium

$$PL^{2n+1}P = 0$$

as follows:

Recall that

$$iL = \sum_j\left(\frac{\underline{p}_j}{m_j}\cdot\frac{\partial}{\partial\underline{q}_j}+\underline{F}_j\cdot\frac{\partial}{\partial\underline{p}_j}\right) .$$

We showed earlier in this chapter that

$$P\psi(\underline{\Gamma}) = \rho_0(\underline{\Gamma})\frac{\psi(\underline{p}_1)}{M(p_1)}$$

where

$$\psi(\underline{p}_1) = \int d^N\underline{Q}\int d^{N-1}\underline{P}\;\psi(\underline{\Gamma}) .$$

$$P(iL)^M P\psi(\underline{\Gamma}) = \frac{\rho_0(\underline{\Gamma})}{M(p_1)}\int d^N\underline{Q}\int d^{N-1}\underline{P}\prod_{i=1}^{M}\left\{\sum_{k_i=1}^{N}\left(\frac{\underline{p}_{k_i}}{m_{k_i}}\cdot\frac{\partial}{\partial\underline{q}_{k_i}}-\frac{\partial U}{\partial\underline{q}_{k_i}}\cdot\frac{\partial}{\partial\underline{p}_{k_i}}\right)\right\}$$

$$\times\;\rho_0(\underline{\Gamma})\frac{\psi(\underline{p}_1)}{M(p_1)} .$$

When the product is expanded, each term contains M gradient operators in $\underline{q}$ operating on $U(\underline{Q})$ and $\rho_0(\underline{Q})$ (which is also a function of U). Since U is invariant under-coordinate reflection, it is clear that those terms with the odd number of gradients vanish upon integration.

Thus

$$PLe^{itL}LP = PL^2P - \frac{t^2}{2!} PL^4P + \frac{t^4}{4!} PL^6P + \dots$$

and expansion of such terms as

$$\frac{1}{s} PL \frac{1}{s-iL} LP \frac{1}{s} PL \frac{1}{s-iL} LP\, PL \frac{1}{s-iL} LP$$

produces products of operators of the form $PL^{2m}P$. Thus $PLe^{it(1-P)L}LP$ is composed of building blocks of the form $PL^{2k}P$. Our investigation focuses on these operators. One of the easy fundamental properties of $PL^{2k}P$ concerns the L immediately following the leftmost P.

$PL^{2k}P$ is related to

$$\int d^NQ \int d^{N-1}\underline{P}\, L\, L^{2k-1} \prod_{j=2}^{N} M(p_j)\rho_0(\underline{Q}) .$$

Again we make use of the fact that

$$iL = \sum_{j=1}^{N} \left(\frac{\underline{p}_j}{m_j} \cdot \frac{\partial}{\partial \underline{q}_j} + \underline{F}_j \cdot \frac{\partial}{\partial \underline{p}_j} \right).$$

Due to the boundary conditions, the $\partial / \partial \underline{q}_j$ part is integrated out by the P operator to yield zero. Similarly for j other than 1, the momentum-dependent part of $\sum_j \underline{F}_j \cdot \partial / \partial \underline{p}_j$ will yield a zero contribution. This leads us to the conclusion that the L immediately following the leftmost P must be $-i\underline{F}_1 \cdot \partial / \partial \underline{p}_1$ and

$$PL^{2k}P = -iP\underline{F}_1 \cdot \frac{\partial}{\partial \underline{p}_1} L^{2k-1} P .$$

Consider now the rightmost L in $PL^{2k}P\psi(\underline{\Gamma})$. We are then interested in the behavior of

$$iLP\psi(\underline{\Gamma}) = iL\rho_0(\underline{\Gamma})\frac{\psi(\underline{p}_1)}{M(p_1)}$$

Since $iL\rho_0(\underline{\Gamma}) = 0$,

$$\begin{aligned} iLP\psi(\underline{\Gamma}) &= \rho_0(\underline{\Gamma})iL\frac{\psi(\underline{p}_1)}{M(p_1)} \\ &= \rho_0(\underline{\Gamma})\underline{F}_1 \cdot \frac{\partial}{\partial \underline{p}_1}\frac{\psi(\underline{p}_1)}{M(p_1)} \\ &= \frac{\rho_0(\underline{\Gamma})}{M(p_1)}\left[\underline{F}_1 \cdot \frac{\partial}{\partial \underline{p}_1} + \underline{F}_1 \cdot \frac{\beta \underline{p}_1}{m_1}\right]\psi(\underline{p}_1) \\ &= \left[\underline{F}_1 \cdot \frac{\partial}{\partial \underline{p}_1} + \underline{F}_1 \cdot \frac{\beta \underline{p}_1}{m_1}\right]P\psi(\underline{\Gamma}) . \end{aligned}$$

We have shown, then, that

$$PL^{2k}P = -P\left[\left(\underline{F}_1 \cdot \frac{\partial}{\partial \underline{p}_1}\right)L^{2k-2}\left(\underline{F}_1 \cdot \left(\frac{\partial}{\partial \underline{p}_1} + \frac{\beta \underline{p}_1}{m_1}\right)\right)\right] P .$$

We introduce the notation $f(x) = O(k)$ where k is a parameter. $f(x)$ is $O(k)$ for x in a specified interval, if there exists some constant M such that $|f(x)| \leq Mk$ for all x in the interval.[d] If we denote the interaction strength between all particles by λ, then $PL^{2k}P$ is $O(\lambda^2)$. Since $PLe^{itL}LP = \sum_{n=0}^{\infty} P[itL]^{2n} L^2P$, $PLe^{itL}LP$ is $O(\lambda^2)$, and $PLe^{it(1-P)L}LP = PLe^{itL}LP + O(\lambda^4)$.

If we would take the thermodynamic limit, where $N \to \infty$ and $\Omega \to \infty$ in such a way that $\frac{N}{\Omega} = n$, $PLe^{itL}LP$ would also have a density dependence. To extract the appropriate dependence we will make use of the Binary Collision Expansion.[14][20]

Define

$$G(s) = \frac{1}{s - iL}$$

and

$$G_\alpha(s) = \frac{1}{s - iL_0 - iF_\alpha \cdot \left(\frac{\partial}{\partial \underline{p}_{\alpha_1}} - \frac{\partial}{\partial \underline{p}_{\alpha_2}}\right)}$$

where

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

and α is a specified pair of particles. For our convenience we will choose α to be particle one, the test particle, and particle two, some specified bath particle; $\alpha_1 = 1$, $\alpha_2 = 2$. The binary collision expansion is concerned with expanding the full N-particle time evolution operator $\frac{1}{s-iL}$ in terms of the G_α's, and binary collision operators T_α.

T_α operating on a function of $\underline{\Gamma}$ describes that motion in which all particles stream freely except for the pair α which collide. The T_α's were first used in connection with fluid motion by Zwanzig.[14] In his paper Method of Finding the Density Expansion of Transport Coefficients in Gases, he discusses many of the important properties of these operators. A form of the binary collision expansion is

$$G(s) = G_\alpha(s) + \sum_{\substack{\beta \\ \beta \neq \alpha}} G_\alpha T_\beta G_\alpha + \sum_{\substack{\beta, \gamma \\ \alpha \neq \beta \neq \gamma}} G_\alpha T_\beta G_\alpha T_\gamma G_\alpha + \ldots\ldots$$

As one can see, the higher order terms involve progressively more collision operators.

With this insight into the behavior of G(s), $PL\frac{1}{s-iL}LP$ becomes

$$PL\frac{1}{s-iL}LP = \frac{\rho_0(\underline{\Gamma})}{M(p_1)}\int d^N\underline{Q}d^{N-1}\underline{P}\frac{\partial}{\partial\underline{p}_1}\cdot\underline{F}_1\frac{1}{s-iL}\underline{F}_1\cdot\left(\frac{\beta\underline{p}_1}{m_1}+\frac{\partial}{\partial\underline{p}_1}\right)$$

$$\times\frac{\rho_0(\underline{\Gamma})}{M(p_1)}\int d^N Q d^{N-1}\underline{P}\,. \qquad [II\text{-}B]$$

Consider

$$\int d^N Q\,\underline{F}_1\frac{1}{s-iL}\underline{F}_1\,\rho_0(\underline{Q}) = \int d^N Q\,\underline{F}_1 G_\alpha(s)\underline{F}_1\,\rho_0(\underline{Q})$$

$$+\int d^N\underline{Q}\sum_\beta \underline{F}_1 G_\alpha T_\beta G_\alpha \underline{F}_1\,\rho_0(\underline{Q})$$

$$+\,.\,.\,.\,.\,.$$

Working with this kind of expression Kawasaki and Oppenheim[20] were able to show that

$$\int d^N\underline{Q}\,\underline{F}_1 G_\alpha(s)\underline{F}_1\,\rho_0(\underline{Q}) \quad \text{is} \quad O(n)$$

$$\int d^N\underline{Q}\sum_\beta \underline{F}_1 G_\alpha(s)T_\beta(s)G_\alpha(s)\underline{F}_1\,\rho_0(\underline{Q}) \quad \text{is} \quad O(n^2)$$

and all other terms are of higher order in density. Since it is readily verified that all other quantities appearing in [II-B] for $PL\frac{1}{s-iL}LP$ have leading order 1 in density,

$$PL\frac{1}{s-iL}LP \quad \text{is} \quad O(n)$$

and hence $PL\frac{1}{s-iL}LP$ is $O(n\lambda^2)$. As a result, if we wish to examine either the low density $(n\to 0)$ or weakly coupled $(\lambda\to 0)$ form of $PLe^{it(1-P)L}LP$, we deal with

$$\frac{\rho_0(\underline{\Gamma})}{M(p_1)}\int d^N\underline{Q}d^{N-1}\underline{P}\;\; \underline{F}_1\cdot\frac{\partial}{\partial\underline{p}_1}\frac{1}{s-iL_0-i\underline{F}_\alpha\cdot\left(\frac{\partial}{\partial p_{\alpha_1}}-\frac{\partial}{\partial \underline{p}_{\alpha_2}}\right)}$$

$$\times\ \underline{F}_1\cdot\left(\frac{\beta\underline{p}_1}{m_1}+\frac{\partial}{\partial\underline{p}_1}\right)\frac{\rho_0(\underline{\Gamma})}{M(p_1)}\int d^N\underline{Q}d^{N-1}\underline{P}$$

This is, then, $PLe^{it(1-P)L}LP$ to $O(n\lambda^2)$. Using the approximation we can study the low density or weak coupling form of Generalized Kinetic Equations.

Inserting this expression into the Zwanzig equation then yields

$$\frac{\partial f(\underline{p}_1,t)}{\partial t} = \int_0^t d\tau\int d^N\underline{Q}d^{N-1}\underline{P}\,\underline{F}_1\cdot\frac{\partial}{\partial\underline{p}_1}\,e^{i\tau\left[L_0+F_{12}\cdot\left(\frac{\partial}{\partial\underline{p}_1}-\frac{\partial}{\partial\underline{p}_2}\right)\right]}\underline{F}_1\cdot\left(\frac{\beta\underline{p}_1}{m_1}+\frac{\partial}{\partial\underline{p}_1}\right)$$

$$\times\ \frac{\rho_0(\underline{\Gamma})}{M(p_1)}f(\underline{p}_1,t-\tau)$$

With this form of the Zwanzig equation we are now in a position to make contact with the equations of Forster and Martin,(11) Boley,(13) and Mazenko.(12) In the Forster-Martin equation, the integral kernel is proportional to precisely $n\lambda^2$. Since we have already seen that each $\underline{F}_1$, contributes a power of λ to our kernel we must consider further the terms $\rho_0(\underline{Q})$ and $e^{it\left[L_0+\underline{F}_{12}\cdot\left(\frac{\partial}{\partial\underline{p}_1}-\frac{\partial}{\partial\underline{p}_2}\right)\right]}$ to maintain this proportionality. To lowest order in λ

$$e^{it\left[L_0+\underline{F}_{12}\cdot\left(\frac{\partial}{\partial\underline{p}_1}-\frac{\partial}{\partial\underline{p}_2}\right)\right]} = e^{itL_0}$$

Similarly, since

$$e^{-\beta U(\underline{Q})} = 1 - \lambda\beta \sum_{i \neq j} v(|\underline{q}_i - \underline{q}_j|) + O(\lambda^2) \quad ,$$

to maintain the kernel to $O(\lambda^2)$ we use

$$\frac{e^{-\beta U(\underline{Q})}}{\int d^N \underline{Q} e^{-\beta U(\underline{Q})}} = \frac{1}{\Omega^N} \quad .$$

We obtain

$$\frac{\partial f(\underline{p}_1, t)}{\partial t} = \int_0^t d\tau \int \frac{d^N \underline{Q}}{\Omega^N} \, d^{N-1}\underline{P} \;\; \underline{F}_1 \cdot \frac{\partial}{\partial \underline{p}_1} e^{i\tau L_0}$$

$$\underline{F}_1 \cdot \left(\frac{\partial}{\partial \underline{p}_1} + \frac{\beta \underline{p}_1}{m_1} \right) \prod_{j=2}^{N} M(p_j) f(\underline{p}_1, t-\tau) + O(\lambda^3) \quad .$$

Since we are considering two-body forces, $\underline{F}_1 = \sum_k \underline{F}_{1k}$ and

$$\frac{\partial f(\underline{p}_1, t)}{\partial t} = N \int_0^t d\tau \int \frac{d^N \underline{Q}}{\Omega^N} \, d^{N-1}\underline{P} \;\; \underline{F}_{12} \cdot \frac{\partial}{\partial \underline{p}_1} e^{i\tau L_0}$$

$$\underline{F}_{12} \cdot \left(\frac{\partial}{\partial \underline{p}_1} + \frac{\beta \underline{p}_1}{m_1} \right) \prod_{j=2}^{N} M(\underline{p}_j) f(\underline{p}_1, t-\tau)$$

$$+ N^2 \int_0^t d\tau \int \frac{d^N \underline{Q}}{\Omega^N} \, d^{N-1}\underline{P} \;\; \underline{F}_{12} \cdot \frac{\partial}{\partial \underline{p}_1} e^{i\tau L_0}$$

$$\underline{F}_{13} \cdot \left(\frac{\partial}{\partial \underline{p}_1} + \frac{\beta \underline{p}_1}{m_1} \right) \prod_{j=2}^{N} M(p_j) f(\underline{p}_i, t-\tau)$$

The term of $O(N^2)$ can be seen to vanish because of the odd symmetry under reflection of $\underline{F}_{12} \, \underline{F}_{13}$. Since $\frac{\partial}{\partial \underline{q}_3} \cdots \frac{\partial}{\partial \underline{q}_N}$ acting on any function of $\underline{q}_1$ and $\underline{q}_2$ only yields zero, the integral kernel becomes

$$n\int \frac{d^3\underline{q}_1 d^3\underline{q}_2}{\Omega}\, d^3\underline{p}_2\, M(p_2)\, \underline{F}_{12}\cdot\frac{\partial}{\partial\underline{p}_1}\, \frac{1}{s+i\,\dfrac{\underline{p}_1}{m_1}\cdot\dfrac{\partial}{\partial\underline{q}_1}+\dfrac{\underline{p}_2}{m_2}\cdot\dfrac{\partial}{\partial\underline{q}_2}}$$

$$\times\, \underline{F}_{12}\cdot\left(\frac{\partial}{\partial\underline{p}_1}+\frac{\beta\underline{p}_1}{m_1}\right) .$$

We compare this with the Forster-Martin[11] kernel for self-correlations (for spatially uniform solutions) their $k_1(\underline{p}_1, \underline{p})$ satisfies

$$k_1(\underline{p}_1, \underline{p}) = n\int d^3\underline{p}' d^3\underline{p}_2\, \frac{d^3\underline{q}_1 d^3\underline{q}_2}{\Omega}\, M(p_1)M(p_2)$$

$$\times\left[\frac{\partial v(|\underline{q}_1-\underline{q}_2|)}{\partial\underline{q}_1}\cdot\frac{\partial}{\partial\underline{p}_1}\,\delta^3(\underline{p}'-\underline{p}_1)\right]\frac{1}{s+iL_0(\underline{p}_1, \underline{q}_1, \underline{p}_2, \underline{q}_2)}$$

$$\times\left[\frac{\partial v(|\underline{q}_1-\underline{q}_2|)}{\partial\underline{q}_1}\cdot\frac{\partial}{\partial\underline{p}_1}\,\delta^3(\underline{p}-\underline{p}_1)\right]\frac{1}{M(p')} .$$

Integrating by parts and carrying out the $\underline{p}'$ differentiation

$$k_1(\underline{p}_1, \underline{p}) = n\int d^3\underline{p}'\int \frac{d^3\underline{q}_1 d^3\underline{q}_2}{\Omega}\, d^3\underline{p}_2\, M(p_1)M(p_2)\,\frac{\partial v(|\underline{q}_1-\underline{q}_2|)}{\partial\underline{q}_1}$$

$$\times\, \delta^3(\underline{p}'-\underline{p}_1)\,\frac{1}{s+iL_0(\underline{p}_1, \underline{p}_2, \underline{q}_1, \underline{q}_2)}\cdot\frac{\partial v(|\underline{q}_1-\underline{q}_2|)}{\partial\underline{q}_1}\cdot\frac{\partial}{\partial\underline{p}}\,\delta^3(\underline{p}_1-\underline{p})$$

$$\times\,\frac{1}{M(p')}\cdot\left[\frac{\partial}{\partial\underline{p}'}+\frac{\beta\underline{p}'}{m}\right] .$$

Carrying out the $\underline{p}'$ integration yields the same form, with $\underline{p}_1$ in place of p' everywhere. The $\underline{p}_1$ Maxwell distributions in numerator and denominator cancel, integrating $\frac{1}{s+iL_0}$ by parts then yields

$$n \frac{\partial}{\partial \underline{p}} \int d^3 \underline{p}_2 \frac{d^3 \underline{q}_2 d^3 \underline{q}_1}{\Omega} \frac{\partial v(|\underline{q}_1 - \underline{q}_2|)}{\partial \underline{q}_1} M(p_2) \frac{1}{s + i\left[\frac{p_1}{m_1} \cdot \frac{\partial}{\partial \underline{q}_1} + \frac{p_2}{m_2} \cdot \frac{\partial}{\partial \underline{q}_2}\right]}$$

$$\times \frac{\partial v(|\underline{q}_1 - \underline{q}_2|)}{\partial \underline{q}_1} \cdot \left(\frac{\partial}{\partial \underline{p}} + \frac{\underline{p}}{mkT}\right) .$$

This is easily seen to be the same as the expression we derived directly from the Zwanzig equation.

Using similar techniques we can reduce the Zwanzig equation to the Mazenko equation. In this case we are able to keep powers of λ higher than the second, as long as we keep the kernel proportional to n. Since in the thermodynamic limit $\rho_0(\underline{\Gamma}) = \frac{1}{\Omega} + O(n)$, the only difference in re-deriving the Boley form of the Mazenko kernel [12] comes from using the full $\frac{1}{s - iL_0 - i\underline{F}_{12} \cdot \left(\frac{\partial}{\partial \underline{p}_1} - \frac{\partial}{\partial \underline{p}_2}\right)}$ operator, instead of its weakly coupled form.

Further investigation will involve use of our form of the Forster-Martin equation. From this point on we will use dimensionless variables unless stated otherwise. Our form of the Forster-Martin self-correlation equation in dimensionless variables is

$$\frac{\partial f(u, t)}{\partial t} = \int_0^t \frac{\partial}{\partial \underline{u}} \cdot \epsilon \underline{\underline{\mathfrak{D}}}(u, t-\tau) \cdot \left(\frac{\partial}{\partial \underline{u}} + \underline{u}\right) f(\tau, u) d\tau$$

where $\widetilde{\underline{\underline{\mathfrak{D}}}}(u, t-\tau) = \langle \underline{F}_1 \frac{1}{s - iL_0} \underline{F}_1 \rangle$

$$s' = \frac{as}{v_0} , \quad \epsilon = na^3 \left(\frac{\lambda}{kT}\right)^2 , \quad |\underline{u}| = \left|\frac{\underline{v}}{\underline{v}_0}\right|$$

$v_0 = \sqrt{\frac{k_B T}{m}}$ and a is the range of force. The force is taken to be purely repulsive.

In this context of weak-coupling the symbol

$$\langle X(\underline{\Gamma}) \rangle = \frac{1}{\Omega^N} \int d^N\underline{Q}\, d^N\underline{P} \;\; X(\underline{\Gamma}) \prod_{j=1}^{N} M(p_j) .$$

This new use of the average symbol will be carried throughout the remainder of our investigation.

III. ANALYSIS OF THE WEAKLY COUPLED EQUATION

A. $\mathcal{D}_{\parallel}$ and $\mathcal{D}_{\perp}$

As we saw in the last section

$$\frac{\partial f(\underline{u}, t)}{\partial t} = \int_0^t d\tau \frac{\partial}{\partial \underline{u}} \cdot \epsilon \underset{\sim}{\mathcal{D}}(\underline{u}, t-\tau) \cdot \left(\frac{\partial}{\partial \underline{u}} + \underline{u}\right) f(\underline{u}, \tau)$$

where

$\underset{\sim}{\mathcal{D}}(\underline{u}, \tau)$

$$= \frac{1}{a^3} \int d^3 \underline{q}_{12} \int d^3 \underline{u}_2 M(u_2) \underline{F}_{12}\left(\left|\frac{\underline{q}_{12}}{a}\right|\right) \exp\left[ita\left(\underline{u} \cdot \frac{\partial}{\partial \underline{q}_1} + \underline{u}_2 \cdot \frac{\partial}{\partial \underline{q}_2}\right)\right] \underline{F}_{12}\left(\left|\frac{\underline{q}_{12}}{a}\right|\right)$$

and $\underline{q}_{12} = \underline{q}_1 - \underline{q}_2$. $\underset{\sim}{\mathcal{D}}(u, t)$ is a second rank tensor function of $\underline{u}$. For this particular kind of tensor, where $\underset{\sim}{\mathcal{D}}(\underline{u}, t) = \underset{\sim}{\mathcal{D}}(u^2, t)$,

$$\mathcal{D}_{kj}(u^2, t) = \mathcal{D}_{\perp}(u^2, t)\left[\delta_{kj} - \frac{u_k u_j}{u^2}\right] + \mathcal{D}_{\parallel}(u^2, t) \frac{u_k u_j}{u^2} .$$

$$\mathcal{D}_{\parallel}(u^2, t) = \frac{\underline{u} \cdot \underset{\sim}{\mathcal{D}}(u^2, t) \cdot \underline{u}}{u^2}$$

is known as the longitudinal component of $\underset{\sim}{\mathcal{D}}$.

$$\mathcal{D}_{\perp}(u^2, t) = \frac{1}{2}\left[\mathrm{Tr}\, \underset{\sim}{\mathcal{D}}(\underline{u}, t) - \mathcal{D}_{\parallel}(\underline{u}, t)\right]$$

is the transverse component.

One can easily verify that

$$\frac{\partial}{\partial \underline{u}} \cdot \underset{\sim}{\mathcal{D}}(u^2, t) \cdot \left(\frac{\partial}{\partial \underline{u}} + \underline{u}\right) = \frac{1}{u^2} \frac{\partial}{\partial u} u^2 \mathcal{D}_{\parallel}(u, t)\left(\frac{\partial}{\partial u} + u\right) + \frac{1}{u^2} \mathcal{D}_{\perp}(u, t) L^2$$

where

$$L^2 = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2}$$

$$\frac{\partial f(\underline{u},t)}{\partial t} = \epsilon \int_0^t d\tau \left\{ \frac{1}{u^2}\frac{\partial}{\partial u} u^2 \mathscr{D}_{\parallel}(u^2,\tau)\left(\frac{\partial}{\partial u}+u\right) + \frac{1}{u^2}\mathscr{D}_{\perp}(u^2,\tau)L^2 \right\} f(u,t-\tau) . \tag{III-A}$$

It is worth noting that

$$\int d^3\underline{u}_1 M(u_1) \mathrm{Tr}\, \underset{\sim}{\mathscr{D}}(\underline{u}_1, t)$$

$$= \frac{1}{\Omega^N}\int d^3\underline{u}_1 M(\underline{u}_1)\int d^3\underline{u}_2 \ldots d^3\underline{u}_N \prod_{j=2}^{N} M(\underline{u}_j)\int d^N\underline{Q}\, \underline{F}_1 e^{itL_0} \cdot \underline{F}_1$$

is the weakly coupled limit of

$$\langle \underline{F}_1(0)\cdot\underline{F}_1(t)\rangle = \frac{1}{\Omega^N}\int d^N\underline{Q}\int d^3\underline{u}_1 \ldots d^3\underline{u}_N \prod_{j=1}^{N} M(\underline{u}_j)\underline{F}_1(\Gamma)e^{itL}\cdot\underline{F}_1(\Gamma)e^{-\beta U(\Gamma)} .$$

The proof follows using the methods of Chapter II.

We consider shortly which forces are reasonable in a weakly coupled situation.

B. Conservation Laws

If we consider particle one to be a "test particle" moving through the bath of the other particles, we are dealing with a two component system. We do not expect the momentum and energy of the test particle to remain constant upon colliding with the other particles. We do, however, expect the total number of particles to remain the same.

This is readily verified for our equation since as we shall show, $\underset{\sim}{\mathscr{D}}(\underline{u},t)$ vanishes as $|\underline{u}|\to\infty$, as does $f(\underline{u},t)$ and its gradient. Hence,

$$\frac{\partial}{\partial t}\int d^3\underline{u} f(\underline{u},t) = \int_0^t d\tau \left\{ \int d^3\underline{u} \frac{\partial}{\partial \underline{u}} \cdot \underset{\sim}{\mathscr{D}}(\underline{u}, t-\tau)\cdot\left(\frac{\partial}{\partial \underline{u}}+\underline{u}\right) f(\underline{u},\tau) \right\} = 0$$

We also expect a Maxwell-Boltzmann distribution of test particles to remain stationary. This is easily seen since

$$\left(\frac{\partial}{\partial \underline{u}} + \underline{u}\right)e^{-u^2/2} = 0 \ .$$

C. The Diffusion Tensor for a Weakly Interacting Brownian Particle

The physical situation of Brownian motion is that of a heavy, nearly stationary, test particle being constantly bombarded by very light bath particles. In this case $\underline{u}$ is nearly zero and

$$\underset{\sim}{\mathcal{D}}(\underline{u}, t) = \frac{1}{\Omega^N}\int d^N\underline{Q}\int d^{N-1}\underline{u}\prod_{i=2}^{N} M(u_i)\underline{F}_1 e^{ita\left[\underline{u}\cdot\frac{\partial}{\partial \underline{q}_1}+\ldots+\underline{u}_N\cdot\frac{\partial}{\partial \underline{q}_N}\right]}\underline{F}_1$$

becomes

$$\underset{\sim}{\mathcal{D}}(\underline{u}, t) \doteq \underset{\sim}{\mathcal{D}}(t) \ .$$

Denoting the resultant isotropic tensor by $\underset{\sim}{\mathcal{D}}_\infty(t)$, the test particle equation becomes

$$\frac{\partial f(\underline{u}, t)}{\partial t} = \int_0^t d\tau \frac{\partial}{\partial \underline{u}} \cdot \underset{\sim}{\mathcal{D}}_\infty(t-\tau)\cdot\left(\frac{\partial}{\partial \underline{u}} + \underline{u}\right) f(\underline{u}, \tau)$$

This is an equation of the form studied by Lebowitz, Percus and Sykes. The reader is referred to (16) and (18) for an excellent analysis of this equation.

D. The Diffusion Tensor for a Weakly Interacting Test Particle in a Lorentz Gas

As we have seen, the physical situation of a test particle in a Lorentz Gas is that of a very light particle moving through a medium of heavy stationary particles. In such a situation

$$iL_0 = a \sum_{k=1}^{N} \underline{u}_k \cdot \frac{\partial}{\partial \underline{q}_k}$$

becomes

$$iL_0 = a\,\underline{u} \cdot \frac{\partial}{\partial \underline{q}_1} \quad .$$

Thus,

$$\underset{\sim}{\mathcal{D}}(\underline{u}, s') = \langle \underline{F}_1 \frac{1}{s' + a \sum_{k=1}^{N} \underline{u}_k \cdot \frac{\partial}{\partial \underline{q}_k}} \underline{F}_1 \rangle$$

$$= \frac{1}{\Omega} \int d^3 \underline{q}_{12}\, \underline{F}_{12}\left(\left|\frac{\underline{q}_{12}}{a}\right|\right) \frac{1}{s' + a\underline{u} \cdot \frac{\partial}{\partial \underline{q}_{12}}} \underline{F}_{12}\left(\left|\frac{\underline{q}_{12}}{a}\right|\right)$$

Further calculations are most conveniently carried out in Fourier transform space. For convenience we continue to use dimensionless variables. Since

$$\underline{F}_{12}\left(\frac{\underline{q}_{12}}{a}\right) = -a \frac{\partial}{\partial \underline{q}_{12}} v\left(\frac{|\underline{q}_{12}|}{a}\right) = \frac{-i}{(2\pi)^3} \int d^3 \underline{k}\, e^{\frac{i}{a}\underline{k} \cdot \underline{q}_{12}}\, \underline{k}\tilde{v}(k)$$

we restrict ourselves to considering only Fourier transformable potentials. Even more restrictive, we will limit ourselves in this investigation to those potentials which are entire functions. Then,

$$\mathcal{D}(\underline{u}, s') = \langle \underline{F}_{12} \frac{1}{s' + a\underline{u} \cdot \frac{\partial}{\partial \underline{q}_{12}}} \underline{F}_{12} \rangle = \frac{1}{(2\pi)^3} \int d^3 \underline{k} \left[\underline{k}\tilde{v}(\underline{k}) \frac{1}{s' + i\underline{u} \cdot \underline{k}} \underline{k}\tilde{v}(k) \right]$$

$$\mathcal{D}_{\parallel}(\underline{u}, s') = \frac{1}{(2\pi)^3} \int d^3 \underline{k}\, \frac{(\underline{k} \cdot \underline{u})^2}{u^2} \frac{[\tilde{v}(k)]^2}{s' + i\underline{u} \cdot k} = \frac{1}{(2\pi)^2} \int_0^{\infty} dk\, k^4 [\tilde{v}(k)]^2 \int_{-1}^{1} \frac{d\eta\, \eta^2}{s + iku\eta}$$

and

$$\mathrm{Tr}\underset{\sim}{\mathcal{D}}(\underline{u}, s') = \frac{1}{(2\pi)^2}\int_0^\infty dk\, k^3[\tilde{v}(k)]^2 \int_{-k}^{k} \frac{dy}{s'+iuy} .$$

To simplify the trace term further, we integrate by parts. Define by $\Phi_n(k)$

$$\Phi_n(k) = \int_k^\infty dk\, k^n[\tilde{v}(k)]^2 .$$

Then

$$\mathrm{Tr}\underset{\sim}{\mathcal{D}}(\underline{u}, s') = \frac{1}{(2\pi)^2}\int_0^\infty dk\, \Phi_3(k)\left[\frac{1}{s'+iuk} - \frac{1}{s'-iuk}\right] .$$

If we extend the definition to include negative (real) k we see that for n odd, $\Phi_n(k)$ is even, and for n even $\Phi_n(k)$ is odd. Thus,

$$\mathrm{Tr}\underset{\sim}{\mathcal{D}}(\underline{u}, s') = \frac{s'}{2\pi^2}\int_0^\infty dk' \frac{\Phi_3(k)}{s'^2+u^2k^2} .$$

Similar calculations show that

$$\mathcal{D}_{\parallel}(\underline{u}, s) = \frac{s'}{2\pi^2 u^2}\left[\Phi_2(0) - s'^2\int_0^\infty dk \frac{\Phi_1(k)}{s'^2+u^2k^2}\right]$$

and

$$\mathcal{D}_{\perp}(\underline{u}, s') = \frac{1}{2}\left[\mathrm{Tr}\underset{\sim}{\mathcal{D}} - \mathcal{D}_{\parallel}\right] = \frac{s'}{(2\pi)^2}\int_0^\infty dk \frac{\Phi_3(k) + \frac{s'^2}{u^2}\Phi_1(k)}{s'^2+u^2k^2} - \frac{s'}{(2\pi)^2}\frac{\Phi_2(k=0)}{u^2} .$$

E. <u>A Theorem Due to Corngold</u>

The two seemingly independent components of the tensor, $\mathcal{D}_{\parallel}$ and $\mathcal{D}_{\perp}$ are connected in a surprising way. Consider

$$\mathcal{D}_{\parallel}(u, s') = \frac{1}{(2\pi)^2}\int_0^\infty dk\, k^4[\tilde{v}(k)]^2 \int_{-1}^{1} d\eta \frac{\eta^2}{s'+iku\eta}$$

Upon the change of variables $u\eta = y$ and suitable manipulation with this variable, we see that

$$\frac{1}{u^2}\frac{d}{du}u^3 \mathcal{D}_{\parallel}(u, s') = \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} dk\, \frac{k^4[\tilde{v}(k)]^2}{s'+iku}$$

$$= \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} dk \left[\frac{\Phi_3(k)}{s'+iku} + \Phi_3(k) k \frac{d}{dk}\frac{1}{s+iuk}\right]$$

Since

$$\mathrm{Tr}\underset{\sim}{\mathcal{D}}(u, s') = \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} \frac{\Phi_3(k)dk}{s'+iuk}$$

and

$$k\frac{d}{dk}\frac{1}{s'+iuk} = u\frac{d}{du}\frac{1}{s'+iuk}$$

we have that

$$\boxed{\mathcal{D}_{\parallel} = \mathcal{D}_{\perp} + u\frac{d}{du}\mathcal{D}_{\perp} = \frac{d}{du}(u\mathcal{D}_{\perp})}$$

We also note that

$$\frac{1}{u^2}\frac{d}{du}\left(u^3 \mathcal{D}_{\perp}(u, s')\right) = \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} dk\, \frac{\Phi_3(k)}{s'+iku} \quad .$$

F. <u>General Properties of $\underset{\sim}{\mathcal{D}}$</u>

$$\Phi_3(k) = \int_k^{\infty} dk\, k^3[\tilde{v}(k)]^2 \, .$$

For k real and positive, $\Phi_3(k)$ is positive. Thus

$$\mathrm{Tr}\underset{\sim}{\mathcal{D}}(u, s') = \frac{s'}{2\pi^2}\int_0^{\infty} dk\, \frac{\Phi_3(k)}{s'^2+u^2k^2}$$

is positive as long as s is real and positive. $\mathrm{Tr}\mathcal{D}(u, s')$ is easily seen to be monotonically decreasing with u.

$$\mathcal{D}_{\parallel} = \frac{1}{(2\pi)^3}\int_0^{\infty} dk\, k^4[\tilde{v}(k)]^2 \int_{-1}^{1} d\eta \frac{\eta^2}{s'+iku\eta}$$

$$= \frac{1}{(2\pi)^2}\int_0^{\infty} dk\, k^4[\tilde{v}(k)]^2 \int_0^{1} \frac{2s'\eta^2}{s'^2+k^2u^2\eta^2}\, d\eta$$

Again, for s' real and positive, $\mathcal{D}_{\parallel}$ is obviously positive. It is also a decreasing function of u. Similar considerations and results apply to $\mathcal{D}_{\perp}$.

G. Series Expansions for $\mathcal{D}_{\parallel}$, $\mathcal{D}_{\perp}$ and Tr$\mathcal{D}$

The combination of variables u/s' turns out to be a convenient grouping for examining the behavior of $\underset{\sim}{\mathcal{D}}$. For $u/s' \ll 1$ we can arrive at the following representations.

$$\mathrm{Tr}\underset{\sim}{\mathcal{D}}(u, s') = \frac{1}{(2\pi)^2}\int_{-1}^{1} d\eta \int_0^{\infty} dk\, k^4[\tilde{v}(k)]^2 \frac{1}{s+iku\eta}$$

$$= \frac{1}{(2\pi)^2}\,\frac{1}{iu}\int_0^{\infty} dk\, k^3[\tilde{v}(k)]^2 \,\ell n\, \frac{1+\frac{iuk}{s}}{1-\frac{iuk}{s}}$$

Expansion of the logarithm in a series in iuk/s and term by term integration produces the asymptotic series

$$\mathrm{Tr}\underset{\sim}{\mathcal{D}}(u, s') = \frac{1}{2\pi^2}\left[\frac{\Phi_4(0)}{s'} - \frac{\Phi_6(0)u^2}{3s'^3} + \frac{\Phi_8(0)u^4}{5s'^5} - + \dots\right]$$

By making direct use of the integral expressions for $\mathcal{D}_{\parallel}$ and $\mathcal{D}_{\perp}$, integrating over the k variable and expanding the resulting logarithmic term, one can also deduce

$$\mathcal{D}_{\parallel} = \frac{1}{2\pi^2}\left[\frac{\Phi_4(0)}{3s'} - \frac{u^2}{s'^3}\frac{\Phi_6(0)}{5} + \frac{u^4\Phi_8(0)}{s'^5 7} - + \dots\right]$$

and

$$\mathcal{D}_{\perp} = \frac{1}{2\pi^2}\left[\frac{\Phi_4(0)}{3s'} - \frac{u^2}{s'^3}\frac{\Phi_6(0)}{15} + \dots\right]$$

Whenever the first term of the $\mathcal{D}_{\parallel}$ and $\mathcal{D}_{\perp}$ series approximates the sum of the series, $\underset{\sim}{\mathcal{D}}$ becomes

$$\underset{\sim}{\mathcal{D}} = \frac{\Phi_4(0)}{6\pi^2 s'}\,\underset{\sim}{1}$$

But this is the type of momentum independent isotropic diffusion tensor which has been studied by Lebowitz and others.[17] Recall that their conjecture was that the diffusion tensor depends only on s'. We see that for the weakly coupled Lorentz Gas, this conjecture holds only at short times or small test-particle velocities.

The long time $(s' \to 0)$ limit is messier. Consider

$$\mathrm{Tr}\underset{\sim}{\mathcal{D}}(u, s') = \frac{s'}{2\pi^2}\int_0^\infty dk\, k^4[\tilde{v}(k)]^2 \int_{-1}^{1} \frac{d\eta}{s'+iku\eta}$$

The η integral is a usual Cauchy integral and exists for all u and $s' > 0$. If we expand in s'/ku and integrate over k, we find that some of the higher order terms in the series are difficult to compute. Fortunately, the first two terms are always easy and suffice, for our analysis

$$\mathrm{Tr}\underset{\sim}{\mathscr{D}}(u, s') = \frac{s'}{2\pi^2 u^2}\int_0^\infty dk\, \frac{\Phi_3(k)}{(s'/u)^2 + k^2}$$

$$= \frac{s'}{2\pi^2 u^2}\int_0^\infty dk \frac{1}{k^2+(s'/u)^2}\left[\Phi_3(0) - \int_0^k dz\, z^3[\widetilde{v}(z)]^2\right]$$

$$= \frac{1}{4\pi}\,\frac{\Phi_3(0)}{u} - \frac{s'}{2\pi^2 u^2}\int_0^\infty \frac{dk}{k^2+(s'/u)^2}\int_0^k dz\, z^3[\widetilde{v}(z)]^2$$

The second term can be expanded in s'/u so that

$$\mathrm{Tr}\underset{\sim}{\mathscr{D}}(u, s') = \frac{\Phi_3(0)}{4\pi u} - \frac{s'}{2\pi u^2}\int_0^\infty \frac{dk}{k^2}\, I(k)$$

where

$$I(k) = \int_0^k dz\, z^2[\widetilde{v}(z)]^2 .$$

Integrating by parts yields

$$\mathrm{Tr}\underset{\sim}{\mathscr{D}}(u, s') = \frac{\Phi_3(0)}{4\pi u} - \frac{s'}{2\pi u^2}\,\Phi_2(0) + \ldots \quad .$$

We can find $\mathscr{D}_{\parallel}$ and $\mathscr{D}_{\perp}$ by using Corngold's theorem. Thus,

$$3\mathscr{D}_{\perp} + u\,\frac{d\mathscr{D}_{\perp}}{du} = \frac{\Phi_3(0)}{4\pi u} - \frac{s'}{2\pi^2}\,\frac{\Phi_2(0)}{u^2} + \ldots \quad .$$

and solving the differential equation term by term one gets

$$\mathscr{D}_{\perp} = \frac{\Phi_3(0)}{8\pi u} - \frac{1}{2\pi^2}\,\frac{\Phi_2(0)s'}{u^2} + \ldots$$

which implies that

$$\mathscr{D}_{\parallel} = \frac{s'\Phi_2(0)}{2\pi^2 u^2} + \ldots \quad .$$

H. $\underset{\sim}{\mathcal{D}}$ for a Gaussian Potential

To make further progress it is convenient to focus on a specific potential. Because of its analytic properties we choose to study a Gaussian potential

$$v(r) = \lambda e^{-(r^2/a^2)} \qquad \tilde{v}(k) = \lambda \pi^{\frac{3}{2}} a^3 e^{-(k^2 a^2/4)}$$

$$\Phi_3(k) = \lambda \pi^3 a^2 e^{-(k^2 a^2/2)} [2 + k^2 a^2]$$

The Gaussian potential is not a good approximation to the true intermolecular potential. It is purely repulsive, it doesn't diverge at the origin. Nevertheless, it is a kind of weak version of the hard core potential, particularly if its peak is high. Such a function can give us some insight into this weakly coupled model and can yield some physically meaningful results for test particle motion in a Lorentz Gas.

By directly integrating the definition of $\mathcal{D}_{\parallel}$ and $\mathcal{D}_{\perp}$ we find that

$$\mathcal{D}_{\parallel}(u, s') = \left(\frac{\pi}{2}\right)^{\frac{3}{2}} \frac{s'}{u^2} \left[1 - \sqrt{\pi} \frac{s'}{\sqrt{2}u} e^{(s'/\sqrt{2}u)^2} \operatorname{erfc}\left(\frac{s'}{\sqrt{2}u}\right)\right]$$

$$\mathcal{D}_{\perp}(u, s') = \frac{\pi^2}{4} \frac{1}{u} e^{(s'/\sqrt{2}u)^2} \operatorname{erfc}\left(\frac{s'}{\sqrt{2}u}\right)$$

The time dependent $\mathcal{D}_{\parallel}$ and $\mathcal{D}_{\perp}$ are

$$\mathcal{D}_{\parallel} = -\frac{d^2}{dt^2} \left(\frac{\pi}{2}\right)^{\frac{3}{2}} \frac{1}{u^2} e^{-(u^2 t^2/2)}$$

and

$$\mathcal{D}_{\perp} = \left(\frac{\pi}{2}\right)^{\frac{3}{2}} e^{-(u^2 t^2/2)}$$

We notice that the combination of variables $s'/\sqrt{2}u$ appears naturally in $\mathcal{D}_{\parallel}(u, s')$ and $\mathcal{D}_{\perp}(u, s')$. Equation [III-A] can be rewritten in terms of this variable $x = s'/\sqrt{2}u$.

$$\epsilon \frac{d}{dx} e^{-(s'^2/4x^2)} \mathcal{D}_{\parallel}(x) \frac{d}{dx} g(x) - \left[\frac{s'^3}{2x^4} + \frac{\ell(\ell+1)}{x^2} \epsilon \mathcal{D}_{\perp}(x)\right] e^{-(s'^2/4x^2)} g(x)$$

$$= \frac{-s'^2}{2x^4} f_{0\ell}(x) .$$

$$\mathcal{D}_{\parallel}(x) = \frac{\pi^{\frac{3}{2}}}{\sqrt{2}} \frac{x^2}{s'} \left[1 - \sqrt{\pi}\, x e^{x^2} \operatorname{erfc}(x)\right]$$

and

$$\mathcal{D}_{\perp}(x) = \frac{\pi^2}{2^{\frac{3}{2}}} \frac{x}{s'} e^{x^2} \operatorname{erfc}(x) .$$

See Figure (III-1).

I. Autocorrelation Functions

$$\operatorname{Tr}\underset{\sim}{\mathcal{D}}(u, s') = \frac{s'}{2\pi^2} \int_0^\infty dk \frac{\Phi_3(k)}{s'^2 + u^2 k^2}$$

we have seen previously that

$$\frac{1}{(2\pi)^{\frac{3}{2}}} \int e^{-(u^2/2)} \operatorname{Tr}\underset{\sim}{\mathcal{D}}(u, s') d^3\underline{u} = \langle \widetilde{\underline{F}(0) \cdot \underline{F}(s')} \rangle .$$

Hence,

$$\langle \widetilde{\underline{F}(0) \cdot \underline{F}(s')} \rangle = \frac{s'}{2\pi^2} \int_0^\infty dk \frac{\Phi_3(k)}{k^2} \left[1 - \sqrt{\pi} \frac{s'}{\sqrt{2}k} e^{(s'/\sqrt{2}k)^2} \operatorname{erfc}\left(\frac{s'}{\sqrt{2}k}\right)\right] \quad \text{[III-B]}$$

Then,

$$\langle \underline{F}(0)\cdot\underline{F}(t)\rangle = \frac{1}{2\pi^2}\int_0^\infty dk\,\frac{\Phi_3(k)}{k^2}\,\frac{d^2}{dt^2}e^{-(t^2k^2/2)}$$

$$= \frac{-1}{2\pi^2}\int_0^\infty dk\,\Phi_3(k)\left[1-t^2k^2\right]e^{-(t^2k^2/2)}$$

The long time behavior is particularly interesting. To extract it, let $x = kt$, then

$$\langle \underline{F}(0)\cdot\underline{F}(t)\rangle = \frac{1}{2\pi^2 t}\int_0^\infty dx\,\Phi_3\left(\frac{x}{t}\right)\left[1-x^2\right]e^{-(x^2/2)} .$$

But $\Phi_3(k) = \int_0^k dk\,k^3[\tilde{v}(k)]^2$ and for small k goes as $\frac{1}{4}k^4[\tilde{v}(0)]^2$. By expanding $\Phi_3\left(\frac{x}{t}\right)$ about the origin, we see that the first non-vanishing term will be of order $\left(\frac{x}{t}\right)^4$ and all higher order terms will contain higher powers of t in the denominator. Thus the leading power of t for $\langle \underline{F}(0)\cdot\underline{F}(t)\rangle$ is $\frac{1}{t^5}$.

In the case of a Gaussian potential (using dimensional variables for better physical insight)

$$\langle \underline{F}(0)\cdot\underline{F}(t)\rangle = \frac{12a\lambda^2 n}{\sqrt{\pi}\,v_0^5}\,\frac{1}{\left(\beta m + \frac{t^2}{a^2}\right)^{\frac{5}{2}}}$$

From the well known Kubo relation

$$D = \lim_{s\to 0}\frac{1}{3m^2}\langle \underline{p}(0)\cdot\underline{p}(\tilde{s})\rangle$$

we calculate the diffusion coefficient for the test particle.

Using the Zwanzig equation [I-A]

$$D = \lim_{s\to 0} \frac{1}{3m^2} \langle \underline{p}(0)\cdot\underline{p}(s)\rangle = \lim_{s\to 0} \frac{\left(\frac{k_B T}{m}\right)}{s + \frac{\langle \underline{F}(0)\cdot\underline{F}(s)\rangle}{3mk_B T}}$$

$\langle \underline{F}(0)\cdot\underline{F}(s)\rangle$ is given by [III-B], so that in the case of the Gaussian potential

$$D = \frac{\left(\frac{k_B T}{m}\right)^{\frac{5}{2}}}{n\lambda^2} \sqrt{\frac{18}{\pi m}} \frac{1}{\sigma}$$

where $\sigma = \pi a^2$.

Notice that the parametric dependence is reasonable. D varies inversely with the density and interaction strength as well as the radius of the scattering particles. This agrees with the Chapman Enskog approach.(15) The temperature dependence $D \propto T^{\frac{5}{2}}$ is characteristic of a weak interaction. The weakly coupled autocorrelation function $\langle \underline{p}(0)\cdot\underline{p}(t)\rangle$ and its kernel $\langle F(0)\cdot F(t)\rangle$ are displayed in Figures [III-2] and [III-3].

J. The Weakly Coupled Equation

We have seen that

$$\frac{\partial f(\underline{u}, t)}{\partial t} = \epsilon \int_0^t d\tau \left\{ \frac{1}{u^2} \frac{\partial}{\partial u} u^2 \mathcal{D}_{\parallel}(u^2, \tau)\left(\frac{\partial}{\partial u} + u\right) + \frac{1}{u^2} \mathcal{D}_{\perp}(u^2, \tau) L^2 \right\} f(\underline{u}, t) \ . \quad \text{[III-A]}$$

Expanding $f(\underline{u}, t)$ in spherical harmonics,

$$f(\underline{u}, t) = \sum_{\ell, m} R_{\ell m}(u, t) Y_{\ell m}(\theta, \varphi) \ .$$

Because of axial symmetry,

$R_{\ell m}(u, t) = R_{\ell 0}(u, t)$ and [III-A] becomes

$$\frac{\partial R_\ell(u,t)}{\partial t} = \epsilon\int_0^t d\tau\left\{\frac{1}{u^2}\frac{\partial}{\partial u}u^2\mathscr{D}_{\parallel}(u^2,\tau)\left(\frac{\partial}{\partial u}+u\right)-\frac{1}{u^2}\mathscr{D}_{\perp}(u^2,\tau)\ \ell(\ell+1)\right\}R_\ell(u,t-\tau).$$

This scalar form of [III-A] is most convenient, for upon taking the Laplace transform we reduce [III-A] to the ordinary differential equation

$$s'R_\ell(u,s') - \epsilon\left\{\frac{1}{u^2}\frac{\partial}{\partial u}u^2\mathscr{D}_{\parallel}(u^2,s')\left(\frac{\partial}{\partial u}+u\right)+\frac{1}{u^2}\mathscr{D}_{\perp}(u^2,s')\ell(\ell+1)\right\}R_\ell(u,s')$$

$$= R_\ell(u,t=0)\ . \qquad \text{[III-C]}$$

At times it will be convenient to make the change of variables

$$R_\ell(u,s') = e^{-(u^2/2)}g_\ell(u,s')$$

in which case the equation becomes

$$\epsilon\frac{\partial}{\partial u}u^2e^{-(u^2/2)}\mathscr{D}_{\parallel}(u,s')\frac{\partial}{\partial u}g(u,s') - (s'u^2+\ell(\ell+1)\epsilon\mathscr{D}_{\perp}(u,s'))e^{-(u^2/2)}g(u,s')$$

$$= -u^2f_{0\ell}(u,t=0)\ .$$

IV. APPROXIMATE SOLUTIONS

A. $\ell > 0$

In this section we take $\ell > 0$.

Although solving

$$\epsilon \frac{d}{du} u^2 e^{-(u^2/2)} \mathcal{D}_{\parallel}(u, s') \frac{d}{du} g_\ell(u, s')$$

$$- \left(s'u^2 + \ell(\ell+1)\epsilon\, \mathcal{D}_{\perp}(u, s') \right) e^{-(u^2/2)} g_\ell(u, s') = -u^2 f_\ell(t=0, u) \qquad \text{[IV-A]}$$

exactly is a formidable undertaking, we can use a number of methods to obtain approximate solutions. In the course of this investigation we will focus on the Gaussian potential as illuminating example.

We begin by noting that this problem contains two natural time scales. The dimensionless inverse time which we will call frequency is $s' = as/v_0$ (a being the range of force and $v_0 = \sqrt{\frac{k_B T}{m}}$). This dimensionless frequency measures time in units of the time needed to complete a collision. The other time scale is related to the mean free path of the bath. Since the mean free path is equal to $\approx 1/na^2$, a particle traveling with speed v_0 will experience an elapsed time of $1/na^2 v_0$ between collision. The corresponding frequency, s', in this case is na^3. In a gas $na^3 \leq 10^{-2}$. Considering test particle motion in a moderately dilute gas will then mean studying those motions which occur when $s' \ll 1$.

Another dimensionless parameter $\epsilon = na^3(\lambda/k_B T)^2$ is the product of "weak coupling" $\lambda/k_B T$ and "low density" na^3. That ϵ is the product of these two small quantities makes sense since the weakly coupled equation (Forster-Martin) is a special case of the low density equation (Mazenko, Boley and Desai). ϵ is also much less than unity.

To begin our analysis, we study the solutions to the associated homogeneous equation. Expanding $f(\underline{u}, s')$ in spherical harmonics we have

$$f(u, \theta, \varphi, s') = e^{-(u^2/2)} g(u, \theta, \varphi, s') = \sum_{\ell} R_{\ell}(u, s') Y_{\ell o}(\theta, \varphi)$$

By making the change of variables

$$R_{\ell}(u, s') = \frac{1}{\sqrt{\mathscr{D}_{\parallel}(u, s')u^2}} e^{-(u^2/4)} h_{\ell}(u, s')$$

the homogeneous equation related to [IV-A] is

$$\frac{d^2 h_{\ell}(u, s')}{du^2} + v(u, s') h_{\ell}(u, s') = 0 \; . \qquad \text{[IV-B]}$$

$v(u, s')$ can be expressed in many ways. Denoting $u^2 \mathscr{D}_{\parallel}(u, s') e^{-(u^2/2)}$ by Δ we can express $v(u, s')$ as

$$-v(u, s') = \frac{s'}{\epsilon \mathscr{D}_{\parallel}} + \frac{\ell(\ell+1)}{u^2} \frac{\mathscr{D}_{\perp}(u, s')}{\mathscr{D}_{\parallel}(u, s')} + \frac{(\sqrt{\Delta})''}{(\sqrt{\Delta})} \; .$$

If we carry out the differentiations in $(\sqrt{\Delta})''$ we obtain

$$v(u, s') = -\frac{u^2}{4} - \frac{1}{2} \frac{\mathscr{D}''_{\parallel}}{\mathscr{D}_{\parallel}} - \frac{\mathscr{D}'_{\parallel}}{\mathscr{D}_{\parallel} u} + \frac{1}{4} \left[\frac{\mathscr{D}'_{\parallel}}{\mathscr{D}_{\parallel}} \right]^2 + \frac{\mathscr{D}'_{\parallel} u}{2 \mathscr{D}_{\parallel}} + \frac{3}{2} - \frac{s'}{\epsilon \mathscr{D}_{\parallel}} - \frac{\ell(\ell+1) \mathscr{D}_{\perp}}{u^2 \mathscr{D}_{\parallel}}$$

For fixed s' and extremely small u, we have shown that

$$\mathscr{D}_{\parallel}(u, s') = \frac{\Phi_4(0)}{6\pi^2 s'} - \frac{\Phi_6(0) u^2}{10\pi^2 s'^3} + \ldots = \frac{c_4}{s'} - \frac{c_6 u^2}{s'^3} + \ldots$$

$$\mathcal{D}_{\perp}(u, s') = \frac{\Phi_4(0)}{6\pi^2 s'} - \frac{\Phi_6(0)u^2}{30\pi^2 s'^3} + \ldots = \frac{c_4}{s'} - \frac{c_6 u^2}{3s'^3} + \ldots$$

and hence

$$\mathcal{D}'_{\parallel}(u, s') = - \frac{2c_6 u}{s'^3} + \ldots$$

$$\mathcal{D}''_{\parallel}(u, s') = - \frac{2c_6}{s'^3} + \ldots$$

By substituting $\mathcal{D}_{\parallel} = \frac{c_4}{s'}$, $\mathcal{D}_{\perp} = \frac{c_4}{s'}$, $\mathcal{D}'_{\parallel} = -\frac{2c_6 u}{s'^3}$ and $\mathcal{D}''_{\parallel} = -\frac{2c_6}{s'^3}$ into our expression for $v(u, s')$ we see that $v(u, s')$ becomes

$$v(u, s') = - \frac{\ell(\ell+1)}{u^2} + O(1)$$

For extremely small u then, the functional form of $v(u, s')$ is independent of both s' and ϵ. However, the range of u over which this expression is valid will depend on both parameters.

Consider now extremely large u. In this case

$$\mathcal{D}_{\parallel}(u, s') = \frac{s'\Phi_2(0)}{2\pi^2 u^2} + \ldots$$

$$\mathcal{D}'_{\parallel}(u, s') = - \frac{s'\Phi_2(0)}{\pi^2 u^3} + \ldots$$

$$\mathcal{D}''_{\parallel}(u, s') = \frac{3s'\Phi_2(0)}{\pi^2 u^4} + \ldots$$

and

$$\mathcal{D}_{\perp}(u, s') = \frac{\Phi_3(0)}{8\pi u} + \ldots$$

Now

$$v(u, s') = -\frac{2\pi^2 u^2}{\epsilon \Phi_2(0)} + O(1)$$

A common technique for studying the solutions to

$$y''(x) + a(x)y'(x) + b(x)y(x) = 0$$

in the limiting situtations $x \to \infty$ and $x \to 0$ is to assert that $\lim\limits_{\substack{x\to\infty \\ x\to 0}} y(x)$ is the solution to

$$y''(x) + \left[\lim_{\substack{x\to\infty \\ x\to 0}} a(x)\right] y'(x) + \left[\lim_{\substack{x\to\infty \\ x\to 0}} b(x)\right] y(x) = 0 . \quad (21)$$

Thus, the solutions to [IV-A] as $u \to 0$ are the solutions to

$$\frac{d^2 h_\ell^{(u)}}{du^2} - \frac{\ell(\ell+1)}{u^2} h_\ell(u) = 0 .$$

That is,

$$h_\ell^{(u)} \sim u^{(\ell+1)}, \ u^{-\ell} \quad \text{as} \quad u \to 0$$

As $u \to \infty$ [IV-A] becomes

$$\frac{d^2 h_\ell(u)}{du^2} - \alpha_2 u^2 h_\ell(u) = 0 .$$

where $\alpha_2 = 2\pi^2 / \epsilon \Phi_2(0)$. Then

$$h_\ell(u) \sim \sqrt{u}\, K_{\frac{1}{4}}\left(\sqrt{\alpha_2}\, \frac{u^2}{2}\right) , \quad \sqrt{u}\, I_{\frac{1}{4}}\left(\sqrt{\alpha_2}\, \frac{u^2}{2}\right) \quad \text{for large } u .$$

Intermediate values of u are much more difficult to discuss for an arbitrary potential. Hence, we might best examine the behavior of v(u, s′) in specific instances. For the Gaussian potential our equation becomes particularly simple. We shall show that $v(u, s')$ is negative for all u and $s' > 0$. Thus, one can use a single WKB approximation for solutions. This we do later. We also consider the following more intuitive "regional" approach.

As we have seen, $v(u, s')$ is an unwieldy function of u and s' except in certain limiting cases, However, experience with the Gaussian potential shows that for fixed s', at any value of u, one simple part of $v(u, s')$ is dominant. For example, for extremely small $u \ll 1$, we will see that $v(u, s')$ is dominated by the term $-\frac{\ell(\ell+1)\mathcal{D}_\perp}{u^2 \mathcal{D}_\parallel}$.
For extremely large $u \gg 1$ the term $\frac{-s'}{\epsilon \mathcal{D}_\parallel}$ dominates and so on. This leads us to believe that we may be able to approximate the true potential by a simpler analytical form and still retain its significant properties.

Consider the exact expressions for $\mathcal{D}_\parallel$ and $\mathcal{D}_\perp$ in the Gaussian case. As we showed in Chapter III

$$\mathcal{D}_\parallel(u, s') = \left(\frac{\pi}{2}\right)^{\frac{3}{2}} \frac{s'}{u^2}\left[1 - \sqrt{\pi}\frac{s'}{\sqrt{2}\,u}\, e^{(s'/\sqrt{2}u)^2} \operatorname{erfc}\left(\frac{s'}{\sqrt{2}\,u}\right)\right] \qquad [\text{IV-C}]$$

$$\mathcal{D}_\perp(u, s') = \frac{\pi^2}{4}\frac{1}{u}\, e^{(s'/\sqrt{2}u)^2} \operatorname{erfc}\left(\frac{s'}{\sqrt{2}\,u}\right) \qquad [\text{IV-D}]$$

Then, by direct differentiation

$$\left(\frac{2}{\pi}\right)^{\frac{3}{2}} \frac{d\mathcal{D}_\parallel}{du}(u, s') = \frac{s'}{u^3} - \left(\frac{3s'}{u^3} + \frac{s'^3}{u^5}\right)\left(1 - \sqrt{\pi}\frac{s'}{\sqrt{2}\,u}\, e^{(s'/\sqrt{2}u)^2} \operatorname{erfc}\left(\frac{s'}{\sqrt{2}\,u}\right)\right) \qquad [\text{IV-E}]$$

and

$$\left(\frac{2}{\pi}\right)^{\frac{3}{2}} \frac{d^2\mathcal{D}_{\parallel}(u, s')}{du^2} = -\frac{6s'}{u^4} - \frac{s'^3}{u^6}$$

$$+\left(12\frac{s'}{u^4} + \frac{9s'^3}{u^6} + \frac{s'^5}{u^8}\right)\left(1 - \sqrt{\pi}\,\frac{s'}{\sqrt{2}\,u}\, e^{(s'/\sqrt{2}\,u)^2} \operatorname{erfc}\left(\frac{s'}{\sqrt{2}\,u}\right)\right) \qquad \text{[IV-F]}$$

It is interesting to note that these last two expressions imply that $\mathcal{D}_{\parallel}(u, s')$ satisfies two simple differential equations. Namely,

$$\frac{d\mathcal{D}_{\parallel}}{du}(u, s') = \left(\frac{\pi}{2}\right)^{\frac{3}{2}} \frac{s'}{u^3} - \left(\frac{3}{u} + \frac{s'^2}{u^3}\right) \mathcal{D}_{\parallel}(u, s')$$

and

$$\frac{d^2}{du^2}\,\mathcal{D}_{\parallel}(u, s') = -\left(\frac{\pi}{2}\right)^{\frac{3}{2}}\left[\frac{6s'}{u^4} + \frac{s'^3}{u^6}\right] + \left(\frac{12}{u^2} + \frac{9s'^2}{u^4} + \frac{s'^4}{u^8}\right)\mathcal{D}_{\parallel}(u, s') \,.$$

We now determine the form of $v(u, s')$ for small u. The function $\sqrt{\pi}\,\frac{s'}{\sqrt{2}\,u}\, e^{(s'/\sqrt{2}\,u)^2} \operatorname{erfc}\left(\frac{s'}{\sqrt{2}\,u}\right)$ which determines the behavior of $\mathcal{D}_{\parallel}$ and $\mathcal{D}_{\perp}$ has an important asymptotic expansion in this region. As u/s becomes small, we have

$$\sqrt{\pi}\,\frac{s'}{\sqrt{2}\,u}\, e^{(s'/\sqrt{2}\,u)^2} \operatorname{erfc}\left(\frac{s'}{\sqrt{2}\,u}\right) \rightarrow 1 - \frac{u^2}{s'^2} + 3\frac{u^4}{s'^4} - \frac{15u^6}{s'^6} + \ldots$$

This asymptotic limit is reached rather quickly. From numerical studies(2) it turns out that the expansion is useful for $s'/\sqrt{2}\,u \geq 6$. Making use of this expansion, using the small u/s' form of $\mathcal{D}_{\perp}$, $\mathcal{D}_{\parallel}$, and its derivatives, and putting these values into our expression for $v(u, s')$, we obtain

$$v(u, s') \to -\frac{\ell(\ell+1)}{u^2} + \varphi(s') + R(u)$$

where $\varphi(s') = \frac{14}{s'^2} - \frac{s'^2}{\epsilon} + \frac{3}{2}$ and $|R(u)| \ll \varphi(s')$, $u > \frac{s'}{10}$. This is region I.

We have seen that $\sqrt{\pi}\,\frac{s'}{\sqrt{2}\,u}\,e^{(s'/\sqrt{2}\,u)^2}\,\mathrm{erfc}\left(\frac{s'}{\sqrt{2}\,u}\right)$ rapidly approaches its asymptotic form as $u/s' \to 0$. In the opposite case, as u becomes greater than s' this function becomes much less than unity. For example, $u = \frac{10s'}{\sqrt{2}}$ implies $\sqrt{\pi}\,\frac{s'}{\sqrt{2}\,u}\,e^{(s'/\sqrt{2}\,u)^2}\,\mathrm{erfc}\left(\frac{s'}{\sqrt{2}\,u}\right) = 0.1$. In this region

$$\mathcal{D}_{\parallel} \to \left(\frac{\pi}{2}\right)^{\frac{3}{2}} \frac{s'}{u^2}$$

$$\mathcal{D}'_{\parallel} \to -\left(\frac{\pi}{2}\right)^{\frac{3}{2}} \frac{2s'}{u^3}$$

$$\mathcal{D}''_{\parallel} \to \left(\frac{\pi}{2}\right)^{\frac{3}{2}} \frac{6s'}{u^4}$$

and

$$\mathcal{D}_{\perp} \to \frac{\pi^2}{4u}$$

As we have already seen, for a moderately dense gas $s' = 10^{-2}$ by the time a mean free path has been traversed by a test particle with speed v_0. Much of the physically interesting phenomena in our system occurs when $s' \ll 1$. Consider small s' for the moment. Under this constraint, and for $u > 10s'$, we substitute the approximate values for $\mathcal{D}_{\perp}$, $\mathcal{D}_{\parallel}$ and its derivatives shown above into $v(u, s')$. The resulting

$v(u, s')$ is again dominated for a range of u by $\frac{-\ell(\ell+1)\mathcal{D}_\perp}{u^2 \mathcal{D}_\parallel}$. For $u \gg s'$, however, the form of this term becomes

$$\frac{-\ell(\ell+1)\mathcal{D}_\perp}{u^2 \mathcal{D}_\parallel} \cong \frac{-\ell(\ell+1)}{us} \sqrt{\frac{\pi}{2}} \ .$$

Of course, there is a smooth transition between $\frac{\ell(\ell+1)\mathcal{D}_\perp}{u^2 \mathcal{D}_\parallel}$ as u goes from less than $s'/10$ to greater than $10s'$. The functional form in the transition region is somewhat complicated as we shall see.

Where $u \geq 10s'$

$$v(u, s') \to \frac{-\ell(\ell+1)}{us} \sqrt{\frac{\pi}{2}} - u^2\left(\frac{1}{\epsilon} + \frac{1}{4}\right) + \frac{1}{2} \ .$$

That $\frac{-\ell(\ell+1)}{us} \sqrt{\frac{\pi}{2}}$ dominates $v(u, s')$ for a range of u is due primarily to the fact that this term is the only term where s' appears uncancelled in the demoninator. We refer to the region where $u > 10s'$, and where $\frac{-\ell(\ell+1)\mathcal{D}_\perp}{u^2 \mathcal{D}_\parallel}$ dominates $v(u, s')$, as region II.

In the preceeding discussion of Region II we have assumed that $s' < 1$. For values of the frequency, $s' \geq 1$, region II simply doesn't appear. For all values of $u \gg s'$ (and hence $\gg 1$) the term $-u^2/\epsilon$ will be the largest.* However, we should point out that for these large frequencies our v_0 speed particle has not yet had time to complete even a single collision. For the remainder of our investigation we will restrict s' to be $s' < 1$.

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*When $\ell(\ell+1)$ is extremely large, region II will appear for a small domain of u.

Even for the smallest s', the term $-s'/\epsilon\mathcal{D}_{\parallel}$ becomes dominant at very large u. This occurs when

$$\frac{-\ell(\ell+1)}{s'u}\sqrt{\frac{\pi}{2}} < \frac{-u^2}{\epsilon}$$

or

$$u > \sqrt[3]{\ell(\ell+1)\sqrt{\frac{\pi}{2}}\,\frac{\epsilon}{s'}} \equiv \beta_\ell(s')$$

This is region III.

In summary then,

	Leading Terms	Approximate $v(u, s')$	Range of Validity
$v(u, s') =$	$\dfrac{-\ell(\ell+1)\mathcal{D}_\perp}{u^2\mathcal{D}_\parallel} - \dfrac{\mathcal{D}'_\parallel}{\mathcal{D}_\parallel u}$	$\dfrac{-\ell(\ell+1)}{u^2} + \varphi(s')$	$0 < u < \dfrac{s'}{10}$
	$\dfrac{-\ell(\ell+1)\mathcal{D}_\perp}{\mathcal{D}_\parallel u^2}$	$\dfrac{-\ell(\ell+1)}{us}\sqrt{\dfrac{\pi}{2}}$	$10s' < u < \beta_\ell(s')$
	$\dfrac{-s'}{\epsilon\mathcal{D}_\parallel}$	$-\dfrac{u^2}{\epsilon}$	$\beta_\ell(s') < u$

where

$$\varphi(s') = \frac{9}{s'^2} - \frac{s'^2}{\epsilon} + \frac{3}{2}$$

$$\beta_\ell(s') = \sqrt{\ell(\ell+1)\sqrt{\pi/2}\,\epsilon/s'}$$

A few remarks concerning this summary are appropriate. The comments made here do not hold for $\ell = 0$ which will be treated later as a separate case. Notice that the bounds of the regions are s' dependent. Region I shrinks as $s' \to 0$. For certain values of s' region II cannot exist because s' is not sufficiently small to satisfy the inequality $s' < \beta_\ell(s')$. As $s' \to 0$, however, region II not only exists but covers the entire u axis.

We must also point out that we have made no approximation to $v(u, s')$ for $s'/10 \le u \le 10s'$. We have done this because the potential does not exhibit any easy behavior in this domain. The detailed behavior of the true $v(u, s')$ is discussed shortly. As $s' \to 0$, this region becomes small.

We now show that the exact $v(u, s')$ is everywhere negative. This is significant for two reasons. First, this is a principal feature of our approximation to $v(u, s')$, and as such should agree with the exact answer. Second, it is a necessary condition for applying a simple WKB technique to solve the equation. For such a $v(u, s')$ the WKB solution will exhibit no turning points.

$$v(u, s') = \frac{-u^2}{4} - \frac{1}{2}\frac{\mathcal{D}''_{\parallel}}{\mathcal{D}_{\parallel}} - \frac{\mathcal{D}'_{\parallel}}{\mathcal{D}_{\parallel} u} + \frac{1}{4}\left[\frac{\mathcal{D}'_{\parallel}}{\mathcal{D}_{\parallel}}\right]^2 + \frac{\mathcal{D}'_{\parallel} u}{2\mathcal{D}_{\parallel}} + \frac{3}{2} - \frac{s'}{\epsilon \mathcal{D}_{\parallel}} - \frac{\ell(\ell+1)\mathcal{D}_{\perp}}{u^2 \mathcal{D}_{\parallel}}$$

$\mathcal{D}_{\perp}$, $\mathcal{D}_{\parallel}$ and its derivatives are functions of u and s' defined in Equations [IV-C] to [IV-F]. Let us make the change of variables $x = s'/\sqrt{2}u$, and let us define the function $\theta(x)$ to be

$$\theta(x) = 1 - \sqrt{\pi}\, x\, e^{x^2} \operatorname{erfc}(x) .$$

Then

$$\frac{\mathcal{D}''_{\parallel}}{\mathcal{D}_{\parallel}} = \frac{1}{u^2}\left(\frac{1}{\theta(x)}\left[-6-2x^2+(12+18x^2+4x^4)\theta\right]\right)$$

$$\frac{\mathcal{D}'_{\parallel}}{\mathcal{D}_{\parallel}} = \frac{1}{u}\left(\frac{1}{\theta(x)}\left[1-(3+2x^2)\theta(x)\right]\right)$$

and

$$\frac{\mathcal{D}_{\perp}}{\mathcal{D}_{\parallel}} = \frac{\sqrt{\pi}}{2}\,\frac{e^{x^2}\,\mathrm{erfc}(x)}{x\theta(x)} = \frac{1-\theta(x)}{2x^2\theta(x)}$$

$v(u, s')$ becomes $\tilde{v}(u, x)$. For any fixed x

$$v(u, x) = \frac{1}{u^2}\left[a_1(x)+a_2(x)u^2+a_3(x)u^4\right]$$

where

$$a_1(x) = \frac{-\ell(\ell+1)[1-\theta(x)]}{2x^2\theta(x)} + \frac{1}{\theta(x)}\left[3+x^2-(6+9x^2+2x^4)\theta(x)\right] \qquad \text{[IV-G]}$$

$$+\frac{1}{4}\left[\frac{1}{\theta(x)}(1-(3+2x^2)\theta(x))\right]^2 - \frac{1-(3+2x^2)\theta(x)}{\theta(x)}$$

$$a_2(x) = \frac{3}{2} + \frac{1}{2\theta(x)}\left[1-(3+2x^2)\theta(x)\right] \qquad \text{[IV-H]}$$

and

$$a_3(x) = -\frac{1}{4} - \frac{1}{\bar{\epsilon}\,\theta(x)} \qquad \text{[IV-I]}$$

where

$$\bar{\epsilon} = \left(\frac{\pi}{2}\right)^{\frac{3}{2}}\epsilon\,.$$

It is remarkable that this change of variables causes u and x to separate so that

$$\tilde{v}(u, x) = \sum_{i=1}^{3}\varphi_i(x)\psi_i(u)\,.$$

A way to show that $\tilde{v}(u, x)$ is everywhere negative is to show that $\tilde{v}(u, x)$ never vanishes. That is, for fixed x

$$u^2 = \frac{-a_2(x)\pm\sqrt{[a_2(x)]^2-4a_1(x)a_3(x)}}{2a_1(x)}$$

is such that u is never real and positive.

Alternatively, we can examine the behavior of $a_1(x)+a_2(x)u^2+a_3(x)u^4$ by making use of the asymptotic forms of the $a_i(x)$'s when appropriate, and using numerical techniques where asymptotic considerations aren't sufficiently accurate. We choose to follow this alternate approach.

Consider any $x > 10$. For such an x we can employ the asymptotic expansion

$$\theta(x) \sim \frac{1}{2x^2} - \frac{3}{4x^4} + \frac{15}{8x^6} - \frac{105}{16x^8} + \cdots$$

Using this expression in $\tilde{v}(u, x)$ we have

$$\tilde{v}(u, x) = \frac{1}{u^2}\left[a_1(x)+a_2(x)u^2+a_3(x)u^4\right]$$

where

$$a_1(x) \sim -\ell(\ell+1) + \frac{1}{4x^2}[23+2\ell(\ell+1)] + 0\left(\frac{1}{x^4}\right)$$

$$a_2(x) \sim \frac{3}{2}\left(1 + \frac{1}{x^2} + 0\left(\frac{1}{x^4}\right)\right)$$

$$a_3(x) \sim -\frac{2x^2}{\epsilon} - \frac{1}{4} - \frac{1}{x^2} + O\left(\frac{1}{x^4}\right)$$

For $u \geqslant 1$ and any reasonable ℓ, $a_3(x)$ causes $\tilde{v}(u, x)$ to be negative. For large ℓ and $u \geqslant 1$, or for arbitrary ℓ and any of the values of u not already considered $a_1(x)$ causes $\tilde{v}(u, x)$ to be negative.

For $x < \frac{1}{10}$.

$$\theta(x) \doteq 1 - \sqrt{\pi}\, x$$

$$a_1(x) = \frac{-\ell(\ell+1)\sqrt{\pi}}{2x} - \frac{\ell(\ell+1)\pi}{2} + \ell(\ell+1)\sqrt{\pi}\,x + \sqrt{\pi}\,x + O(x^2)$$

$$a_2(x) = \frac{1}{2} + \frac{\sqrt{\pi}\,x}{2} + O(x^2)$$

and

$$a_3(x) = -\frac{1}{4} - \frac{1}{\bar{\epsilon}}(1 + \sqrt{\pi}\,x) + O(x^2)$$

Again for $u \geqslant 1$ and reasonable ℓ, $a_3(x)$ causes $\tilde{v}(u, x)$ to be negative. For large ℓ and $u \geqslant 1$, or for arbitrary ℓ and any u not already considered $a_1(x)$ causes $\tilde{v}(u, x)$ to be negative.

This leaves the region $0.1 < x < 10$. Here asymptotic arguments are inadequate and careful numerical studies of the coefficients must be made. These studies have been carried out. For $u \geqslant 1$, $a_3(x)$ causes $\tilde{v}(u, x)$ to be negative. For small u, or large ℓ, $a_1(x)$ still maintains $\tilde{v}(u, x)$ negative.[b]

The sets of graphs (IV 1-4) show the frequency (s') dependence of the exact $v(u, s')$. The first set was drawn for $\bar{\epsilon} = 10^{-6}$, the second $\bar{\epsilon} = 10^{-3}$. The smaller ϵ is for a more dilute system. ℓ is taken to be 3. The frequencies studied were $s' = 1$, 10^{-2}, 10^{-4} and 10^{-6}. $s' = 1$ corresponds to the inverse of the time needed to complete a collision for a v_0 speed particle. $s' = 10^{-2}$ corresponds to the inverse of the time needed to traverse of mean free path for the moderately dense gas $\bar{\epsilon} = 10^{-3}$, while $s' = 10^{-4}$ is the frequency corresponding to the traverse of a mean free path for a v_0 speed particle in the $\bar{\epsilon} = 10^{-6}$ system. $s' = 10^{-6}$ is a frequency corresponding to a long time in both systems.

The agreement between the exact $v(u, s')$ and our approximate $v(u, s')$ is extremely good. For high frequencies, of course, the approximate $v(u, s')$ is defined only at high and low u. However, by the time a single mean free path is traversed the approximate $v(u, s')$ describes the behavior over nearly all u. Notice, particularly, the growing region II, corresponding to $v(u, s') = \frac{-\ell(\ell+1)}{us'}\sqrt{\frac{\pi}{2}}$.

Let us once again emphasize the effect of density on the behavior of $v(u, s')$. This is done in a final graph showing $v(u, s')$ for $\ell = 3$ and $s' = 10^{-4}$ done for different values of $\epsilon = na^3(\lambda/k_B)^2$ (see Fig. (IV-5)).

Now that we have some feel for the structure of our equation, we are in a position to find approximate solutions. Since we are dealing with a relatively simple physical situation, we can infer many of the properties of the solution before solving our equation.

Classical mechanics shows that upon the completion of a collision between a light incoming particle and an infinitely heavy stationary particle there is no energy transfer. During a collision, on the other hand, the particle will slow down as it penetrates into the repulsive energy region, and speeds up as it leaves. By considering a Gaussian potential with a peak energy λ, and by recognizing that in our low density regime it is highly probable that our test particle collides with only one other particle at a time; we expect our solution to predict that the test particle's kinetic energy will lie in a small range of values — of approximate size λ — about its initial value.

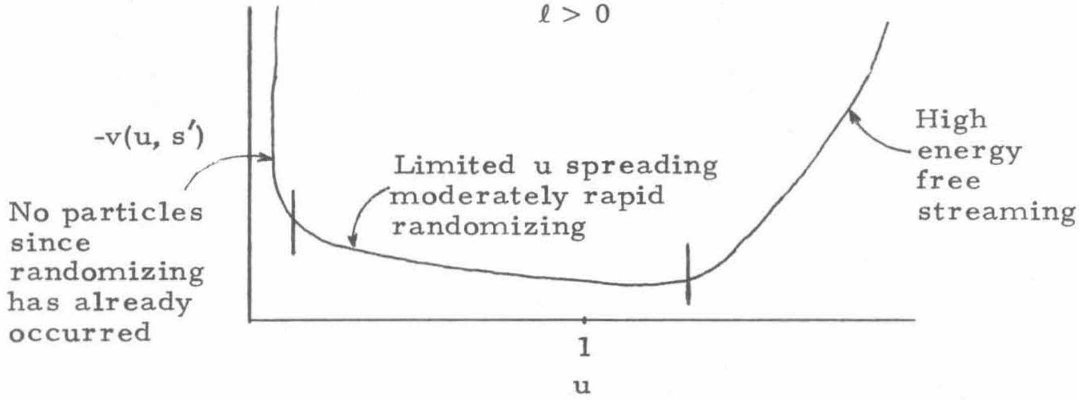
The direction of travel of a particle will be changed by a collision. As time goes on, the direction of travel becomes randomized. If the test particle starts off traveling to the right, after many collisions it is equally probably that it is traveling in any direction. More precisely, if we expand our distribution function in spherical harmonics, the $\ell > 0$ terms will die out in time, leaving the distribution isotropic. In our treatment of the approximate solutions we do the cases $\ell > 0$ and $\ell = 0$ separately.

Since a test particle is trapped in a rather narrow energy band, it is appropriate to consider the differences in behavior of test particles with differing initial energies. As we have seen, a test particle with energy $\frac{3}{2}\beta^{-1}$ has speed $v_0 = \sqrt{\frac{3}{m\beta}}$. Since $u = v/v_0$, this means that a test particle with dimensionless speed $u = 1$ is such that its kinetic energy $\gg \lambda$. Such a particle will need several collisions to change its trajectory and cause its distribution function to become isotropic.

Consider a particle with an original speed $\gg v_0$, that is, $u \gg 1$. Instead of such a particle needing several collisions to appreciably change its trajectory, it may take hundreds of collisions. Similarly, for u on the order of 10^{-4} or even lower, the energy of the corresponding test particle $\ll \frac{3}{2}\beta^{-1}$. Here we can no longer validly claim our system is weakly coupled. In fact, the coupling for these lethargic particles is rather strong, and instead of needing several collisions to become randomized, these particles will be randomized almost instantaneously.

These three energy regions correspond roughly to the three regions in $v(u, s')$ for s' small. In the region closest to the origin we should expect extremely rapid randomizing, in the second a slowly growing region where randomizing takes several collisions to occur, and in the third, high energy region, we expect essentially free streaming until enough time has elapsed that region II has spread to those large values of u and randomizing begins.

For small s′ we expect



The solutions to the equation do have these properties.

Now that we have studied v(u, s′) and have a good idea of what properties our solution must have, we reconsider

$$\frac{d^2h_\ell(u, s')}{du^2} + v(u, s')h_\ell(u, s') = 0 .$$

In region I our equation becomes

$$h_\ell''(u, s') + \left[-\frac{\ell(\ell+1)}{u^2}\right]h_\ell(u, s') = 0 .$$

Whose solution is

$$h_\ell(u, s') = Au^{\ell+1} + Bu^{-1} .$$

In the second region

$$h_\ell''(u, s') - \frac{\alpha_\ell^2 h(u, s')}{4us'} = 0 .$$

where

$$\alpha_\ell^2 = 4\ell(\ell+1)\sqrt{\frac{\pi}{2}}$$

Here

$$h_\ell(u, s') = A\sqrt{u}\, I_1\left(\alpha_\ell\sqrt{\frac{u}{s'}}\right) + B\sqrt{u}\, K_1\left(\alpha_\ell\sqrt{\frac{u}{s'}}\right)$$

And in the third region

$$h_\ell''(u, s') - \frac{u^2}{\bar{\epsilon}}\, h_\ell(u, s') = 0$$

yields

$$h_\ell(u, s') = A\sqrt{u}\, K_{\frac{1}{4}}\left(\sqrt{\frac{1}{\bar{\epsilon}}}\,\frac{u^2}{2}\right) + B\sqrt{u}\, I_{\frac{1}{4}}\left(\sqrt{\frac{1}{\bar{\epsilon}}}\,\frac{u^2}{2}\right).$$

We will soon be comparing our regional solution to WKB solutions. To facilitate this comparison and to examine limiting cases we list here various limiting forms of the regional solutions. In region I for small u

$$Au^{\ell+1} + Bu^{-\ell} \rightarrow Au^{\ell+1}.$$

In region II, whenever $\alpha_\ell\sqrt{\frac{u}{s'}}$ is large (which occurs for large ℓ, large u, or small s')

$$\sqrt{u}\, I_1\left(\alpha_\ell\sqrt{\frac{u}{s'}}\right) \rightarrow \frac{\sqrt[4]{us'}}{(2\pi\alpha_\ell)^{\frac{1}{2}}}\, e^{\alpha_\ell\sqrt{u/s'}}$$

and

$$\sqrt{u}\, K_1\left(\alpha_\ell\sqrt{\frac{u}{s'}}\right) \rightarrow \left[\frac{\pi\sqrt{us'}}{2\alpha_\ell}\right]^{\frac{1}{2}} e^{-\alpha_\ell\sqrt{u/s'}}$$

In region III since $\bar{\epsilon}$ is small and u is large, good approximations to $K_{\frac{1}{4}}(u^2/2\sqrt{\epsilon})$ and $I_{\frac{1}{4}}(u^2/2\sqrt{\epsilon})$ are

$$\sqrt{u}\,K_{\frac{1}{4}}\left(\frac{u^2}{2\sqrt{\bar{\epsilon}}}\right) \doteq \sqrt{\frac{\pi}{u}}\;\sqrt[4]{\epsilon}\;e^{-(u^2/2\sqrt{\bar{\epsilon}})}$$

$$\sqrt{u}\;I_{\frac{1}{4}}\left(\frac{u^2}{2\sqrt{\bar{\epsilon}}}\right) \doteq \frac{\sqrt[4]{\bar{\epsilon}}}{\sqrt{\pi u}}\;e^{u^2/2\sqrt{\bar{\epsilon}}}$$

An alternate, more systematic, approach toward finding approximate solutions to [IV-A] is to use the WKB method. Because $v(u, s')$ is negative for all u and $s' > 0$, the method is particularly appropriate. There will be no turning points, and no need to use connection formulae.

We approximate the solution to

$$h_\ell''(u, s') + v(u, s')h_\ell(u, s') = 0$$

by

$$h_\ell(u, s') = \frac{1}{\sqrt[4]{|v(u, s')|}}\;\exp \pm \int du \sqrt{|v(u, s')|}\quad .$$

We can now use the same arguments about $v(u, s')$ as we have used all along to simplify the solution. Instead of using the exact unwieldy $v(u, s')$ to find $h_\ell(u, s')$ explicitly, we use an approximate $v(u, s')$. This yields

WKB Solutions

$v(u, s')$	$h_\ell(u, s')$	Region
$-\frac{\ell(\ell+1)}{u^2}$	$\frac{\sqrt{u}}{\sqrt[4]{\ell(\ell+1)}}\;[u]^{\pm\sqrt{\ell(\ell+1)}}$	I
$-\frac{\alpha_\ell^2}{4us'}$	$\frac{\sqrt[4]{4us'}}{\sqrt{\alpha_\ell}}\exp \pm \left(\alpha_\ell \sqrt{\frac{u}{s'}}\right)$	II
$-\frac{u^2}{\bar{\epsilon}}$	$\frac{\sqrt[4]{\bar{\epsilon}}}{\sqrt{u}}\exp \pm \left(\frac{u^2}{2\sqrt{\bar{\epsilon}}}\right)$	III

We present a comparison of the WKB solutions vs. the regional solutions in their limiting forms.

Limiting Regional Solution	WKB	Ratio of $\frac{\text{WKB}}{\text{Regional}}$	Region
$u^{\ell+1}$	$\frac{1}{\sqrt[4]{\ell(\ell+1)}} u^{\sqrt{\ell(\ell+1)}-\frac{1}{2}}$	$\frac{1}{\sqrt[4]{\ell(\ell+1)}} u^{\left[\sqrt{\ell(\ell+1)} - (\ell+\frac{1}{2})\right]}$	I
$\frac{\sqrt[4]{us'}}{[2\pi\alpha_\ell]^{\frac{1}{2}}} e^{\alpha_\ell\sqrt{u/s'}}$	$\frac{\sqrt[4]{4us'}}{\sqrt{\alpha_\ell}} e^{\alpha_\ell\sqrt{u/s'}}$	$2\sqrt{\pi}$	II
$\left[\frac{\pi\sqrt{us'}}{2\alpha_\ell}\right]^{\frac{1}{2}} e^{-\alpha_\ell\sqrt{u/s'}}$	$\frac{\sqrt[4]{4us'}}{\sqrt{\alpha_\ell}} e^{-\alpha_\ell\sqrt{u/s'}}$	$2\sqrt{\pi}$	II
$\sqrt{\frac{\pi}{u}}\sqrt[4]{\epsilon}\; e^{-(u^2/2\sqrt{\epsilon})}$	$\frac{\sqrt[4]{\epsilon}}{\sqrt{u}} e^{-(u^2/2\sqrt{\epsilon})}$	$\frac{1}{\sqrt{\pi}}$	III
$\frac{\sqrt[4]{\epsilon}}{\sqrt{\pi u}} e^{u^2/2\sqrt{\epsilon}}$	$\frac{\sqrt[4]{\epsilon}}{\sqrt{u}} e^{u^2/2\sqrt{\epsilon}}$	$\sqrt{\pi}$	III

We see that the WKB solution is an adequate representation of the true solution in all regions. Although the WKB solutions are essentially equivalent to the regional solutions, we find it convenient to continue by using the limiting forms of the regional solutions.

To deal properly with the inhomogeneous equation we use Green's function

$$\mathcal{G}(\underline{u}, \underline{u}', t) = M^{-1}(\underline{u})K(\underline{u}, \underline{u}', t) .$$

$$f(u,t) \equiv \int d^3\underline{u}'\ M^{-1}(\underline{u}')K(\underline{u},\underline{u}',t)f(\underline{u}',t=0)\ .$$

By substituting this expression for f(u, t) into equation [III- C] we see that K(u, u′, s′) satisfies

$$s'K(\underline{u},\underline{u}',s') - \frac{\partial}{\partial\underline{u}}\cdot\underline{\underline{\mathcal{D}}}(\underline{u},s')\cdot\left(\frac{\partial}{\partial\underline{u}}+\underline{u}\right)K(\underline{u},\underline{u}',s') = M(u)\delta(\underline{u}-\underline{u}')$$

The solution to Green's function problem is significant in itself in that it tells us what happens if we start a test particle with a particular velocity $\underline{u}'$.

To solve for $K(\underline{u},\underline{u}',t)$ we use much the same technique as before. Expand $K(\underline{u},\underline{u}',t)$ in spherical harmonics.

$$K(\underline{u},\underline{u}',t) = \sum_{\ell,m} R_\ell(u,u',t)Y_{\ell m}(\hat{u})Y^*_{\ell m}(\hat{u}')$$

Then

$$R_\ell(u,u',0) = \frac{\delta(u-u')M(u)}{u^2}$$

and $R_\ell(u,u',t)$ satisfies [III- C].

By making the change of variables

$$R_\ell(u,u',s') = \frac{G_\ell(u,u',s')}{\epsilon(2\pi)^{\frac{3}{2}}}\frac{1}{\sqrt{\Delta(u)\Delta(u')}}$$

we have that

$$\frac{d^2G_\ell(u,u',s')}{du^2} + v(u,u',s')G_\ell(u,u',s') = \frac{\delta(u-u')M^{-1}(u)\epsilon(2\pi)^{\frac{3}{2}}\sqrt{\Delta(u)\Delta(u')}}{u^2\epsilon\mathcal{D}_{\parallel}} = \delta(u-u')$$

Note that $G_\ell(u,u',s')$ is an ordinary Green's function and hence is symmetric in u and u′. The change of variable is made in such a way that $R_\ell(u,u',s')$ is also symmetric in u and u′.

Consider the Green's function in the limit of small ϵ.

$$G_\ell(u, u', s') = \frac{1}{W(g_1, g_2)}[g_1(u)g_2(u')H(u-u') + g_1(u')g_2(u)H(u'-u)]$$

where $H(u-u')$ is the Heaviside step function. $W(g_1, g_2)$ is the Wronskian of the two independent solutions to the homogeneous equation g_1 and g_2. As we have done throughout this section, we will continue to consider those frequencies corresponding to times greater than a collision time.

As we have seen, for $\bar{\epsilon}$ small,

$$g_1(u) \to \sqrt{\pi/u}\,\sqrt[4]{\bar{\epsilon}}\, e^{-(u^2/2\sqrt{\bar{\epsilon}})}$$

$$g_2(u') \to \frac{1}{\sqrt{\pi u'}}\sqrt[4]{\bar{\epsilon}}\, e^{(u'^2/2\sqrt{\bar{\epsilon}})}$$

and

$$W(g_1, g_2) \to 2 .$$

For $u \geq s'$

$$K_\ell(u, u', s') \to \frac{e^{-[(u^2+u'^2)/4]}}{(2\pi)^{\frac{3}{2}}}\frac{1}{2s'}\frac{1}{\sqrt{\epsilon}}\frac{1}{\sqrt{u'u}}\, e^{-[|(u^2-u'^2)/\sqrt{\epsilon}|]}$$

We see, then, that a particle starting off with a speed u' will have a distribution function independent of time and confined to the band of energies

$$e^{-[(|u^2-u'^2|)/2\sqrt{\epsilon}]}$$

The particle will make collisions, speed up and slow down, but will be confined to an energy band whose width is determined by $na^3(\lambda/\beta)^2$. Since $K_\ell(u, u', s')$ is independent of ℓ in this approximation, the angular part of the problem sums to $\delta(\hat{\Omega}-\hat{\Omega}')$. That is,

$$K(\underline{u}, \underline{u}', s') = K(u, u', s')\delta(\hat{\Omega}-\hat{\Omega}') .$$

This is physically a contradiction. We cannot have energy changes without angular changes. This contradiction arises from our suppression of the ℓ-dependent part of $v(u, s')$. This part of $v(u, s')$ which is smaller than $-(u^2/\overline{\epsilon})$ in region III is hard to take into consideration without making the mathematics much more difficult.

As $\epsilon \to 0$ we expect free streaming to set in.

$$K(u, u', s) \doteq \frac{e^{-(u^2+u'^2/4)}}{(2\pi)^{\frac{3}{2}}} \frac{1}{s'uu'}\left[\frac{1}{2}\sqrt{\frac{uu'}{\epsilon}}\, e^{-(\sqrt{uu'}\,|u-u'|/\sqrt{\epsilon})}\right] .$$

Using the representation

$$\delta(x) = \lim_{\lambda\to\infty} \frac{\lambda}{2} e^{-\lambda|x|}$$

we have

$$K(u, u', s') = \frac{1}{s'} \frac{M(u)}{u^2} \delta(u-u') .$$

Thus

$$f(u, s') = \int du' u'^2 M^{-1}(u') \frac{1}{s'} \frac{M(u')}{u'^2} \delta(u-u') f(u', t=0)$$

becomes

$$f(u, s') = \frac{1}{s'} f(u, t=0) .$$

Consider next an $s' \to 0$ situation. The second region takes up most of the u axis, certainly that part of the u axis in which most of the particles of any reasonable initial and evolved distributions are included.

$$R_\ell(u, u', s') = \frac{1}{(2\pi)^{\frac{3}{2}} \epsilon\sqrt{\Delta(u)\Delta(u')}} \frac{\sqrt{s'}}{\alpha_\ell} \sqrt[4]{uu'}\, e^{-(\alpha_\ell\,|\sqrt{u}-\sqrt{u'}|/\sqrt{s'})} .$$

Since $\mathcal{D}_{11}(u, s') \to \frac{s'}{u^2}$ as $s' \to 0$,

$$R_\ell(u, u', s') = \frac{\sqrt{M(u)M(u')}}{(2\pi)^{\frac{3}{2}}\epsilon\sqrt{s'}} \frac{\sqrt[4]{uu'}}{\alpha_\ell} e^{-(\alpha_\ell |\sqrt{u} - \sqrt{u'}| / \sqrt{s'})}$$

Again, it would be of interest to understand this Green's function's behavior in t space. Corngold[(7)] has shown that for large γt,

$$R_\ell(u, u', t) \sim \frac{\sqrt{M(u)M(u')}}{(2\pi)^{\frac{3}{2}}\epsilon} \frac{\sqrt[4]{uu'}}{\alpha_\ell} \frac{2}{\pi\sqrt{6t}} e^{-[\frac{3}{4}\gamma^{\frac{2}{3}}(2t)^{\frac{1}{3}}]} \cos\left[\frac{3}{4}\sqrt{3}\gamma^{\frac{2}{3}}(2t)^{\frac{1}{3}}\right]$$

where

$$\gamma = \alpha_\ell |\sqrt{u} - \sqrt{u'}| .$$

Notice this predicts an exponentially damped oscillatory solution with the period increasing in time.

We can invert $R_\ell(u, u', s')$ exactly. For $\alpha > 0$

$$\mathcal{L}^{-1}\left\{\frac{1}{s^\alpha} e^{-(\gamma/s)}\right\} = \left(\frac{t}{\gamma}\right)^{\frac{\alpha-1}{2}} J_{\alpha-1}(2\sqrt{\gamma t})$$

Since we are dealing with $1/s^\alpha e^{-(\gamma/\sqrt{s})}$, we must in addition make use of the formula

$$\mathcal{L}^{-1}\{g(\sqrt{s})\} = \frac{1}{2\pi t^{\frac{3}{2}}} \int_0^\infty u\, e^{-(u^2/4t)} f(u) du$$

where

$$\mathcal{L}[f(u)] = g(s) .$$

Inverting into t space, the time behavior is

$$R_\ell(u, u', t) = \frac{e^{-[(u^2+u'^2)/4]}}{(2\pi)^{\frac{3}{2}}} \frac{\sqrt[4]{uu'}}{\alpha_\ell} \frac{1}{2\pi t^{\frac{3}{2}}} \int_0^\infty dx\, x J_0(2\sqrt{\alpha_\ell |\sqrt{u} - \sqrt{u'}|x}) e^{-(x^2/4t)}$$

Figures [IV-6] through [IV-8] show the time behavior of $\frac{1}{t^{\frac{3}{2}}}\int_0^\infty dx\, x\, e^{-(x^2/4t)} J_0(2\sqrt{\gamma x})$. Notice that as γt becomes large (≥ 30), the curves agree with the asymptotic prediction. There is an exponential damping of oscillatory solutions with variable period. Recall that this form of the Green's function is achieved in the $s' \to 0$ limit. The Tauberian theorems predict this corresponds to long times, thus, we should believe our answers only after a few collision times have past, say for $t > 4$.

Figure [IV-9] shows $R_\ell(\gamma, t)$ as a function of γ for several fixed times.

From the figures we see that the Green's function vanishes as $t \to \infty$. Physically this corresponds to the "randomizing" of the distribution function. All spherical harmonics with $\ell > 0$ are damping out, and as we shall soon show, only the $\ell = 0$ component remains. Figures [IV-6] through [IV-8] show us that as γ increases, the rate of decrease of $R_\ell(\gamma, t)$ becomes larger. Since γ is proportional to $\ell(\ell+1)|\sqrt{u} - \sqrt{u'}|$ we can infer that for fixed $|\sqrt{u} - \sqrt{u'}|$, the most anisotropic components of the distribution function will decay out the fastest. This also shows that $|\sqrt{u} - \sqrt{u'}|$ cannot be too large. If $|\sqrt{u} - \sqrt{u'}|$ is large, γ is large and at long times (for which the Green's function is valid) the distribution function is zero. This is related to the band of energies effect.

Finally, we consider the region $u < s'$, that is, extremely low energy particles. Here

$$G(u, u', s') = \frac{1}{\sqrt{\Delta(u)\Delta(u')}} \frac{1}{(2\pi)^{\frac{3}{2}}\epsilon} \frac{1}{2}\left[u^{\ell+1} u'^{-1} H(u'-u) + u^{-\ell} u'^{\ell+1} \; H(u-u')\right]$$

In this region $\mathcal{D}_{\parallel} \rightarrow c_4/s'$. The time behavior of this function is the highly singular $\delta'(t)$. That is, all of the randomizing in this region occurs at an early instant, and after even a single collision time its distribution function contains no terms with $\ell > 0$.

B. $\underline{\ell = 0}$.

The isotropic, or $\ell = 0$ component of the one particle distribution function can be analyzed in a manner similar to that used for the anisotropic components. The $\ell = 0$ component of $f(\underline{u}, s')$ is $R_{\ell=0}(u, s')$.

$$R_{\ell=0}(u, s') = \frac{1}{\sqrt{\Delta(u, s')}} h_{\ell=0}(u, s')$$

where

$$\frac{d^2 h_0(u, s')}{du^2} + v_{\ell=0}(u, s') h_0(u, s') = 0 \; .$$

$v_{\ell=0}(u, s')$ is now

$$v_{\ell=0}(u, s') = -\frac{u^2}{4} - \frac{1}{2}\frac{\mathcal{D}''_{\parallel}}{\mathcal{D}_{\parallel}} - \frac{\mathcal{D}'_{\parallel}}{\mathcal{D}_{\parallel} u} + \frac{1}{4}\left[\frac{\mathcal{D}'_{\parallel}}{\mathcal{D}_{\parallel}}\right]^2 + \frac{\mathcal{D}'_{\parallel} u}{\mathcal{D}_{\parallel}} + \frac{3}{2} - \frac{s'}{\epsilon \mathcal{D}_{\parallel}} \; .$$

Figure [IV-10] shows $v(u, s')$ for various values of s'. Notice that unlike the $\ell > 0$ case, $-v(u, s')$ is not everywhere negative. As $s' \rightarrow 0$, $-v(u, s')$ develops a turning point. Since the small s' and large s' behavior of $v(u, s')$ differ, it is important to study both limits.

We change variables from u and s', to u and x with $x = s'/\sqrt{2}u$. We study the $x \rightarrow 0$ and $x \rightarrow \infty$ limits. Writing $v(u, s')$ as $\tilde{v}(u, x)$

$$\tilde{v}(u, x) = \frac{1}{u^2}\left[a_1(x) + a_2(x)u^2 + a_3(x)u^4\right].$$

where $z_1(x)$ is the same as [IV-G] now with $\ell = 0$, $a_2(x)$ and $a_3(x)$ are precisely as [IV-H] and [IV-I] respectively. Consider the limit $x \to 0$.

$$a_1(x) \to 0$$

$$a_2(x) \to \frac{1}{2}$$

and

$$a_3(x) \to -\frac{1}{\epsilon}.$$

Considering the resultant differential equation we have

$$\frac{d^2h(u)}{du^2} + \left(\frac{1}{2} - \frac{u^2}{\epsilon}\right)h(u) = 0$$

Mazo[18] was the first to study such equations in the context of modern kinetic theory. The solution to our particular equation is

$$h_0(u, s') = AD_0\left(\frac{\sqrt{2}\,u}{\sqrt{\epsilon}}\right) + BD_0\left(\frac{i\sqrt{2}\,u}{\sqrt{\epsilon}}\right).$$

where $D_{-a}(y)$ is the Weber function of index a.

Mazo has shown that $D_{-a}(y)$ is entire in a and y. Further, for large values of y

$$D_{-a}(y) \sim y^a e^{-(y^2/4)}.$$

The Wronskian is $\sqrt{2\pi}/\Gamma(a)$. Since $\bar{\epsilon}$ is small, for all but extremely small u, our Green's function is proportional to

$$\frac{e^{-[|(u^2-u'^2)/\sqrt{\epsilon}|]}}{s'}$$

As we saw before in some detail this corresponds to the test particle being trapped in an energy band determined by the interaction strength, and density of the both. Unlike $\ell > 0$, however, this is true in the $\lim s' \to 0$. At long times the test particle's distribution function is isotropic and is determined by the initial conditions as shown above.

Consider the short time limit, that is, $s' \to \infty$. Now

$$a_1(x) \to 0$$

$$a_2(x) \to \frac{3}{2}$$

and

$$a_3(x) \to -\frac{2x^2}{\overline{\epsilon}} - \frac{1}{4}.$$

Our equation becomes

$$\frac{d^2 h(u, s')}{du^2} - \left(\frac{s'^2}{\overline{\epsilon}} - \frac{3}{2} + \frac{u^2}{4}\right) h = 0$$

The solution is $A D_{-(s'^2/\overline{\epsilon})+1}(u) + B D_{-(s'^2/\overline{\epsilon})+1}(-u)$. The Green's function can be expressed as

$$G(u, u', s') = \frac{\Gamma\left(\frac{s'}{\overline{\epsilon}} - 1\right)}{\sqrt{2\pi}} \frac{1}{\sqrt{\Delta(u)\Delta(u')}} \frac{1}{(2\pi)^{\frac{3}{2}}\epsilon} \Big[D_{-(s'^2/\overline{\epsilon})+1}(u) \overline{D}_{-(s'^2/\overline{\epsilon})+1}(-u') H(u-u')$$
$$+ D_{-(s'^2/\overline{\epsilon})+1}(u') \overline{D}_{-(s'^2/\overline{\epsilon})+1}(-u) H(u'-u) \Big]$$

Consider now the difficult problem of inverting into t space. Since $D_a(x)$ is entire, and $\mathcal{D}_{\parallel} \to c_4/s'$ as $x \to \infty$, the only singularities in this problem come from $\Gamma((s'^2/\overline{\epsilon}) - 1)$. The Gamma function is singular whenever

$$s'^2 = (1 - n)\overline{\epsilon} \qquad n = 0, 1, 2, \ldots \quad .$$

All singularities for s' large occur on the imaginary axis. (Since we are considering a large s' limit, those singularities occurring for

$|s'| \ll 1$ are suspect.) At extremely short times the distribution function is described by a superposition of periodic motions.

In this research we have derived and solved an equation describing test particle motion in a Lorentz Gas. Within the weakly coupled description, we find that the distribution function describing the test particle becomes isotropic at a rate which depends on the density and interaction strength of the system. We have solved our equation for the asymptotic forms of the Green's function in several interesting limits.

This work can be extended in a number of directions. One of the most promising possibilities is the relaxation of the assumption about mass ratios. By allowing an arbitrary ratio of the mass of the test particle to the mass of a bath particle, we consider a rather general test particle problem. The mathematical consequences of an arbitrary mass ratio will stem from the different $\underset{\sim}{\mathfrak{D}}$ tensor in the equation for $f(\underline{p}, t)$.

Another area that needs further work is in finding ways of extracting more detailed information from solutions to our equation. While our intuitive regional approximation scheme will give us clues as to the asymptotic behavior of $f(p, t)$, more detailed information awaits systematic developments.

The $\underset{\sim}{\mathfrak{D}}$ tensor is sensitive to the interaction potential used. We have found that $\underset{\sim}{\mathfrak{D}}$ develops singularities whenever the interaction potential is not an entire function. Why? What are the properties of $\underset{\sim}{\mathfrak{D}}$ common to all repulsive potentials? And so on.

We have noticed that the destruction fragment vanishes when we choose our particular Projection Operator. This raises questions as to the physical significance of this term. Quite possibly the destruction fragment contains information concerning collective motion.

These are some of the most obvious extensions of this research. There are many others. The Zwanzig approach toward solution of the N-body problem seems to hold tantalizing possibilities.

NOTES

(a) In this limit, the bath particles becomes infinitely massive but T remains constant.

(b) This is true for ϵ small which is one of our assumptions.

(c) Particles 2 through N are considered to form an equilibrium bath.

(d) f(x) will be considered dependent parametrically on k.

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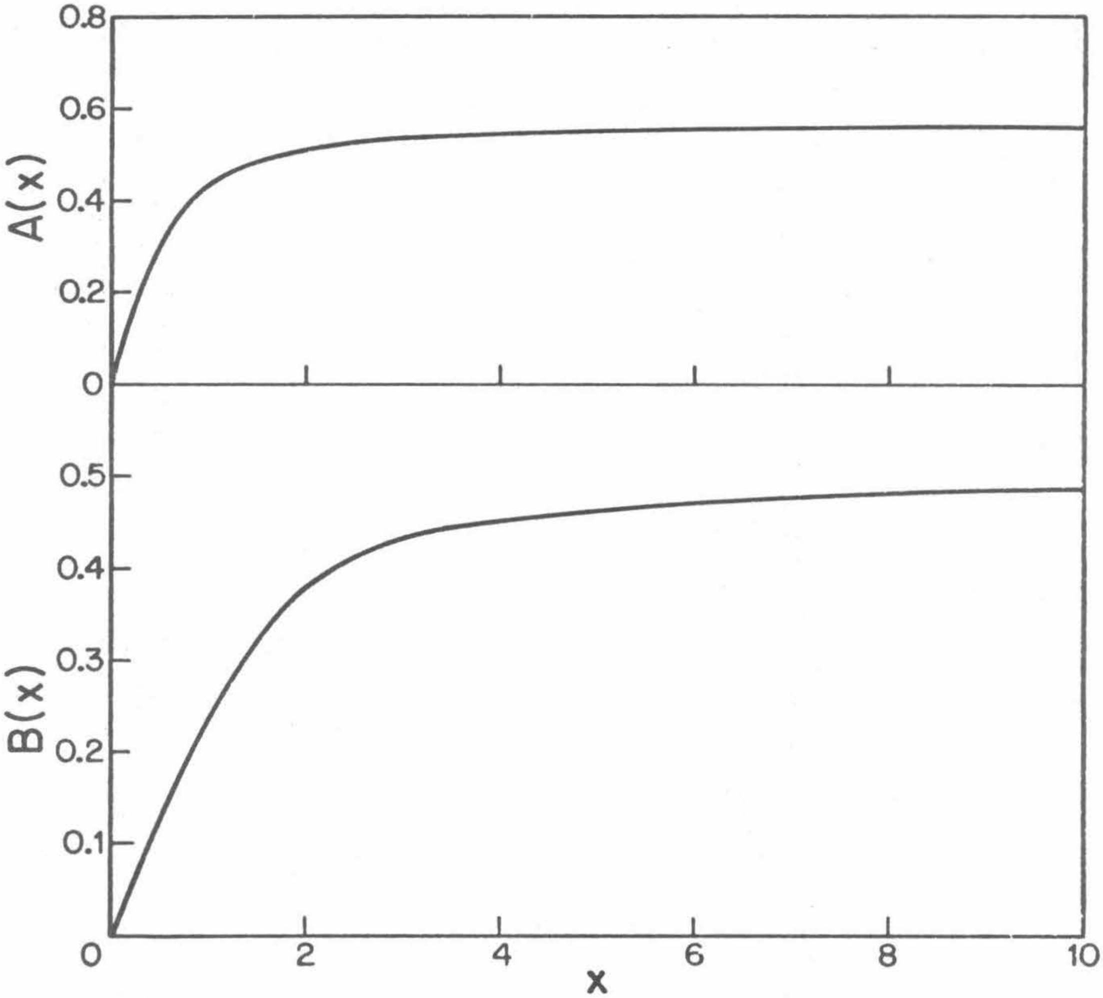

Figure [III-1].

$$A(x) = \mathcal{D}_{\perp}(x)\,\frac{2^{\frac{3}{2}}}{\pi^{2}}\,s' \qquad B(x) = \mathcal{D}_{\parallel}(x)\,\frac{\sqrt{2}}{\pi^{\frac{3}{2}}}\,s'$$

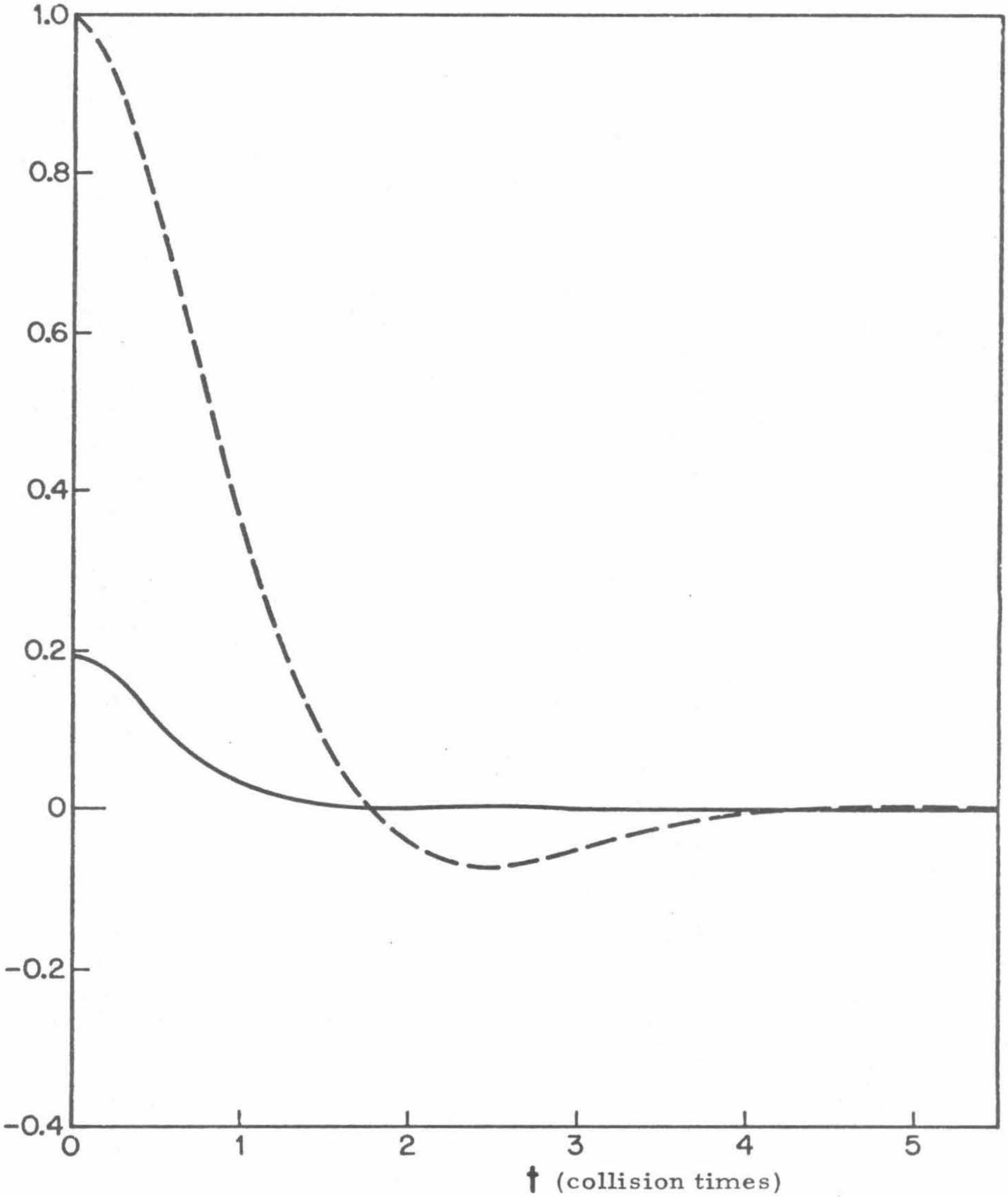

Figure [III-2].

---- velocity autocorrelation function; —— 10 × kernel; $\epsilon = \frac{\sqrt{\pi}}{2}$

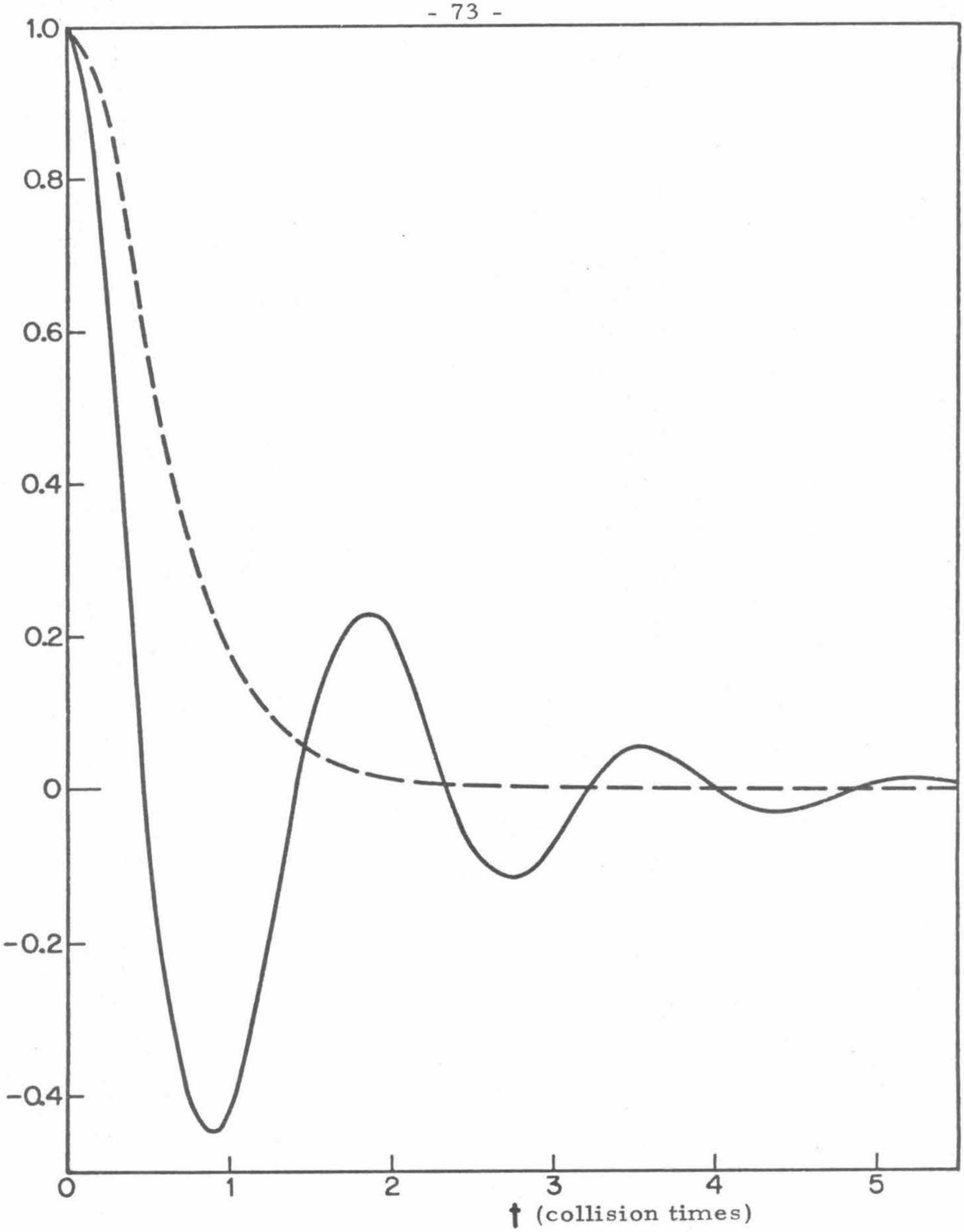

Figure [III-3].

—— velocity autocorrelation function; - - - - 10 × kernel; $\epsilon = \frac{5\sqrt{\pi}}{2}$

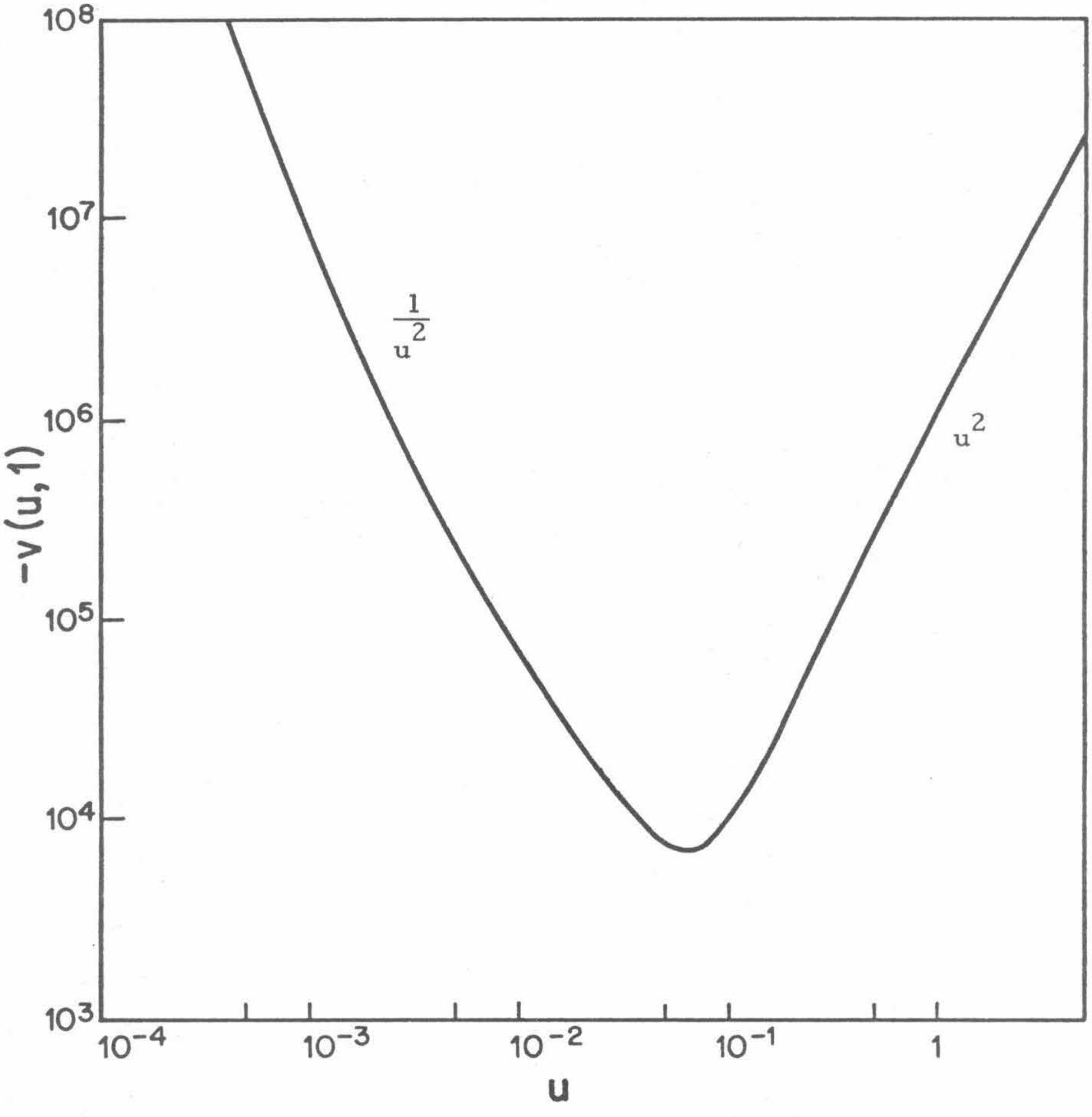

Figure [IV-1]. $s' = 1$; $\varepsilon = 10^{-6}$

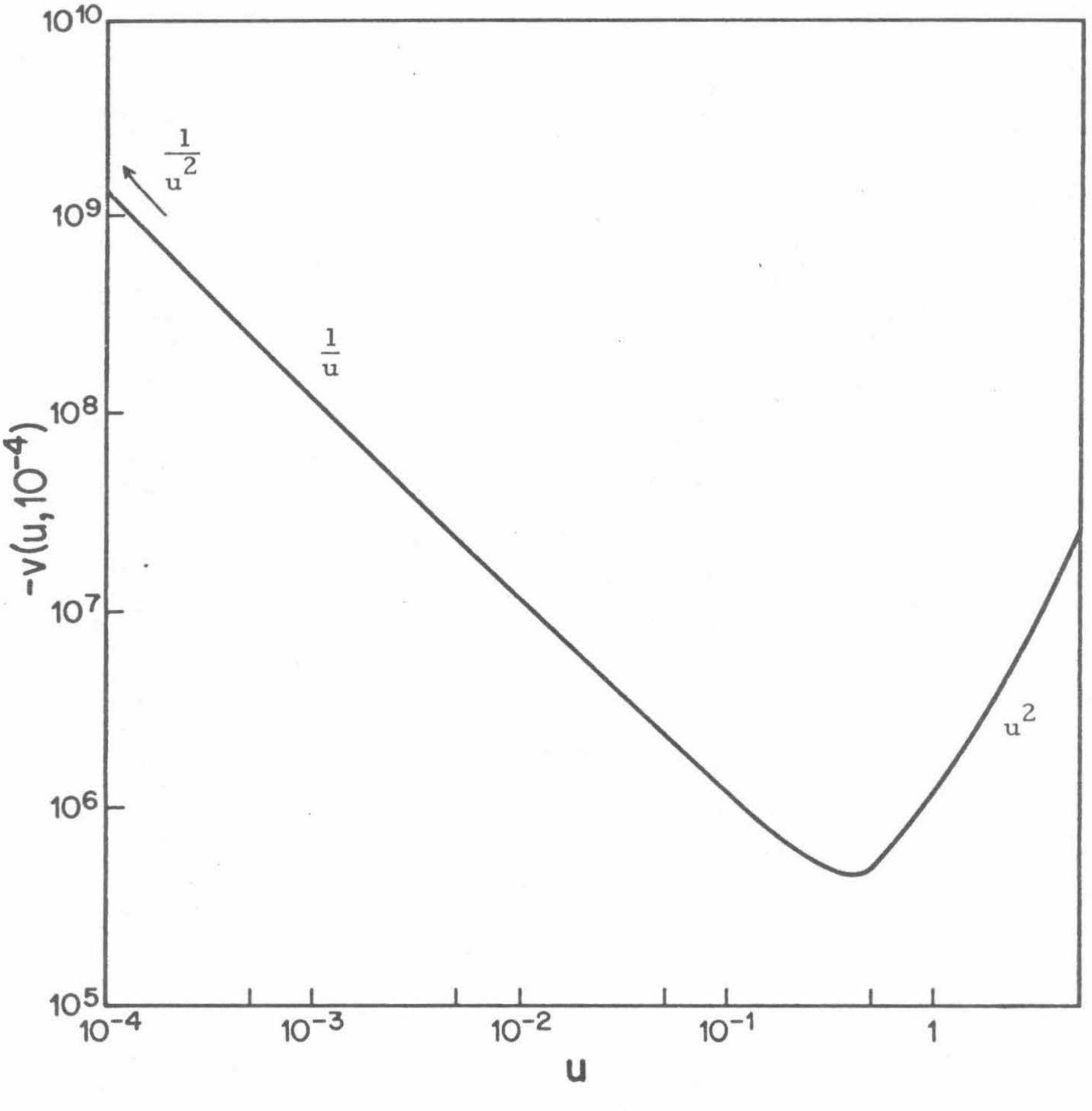

Figure [IV-2]. $s' = 10^{-4}$; $\epsilon = 10^{-6}$

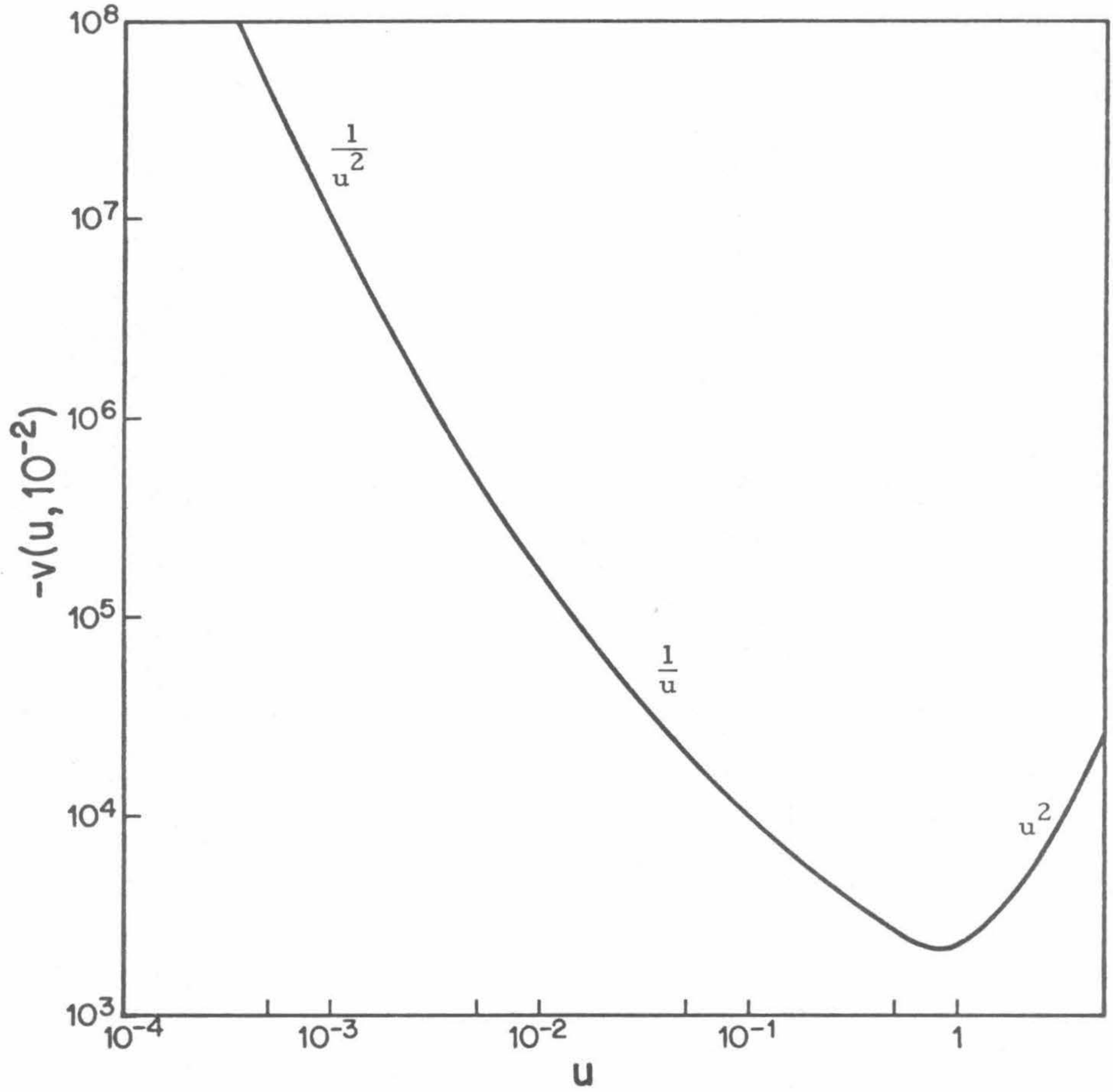

Figure [IV-3]. $s' = 10^{-2}$; $\varepsilon = 10^{-3}$

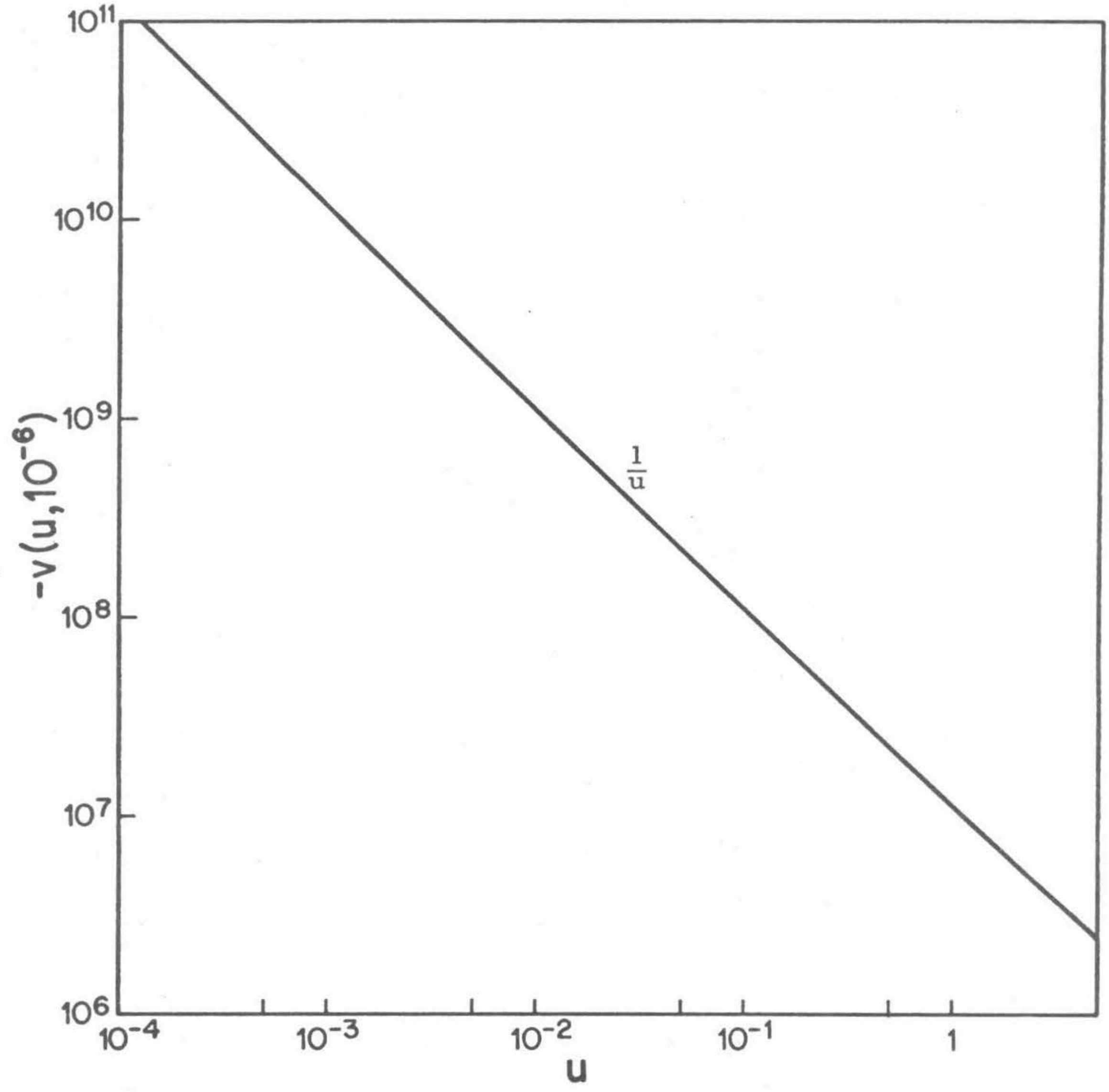

Figure [IV-4]. $s' = 10^{-6}$; $\epsilon = 10^{-3}$

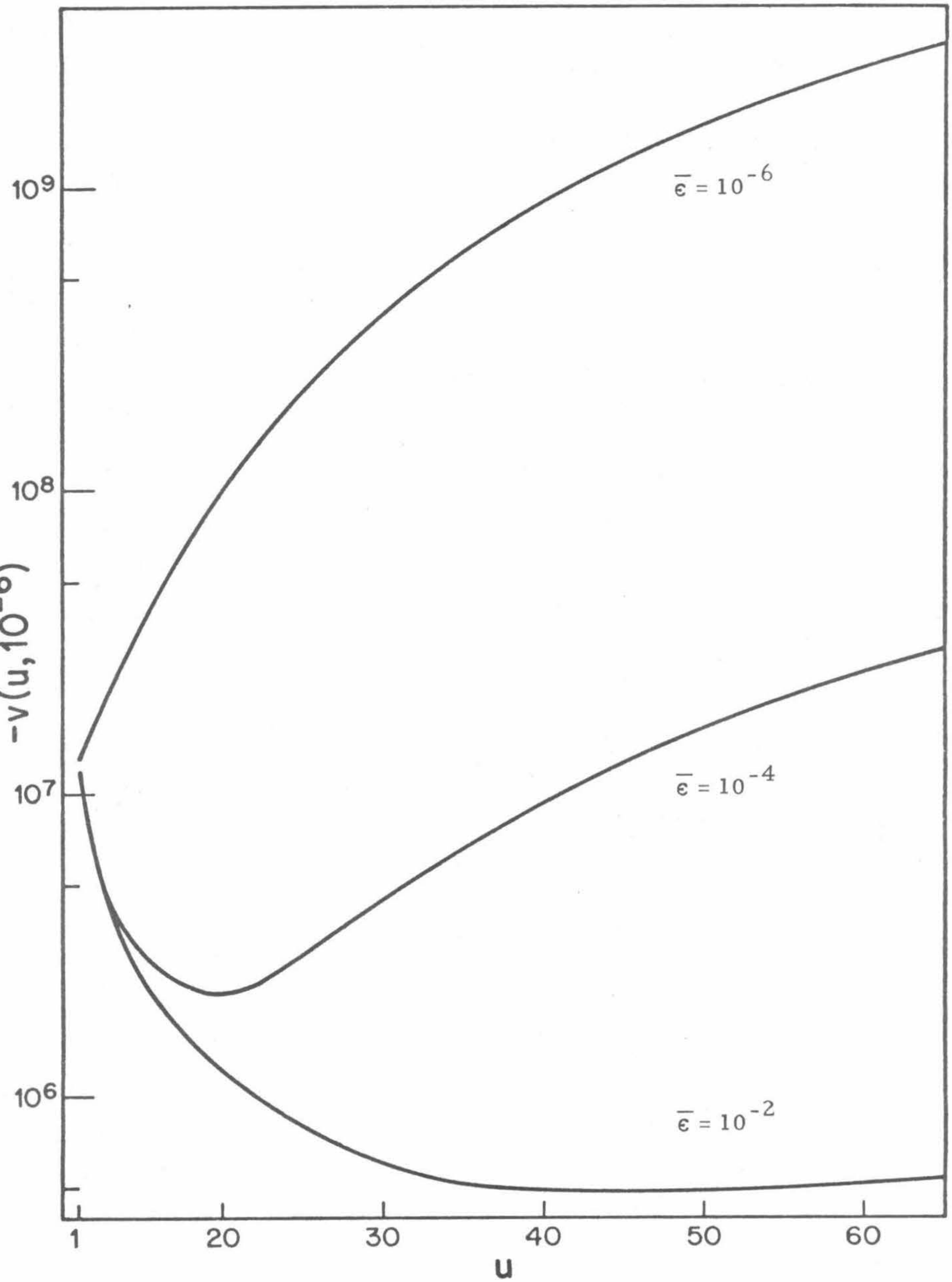

Figure [IV-5].

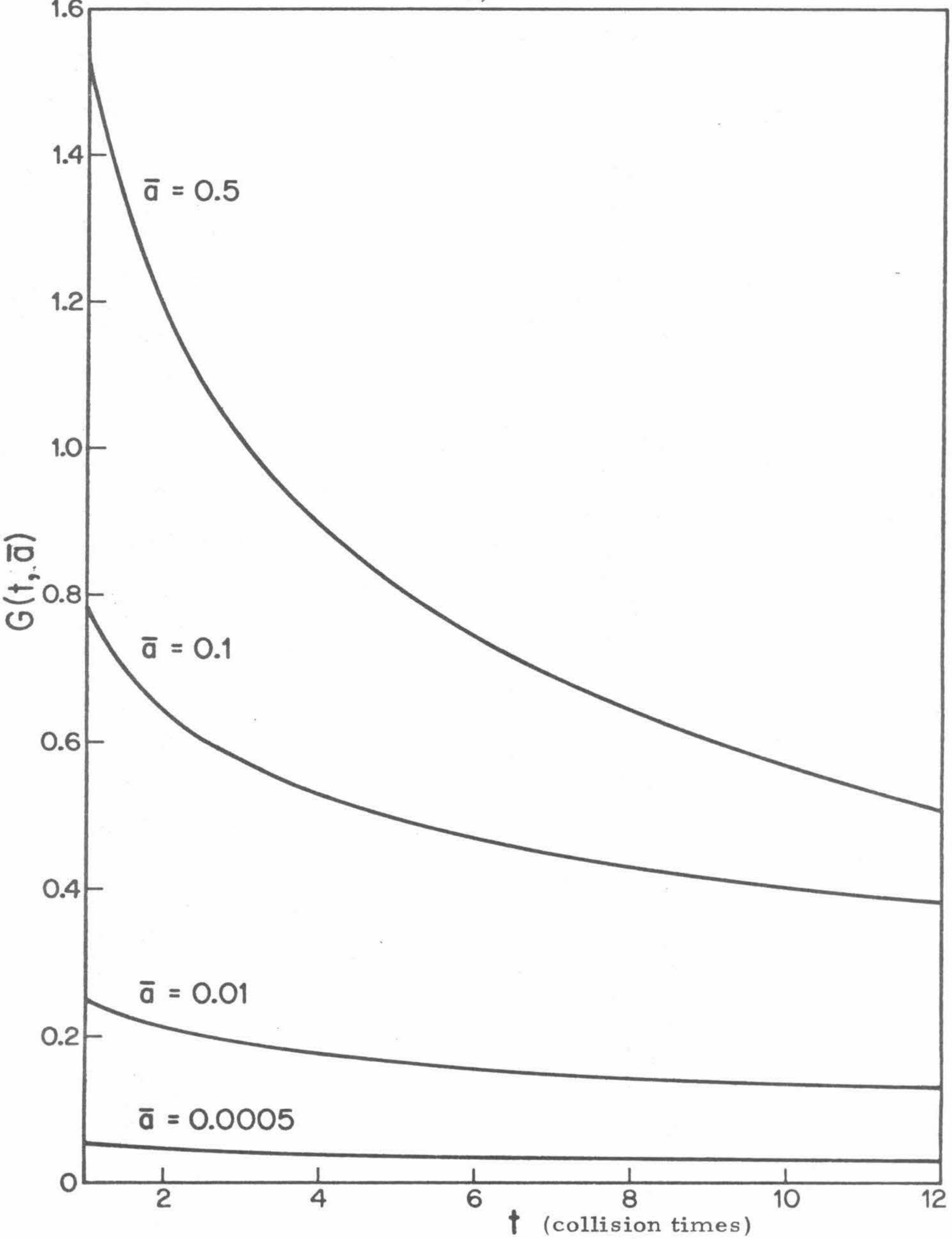

Figure [IV-6]. $(\bar{a} = \gamma)$

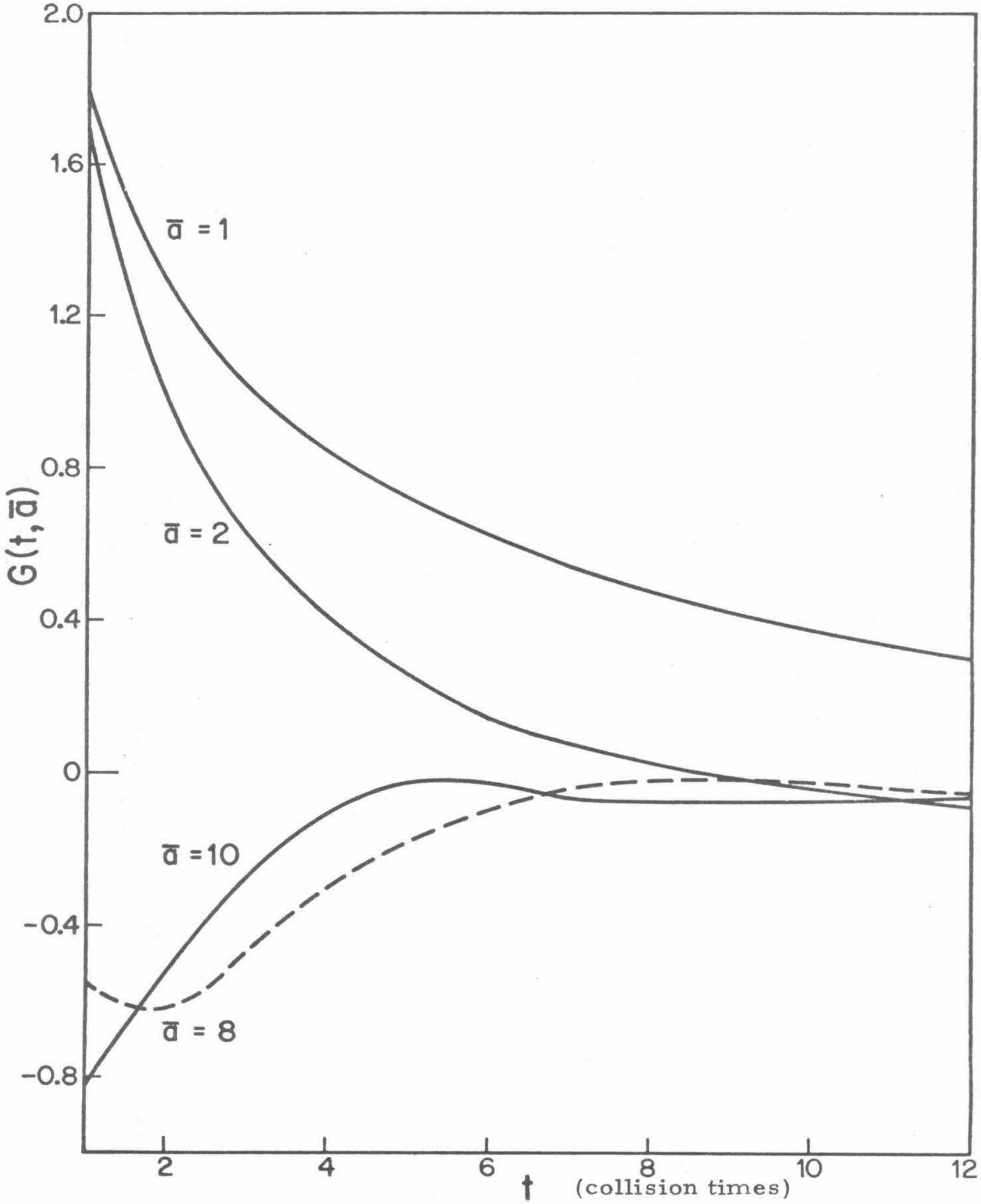

Figure [IV-7]. $(\bar{a} = \gamma)$

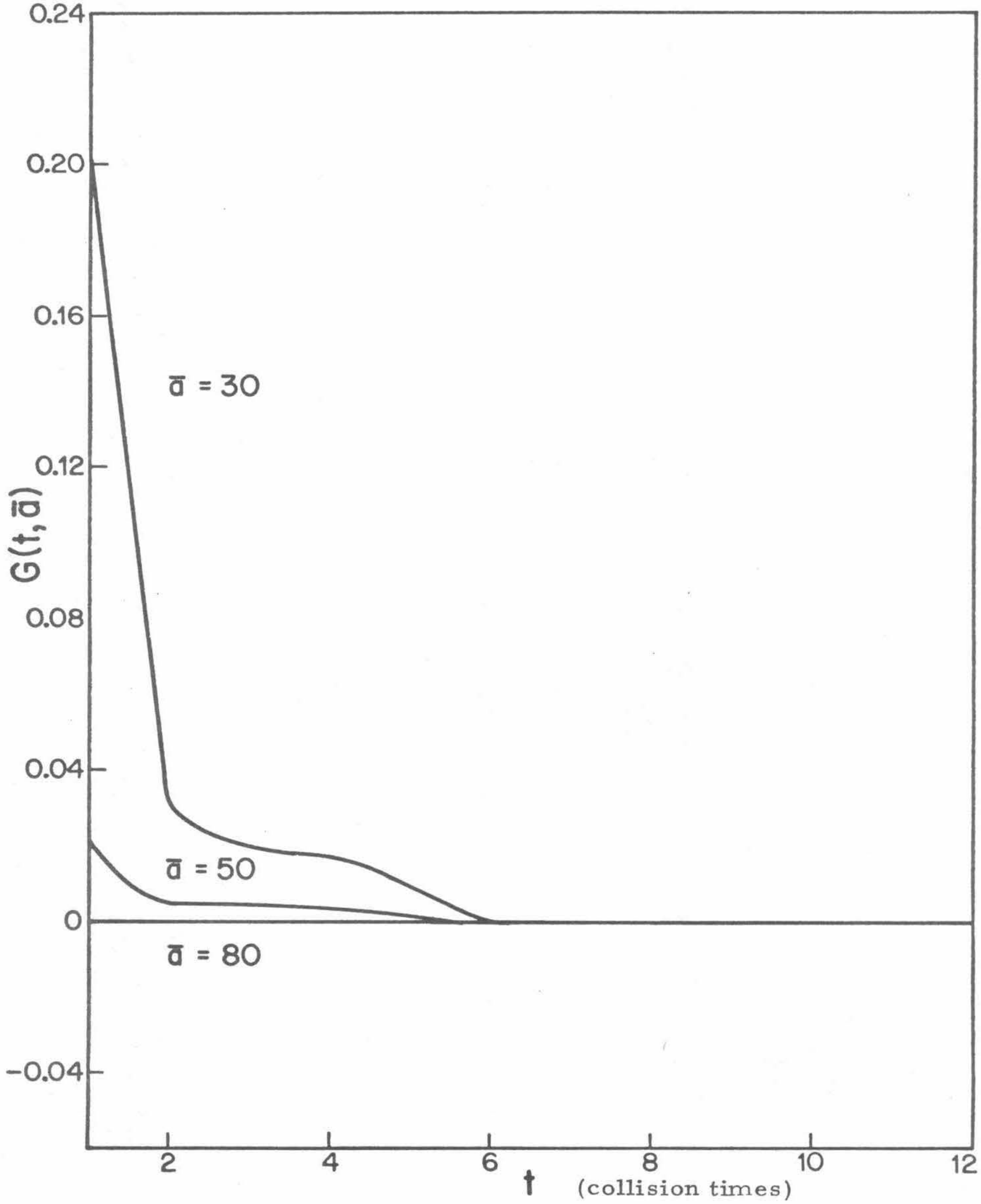

Figure [IV-8]. $(\bar{a} = \gamma)$

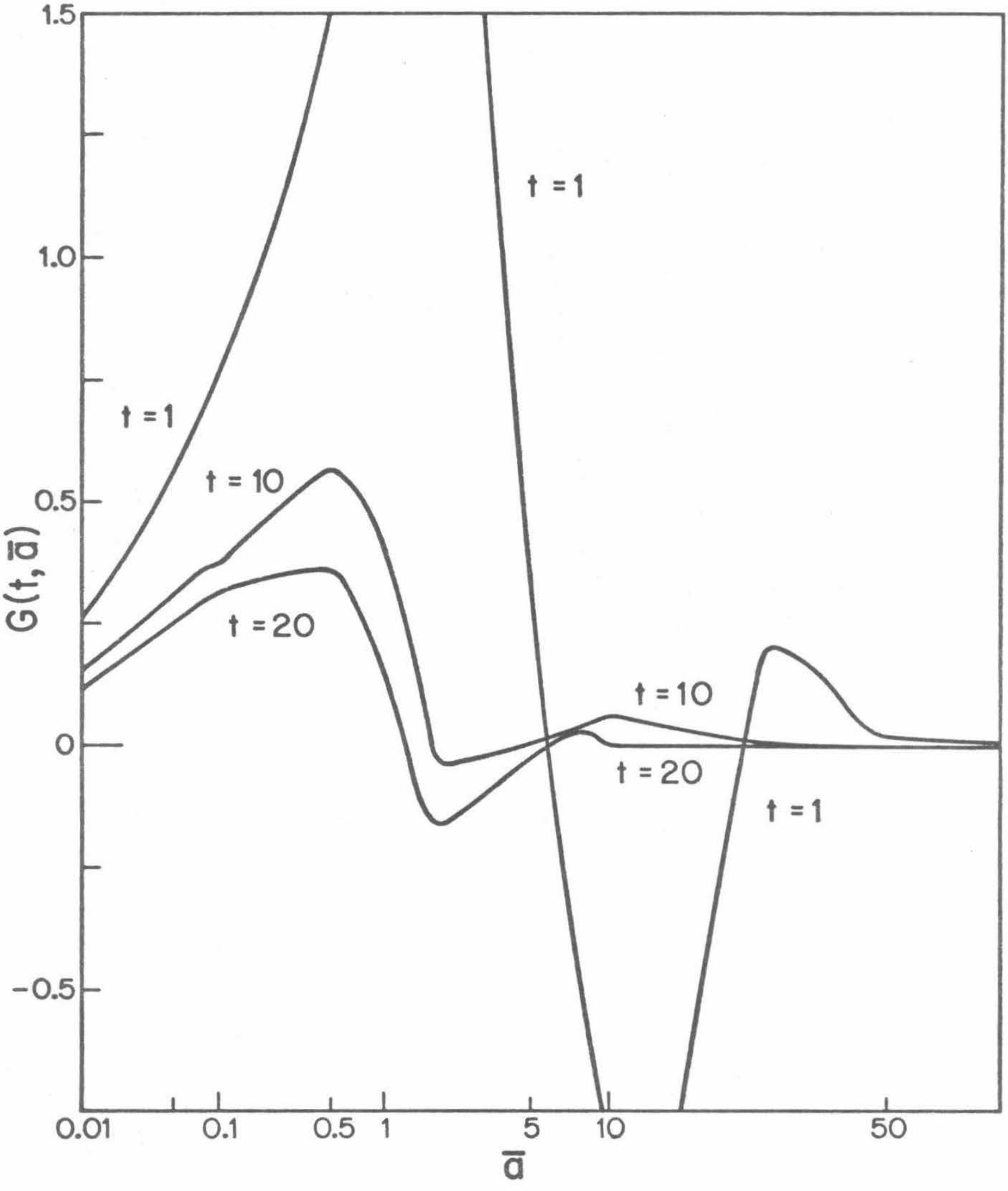

Figure [IV-9]. $(\bar{a} = \gamma)$

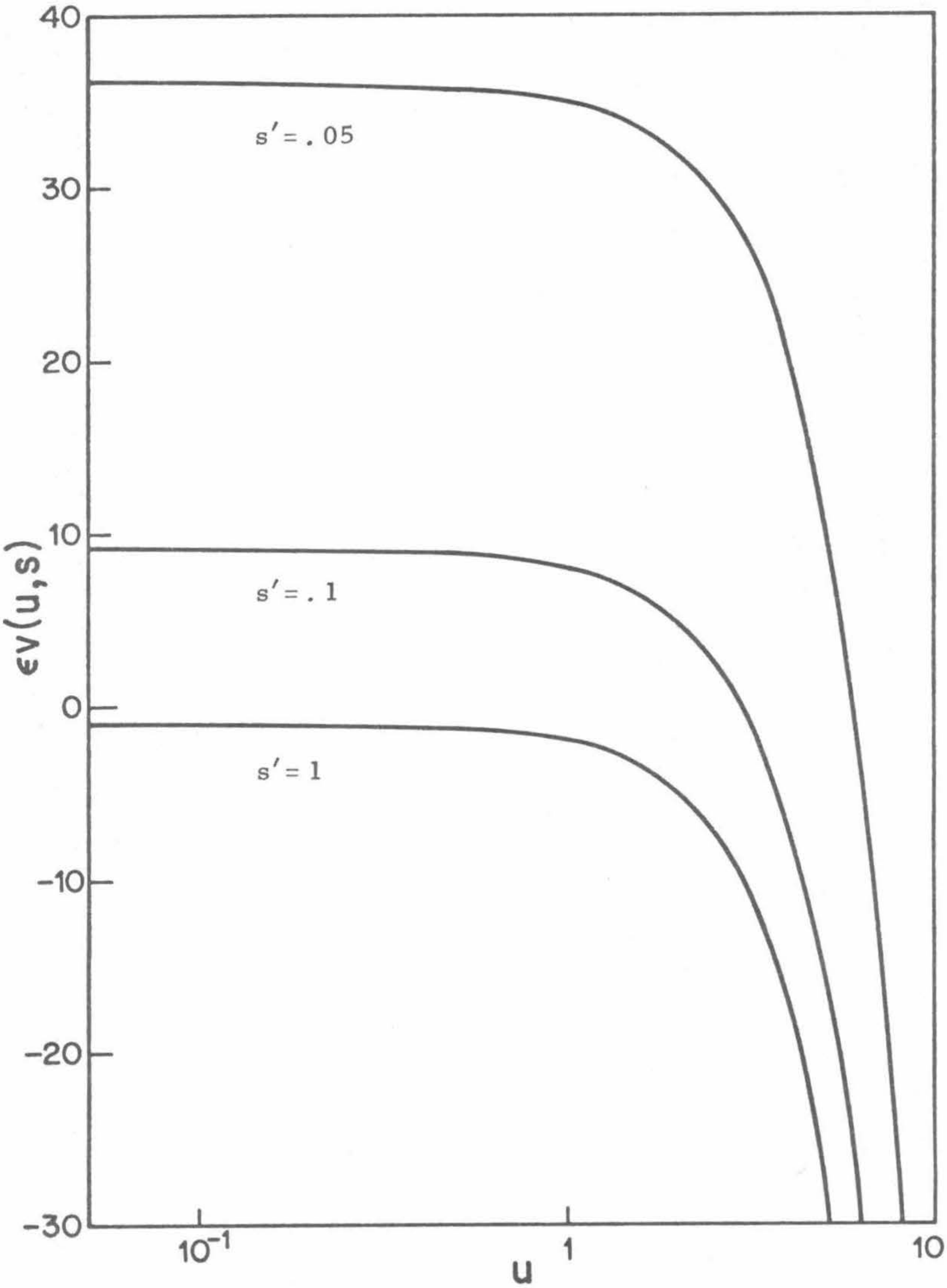

Figure [IV-10]. $\epsilon = 10^{-2}$; $\ell = 0$

Figure Captions

Figure III-1. $\mathcal{D}_{\parallel}(x)$ and $\mathcal{D}_{\perp}(x)$ are plotted as functions of x for the case of a Gaussian potential. Since $x = \frac{s'}{\sqrt{2}\,u}$, we see that for s', $\mathcal{D}_{\parallel}$ and $\mathcal{D}_{\perp}$ are monotonically decreasing functions of u.

Figure III-2. The velocity autocorrelation function and its kernel are shown for the case of a Gaussian potential. These curves are dependent on the assumption of weak coupling. t is measured in units of collision times.

Figure III-3. The same quantities are plotted for a larger $\epsilon = na^3\left(\frac{\lambda}{k_B T}\right)^2$. Notice the increased "structure" of the curve.

Figure IV-1. $-v(u, s')$ is plotted against u for $s' = 1$ and $\epsilon = 10^{-6}$. Notice that there is no region varying as $1/u$ at this high frequency, corresponding roughly to a single col-collision time.

Figure IV-2. Again, $-v(u, s')$ is plotted against u. Now that the frequency is much lower, there is a large region varying as $1/u$. As $s' \to 0$ this region predominates.

Figure IV-3. and Figure IV-4. The same effect as described in IV-1 and IV-2 is shown for a larger value of ϵ

Figure IV-5. In this graph we wish to emphasize the dependent of $v(u, s')$ on ϵ. s' is taken to be 10^{-6}. The $1/u$ dependence is most pronounced for the highest value of ϵ.

Figure IV-6. In this graph we plot the long time behavior of the

Green's function of kinetic Eq. III-C. Our system is a Lorentz gas where the test particle interacts with both particles by means of a Gaussian potential. This first graph in the series covers the range $\overline{a} = \gamma$ between .005 and .5 (see pp. 62 and 63).

Figure IV-7. This graph shows the long time behavior of the Green's function for $\overline{a}$ between 1 and 10. Note that $\overline{a}$ increases as ℓ and $|u-u'|$ increase.

Figure IV-8. This graph shows the long time behavior of the Green's function for large values of $\overline{a}$.

Figure IV-9. In this figure the Green's function of III-C is plotted as a function of $\overline{a}$ for various times (measured in collision times). Note that as $t \to \infty$, the Green's function vanishes for all $\overline{a}$.

Figure IV-10. This is $v(u;s')$ for the special case $\ell = 0$. Notice that $v(u;s')$ does change sign for s' small.