ANALYSIS OF THE GENERALIZED BOLTZMANN EQUATION

by

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ABSTRACT

The generalized Boltzmann equation derived by G.F. Mazenko is used to study the spectrum of density fluctuations in a dilute monoatomic gas of hard spheres.

The method of Kinetic modelling is used to generate numerical solutions to the initial value problem based on the Fourier and Laplace transformed kinetic equation. A set of Hermite polynomial functions, in contrast to the set of Sonine polynomial functions, is used as the basis in formulating the Kinetic modelling. This choice is motivated by the fact that at finite wave number one loses the rotational symmetry in the collision kernel. Kinetic models of different orders were formulated and their convergence properties were examined. It is found that a Kinetic model of order around 40 is sufficient to ensure numerical convergence of the solution.

The effects of the wave number dependence of the collision kernel are explicitly investigated. It is shown that deviations in the spectrum of density fluctuations from the the results of the linearized Boltzmann equation can be as much as 10-20%. Such differences appear to be within the resolutions of a careful inelastic neutron scattering experiment.

Our results also show that the two calculations should not be significantly different for $kr_o \leq 0.005$ where k is the wave number of the density fluctuations and r_o the hard sphere diameter.

It is shown that the self-correlation spectrum is no different from that calculated with the neutron transport equation. This is due to the fact that in the case of the self-correlation there is essentiallly no difference between the kernels of the two equations.

Thesis Suprevisor: Sidney Yip

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CHAPTER 1

Introduction

1-1 Background

It is now generally acknowledged that time correlation functions are the fundamental quantities in the description of transport processes and scattering phenomena(20). The Fluctuation-Dissipation theorem has shown that the linear response of a system to an external disturbance can be expressed in terms of time dependent correlations in the equilibrium ensemble(6). In other words the fluctuation phenomena of a system in equilibrium can be related to the behaviour of the system under an external driving force. Actually, what is normally computed is the space-time Fourier transform of these correlation functions. This is because the Fourier spectrum of certain of these functions can be related to the results of scattering experiments on gases and the following discussion applies primarily to this category of phenomena although the results may also be applied to include other kinds of experiments. We consider only classical correlation functions.

The first such spectrum to be used was the spectrum of the density-density correlation function $G(\underline{r},t)$ (1),

$$G(\underline{r}-\underline{r}', t-t') = \frac{1}{n} \left\langle \sum_{ij} \delta(\underline{r}-\underline{R}_i(t))\, \delta(\underline{r}'-\underline{R}_j(t')) \right\rangle \tag{1-1}$$

where n is the uniform number density and $\langle\ \rangle$ denotes an average of the particle phase co-ordinates over an equilibrium distribution usually taken to be a canonical ensemble.

By invoking the Fluctuation-Dissipation theorem, the correlation function $G(\underline{r},t)$ can be calculated from the density response. This approach implies that the equations describing the behaviour of the system's density are known.

When the long wavelength and small frequency region of the density correlation function is to be examined, the hydrodynamic equations can be used to study $G(\underline{r},t)$ (13). But when the wavelengths become comparable to the molecular mean free path and the frequency becomes comparable to the molecular collision frequency, Kinetic equations have to be used because the continuum description is no longer valid. The Boltzmann equation and the neutron transport equation are such equations and they have been used to compute the spectrums of $G(\underline{r},t)$ and the self correlation function $G_s(\underline{r},t)$ (15,5).

However even these equations break down when the wavelengths are comparable to the particle dimensions and the times are comparable to the collision duration. Mathematically this is due to the fact that the kernels in the collision integrals of those equations are frequency and wavelength independent.

The problem then, is to formulate generalized Kinetic equations which are valid for all wavelengths and all frequencies. This has been done using projection operator techniques (9,11). By applying such techniques to the phase space of the system, the more fundamental* complex fluctuation function

$$S(\underline{k}, \underline{\xi}\,\underline{\xi}', z) = \int \frac{d\omega}{2\pi} \frac{S'(\underline{k}, \underline{\xi}\,\underline{\xi}', \omega)}{(\omega - z)} \tag{1-2}$$

can be shown to satisfy an equation of the form

$$(z - \underline{k}\cdot\underline{\xi}\, v_0)\, S(\underline{k}, \underline{\xi}\,\underline{\xi}', z) - \int d^3\bar{\xi}\, M'(\underline{k}, \underline{\xi}\,\bar{\underline{\xi}}, z)\, S(\underline{k}, \bar{\underline{\xi}}\,\underline{\xi}', z) = -S^{\circ}(\underline{k}, \underline{\xi}\,\underline{\xi}') \tag{1-3}$$

The transformed initial condition $\overset{\circ}{S}(\underline{k}, \underline{\xi}\,\underline{\xi}')$ is given by

$$S^{\circ}(\underline{k}, \underline{\xi}\,\underline{\xi}') = n\left[\Phi(\xi)\, \delta(\underline{\xi} - \underline{\xi}') + \Phi(\underline{\xi})\, n h(k)\, \Phi(\underline{\xi}')\right] \tag{1-4}$$

where we have used the following non-dimensional momentum variables

$$\underline{\xi} = \underline{P} / m v_0 \qquad \text{and} \qquad v_0^2 = (m\beta)^{-1} \tag{1-5}$$

The function

$$\Phi(\underline{\xi}) = (2\pi)^{-3/2} e^{-\xi^2/2} \tag{1-6}$$

---

*G($\underline{r}$,t) can be obtained from this by carrying out the appropriate transform inversions, limiting process and various momentum integrals.

is the Maxwellian velocity distribution, h($\underline{k}$) is the transformed total correlation function and $M'(\underline{k}, \underline{\xi}\,\underline{\xi}', z)$ is the memory function for the one particle distribution function. Before further discussion of equation (1-3), it should be noted that we can relate $S(\underline{k}, \underline{\xi}\,\underline{\xi}', z)$ to a correlation function as

$$S'(\underline{k}, \underline{\xi}\,\underline{\xi}', \omega) = \int d^3(\underline{r}-\underline{r}') \int d(t-t') \Big[S(\underline{r}-\underline{r}', \underline{\xi}\,\underline{\xi}', t-t') \, e^{-i\underline{k}\cdot(\underline{r}-\underline{r}') + i\omega(t-t')} \Big] \qquad (1\text{-}7)$$

where

$$S(\underline{r}-\underline{r}', \underline{p}\,\underline{p}', t-t') = \langle \, (f(\underline{r}\,\underline{p}\,t) - \langle f(\underline{r}\,\underline{p}\,t) \rangle_{eq} \; (f(\underline{r}'\underline{p}'t') - \langle f(\underline{r}'\underline{p}'t')_{eq} \rangle) \, \rangle_{eq} \qquad (1\text{-}8)$$

is the equilibrium fluctuation function of the phase space density operator

$$f(\underline{r}\,\underline{p}\,t) = \sum_{\alpha} \delta(\underline{r} - \underline{r}^{\alpha}(t)) \, \delta(\underline{p} - \underline{p}^{\alpha}(t)) \qquad (1\text{-}9)$$

Equation (1-3) has the form of the desired generalized equation, and the problem is now to find a tractable form for $M'(\underline{k}, \underline{\xi}\,\underline{\xi}', z)$. There are basically two approaches to surmount this obstacle. The first is to postulate phenomenological models (16) and the other is to evaluate the memory function exactly for special systems.

The second approach is what concerns us in this thesis. Upto the present, only two useful approximations to the memory function have been derived. The first is a weak coupling expansion to obtain the memory function to second order in the interaction potential (4,11). This approximation is only good in the case of weakly coupled fluids. Unfortunately weak coupling excludes hard core interactions. So this method cannot be applied to real fluids.

The other procedure, derived by Mazenko, involves an expansion to the lowest order in the density but it is valid for all interactions. It can therefore be applied to real dilute gases. Mazenko has shown that his low density memory function reduces to the linearized Boltzmann collision kernel in the low frequency and long wavelength limit. It also satisfies certain sum rules and is consistent with the conservation laws. In the present work we will be concerned only with the Mazenko equation.

Present Research

In this thesis we apply the Mazenko equation to the analysis of neutron scattering in gases. To obtain the spectrum of the scattered neutron beam we have to calculate the generalized structure factor $S(\underline{k},\omega)$ which is the space-time transform of the two body correlation function of the gas (1). This is the $G(\underline{r},t)$ mentioned earlier.

When the complex fluctuation function is expanded in terms of a modified Hermite polynomial basis, one of the co-efficients of expansion turns out to be $S(k,\omega)$. We therefore expanded equation (1-3) in terms of that basis. This equation was then approximated for computational analysis. The approximation method used was that of Kinetic modelling (3). The linear system of algebraic equations obtained through this approximation was then solved numerically on the computer to yield the desired spectrum $S(k,\omega)$.

Our results should be good for all values of the wavelength and frequency since Mazenko's memory function is the correct wavelength and frequency dependent generalization of the linearized Boltzmann collision operator. In the case of the hard sphere gas it brings in an additional parameter kr_0 which is a measure of the wavelength in terms of the particle dimensions. In the limit where the wavelength is long compared to the particle dimensions our results reduce to those obtained using the Boltzmann equation as they should. But at finite kr_0 where the Boltzmann equation is no longer valid, our results do show significant deviations from Sugawara's results (13). Thus within the restriction of low density, we are able to delineate the region of validity for the Boltzmann equation and obtain quantitative corrections for wavelengths outside this region.

Besides the spectrum of the density correlation function, we have also obtained the spectrum for the Van-Hove self-correlation. This function appears in the theory of incoherent neutron scattering and it is related to the phenomenon of diffusion in the fluid (20). The calculation is a by-product of the density correlation calculation since the memory function for the self-correlation turns out to be the $kr_0 \to \infty$ limit of the homogeneous part of the memory function for the density correlation. Both correlation functions therefore can be obtained from a single calculation.

In the following chapter a classical derivation is given of Mazenko's result for the memory function valid for a general two-body potential. We then discuss the reduction of this memory function to the Boltzmann collision operator in the appropriate limit. The final section of the chapter is devoted to the hydrodynamical description of the continuum region. Certain transport co-efficients are tied in with the solution of the hydrodynamic equations and are specialized to the case of the hard core gas. For eventual comparision purposes the general analytic expressions for $S(k,\omega)$ in the hydrodynamical region is given. Once again we specialize it to the hard core case.

Chapter three sets up in detail the calculations for $S(k,\omega)$ and the self-correlation spectrum $S(k,\omega)$.

The Kinetic model is also discussed in this chapter and particular attention is paid to the fact that our basis is not the conventional Sonine Polynomial. We have chosen to work with a modified version of the Hermite polynomials, thus bringing in questions of convergence to be examined later. The problem of ordering such a truncated basis is touched upon and reasons are given for our various schemes. The last section of this chapter examines the connection and consequences of the different transform definitions used by Mazenko and Sugawara. This is important as we intend to use Sugawara's results as a means of checking our computations.

In chapter four we reduce the general operator derived in chapter two to our special case of the hard core gas. The matrix elements needed for the Kinetic model calculation are also presented in this chapter with an explanatory note on their computation. We also discuss properties of these elements such as the variation with the parameter kr_o.

The numerical results we have obtained are presented and discussed in chapter five. Finally, chapter six summarizes possible experimental work based on our results and also indicates our general plans for future work along these lines.

CHAPTER 2

The Generalized Kinetic equation of Mazenko

2-1 Introduction

We begin this chapter by presenting a derivation of Mazenko's low density memory function $\Sigma(\underline{k},\underline{pp}',z)$ in section 2-2. We will show that it can be written as a sum of two parts

$$\Sigma(\underline{k},\underline{p}\underline{p}',z)=\Sigma^{(s)}(\underline{k},\underline{p}\underline{p}',z)+\Sigma^{(c)}(\underline{k},\underline{p}\underline{p}',z) \qquad (2\text{-}1)$$

$\Sigma^{(s)}(k,pp, z)$ can be thought of as the mean field on one particle due to all the others and is known as the static part of the memory function. $\Sigma^{(c)}(\underline{k},\underline{pp}, z)$ is the collision part. We will show that this part in its turn can be written as a sum of two parts.

$$\Sigma^{(c)}(\underline{k},\underline{p}\underline{p}',z)=\Sigma_{I}^{(c)}(\underline{k},\underline{p}\underline{p}',z)+\Sigma_{H}^{(c)}(\underline{k},\underline{p}\underline{p}',z) \qquad (2\text{-}2)$$

$\Sigma_{I}^{(c)}(\underline{k},\underline{pp},z)$ is what Mazenko (2) calls the inhomogeneous term while $\Sigma_{H}^{(c)}(\underline{k},\underline{pp},z)$ is the homogeneous term.

With the analytic form of $\Sigma(\underline{k},\underline{pp},z)$ in hand, we then show, in section 2-3, that it can be reduced to the linearized Boltzmann collision operator in the long time and long distance limit. This means that our calculations for the density spectrum using Mazenko's generalized Kinetic equation should, in the long time and long distance limit, give the same results as those using the Boltzmann equation.

Finally we conclude the chapter by briefly discussing the hydrodynamic regime[+].

2-2 Derivation of the low density Memory function

Instead of discussing Mazenko's quantum mechanical derivation of his memory function we will follow Boley (8) and give a classical derivation of the low density result.

The classical correlation function $S(\underline{r}-\underline{r}', \underline{pp}, t-t')$ obeys equation (3-1a). If we Fourier and Laplace transform this equation using

$$S(\underline{k}, \underline{p}\underline{p}', t) = \int d^3r\, e^{-i\underline{k}\cdot\underline{r}}\, S(\underline{r}, \underline{p}\underline{p}', t) \qquad (2\text{-}3)$$

$$S(\underline{k}, \underline{p}\underline{p}', z) = i\int_0^\infty dt\, e^{izt}\, S(\underline{k}, \underline{p}\underline{p}', t) \qquad (2\text{-}4)$$

we obtain

$$\begin{aligned}(z - \underline{p}\cdot\frac{\underline{k}}{m})\, S(\underline{k}, \underline{p}\underline{p}', z) &+ S(\underline{k}, \underline{p}\underline{p}', t=0) \\ &= \int d^3\bar{p}\, \Sigma(\underline{k}, \underline{p}\underline{p}'; z)\, S(k, \underline{p}\underline{p}', z)\end{aligned} \qquad (2\text{-}5)$$

Boley's idea was to expand S(k,pp,z) and $\Sigma(\underline{k}, \underline{pp}, z)$ in a fugacity series

$$S(\underline{k}, \underline{p}\underline{p}', z) = y S_1 + y^2 S_2 + O(y^3) \ldots .$$

$$\Sigma(\underline{k}, \underline{p}\underline{p}'\, z) = \Sigma_0 + y\Sigma_1 + O(y^2) \qquad (2\text{-}6)$$

[+] The reader should consult Appendix A if he desires the detailed mathematical steps behind the results quoted in this chapter.

, where y is the fugacity, and use equation (2-5) to relate the coefficients of expansion in the two series.

This method leads to the following equations for S_1 and S_2

$$(z - \underline{k}\cdot\underline{p}/m)\,S_1 + S_1^{\circ} = \int d^3\bar{p}\;\Sigma_0\,S_1 \tag{2-7a}$$

$$(z - \underline{k}\cdot\underline{p}/m)\,S_2 + S_2^{\circ} = \int d^3\bar{p}\;\Sigma_1\,S_1 \tag{2-7b}$$

where S_1° and S_2° are the respective initial conditions. For convenience we do not write out the arguments of S_i, S_i^{0}, and Σ_i, i=1, 2. The relationship between fugacity and density is (26)

$$\left(\beta\frac{h^2}{2\pi m}\right)^{3/2} y = n\left\{1 - n\int d^3r\, f(r) + O(nr_0^3)^2\right\} \tag{2-8a}$$

where $$f(r) = e^{-\beta V(r)} - 1 \tag{2-8b}$$

Thus Σ_1 should also be the memory function to first order in the density.

Now we are left with the problem of calculating the terms S_1 and S_2. We use the grand canonical ensemble to evaluate these terms,

$$\langle F\rangle = P^{-1}(\beta y V)\sum_{N=0}^{\infty}\frac{y^N}{N!\,h^{3N}}\int d1\ldots dN\Big(e^{-\beta H_N(1\ldots N)}\,F(1\ldots N)\Big) \tag{2-9}$$

where $1 = (r_1, p_1)$, H_N is the Hamiltonian of the N particle system, h is Planck's constant, P is the grand partition function and the limit $V\to\infty$ has to be taken to complete the averaging process. The grand canonical ensemble thus leads logically to a fugacity expansion and we find,

$$S_1(\underline{r}, \underline{p}\,\underline{p}', t) = \delta(\underline{r} - \underline{p}t/m)\, \phi(p)\, \delta(\underline{p} - \underline{p}') \qquad (2\text{-}10)$$

$$S_2(\underline{r}, \underline{p}\,\underline{p}', t) = \frac{1}{2!} \int d1\, d2\, \phi(p_1)\, \phi(p_2) \Big\{ e^{-\beta V(r_1 - r_2)} \Big[e^{itL(12)} \sum_{i=1}^{2} \delta(x - x_i) \Big] \sum_{j=1}^{2} \delta(x' - x_j) - \sum_{i=1}^{2} \Big[e^{itL_0(12)} \delta(x - x_i) \Big] \delta(x' - x_j) \Big\} - \phi(p)\, \phi(p') \qquad (2\text{-}11)$$

L is the two-body Liouville operator

$$iL_0(12) = p_1 \cdot \nabla_1 / m + p_2 \cdot \nabla_2 / m \qquad (2\text{-}12)$$

$$iL_1(12) = -\nabla_1 V(\underline{r}_1 - \underline{r}_2) \cdot \big[\partial/\partial \underline{p}_1 - \partial/\partial \underline{p}_2 \big] \qquad (2\text{-}13)$$

$$iL(12) = iL_0(12) + iL_1(12) \qquad (2\text{-}14)$$

The form of S_1 and equation (2-7a) tells us that S_1 evolves by free streaming. Thus Σ_0 is zero.

If we substitute for S_1 in equation (2-7b) we find that

$$\Sigma_1(\underline{k}, \underline{p}\,\underline{p}', z)\, \phi(p') = -[z - \underline{k} \cdot \underline{p}'/m] \big\{ (z - \underline{k} \cdot \underline{p}/m)\, S_2(\underline{k}, \underline{p}\,\underline{p}', z) + S_2^0(\underline{k}, \underline{p}\,\underline{p}') \big\} \qquad (2\text{-}15)$$

To reduce equation (2-13) further we make use of the fact that

$$(\partial/\partial t + \underline{p} \cdot \nabla/m)(\partial/\partial t + \underline{p}' \cdot \nabla/m)\, S_2(\underline{r}, \underline{p}\,\underline{p}', t) = -\frac{1}{2!} \int d1\, d2\, \phi(p_1)\, \phi(p_2)\, e^{-\beta V(r_1 - r_2)} \Big[e^{itL(12)}\, iL_1(12) \sum_{i=1}^{2} \delta(x - x_i) \Big]\, iL_1(12) \sum_{j=1}^{2} \delta(x' - x_j) + R_B \qquad (2\text{-}16)$$

where

$$R_B = \frac{1}{2!} \int d1\, d2\, \phi(p_1)\, \phi(p_2)\, e^{-\beta V(r_1 - r_2)} \Big[-iL_0(12) \sum_{j=1}^{2} \delta(x' - x_j) + \sum_{j=1}^{2} \delta(x' - x_j)\, \underline{p}' \cdot \nabla / m \Big] \Big[e^{itL(12)}\, iL_1(12) \sum_{i=1}^{2} \delta(x - x_i) \Big] \qquad (2\text{-}17)$$

R_B is the difference between our equation (2-16) and Boley's equation (16). However the transform of R_B turns out to be zero.

Using the result proved in equation (2-15), it can be shown that the transform of equation (2-13) is

$$\phi(\underline{p}')\, \Sigma_1(\underline{k}, \underline{p}, \underline{p}', z) = \Big[i\left(\partial/\partial t + i\, \underline{p} \cdot \underline{k}/m \right) S_2(\underline{k}, \underline{p}\, \underline{p}', t) \Big]_{t=0} + i \int_0^\infty dt\, e^{izt} \int d^3 r\, e^{-i\underline{k} \cdot \underline{r}} \left[\text{R.H.S of } (2\text{-}14) \right] \qquad (2\text{-}18)$$

It is clear that the first term on the right hand side of (2-18) forms the static part of the memory function. It can be shown that this part $\Sigma_1^{(s)}$ reduces to

$$\Sigma_1^{(s)}(\underline{k}, \underline{p}) = -\underline{p} \cdot \underline{k}/m\; f(\underline{k})\, \phi(\underline{p}) \qquad (2\text{-}19)$$

The collisional part $\Sigma_1^{(c)}$ of the memory function is given by the transform of the right hand side of equation (2-16).

If we use the following transformation

$$\begin{aligned} \underline{p}_1 + \underline{p}_2 &= 2\, \underline{\alpha} \qquad (2\text{-}20) \\ \underline{p}_1 - \underline{p}_2 &= 2\, \overline{\underline{p}} \\ \underline{r}_1 + \underline{r}_2 &= 2\, \underline{R} \\ \underline{r}_1 - \underline{r}_2 &= \underline{r} \end{aligned}$$

we can reduce $\mathcal{E}_1^{(c)}$ to the following form

$$\begin{aligned} &\mathcal{E}_1^{(c)}(\underline{k}, \underline{p}\, \underline{p}', z)\, \phi(\underline{p}') = \partial/\partial \underline{p}_i\, \partial/\partial \underline{p}_j' \int d^3\alpha\, d^3\bar{P}\, d^3\bar{r} \\ &\left(\frac{\beta}{\pi m}\right)^3 e^{-\beta\alpha^2/m - \beta\bar{P}^2/m} \; g(\underline{\bar{r}})\, \nabla_{\bar{r}} V(\bar{r}) \left[e^{i\underline{k}\cdot\underline{\bar{r}}/2}\, \delta(\underline{p}' - \underline{\alpha} - \underline{\bar{P}}) \right. \\ &\left. - e^{-i\underline{k}\cdot\underline{\bar{r}}/2}\, \delta(\underline{p}' - \underline{\alpha} + \underline{\bar{P}}) \right] \left[z - \underline{\alpha}\cdot\underline{k}/m - i\left(2\underline{\bar{P}}\cdot\nabla_r/m \right.\right. \\ &\left.\left. - \nabla_{\bar{r}} V(\bar{r}) \cdot \partial/\partial\underline{\bar{P}} \right)\right]^{-1} \nabla_{i\bar{r}} V(\bar{r})\, e^{-i\underline{k}\cdot\underline{\bar{r}}/2}\, \delta(\underline{p} - \alpha - \underline{\bar{P}}) \end{aligned} \qquad (2\text{-}21a)$$

where $$g(r) = e^{-\beta V(\underline{r})} \qquad (2\text{-}21b)$$

When we take into account the variable n in the expansion we can see that equation (2-21a) agrees with Mazenko's expression (2).

2-3 Reduction to the linearized Boltzmann Collision Operator

The linearized Boltzmann equation is

$$(\partial/\partial t + \underline{p}\cdot\nabla_r/m)\, f(\underline{r}, \underline{p}, t) = J(f(\underline{r}, \underline{p}, t)) \qquad (2\text{-}22)$$

where J is the collision operator (27),

$$\begin{aligned} J(f(\underline{r}, \underline{p}, t)) = \frac{1}{m} \int d^3p_1 \int d\Omega\; g\, I(g, \theta)\, [\, & f(r, \underline{p}', t) \\ & + f(\underline{r}, \underline{p}_1', t) - f(\underline{r}, \underline{p}, t) - f(r, \underline{p}_1, t)]\, \phi(p_1) \end{aligned} \qquad (2\text{-}23)$$

where

$mg = |\underline{p} - \underline{p}_1| = |\underline{p}' - \underline{p}_1'|$

$I(g, \theta) = b\, db\, d\psi / d\Omega$ is the differential scattering cross-section

b = impact parameter

$d\Omega = \sin\theta\, d\theta\, d\psi$ is a solid angle

θ = the scattering angle

(2-24)

The momentum variables obey the following conservation laws,

$$\underline{p} + \underline{p}_1 = \underline{p}' + \underline{p}_1' \qquad (2\text{-}25)$$

$$p^2 + p_1^2 = p'^2 + p_1'^2 \qquad (2\text{-}26)$$

We now write the following defining equation for the kernel $L_B(\underline{p},\underline{p}'')$

$$\int d^3\bar{p}\, L_B(\underline{p},\bar{\underline{p}})\, f(\underline{r},\underline{p},t) = J(f(\underline{r},\underline{p},t)) \qquad (2\text{-}27)$$

The explicit analytic form of $L_B(\underline{p},\underline{p}'')$ is then

$$\phi(\underline{p}'')L_B(\underline{p},\underline{p}'') = \frac{1}{m}\int d^3p_1 \int d\Omega\; I(\underline{p}-\underline{p}_1,\theta)|\underline{p}-\underline{p}_1|/m$$
$$\phi(p)\phi(p_1)\left[\delta(\underline{p}''-\underline{p}_1)+\delta(\underline{p}''-\underline{p}_1')-\delta(\underline{p}''-\underline{p})-\delta(\underline{p}''-\underline{p}_1)\right] \qquad (2\text{-}28)$$

We would like to show that our memory operator $\Sigma^{(c)}(\underline{r},pp'',t)$‡ derived in section (2-2) reduces to $L(\underline{p},\underline{p}'')$ for long times and long distances.⁺ In transform language, the proposition becomes one of proving

$$\lim_{\underline{k}\to 0,\, z\to i0^+} \Sigma^{(c)}(\underline{k},\underline{p}\underline{p}'',z) = L_B(\underline{p},\underline{p}'') \qquad (2\text{-}29a)$$

We will prove the equivalent statement

$$\lim_{k\to 0,\, z\to i0^+} \phi(p'')\,\Sigma^{(c)}(\underline{k},\underline{p}\underline{p}'',z) = \phi(p'')\,L_B(\underline{p},\underline{p}'') \qquad (2\text{-}29b)$$

⁺The following derivation parallels that of Mazenko(28)

‡We have dropped the subscript 1 from $\Sigma_1^{(c)}$ and will from now on use the symbol $\Sigma^{(c)}$ to represent our low density

The k=0 limit is easy to take. We just set k=0. After some algebraic manipulations we find

$$\begin{aligned}\mathcal{E}^{(c)}(0,\underline{p}\,\underline{p}'',z)\,\phi(p'') = {}& -n^2\,(\beta/\pi m)^3\int d^3\alpha\, d^3r\, d^3\bar{p}\\ & e^{-\frac{\beta}{m}(\alpha^2+\bar{p}^2)}\left[\delta(\underline{\alpha}-\underline{p}''+\underline{\bar{p}})+\delta(\underline{\alpha}-\underline{p}''-\underline{\bar{p}})\right](z+L_0(\underline{r},\underline{\bar{p}}))\\ & \left\{g(r)\left[iz\int_0^\infty dt\, e^{izt}\delta(\underline{p}-\underline{\alpha}-\underline{\bar{p}}(t)+\delta(\underline{p}-\underline{\alpha}-\underline{\bar{p}})\right]\right\}\end{aligned} \qquad (2\text{-}30)^{+}$$

As a digression, it is gratifying to note that the static term vanishes in this limit as it should. Going back to equation (2-30), using mathematical identities proved in appendix A we can write

$$\begin{aligned}\mathcal{E}^{(c)}(0,\underline{p}\,\underline{p}'',z)\,\phi(p'') = {}& -n^2\,(\beta/\pi m)^3\int d^3\alpha\, d^3r\, d^3\bar{p}\\ & e^{-\beta(\alpha^2+\bar{p}^2)/m}\left[\delta(\underline{\alpha}-\underline{p}''+\underline{\bar{p}})+\delta(\underline{\alpha}-\underline{p}''-\underline{\bar{p}})\right]\\ & 2\,\underline{p}\cdot\nabla r/m\left\{g(r)\left[\theta(-\hat{\underline{r}}\cdot\underline{\bar{p}})\left(\delta(\underline{p}-\underline{\alpha}-\underline{\bar{p}})-\delta(\underline{p}-\underline{\alpha}-\underline{\bar{p}}')\right)\right]\right\}\end{aligned} \qquad (2\text{-}31)$$

The step function $\theta(-\hat{\underline{r}}\cdot\bar{\underline{p}})$ has been introduced to take account of the fact that there will be a collision only if $\underline{r}\cdot\bar{\underline{p}} < 0$. Now, for the purposes of the spatial integration, we use the polar co-ordinates bdbdzdψ and set $\bar{\underline{p}}$ along the z-axis. b and ψ are as defined in equation (2-24). The step function enables us to restrict our attention to the $z=-\infty$ surface and we find that

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[‡] memory function.

[+] The interested reader should consult chapter 4 for further details.

$$\Sigma^{(c)}(\underline{p},\underline{p}'')\,\phi(p'') = -in^2(\beta/\pi m)^3\int d^3\alpha\, d^3\bar{p}\; e^{-\beta(\alpha^2+\bar{p}^2)/m}$$
$$2|\bar{p}|/m\,[\,\delta(\underline{\alpha}-\underline{p}''+\underline{\bar{p}})+\delta(\underline{\alpha}-\underline{p}''-\underline{\bar{p}})\,]$$
$$\int_0^\infty b\,db\int_0^{2\pi}d\psi\,[\,\delta(\underline{p}-\underline{\alpha}-\underline{\bar{p}})-\delta(\underline{p}-\underline{\alpha}-\underline{\bar{p}}')\,]$$

(2-32)

Using the definition of the differential scattering cross-section I(g,θ) and integrating over α we are left with

$$\Sigma^{(c)}(\underline{p},\underline{p}'')\,\phi(p'') = -in^2(\beta/\pi m)^3\int d\Omega\, d^3\bar{p}\; 2|\bar{p}|/m$$
$$e^{-\beta\bar{p}^2}\, I(\bar{p},\theta)\,[\,e^{-\beta(\underline{p}-\underline{\bar{p}})^2/m}\,\delta(\underline{p}-\underline{p}'')$$
$$-\,e^{-\beta(\underline{p}-\underline{\bar{p}}')^2/m}\,\delta(\underline{p}-\underline{\bar{p}}'-\underline{p}''+\underline{\bar{p}})+e^{-\beta/m(\underline{p}-\underline{\bar{p}})^2}$$
$$\delta(\underline{p}-2\underline{\bar{p}}-\underline{p}'')-e^{-\frac{\beta}{m}(\underline{p}-\underline{\bar{p}}')^2}\,\delta(\underline{p}-\underline{\bar{p}}'-\underline{p}''-\underline{\bar{p}})\,]$$

(2-33)

We now use the following transformation

$$2\underline{\bar{p}} = \underline{p} - \underline{p}_1 \qquad (2\text{-}34)$$

This transformation in combination with equations (2-24), (2-25) and (2-26) allows us to write

$$\Sigma^{(c)}(\underline{p}\,p'')\,\phi(p'') = i\frac{n^2}{2}\left(\frac{\beta}{\pi m}\right)^3\int d\Omega\, d^3p_1\;|\underline{p}-\underline{p}_1|/m$$
$$I(\underline{p}-\underline{p}_1,\theta)\,e^{-\frac{\beta}{m}(\underline{p}-\underline{p}_1)^2/2}\left\{e^{-\frac{\beta}{m}(\underline{p}_1+\underline{p})^2/2}\,\delta(\underline{p}-\underline{p}'')+\delta(\underline{p}_1-\underline{p}'')\right.$$
$$\left.e^{-(\underline{p}+\underline{p}_1)^2\beta/2m}-\delta(-2\underline{p}_1+\underline{p}'+2\underline{p}_1'-\underline{p}'')\,e^{-(\underline{p}-\frac{1}{2}(\underline{p}'-\underline{p}_1))^2\beta/2m}-\delta(\underline{p}_1'-\underline{p}'')\,e^{-(\underline{p}-\frac{1}{2}(\underline{p}'-\underline{p}_1'))^2}\right\} \quad (2\text{-}35)$$

This can be shown to reduce to

$$\Sigma^{(c)}(\underline{p}\,\underline{p}'')\,\phi(p'') = i\,\phi(p)\int d^3p_1\,d\Omega\;|\underline{p}-\underline{p}_1|/m\; I(\underline{p}-\underline{p}_1,\theta)\,\phi(p_1)$$
$$[\,\delta(\underline{p}''-\underline{p}_1')+\delta(\underline{p}''-\underline{p}')-\delta(\underline{p}''-\underline{p})-\delta(\underline{p}''-\underline{p}_1)\,] \quad (2\text{-}36)$$

When equation (2-36) is compared with equation (2-28), we see that asides from a factor of i the two expressions are identical.

2-4 The Hydrodynamic limit

To provide a sense of completeness, we present a discussion of the hydrodynamic equations in this section. Historically these were the first equations to be used to calculate $S(k,\omega)$. They provide a macroscopic viewpoint and the spectrum so calculated is good only for times and distances long compared with the intercollision time and the mean free path. These equations are stated below with a brief word about their derivation. The derivation enables us to connect the thermal conductivity λ and the shear viscosity η_s with the microscopic properties of the fluid. We then formulate an analytic expression for $S(k,\omega)$ using these equations. This allows us to identify prominent features of the spectrum with certain macroscopic processes. Finally we specialize our expressions to the hard sphere case.

The Chapman-Enskog procedure enables us to derive a set of hydrodynamic equations from the Boltzmann equation. These equations consist of the conservation laws for mass, momentum and energy flux and equations for the heat flux vector and stress tensor. The Chapman-Enskog procedure first makes use of the fact that the Boltzmann collision operator $Q(f(\underline{r},\underline{v},t))$ satisfies the following equation for a set of functions $\{\psi_i(\underline{v})\}$ (12,25),

$$\int d^3v\ \psi_i(\underline{v})\ Q\ (f(\underline{r},\underline{v},t)) = 0 \qquad i=1,..3 \tag{2-37}$$

This set $\{\psi_i(\underline{v})\}$ is known as the set of collisional invariants and consists of $\{u, b\underline{v}, cv^2\}$ where a and c are scalar constants where as b is a constant vector. Equation (2-37) enables us to derive the set of conservation equations for it implies that

$$\int d^3v'\ \psi_i(\underline{v}')\ (\partial/\partial t + \underline{v}'.\nabla)\ f(\underline{r},\underline{v}',t) = 0 \tag{2-38}$$

If the integration in equation (2-38) is carried out for each of the ψ_i we obtain the macroscopic laws for the conservation of number density $\rho(\underline{r},t)$, momentum density $\rho(\underline{r},t)\underline{v}$; and energy density $\rho(r,t)(\frac{1}{2}v^2+ e)$

$$\partial/\partial t(\rho) + \partial/\partial x_i(\rho v_i) = 0 \tag{2-39}$$

$$\partial/\partial t(\rho v_j) + \partial/\partial x_i(\rho v_i v_j + P_{ij}) = 0 \tag{2-40}$$

$$\partial/\partial t[\rho(\tfrac{1}{2}v^2+e)] + \partial/\partial x_i[\rho v_i(\tfrac{1}{2}v^2+e) + P_{ij}v_j + q_i] = 0 \tag{2-41}$$

where the summation convention is used

$$\rho = \int d^3v'\ f(\underline{r},\underline{v}',t)$$

$$(\rho\underline{v}) = \int d^3v'\ f(\underline{r},\underline{v}',t)\ \underline{v}'$$

$P_{ij} = \int d^3v' \, c_i c_j \, f(\underline{r}, \underline{v}', t)$

is the stress tensor

$q_i = \frac{1}{2} \int d^3v' \, c_i c^2 f(\underline{r}, \underline{v}', t)$

is the heat flux vector

$\rho e = \frac{1}{2} \int d^3v' \, c^2 f(\underline{r}, \underline{v}', t)$

is the energy density due to the peculiar velocity $\underline{c}$.

(2-42)

We have dropped the functional dependence on $(\underline{r},t)$ to simplify the notation. Temperature is normally used instead of energy density in equation (2-41). To do so here we would have to use thermodynamic relations and as it is not our intention to get involved with such issues we shall side step the point.

If equations (2-39) - (2-41) are examined carefully it will be seen that we have three equations with five unknowns. Apart from our conserved variables we also have the heat flux vector and the stress tensor. The Chapman-Enskog method allows us to derive equations directly from the Boltzmann equation relating the heat flux vector to the temperature gradient and the pressure tensor to the rate of strain tensor (12). In the process of doing so expressions are obtained relating the thermal conductivity and shear viscosity to the molecular properties of the fluid.

The second order Chapman-Enskog approximation gives us

$$\underline{q} = -\lambda \nabla T(\underline{r},t) \tag{2-43}$$

$$P_{ij} = \rho_0 k_B T(\underline{r},t)\delta_{ij} - \eta_s \left(\tfrac{1}{3} D_{kk}(\underline{r},t)\delta_{ij} - D_{ij}(\underline{r},t) \right) \tag{2-44}$$

where

$D_{ij} = \tfrac{1}{2}\left(\partial u_i/\partial x_j + \partial u_j/\partial x_i \right)$ is the rate of strain tensor (2-45)

η_s = the shear viscosity (2-46)

λ = thermal conductivity (2-47)

The equations for η_s and λ in terms of the molecular properties of the fluid will not be given here as it would lead us into an extensive discussion of the Chapman-Enskog approximation scheme. As we have no intentions of getting involved in such a discussion we will proceed to the calculation of the hydrodynamic density spectrum. Now that we have all of the hydrodynamic equations it is a simple matter to obtain an analytic expression for S(k,W). Our discussion follows Clark's derivation (24).

For long times and long distances G($\underline{r}$,t) becomes

$$G(\underline{r},t) = \tfrac{1}{n} \langle \rho(0,0)\, \rho(\underline{r},t) \rangle \tag{2-48}$$

For small deviations from equilibrium equations (2-39) -

(2-41) can be linearized to give (13),

$$\partial \rho_1 / \partial t + \rho_0 \nabla \cdot \underline{v} = 0 \tag{2-49}$$

$$\rho\, \partial \underline{v} / \partial t + c_0^2/\gamma\, \nabla \rho_1 + c_0^2 \beta \rho_0 \nabla T_1/\gamma - \tfrac{4}{3} \eta_s/m\, \nabla(\nabla \cdot \underline{v}) = 0$$

(Navier-Stokes equation) (2-50)

$$\rho_0 c_v\, \partial T_1/\partial t - c_v/\beta\, (\gamma - 1)\, \partial \rho_1/\partial t - \lambda \nabla^2 T_1 = 0 \tag{2-51}$$

where m= mass per particle

$T = T_0 + T_1$ is the temperature

T_0= equilibrium temperature

ρ_0 = equilibrium density

$\gamma = c_p/c_v$

β = thermal expansion coefficient

c_0 = adiabatic sound velocity

(2-52)

We have made use of equations (2-43) and (2-44) and assumed that local thermodynamic equilibrium holds.

The external force is taken to be zero. The initial condition to be used in conjunction with equations (2-48)-(2-50) to calculate $S(\underline{k}, w)$ is

$$\langle \rho_1(\underline{r}, 0)\, \rho(0,0) \rangle = \delta(\underline{r}) + \rho_0 h(\underline{r}) \tag{2-53}$$

These equations are solved for $n(\underline{k}, s)$ the Fourier-Laplace transform of the density fluctuation

$$n(\underline{k}, s) = \int d^3r \int_0^\infty dt\, \exp(-\underline{k} \cdot \underline{r})\, \exp(-st)\, \rho_1(\underline{r}, t) \tag{2-54}$$

If we subtract out the equilibrium contribution⁺ to the spectrum $S(k,\omega)$ we can relate the resulting spectrum $S_\rho(k,\omega)$ to $n(\underline{k},s)$. Using this relationship it can be shown that (24)

$$S_\rho(k,\omega) = 2\frac{K_T}{K_I}\left\{\frac{(1-1/\gamma)}{\Gamma_c^2+\omega^2}\Gamma_c + \frac{2\Gamma_B\omega_0^2/\gamma - \Gamma_c(\omega^2-\omega_0^2)(1-1/\gamma)}{(\omega^2-\omega_0^2)^2+(2\omega\Gamma_B)^2}\right] \quad (2\text{-}55)$$

where

K_T = isothermal compressibility (2-56a)

$K_I = (\rho_0 k_B T)^{-1}$ isothermal (2-56b)

compressibility of an ideal gas

$$\Gamma_c = \lambda k^2/\rho_0 c_p \quad (2\text{-}57)$$

$$\Gamma_B = \tfrac{1}{2}\left\{\frac{4\eta_s}{3m\rho_0} + (1-1/\gamma)\frac{\lambda}{\rho_0 c_v}\right\}k^2 \quad (2\text{-}58)$$

$$\omega_0 = k c_0 \quad (2\text{-}59)$$

It must be noted that equation (2-55) is an approximation to the exact result. When $\Gamma_c, \Gamma_B \ll \omega_0$, equation (2-55) can be further simplified to the familiar three component spectrum

$$S_\rho(k,\omega) = \frac{K_T}{K_I}\left\{\frac{(1-1/\gamma)2\Gamma_c}{\omega^2+\Gamma_c^2} + \frac{\Gamma_B}{\gamma}\left[\frac{1}{\Gamma_B^2+(\omega-\omega_0)^2} + \frac{1}{\Gamma_B^2+(\omega+\omega_0)^2}\right]\right]\Big\} \quad (2\text{-}60)$$

⁺The equilibrium contribution leads to a $\delta(k)$ term in the spectrum. This term is of no physical interest.

Physically, the Brillouin components of this spectrum centred at $\omega = \pm\, \omega_0$ are due to propagating density fluctuation modes which are simply thermally driven acoustic waves. The central peak is due to the non-propagating thermal diffusion mode.

For a dilute gas of hard spheres of diameter σ (17) we find

$$\begin{aligned} \kappa_T / \kappa_I &\simeq 1 \\ \gamma &= 5/3 \\ \lambda &= 25/32 \left[k_B T / \pi m \right]^{1/2} \left(C_v / \sigma^2 \right) \\ \eta_s &= \left(5/16\, \sigma^2 \right) \left[m k_B T / \pi \right]^{1/2} \\ c_0 &= \left[5 k_B T / 3m \right]^{1/2} \end{aligned} \tag{2-61}$$

With these values the widths Γ_B and Γ_c are

$$\Gamma_c = \left(15 k^2 / 32 \rho_0 \sigma^2 \right) \left[k_B T / \pi m \right]^{1/2} \tag{2-62}$$

$$\Gamma_B = \left(35 k^2 / 96 \rho_0 \sigma^2 \right) \left[k_B T / \pi m \right]^{1/2} \tag{2-63}$$

$$\omega_0 = k \left[5 k_B T / 3m \right]^{1/2} \tag{2-64}$$

So for the hard sphere gas equation (2-60) becomes

$$S_\rho(k,\omega) = \left\{ \frac{4\Gamma_c}{5(\omega^2 + \Gamma_c^2)} + \frac{3}{5}\Gamma_B \left[\frac{1}{\Gamma_B^2 + (\omega - \omega_0)^2} + \frac{1}{\Gamma_B^2 + (\omega + \omega_0)^2} \right] \right\} \tag{2-65}$$

This equation can be used to check our numerical calculations in the long wavelength limit for the hydrodynamical region in the Boltzmann limit.

In closing this chapter we would like to clarify a point of notation. $S(k,\omega)$ is the space-time transform of $G'(r-r', t-t')$ where

$$G'(r-r',t-t') = G(\underline{r}-\underline{r}', t-t') - n \qquad (2\text{-}66)$$

It therefore differs from $S(k,\omega)$ by a constant term. We, however shall use the terms $S(k,\omega)$ and $S_{\rho}(k,\omega)$ as though they were synonymous. The reader should be mentally prepared to use the terms interchangably.

CHAPTER 3

Calculation of the Density Fluctuation Spectrum

3-1 Formulation

The classical correlation function $S(\underline{r}-\underline{r}', \underline{p}\ \underline{p}', t-t')$, defined in chapter 1, satisfies a Boltzmann-like equation of the form (4),

$$(\partial/\partial t + \underline{p}\cdot\nabla/m)\, S(\underline{r}, \underline{p}\underline{p}', t) = \int_0^t d\bar{t} \int d^3\bar{r}\, d^3\bar{p}\; \mathcal{E}(\underline{r}-\bar{\underline{r}}, p\bar{\underline{p}}, t-\bar{t})\, S(\bar{\underline{r}}, \bar{\underline{p}}\,\underline{p}', \bar{t}) \tag{3-1a}$$

with the transformed initial condition,

$$\tilde{S}(\underline{\mathbf{k}}, \underline{p}\underline{p}') = \phi(p)\, \delta(\underline{p}-\underline{p}') + h(k)\, \phi(p)\, \phi(p') \tag{3-1b}$$

where

$$\phi(p) = n\,(2\pi m/\beta)^{-3/2}\, e^{-\beta p^2/2m} \tag{3-1c}$$

is the Maxwellian velocity distribution and

$$\beta = (1/mv_0^2) \tag{3-1d}$$

What is experimentally measured is the spectrum of density fluctuations, $S(k,\omega)$ which is defined as the space time Fourier transform of the correlation function, $G'(\underline{r},t)$

$$G'(\underline{r}, t) = \frac{1}{n} \left\langle \sum_{ij} \delta(\underline{r}_i(0))\, \delta(\underline{r}-\underline{r}_j(t)) \right\rangle - n \tag{3-2}$$

n = uniform number density

$$M\ S(k,\omega) = \lim_{\varepsilon\to 0} \int d^3r\, e^{-i\underline{k}\cdot\underline{r}} \int_{-\infty}^{\infty} dt\, e^{izt}\, G(\underline{r}, t) \tag{3-3}$$

$$z = \omega + i\epsilon, \quad \epsilon > 0$$

Owing to a slight difference in the definitions of the transforms used in Mazenko's thesis (2) and those used in Sugawara's thesis (3), transforms using Mazenko's convention will be denoted by a presubscript M while the ones obtained by using Sugawara's convention will be denoted by a presubscript S. In a later section these two approaches will be reconciled.

From equations (1-8) and (3-2) it can be seen that

$$G'(\underline{r}, t) = \int \frac{d^3p}{n} \int d^3p' \, S(\underline{r}, \underline{p}\,\underline{p}', t) \tag{3-4}$$

Thus the solution to equation (3-1) and the density fluctuation spectrum are related by:-

$$ {}_M S(k,\omega) = \lim_{\epsilon \to 0} \int \frac{d^3r}{n} \, e^{-i\underline{k}\cdot\underline{r}} \int_{-\infty}^{\infty} dt \, e^{izt} \int d^3p \int d^3p' \, S(\underline{r}, \underline{p}\,\underline{p}', t) \tag{3-5}$$

Using various symmetry properties this can be further simplified:-

$$ {}_M S(k,\omega) = \lim_{\epsilon \to 0} 2 \frac{\mathrm{Re}}{n} \int d^3r \, e^{-i\underline{k}\cdot\underline{r}} \int_0^{\infty} dt \, e^{izt} \, S(\underline{r}, t) \tag{3-6}$$

$$ = \lim_{\epsilon \to 0} 2 \frac{\mathrm{Im}}{n} \int d^3p \int d^3p' \, S(\underline{k}, \underline{p}\,\underline{p}', z) \tag{3-7}$$

where

$$ S(\underline{k}, \underline{p}\,\underline{p}', z) = i \int d^3r \, e^{-i\underline{k}\cdot\underline{r}} \int_0^{\infty} dt \, e^{izt} \, S(\underline{r}, \underline{p}\,\underline{p}', t) \tag{3-8}$$

Equation (3-1) is now Fourier-Laplace transformed to yield

$$(z - \underline{k}\cdot\underline{p}/m)\, S(\underline{k}, \underline{p}\,\underline{p}', z) - \int d^3\bar{p}\; \Sigma(\underline{k}, \underline{p}\,\bar{\underline{p}}, z)\, S(\underline{k}, \bar{\underline{p}}\,\underline{p}', z) = -\, \tilde{\hat{S}}_c(\underline{k}, \underline{p}\,\underline{p}') \qquad (3\text{-}9)$$

where:-

$$\Sigma(\underline{k}, \underline{p}\,\underline{p}', z) = i \int d^3r\, e^{-i\underline{k}\cdot\underline{r}} \int_0^\infty dt\, e^{izt}\, \Sigma(\underline{r}, \underline{p}\,\underline{p}', t) \qquad (3\text{-}10)$$

Now integrate over all p′

$$S_n(\underline{k}, \underline{p}, z) = \int d^3p'\, S(\underline{k}, \underline{p}\,\underline{p}', z) \qquad (3\text{-}11)$$

$$(z - \underline{k}\cdot\underline{p}/m)\, S_n(\underline{k}\,\underline{p}\,z) - \int d^3\bar{p}\; \Sigma(\underline{k}, \underline{p}\,\bar{\underline{p}}, z)\, S_n(\underline{k}\,\bar{\underline{p}}\,z) = -\,[\,\phi(p) + h(k)\,\phi(p)\,n\,] \qquad (3\text{-}12)$$

Introduce the non-dimensional variables

$$\begin{aligned} \xi &= \underline{p}/mv_0 \\ S_n(k\,\xi\,z) &= n\, S_n'(\underline{k}\,\underline{p}\,z)/(mv_0)^3 \\ \Phi(\xi) &= e^{-\xi^2/2}/(2\pi)^{3/2} \\ \Sigma(\underline{k}, \underline{\xi}\,\underline{\xi}', z) &= M'(\underline{k}, \underline{\xi}\,\underline{\xi}', z)/(mv_0)^3 \end{aligned} \qquad (3\text{-}13)$$

The $\underline{k}$-direction is now choosen parallel to the ξ_3-axis. Then the dimensionless equation that has to be solved is,

$$(z - kv_0\xi_3)\, S_n'(\underline{k}\,\underline{\xi}\,z) - \int d^3\bar{\xi}\, M'(\underline{k}\,\underline{\xi}\,\bar{\underline{\xi}}\,z)\, S_n'(\underline{k}\,\bar{\underline{\xi}}\,z) = -\,\Phi(\xi)\,[\,1 + n\,h(k)\,] \qquad (3\text{-}14a)$$

$${}_M S(k,\omega) = \lim_{\epsilon\to 0} 2\,\mathrm{Im} \int d^3\xi\, S_n'(\underline{k}\,\underline{\xi}\,z) \qquad (3\text{-}14b)$$

To conclude this section it seems worthwhile to point out the fact that the self-correlation function

$$S_s(\underline{r},\underline{p}\,\underline{p}',t) = \langle \sum_i \delta(\underline{r}-\underline{r}_i(t))\,\delta(\underline{p}-\underline{p}_i(t))\,\delta(\underline{r}_i(0))\,\delta(\underline{p}'-\underline{p}_i(0))\rangle \qquad (3\text{-}15)$$

also satisfies a Boltzmann-like equation similar to equation (3-1) but with a different memory kernel $\mathcal{E}_s$ and a different initial condition. $\mathcal{E}_s$ is essentially a portion of $\mathcal{E}$ and more will be said about this relation in chapter 4.

If we go through the same formalism as we did with $S(\underline{r},\underline{p}\underline{p}',t)$ we find that

$$(z-\underline{k}\cdot\underline{p}/m)\,S_s(\underline{k},\underline{p}\,\underline{p}',z) - \int d^3\bar{p}\;\mathcal{E}_s(\underline{k},\underline{p}\,\bar{\underline{p}},z)\,S_s(\underline{k},\bar{\underline{p}}\,\underline{p}',z) = -\hat{S}_s(\underline{k},\underline{p}\,\underline{p}') \qquad (3\text{-}16)$$

where

$$\tilde{S}_s(\underline{k},\underline{p}\,\underline{p}') = \phi(p')\,\delta(\underline{p}-\underline{p}') \qquad (3\text{-}17)$$

$$S_s(\underline{k},\underline{p}\,\underline{p}',z) = i\int d^3r\; e^{-i\underline{k}\cdot\underline{r}}\int_0^\infty dt\; e^{izt}\,S_s(\underline{r},\underline{p}\,\underline{p}',t) \qquad (3\text{-}18)$$

$$\mathcal{E}_s(\underline{k},\underline{p}\,\underline{p}',z) = i\int d^3r\; e^{-i\underline{k}\cdot\underline{r}}\int_0^\infty dt\; e^{izt}\,\mathcal{E}_s(\underline{r},\underline{p}\,\underline{p}',t) \qquad (3\text{-}19)$$

Integrating over all p and non-dimensionalizing as before, we arrive at,

$$(z-kv_0\xi_3)\,S'_{sn}(\underline{k}\,\underline{\xi}\,z) - \int d^3\bar{\xi}\;M'_s(k,\underline{\xi}\,\bar{\underline{\xi}},z)\;S'_{sn}(\underline{k}\,\bar{\underline{\xi}}\,z) = -\Phi(\xi) \qquad (3\text{-}20)$$

$${}_M S_s(k,\omega) = \lim_{\epsilon\to 0} 2\,\mathrm{Im}\int d^3\xi\; S'_{sn}(\underline{k}\,\underline{\xi}\,z) \qquad (3\text{-}21)$$

To extract the information that we desire, equations (3-14) and (3-20) will have to be approximated by a form more amenable to numerical solution. The approximation technique that we decided to use is the method of Kinetic modelling. The method and its application to this case is discussed in more detail in the next section.

3-2 Kinetic modelling - Formulation

Every bounded linear operator may be represented by a matrix and the matrix representation of the memory operator in equation (3-1) has an infinite number of elements. The method of Kinetic modelling to discussed in this section gives us one means for approximating this infinite matrix (22,23).

We shall discuss this technique by applying it to equation (3-14).

Let $\{\psi_i(\xi)\}$ be a complete orthonormal set of functions with the weighting function $\Phi(\xi)$. We then expand both $M(\underline{k},\underline{\xi}\underline{\xi}', z)$ and $S'_n(\underline{k}\,\underline{\xi}\,z)$ in terms of this set.

$$M'(\underline{k},\underline{\xi}\,\underline{\xi}',z) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \psi_i(\underline{\xi})\,\psi_j^*(\underline{\xi}')\,\Phi(\xi)\,M(i/j) \tag{3-22}$$

$$S'_n(\underline{k}\,\underline{\xi}\,z) = \sum_{i=1}^{\infty} \psi_i(\underline{\xi})\,\Phi(\xi)\,S_i(\underline{k}\,z) \tag{3-23}$$

where by orthonormality,

$$S_i(\underline{k}\,z) = \int d^3\xi\,\psi_i^*(\underline{\xi})\,S'_n(\underline{k}\,\underline{\xi}\,z)$$

$$M(i|j) = \int d^3\xi\, d^3\xi'\, \psi_i^*(\underline{\xi})\, M'(\underline{k},\underline{\xi}\,\underline{\xi}',z)\, \Phi(\xi')\, \psi_j(\xi') \tag{3-24}$$

These expansions are then substituted into (3-14)

$$(z-kv_0\xi_3)\sum_{i=1}^{\infty} S_i(\underline{k}z)\,\psi_i(\underline{\xi})\,\Phi(\xi) - \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\int d^3\bar{\xi}\,\psi_i(\underline{\xi})\,\Phi(\xi)\,M(i/j)\,\psi_j^*(\bar{\underline{\xi}})\,\Phi(\bar{\xi})\sum_{\nu=1}^{\infty}\psi_\nu(\bar{\xi})\,S_\nu(\underline{k}z) = -\Phi(\xi)\,[1+n\,h(k)] \tag{3-25}$$

This reduces to

$$(z-kv_0\xi_3)\sum_{i=1}^{\infty}\psi_i(\underline{\xi})\,\Phi(\xi)\,S_i(\underline{k}z) - \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\psi_i(\underline{\xi})\,\Phi(\xi)\,M(i/j)\,S_j(\underline{k}z) = -\Phi(\xi)\,[1+n\,h(k)] \tag{3-26}$$

Upto this point the equation is still exact but in order to proceed further the infinite sums will now have to be truncated. The method of Kinetic modelling however leaves the free-streaming operator unaltered. Thus one of the advantages of the approximation is that it will give the exact answer in the free-particle limit.

The memory term is truncated by the approximation

$$\begin{aligned} M(i/j) &= M(N+1/N+1)\,\delta_{ij}, \text{ for } i \text{ or } j > N \\ &= -i\,\lambda_N\,\delta_{ij} \end{aligned} \tag{3-28}$$

where $\lambda_N = i\,M(N+1/N+1)$

The Kinetic model is said to of order N.

With this approximation equation (3-26) can be written as:

$$(z - kv_0\xi_3 + i\lambda_N)\sum_{i=1}^{\infty}\psi_i(\underline{\xi})\,\Phi(\xi)\,S_i(\underline{k}\,z) - \sum_{i=1}^{N}\sum_{j=1}^{N}\psi_i(\underline{\xi})\,\Phi(\xi)\,S_j(\underline{k}\,z)(M(i/j) + i\lambda_N\delta_{ij}) = -\Phi(\xi)\,[1 + nh(k)] \tag{3-29}$$

By using the orthonormality of the set $\{\psi_i(\xi)\}$ equation (3-29) can be shown to reduce to the form

$$S_k(\underline{k}z) - y^*\sum_{i=1}^{N}\sum_{j=1}^{N} S_j(\underline{k}z)\,\tilde{C}_{ik}(\underline{k}z)\left(\frac{M(i/j)}{\lambda_N} + i\delta_{ij}\right) = -\frac{y^*}{\lambda_N}\tilde{A}_k(z)\,(1 + nh(k)) \tag{3-30a}$$

If our basis is chosen such that $\psi_1(\xi)=1$, then using (3-14b)

$$_M S(k,\omega) = \lim_{\epsilon\to 0} 2\,\mathrm{Im}\int d^3\xi\sum_{i=1}^{\infty}\Phi(\xi)\,\psi_i(\xi)\,S_i(\underline{k}z)$$

$$= \lim_{\epsilon\to 0} 2\,\mathrm{Im}\,S_1(\underline{k}z) \tag{3-30b}$$

where,

$$\tilde{C}_{is}(z) = \int d^3\xi\,\psi_i(\underline{\xi})\,\Phi(\xi)\,\psi_s^*(\underline{\xi})/(z - \xi_3/\sqrt{2}) \tag{3-31a}$$

$$\tilde{A}_s(z) = \tilde{C}_{1s}(z) = \int d^3\xi\,\psi_s^*(\underline{\xi})\,\Phi(\xi)/(z - \xi_3/\sqrt{2}) \tag{3-31b}$$

$$x = z/\sqrt{2}\,kv_0 \tag{3-31c}$$

$$y^* = \lambda_N/\sqrt{2}\,kv_0 \tag{3-31d}$$

$$Z = x + iy^* \tag{3-31e}$$

One of the above parameters, y*, can be related to an experimentally measurable quantity, the shear viscosity η_s. It has been shown that,

$$\eta_s = m n v_0^2 / \lambda_a \qquad (3\text{-}32a)$$

where $\lambda_a = i M(a/a)$ (3-32b)

If we introduce the parameter

$$y = \lambda_a / \sqrt{2} k v_0 \qquad (3\text{-}32c)$$

we see that from (3-32a) that

$$\eta_s = m n v_0 / \sqrt{2} k y \qquad (3\text{-}32d)$$

and as $y^* = y \lambda_N / \lambda_a$ (3-33)

we have a means of relating our parameter y^* to experimental conditions.

A more detailed discussion regarding the number of independent parameters and their relation to experimentally measurable quantities is given in chapter 5.

Equation (3-21) for the self-correlation function can also be reduced to a form similar to that of equation (3-30a) if we repeat the above procedure,

$$S_{sk}(\underline{k} z) - y^* \sum_{i=1}^{N} \sum_{j=1}^{N} S_{sj}(\underline{k} z) \tilde{C}_{ik}(z) \left(M_s(i/j)/\lambda_N + i \delta_{ij} \right) = - \frac{y^*}{\lambda_N} \tilde{A}_k(\underline{k} z) \qquad (3\text{-}34a)$$

$$_M S_s(k, \omega) = \lim_{\epsilon \to 0} 2 \, \mathrm{Im} \, S_{s1}(\underline{k} z) \qquad (3\text{-}34b)$$

3-3 Kinetic modelling - Accuracy

As has been noted in section 3-2 the method will certainly give us the correct spectrum in the free particle limit regardless of the order of the model, but one is still left with the question concerning the error over the other regimes.

If equation (3-30a) is written in matrix form it can be seen that the method has essentially replaced the infinite matrix form of the memory operator with a matrix $\left[\begin{array}{c|c} A_N & 0 \\ \hline 0 & \begin{matrix} \lambda_N & & \\ & \ddots & \\ & & \lambda_N \end{matrix} \end{array}\right]$ where $\left[\begin{array}{c|c} A_N & B \\ \hline C & D \end{array}\right]$ is the exact representation. Thus the approximate solution should converge to the exact solution for all regimes when the order of the model N approaches infinity. Thus questions about the accuracy of the situation become ones about the convergence behaviour of the solution. On the basis of this result, Sugawara has examined the accuracy of the Kinetic modelling method when a Sonine polynomial basis is used, by numerically studying the convergence behaviour of the solution as N is varied (3). As will be seen in chapter five our work with the modified Hermite polynomials as the basis is also based on this result and in this section we will attempt to present a general discussion of the convergence problem.

Given that N is finite one has to resort to physical reasoning to improve the convergence behaviour with respect to rate and smoothness. It appeals to the physical intuition to think of the set $\{\Psi_i\}$ as relaxation modes as we know that the eigenvalues of the collision operator in the linearized Boltzmann equation are indeed the decay constants for the spatially uniform initial problem.

We know that the elements corresponding to the conservation laws will have to be present in A if the correct hydrodynamic behaviour is to be obtained. By including these elements we have essentially incorporated the hydrodynamical relaxation modes into our equation. So we expect that our results in the hydrodynamical region will be those obtained by making direct use of the hydrodynamical equations.

If the set $\{\psi_i\}$ are the eigenvectors of the memory operator then the off-diagonal elements are indeed zero and the approximation will be more accurate but even in this case the decay modes are still coupled together by the streaming term.

The approximation on the other hand decouples the higher modes from the relaxation processes influencing the density function spectrum. It does however leave the lower modes coupled. The ordering of the set should therefore be expected to play an important role in the convergence behaviour of the solution.

3-4 Relation between ${}_S S(k,w)$ and ${}_M S(k,w)$:-

As we intend to compare the results of the present work in the Boltzmann equation with those obtained by Sugawara it would be appropriate at this stage to indicate the connection between ${}_S S(k,w)$ and ${}_M S(k,w)$.

From Sugawara's thesis,

$$ {}_S S(k,\omega) = \int_{-\infty}^{\infty} dt \int d^3r \, e^{i(\underline{k}\cdot\underline{r} - \omega t)} G(\underline{r},t) \qquad (3\text{-}35) $$

Comparing this with equation (3-2) we see that

$$ {}_S S(k,\omega) = {}_M S(-k,-\omega) \qquad (3\text{-}36) $$

Since the definitions of x and y used in Sugawara's thesis and ours are identical we have

$$ {}_S S(x,y) = {}_M S(x,-y) \qquad (3\text{-}37) $$

CHAPTER 4

The Memory Operator

4-1 Reduction to Hard Sphere case:-

In this chapter we will devote our attention to the evaluation of the matrix elements $M(i/j)$ used in equations (3-30a) and (3-34a). As can be seen from equation (2-21a) the general form of the memory operator requires a knowledge of the interatomic potential $V(\underline{r})$[+]. For this work we restrict our attention to the hard sphere potential

$$V(\underline{r}) = \begin{cases} 0 & |\underline{r}| > r_0 \\ \infty & |\underline{r}| \leq r_0 \end{cases} \qquad (4-1)$$

where r_0 = hard sphere diameter (4-2)

The memory function can be written as a sum of a static part $\Sigma^{(s)}(\underline{k}\,\underline{p})$ and a collision part $\Sigma^{(c)}(\underline{k},\underline{p}\,\underline{p}',z)$ and to simplify the algebra we shall make use of that fact and treat the two parts separately

$$\Sigma(\underline{k},\underline{p}\,\underline{p}',z) = \Sigma^{(s)}(\underline{k}\,\underline{p}) + \Sigma^{(c)}(\underline{k},\underline{p}\,\underline{p}',z) \qquad (4-3)$$

Non-dimensionalizing we obtain

$$M'(\underline{k},\underline{p}\,\underline{p}',z) = M'^{(s)}(\underline{k}\,\underline{\xi}) + M'^{(c)}(\underline{k},\underline{\xi}\,\underline{\xi}',z) \qquad (4-4)$$

From equation (2-19) it can be seen that

$$M'^{(s)}(\underline{k}\,\underline{\xi}) = -k V_0 \xi_3 C(k)\, \Phi(\xi)\, n$$

[+] In this chapter position variables are all relative.

$$= -k V_0 \xi_3 n h(k) \Phi(\xi) \tag{4-5}$$

The collision part of the memory function is more difficult to evaluate as it depends upon the dynamical behaviour of the system.

The non-dimensional form of equation (2-21a) is evidently

$$\begin{aligned} M'^{(c)}(\underline{k}, \underline{\xi}\, \underline{\xi}', z)\,\Phi(\xi') &= \frac{n}{(\pi)^3} \nabla^i_{\xi} \nabla^j_{\xi'} \int d^3\alpha\, d^3r\, d^3\bar{\xi} \\ & e^{-\alpha^2} e^{-\bar{\xi}^2} g(r)\, \nabla^j_r V(r) \left[e^{i\underline{k}\cdot\underline{r}/2} \delta(\underline{\alpha} - \underline{\xi}' + \underline{\bar{\xi}}) \right. \\ & \left. - e^{-i\underline{k}\cdot\underline{r}/2} \delta(\underline{\alpha} - \underline{\xi}' - \underline{\bar{\xi}}) \right] \left[z - \underline{k}\cdot V_0 \underline{\alpha} + L(\underline{r}, \underline{\bar{\xi}}) \right]^{-1} \\ & \nabla^i_r V(\underline{r})\, e^{-i\underline{k}\cdot\underline{r}/2} \quad \delta(\underline{\xi} - \underline{\alpha} - \underline{\bar{\xi}}) \end{aligned} \tag{4-6}$$

where $$g(r) = e^{-\beta V(r)} \tag{4-7a}$$

$$L(\underline{r}, \underline{\bar{P}}) = -2i\, \underline{\bar{P}}\cdot\nabla_{\underline{r}} / m + i \nabla_{\underline{r}} V(r) \cdot \nabla_{\underline{\bar{P}}} \tag{4-7b}$$

To reduce equation (4-6) to a more manageable form we have to carry out a number of algebraic manipulations. In this section we will restrict ourselves to certain important steps of the reduction. The necessary algebraic identities are quoted below but the mathematical proof is left to Appendix B.

To simplify the notation we define (28),

$$\rho_k(\underline{\bar{P}}) = e^{-i\underline{k}\cdot\underline{r}/2} \delta(\underline{P} - \underline{\alpha} - \underline{\bar{P}}) \tag{4-8}$$

$$\rho_k'(\underline{\bar{P}}) = e^{i\underline{k}\cdot\underline{r}/2} \delta(\underline{\alpha} - \underline{P}' + \underline{\bar{P}}) + e^{-i\underline{k}\cdot\underline{r}/2} \delta(\underline{\alpha} - \underline{P}' - \underline{\bar{P}}) \tag{4-9}$$

This allows us to write $\mathcal{E}^{(c)}(\underline{k},\underline{p}\underline{p},z)$ as

$$\mathcal{E}^{(c)}(\underline{k},\underline{p}\,\underline{p}',z)\,\phi(p') = -n^2(\beta/\pi m)^3\int d^3\alpha\, d^3r\, d^3\bar{p}$$
$$e^{-\beta(\alpha^2+\bar{p}^2)/m}\, g(r)\,(L_I(\underline{r},\underline{\bar{p}})\,\rho'_k(\underline{\bar{p}}))\,[z-\underline{k}\cdot\underline{\alpha}/m$$
$$+L(\underline{r},\underline{\bar{p}})]^{-1}L_I(\underline{r},\underline{\bar{p}})\,\rho_k(\underline{\bar{p}}) \tag{4-10}$$

If we integrate by parts over $\underline{p}$ and use the identities (B- 1) and (B- 4) we can show that,

$$\mathcal{E}^{(c)}(\underline{k},\underline{p}\,\underline{p}',z)\,\phi(p') = \{\mathcal{E}^{(c)}_I(\underline{k},\underline{p}\,\underline{p}',z) + \mathcal{E}^{(c)}_H(\underline{k},\underline{p}\,\underline{p}',z)\}\,\phi(p') \tag{4-11}$$

where

$$\mathcal{E}^{(c)}_H(\underline{k},\underline{p}\,\underline{p}',z)\,\phi(p') = -n^2(\beta/\pi m)^3\int d^3\alpha\, d^3r\, d^3\bar{p}\;\rho'_k(\underline{\bar{p}})$$
$$e^{-\beta(\alpha^2+\bar{p}^2)/m}\,[z-\underline{k}\cdot\underline{\alpha}/m+L_0(\underline{r},\underline{\bar{p}})]\,\{g(r)[z-\underline{k}\cdot\underline{\alpha}/m$$
$$+L(\underline{r},\underline{\bar{p}})]^{-1}L_I(\underline{r},\underline{\bar{p}})\,\rho_k(\underline{\bar{p}})\} \tag{4-12}$$

$$\mathcal{E}^{(c)}_I(\underline{k},\underline{p}\,\underline{p}',z)\,\phi(p') = n^2(\beta/\pi m)^3\int d^3\alpha\, d^3r\, d^3\bar{p}\;\rho'_k(\bar{p})$$
$$g(r)\,e^{-\beta(\alpha^2+\bar{p}^2)/m}\,L_I\,\rho_k(\bar{p}) \tag{4-13}$$

Let us consider the $\mathcal{E}^{(c)}_I(\underline{k},\underline{p}\underline{p},z)$ part first. We use the identity (B-2) and integrate by parts over the spatial co-ordinates to obtain

$$\mathcal{E}^{(c)}_I(\underline{k},\underline{p}\,\underline{p}',z)\,\phi(p') = \frac{n^2}{\beta}(\beta/\pi m)^3\, i\int d^3\alpha\, d^3\bar{p}\, d^3r$$
$$h(r)\,e^{-\beta(\alpha^2+\bar{p}^2)/m}\,\nabla_r\,(\rho'_k(\bar{p})\,\nabla_{\bar{p}}\,\rho_k(\bar{p})) \tag{4-14}$$

When $\nabla_{\bar{p}}$ is interchanged with $-\nabla_p$ and the integrations are carried out we find

$$\Sigma_{I}^{(c)}(\underline{k},\underline{p}\,\underline{p}')\,\phi(p') = \frac{\underline{k}\cdot\underline{p}'}{m}\,h(k)\,\phi(p)\,\phi(p') \tag{4-15}$$

Now we shall consider the other part of the memory function.

Using (B-8) in (4-12) we see that

$$\begin{aligned}\Sigma_{H}^{(c)}(\underline{k},\underline{p}\,\underline{p}',z)\,\phi(p') = {} & -n^2(\beta/\pi m)^3 \int d^3\alpha\, d^3r\, d^3\bar{p}\, \Big[\\ & e^{i\underline{k}\cdot\underline{r}/2}\,\delta(\underline{\alpha}-\underline{p}'+\bar{\underline{p}}) + e^{-i\underline{k}\cdot\underline{r}/2}\,\delta(\underline{\alpha}-\underline{p}'-\bar{\underline{p}})\Big]\, e^{-\beta(\alpha^2+\bar{p}^2)/m} \\ & \big[z-\underline{k}\cdot\underline{\alpha}/m + L_0(\underline{r},\bar{\underline{p}})\big]\Big\{g(r)\Big[i(z-\underline{k}\cdot\underline{p}/m)\int_0^\infty dt \\ & e^{i(z-\underline{k}\cdot\underline{\alpha}/m)t}\, e^{-i\underline{k}\cdot\underline{r}(t)/2}\,\delta(\underline{p}-\underline{\alpha}-\bar{\underline{p}}(t)) + \\ & e^{-i\underline{k}\cdot\underline{r}/2}\,\delta(\underline{p}-\underline{\alpha}-\bar{\underline{p}})\Big]\Big\}\end{aligned} \tag{4-16}$$

We will concentrate our attention on

$$Q = i(z-\underline{k}.\underline{p}/m)\int_0^\infty dt\, e^{i(z-\underline{k}\cdot\underline{\alpha}/m)t}\, e^{-i\underline{k}\cdot\underline{r}(t)}\,\delta(\underline{p}-\underline{\alpha}-\bar{\underline{p}}(t)) \tag{4-17}$$

$$\begin{aligned} = {} & \int_0^\infty dt\, e^{i(z-\underline{k}\cdot\underline{\alpha}/m)t}\,\delta(\underline{p}-\underline{\alpha}-\bar{\underline{p}}(t))\,\big[z-\underline{k}\cdot\underline{\alpha}/m \\ & -i\,d/dt\big]\, e^{-i\underline{k}\cdot\underline{r}(t)/2}\end{aligned} \tag{4-18}$$

Equation (4-18) when integrated by parts gives us

$$\begin{aligned} Q = {} & -\delta(\underline{p}-\underline{\alpha}-\bar{\underline{p}})\, e^{-i\underline{k}\cdot\underline{r}/2} - \int_0^\infty dt\, e^{-i\underline{k}\cdot\underline{r}(t)/2} \\ & e^{i(z-\underline{k}\cdot\underline{\alpha}/m)t}\,\frac{d}{dt}\,\delta(\underline{p}-\underline{\alpha}-\bar{\underline{p}}(t))\end{aligned} \tag{4-19}$$

This result enables us to get rid of the free particle part in $\Sigma^{(c)}$.

$$Q' = Q + e^{-ik\underline{r}\cdot\underline{r}/2}\,\delta(\underline{p}-\underline{\alpha}-\underline{\bar{p}})$$

$$= -\int_0^\infty dt\, e^{-i\underline{k}\cdot\underline{r}(t)/2}\, e^{i(z-\underline{k}\cdot\underline{\alpha}/m)t}\,\frac{d}{dt}\delta(\underline{p}'-\underline{\alpha}-\underline{\bar{p}}(t))$$

(4-20)

To proceed any further we have to analyse the collision dynamics. If we use the results proved in Appendix B we find that

$$Q' = -\int_0^\infty dt\, e^{i(z-\underline{k}\cdot\underline{\alpha}/m)t}\, e^{-i\underline{k}\cdot\underline{r}(t)/2}\,\theta(r_0^2-b^2)$$

$$\theta_-(\hat{r}\cdot\underline{\bar{p}})\,\delta(t-\tau)\,[\delta(\underline{p}_1-\underline{\alpha}-\underline{\bar{p}}^*)-\delta(\underline{p}_1-\underline{\alpha}-\underline{\bar{p}})]$$

$$= e^{i(z-\underline{k}\cdot\underline{\alpha}/m)\tau}\, e^{-i\underline{k}\cdot\hat{\rho}r_0/2}\,\theta(r_0^2-b^2)\,\theta_-(\hat{r}\cdot\hat{\bar{p}})$$

$$[\delta(\underline{p}'-\underline{\alpha}-\underline{\bar{p}})-\delta(\underline{p}'-\underline{\alpha}-\underline{\bar{p}}^*)] \qquad (4\text{-}21)$$

When this is used in equation (4-16) it can be shown that

$$\Sigma_H^{(c)}(\underline{k},\underline{p}\underline{p}',z)\,\phi(p') = -n^2(\beta/\pi m)^3\int d^3\alpha\, d^3r\, d^3\bar{p}$$

$$[e^{i\underline{k}\cdot\underline{r}/2}\,\delta(\underline{\alpha}-\underline{p}+\underline{\bar{p}})+e^{-i\underline{k}\cdot\underline{r}/2}\,\delta(\underline{\alpha}-\underline{p}-\underline{\bar{p}})]$$

$$e^{-\beta(\alpha^2+\bar{p}^2)/m}\,[z-\underline{k}\cdot\underline{\alpha}/m+L_0(\underline{r},\underline{\bar{p}})]$$

$$\{g(r)\, e^{i(z-\underline{k}\cdot\underline{\alpha})\tau}\, e^{-i\underline{k}\cdot\hat{\rho}r_0/2}\,\theta(r_0^2-b^2)\,\theta_-(\hat{r}\cdot\underline{\bar{p}})$$

$$[\delta(\underline{p}'-\underline{\alpha}-\underline{\bar{p}})-\delta(\underline{p}'-\underline{\alpha}-\underline{\bar{p}}^*)]\}$$

(4-22)

Appendix B shows that

$$[\, z - \underline{k}\cdot\underline{\alpha}/m + L_0(\underline{r}, \bar{\underline{p}})\,]\,[\, g(r)\, e^{i(z-\underline{k}\cdot\underline{\alpha}/m)\tau}\,] = e^{i(z-\underline{k}\cdot\underline{\alpha}/m)\tau}\, L_0(\underline{r}, \bar{\underline{p}})\, g(r)$$

(4-23)

we then have

$$\begin{aligned}\mathcal{E}_H^{(c)}(\underline{k}, \underline{p}\,\underline{p}', z)\,\phi(\underline{p}') = -n^2 (\beta/\pi m)^3 \int d^3\alpha\, d^3r\, d^3\bar{p} \\ [\, e^{i\underline{k}\cdot\underline{r}/2}\, \delta(\underline{\alpha} - \underline{p} + \bar{\underline{p}}) + e^{-i\underline{k}\cdot\underline{r}/2}\, \delta(\underline{\alpha} - \underline{p} - \bar{\underline{p}}^*)\,] \\ e^{-\beta(\alpha^2+\bar{p}^2)/m}\, e^{i(z-\underline{k}\cdot\underline{\alpha}/m)\tau}\, e^{-i\underline{k}\cdot\hat{r}\, r_0/2}\, \theta(r_0^2 - b^2) \\ \theta_-(\hat{r}\cdot\vec{\bar{p}})\, [\, \delta(\underline{p}' - \underline{\alpha} - \bar{\underline{p}}) - \delta(\underline{p}' - \underline{\alpha} - \bar{\underline{p}}^*)\,] \\ L_0(\underline{r}, \bar{p})\, g(r)\end{aligned}$$

(4-24)

Now we do the spatial integration. Equation (B-2) allows us to restrict our attention to the surface of the sphere $r=r_0$. We find,

$$\begin{aligned}\mathcal{E}_H^{(c)}(\underline{k}, \underline{p}\,\underline{p}', z)\,\phi(p') = i n^2 (\beta/\pi m)^3 \int d^3\alpha\, d^3r\, d^3\bar{p} \\ [\, \delta(\underline{\alpha} - \underline{p} + \bar{\underline{p}}) + e^{-i\underline{k}\cdot\hat{r}\, r_0/2}\, \delta(\underline{\alpha} - \underline{p} - \bar{\underline{p}})\,] \\ e^{-\beta(\alpha^2+\bar{p}^2)/m}\;\; 2\, \bar{\underline{p}}\cdot\frac{\hat{r}}{m}\, \delta(r - r_0)\, \theta_-(\hat{r}\cdot\hat{p}) \\ [\, \delta(\underline{p}' - \underline{\alpha} - \bar{\underline{p}}) - \delta(\underline{p}' - \underline{\alpha} - \bar{\underline{p}}^*)\,]\end{aligned}$$

$$= r_0^2\, i n^2 (\beta/\pi m)^3 \int d\Omega\, d^3\alpha\, d^3\bar{p}\; 2\, \bar{\underline{p}}\cdot\hat{r}/m$$

$$e^{-\beta(\alpha^2+\bar{p}^2)/m}\,\theta_-(\hat{r}\cdot\hat{p})\,\delta(\underline{\alpha}-\underline{p}+\underline{\bar{p}})\{\delta(\underline{p}'-\alpha-\underline{\bar{p}})$$
$$-\,\delta(p'-\underline{\alpha}-\underline{\bar{p}}^{*}) + e^{-i\underline{k}\cdot\hat{r}r_0}\,(\delta(\underline{p}'-\underline{\alpha}+\underline{\bar{p}})$$
$$-\,\delta(\underline{p}'-\underline{\alpha}+\underline{\bar{p}}^{*}))\}$$

(4-25)

where $d\Omega_r$ = infinitesimal solid angle

Note that we have performed the transformation $\underline{r}\rightarrow -\underline{r}$, $\underline{p}\rightarrow -\underline{p}$ in the term proportional to $e^{-i\underline{k}\cdot\hat{r}r_0}$

On non-dimensionalizing equations (4-25) and (4-15) we find

$$M'^{(c)}_{H}(\underline{k},\underline{\xi}\xi')\,\Phi(\xi') = 16\frac{i n r_0^2 v_0}{(2\pi)^3}\int d^3\alpha\, d^3\bar{\xi}\, d\Omega_r\, e^{-(\alpha^2+\bar{\xi}^2)}$$
$$\theta_-(\hat{r}\cdot\underline{\bar{\xi}})\,\hat{r}\cdot\underline{\bar{\xi}}\;\delta(\underline{\alpha}-\underline{\xi}+\underline{\bar{\xi}})\,[\,\delta(\underline{\xi}'-\underline{\alpha}-\underline{\bar{\xi}})-\delta(\underline{\xi}-\underline{\alpha}-\underline{\bar{\xi}}^{*})$$
$$+\,e^{i\underline{k}\cdot r_0\hat{r}}\{\delta(\underline{\xi}'-\underline{\alpha}+\underline{\xi})-\delta(\underline{\xi}'-\underline{\alpha}+\underline{\bar{\xi}}^{*})\}\,]$$

(4-26)

$$M'^{(cc)}_{I}(\underline{k},\underline{\xi}\,\underline{\xi}')\,\Phi(\xi') = -4\pi n r_0^2 V_0\, j_1(kr_0)\,\hat{k}\cdot\underline{\xi}'\,\frac{e^{-(\xi^2+\xi'^2)/2}}{(2\pi)^3}$$

(4-27)

This is as far as we will carry the analytic approach. Equations (4-26) and (4-27) are in a form more amenable to numerical analysis. In the next section we will calculate the matrix elements M(i/j) using the equations.

$^{+}j_1(kr_0)$ is the first order Spherical Bessel function -

4-2 Matrix Element calculation

The orthonormal basis we decided to use is essentially the Hermite polynomials,

$$\psi_i(\underline{\xi}) = \psi_{\ell m n}(\underline{\xi}) = \bar{H}_\ell(\xi_1)\,\bar{H}_m(\xi_2)\,\bar{H}_n(\xi_3) \Big/ (\ell!\,m!\,n!)^{1/2} \tag{4-28}$$

where $\bar{H}_\ell(\xi) = H_\ell(\xi/\sqrt{2}) \Big/ (2^{\ell/2})$ (4-29)

$H_\ell(\xi)$ is the Hermite polynomial as defined in Morse and Feshbach (29). As a matter of nomenclature we shall call our basis the modified Hermite polynomials.

To facilitate the mathematical analysis it is desirable to consider separately the static part, the inhomogeneous collision part and the homogeneous collision part.

Using equations (4-5), (4-26), (4-27) and (3-24) we see that:-

$$\begin{aligned} M^{(s)}(i|j) &= 4\pi n r_0^2 v_0 \quad j_1(kr_0)\,\delta_{0\ell'}\delta_{0m'}\delta_{0n'}\delta_{0\ell}\,\delta_{0m}\,\delta_{1n} \\ &= M^{(s)}(\ell m n\,|\,\ell' m' n') \end{aligned} \tag{4-30}$$

$$\begin{aligned} \frac{M}{2}{}_{I}^{(c)}(i|j) &= -2 n r_0^2 v_0 \pi\, j_1(kr_0)\,\delta_{0\ell'}\delta_{0m'}\delta_{1n'}\delta_{0\ell}\,\delta_{0m}\,\delta_{0n} \\ &= M_{I}^{(c)}(\ell m n\,|\,\ell' m' n')/2 \end{aligned} \tag{4-31}$$

$$\frac{M}{2}{}_{H}^{(c)}(i|j) = 8\frac{i n}{(2\pi)^3} r_0^2 v_0 \int d^3\xi\, d^3\bar{\xi}\, d\Omega_r\, e^{-(\xi-\bar{\xi})^2} e^{-\bar{\xi}^2}$$

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[1] Handbook of Mathematical functions' U.S. Commerce Department.

$$\hat{r}\cdot\bar{\underline{\xi}}\,[1-\theta(\hat{r}\cdot\bar{\underline{\xi}})]\,\psi_i(\underline{\xi})\{\psi_j(\underline{\xi})-\psi_j(\underline{\xi}-2\hat{r}(\\ \hat{r}\cdot\bar{\underline{\xi}}))+e^{i\underline{k}\cdot r_0\hat{r}}(\psi_j(\underline{\xi}-2\bar{\underline{\xi}})-\psi_j(\underline{\xi}-2\bar{\underline{\xi}}+\\ 2\hat{r}(\hat{r}\cdot\bar{\underline{\xi}}))\} \qquad (4\text{-}32)$$

Equations (4-30) and (4-31) are in a form that can be directly programmed, but equation (4-32) has to be simplified further.

The computer program 'Matrix'[+] calculates $M_{H}^{(c)}(i/j)/2$ which is relatively more complicated than either equation (4-30) or equation (4-31). These expressions for $M_{I}^{(c)}(i/j)/2$ and $M^{(s)}(i/j)/_{2}$ are directly incorporated into the program 'Dispersion'.

To check 'Matrix' some of the lower order elements were worked out by hand and compared with the program output for various values of the parameter kr_0[‡].

As a final touch, a number of the lower order elements for $kr_0=0.0$ were linearly combined to form the equivalent elements for a Sonine polynomial basis*. These were checked against Sugawara's (3) and Mott-Smith's matrix elements (7). As was noted in an earlier chapter

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[+] For a more comprehensive description of the various computer programs used, see appendix D.

[‡] The interested reader will find analytic expressions for these in Mazenko's thesis.

*A general transformation between the Hermite basis and the Sonine basis is given in appendix C.

the kr_0 =0.0 limit of the generalized equation is the linearized Boltzmann equation and thus we would expect that our test would yield identical values for the three sets of matrix elements.

What we do find is that they are off by constant factors. This was expected in the case of Mott-Smith's numbers as his matrix elements are derived in terms of a certain bracket integral. This was however not expected of Sugawara's matrix elements. On closer examination it was discovered that a factor of $8\sqrt{\pi}$ had been dropped in his program for calculating the matrix elements.

Taking into account the factor that Sugawara dropped the factor of $8\sqrt{\pi}$ the two sets of numbers are, within roundoff error, identical.

It should be noted that constant factors in the expressions for the matrix elements have no effect on the spectrum calculations as we are only concerned with the ratios of these elements.

Finally with the basis we have chosen it can be shown that the elements with odd l or m index do not enter into our spectrum calculations so we only need to compute the elements with even l and even m indices.

4-3 Self-Correlation operator (Memory)

The memory function $\mathcal{E}_s(\xi\xi')$ for the self-correlation function is obtained by simply ignoring the dynamic correlations between different particles in the collision part of the total memory function $\Sigma(\underline{k}, \underline{\xi}\,\underline{\xi}', z)$. That is to say we drop the terms involving the exponential $e^{-i\underline{k}r_0\cdot\hat{r}}$ in equation (4-26). One also drops the static part. After going through the same manipulative procedures of section (4-1) we arrive at the result that:

$$M'_s(\underline{k}, \underline{\xi}\,\underline{\xi}')\,\Phi(\xi') = \frac{16\, i\, n r_0^2 v_0}{(2\pi)^3}\int d^3\alpha\, d^3\bar{\xi}\, d\Omega_r$$

$$\hat{r}\cdot\bar{\underline{\xi}}\; e^{-(\alpha^2+\bar{\xi}^2)}\,[1-\theta(\hat{r}\cdot\bar{\underline{\xi}})]\,\{\delta(\underline{\xi}'-\alpha-\underline{\xi})$$

$$- \delta(\underline{\xi}-\underline{\alpha}-\bar{\underline{\xi}}')\}\,\delta(\underline{\alpha}-\underline{\xi}+\bar{\underline{\xi}}) \qquad (4-33)$$

This is the wavelength and frequency dependent generalization of the neutron transport kernel (15).

Thus it can be seen that the self-correlation memory function is just part of the two-body memory function and the 'Matrix' program is easily modified to seperate out that part. This part does not depend upon kr_0 at all and in fact for the hard sphere case

$$\Sigma_s(\underline{\xi}\,\underline{\xi}') = \lim_{kr_0\to\infty} \Sigma^{(c)}(\underline{k}, \underline{\xi}\,\underline{\xi}') \qquad (4-34)$$

This can be seen by expanding $e^{-i\underline{k}r_0\cdot\hat{r}}$ in terms of spherical Bessel functions. One could speculate that this is true in the general case.

4-4 Properties of the matrix Elements

The matrix elements of the homogeneous collision memory function have a number of general properties which are very useful in reducing the amount of computation required. They are useful also in checking the 'Matrix' program.

(a) If $l+l'$ or $m+m'$ are odd, then the matrix element is zero.

(b) If $(n+n')$ is odd, then the matrix element is real and approaches zero as k goes to zero.

(c) If $(n+n')$ is even then the matrix element is pure imaginary and approaches a constant as k goes to zero.

(d) The matrix element is symmetric under the transformation $l \rightleftarrows m$ and $l' \rightleftarrows m'$.

(e) The diagonal matrix elements are purely imaginary and their imaginary part is negative.

(f) The off-diagonal elements are small in magnitude compared to the diagonal matrix elements.

Properties (a) and (d) cut down tremendously the number of elements that have to be computed while property (f) ensures that Kinetic modelling can be used.

The matrix elements of the self memory function, on

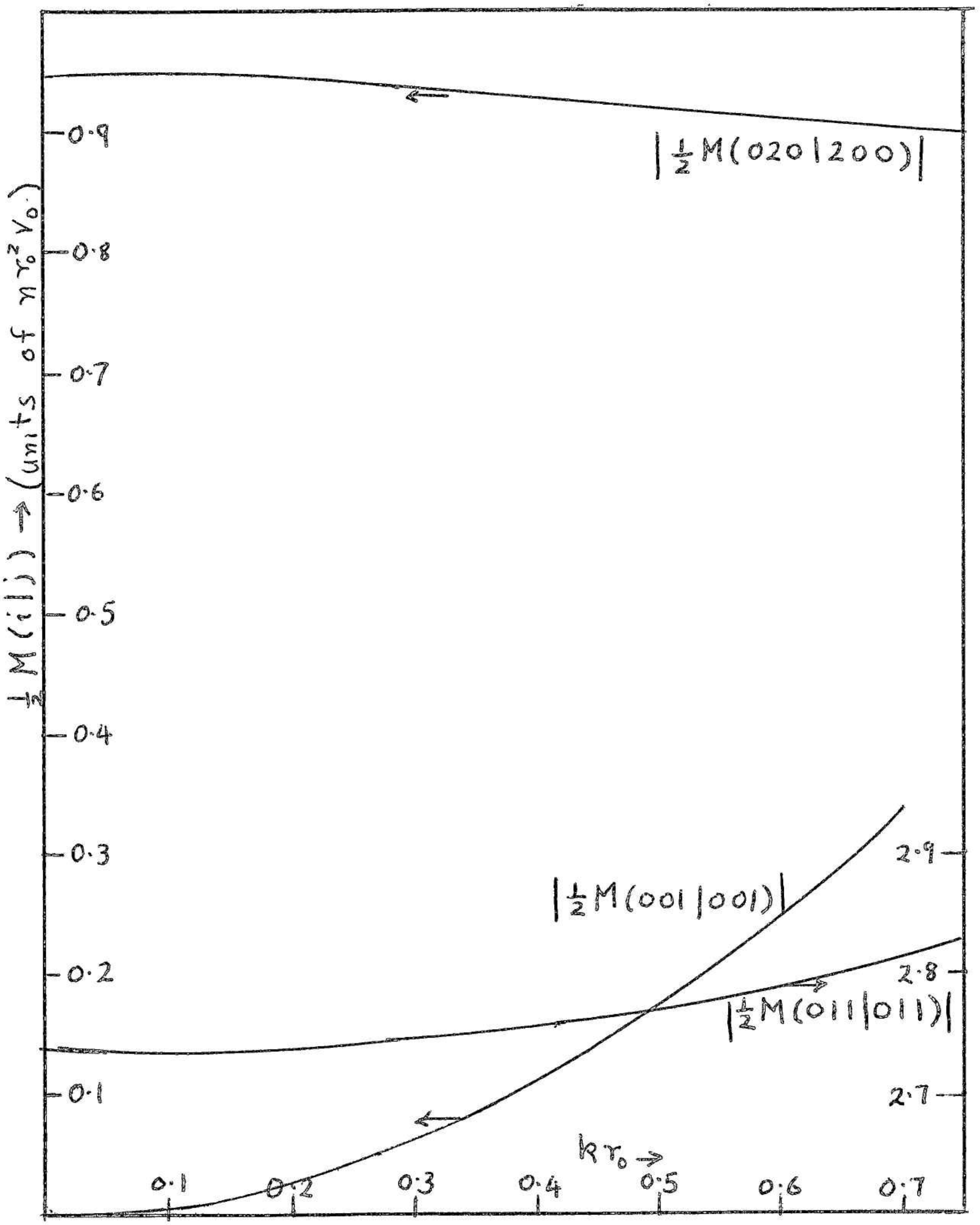

FIG. 4.1 DEPENDENCE OF MATRIX ELEMENTS ON kr_0

the other hand obey rules (a), (d), (e) and (f). In addition to those properties they have the property that

(g) If $(n+n')$ is odd the element is zero.

Table 4-1 is a list of some of the diagonal elements for the two-particle memory function. These are the important elements as we need them to arrange the modes in the λ-ordering scheme^{+}. Table 4-2 is a list of the corresponding numbers for the self-correlation memory function.

We also show the variation of element M(011/011) with the parameter kr_0 in Figure 4-1. This gives a general illustration of how the diagonal elements vary with kr_0. The M(011/011) element is important because it is the element related to the shear viscosity through equation (3-32c).

What is more interesting is the behaviour of the so-called 'conservation' elements. These are M(lmn/000), M(lmn/001) and the linear combination (M(lmn/002)+M(lmn/020)+M(lmn/200)).

In the Boltzmann equation region namely $kr_0=0$ these elements are zero, implying the conservation of number density, momentum in the ξ_3-direction and energy. We expect this as the Boltzmann collision operator is known to conserve these quantities. However for non-zero values

		kr_o					
No	lmn	0.0	0.1	0.3	0.7	1.0	∞
1	000	0.0	0.0	0.0	0.0	0.0	0.0
2	001	0.0	0.007	0.063	0.33	0.66	2.36
3	002	1.89	1.896	1.93	2.13	2.36	3.30
4	020	1.89	1.89	1.90	1.94	1.99	3.31
5	200	1.89	1.89	1.90	1.94	1.99	3.31
6	003	2.83	2.84	2.87	3.04	3.24	3.97
7	004	3.53	3.54	3.56	3.72	3.90	4.51
8	040	3.53	3.53	3.53	3.55	3.57	4.51
9	400	3.53	3.53	3.53	3.55	3.57	4.51
10	021	3.78	3.78	3.79	3.84	3.89	4.46
11	201	3.78	3.78	3.79	3.84	3.89	4.46
12	005	4.10	4.11	4.14	4.28	4.45	4.98
13	022	4.55	4.56	4.57	4.61	4.67	5.06
14	202	4.55	4.55	4.57	4.61	4.67	5.06
15	220	4.55	4.56	4.55	4.56	4.58	5.06
16	006	4.60	4.61	4.63	4.76	4.92	5.41
17	060	4.60	4.61	4.60	4.61	4.61	5.41
18	600	4.60	4.61	4.60	4.61	4.61	5.41
19	041	4.95	4.95	4.95	4.95	4.95	5.41
20	401	4.95	4.95	4.95	4.95	4.95	5.41
21	007	5.05	5.05	5.08	5.20	5.35	5.79
22	023	5.12	5.12	5.13	5.17	5.23	5.54
23	203	5.12	5.12	5.13	5.17	5.23	5.54
24	008	5.45	5.46	5.48	5.60	5.74	6.15
25	080	5.45	5.45	5.45	5.46	5.45	6.15
26	800	5.45	5.45	5.45	5.46	5.45	6.15
27	221	5.48	5.49	5.48	5.48	5.48	5.73
28	024	5.58	5.59	5.60	5.64	5.69	5.95
29	042	5.58	5.59	5.58	5.58	5.58	5.95
30	204	5.58	5.59	5.60	5.64	5.69	5.95

TABLE. 4.1 DEPENDENCE OF $\frac{1}{2}$ M(i/i) ON kr_o - λ-ORDER (Cont.)

		kr_o					
No	lmn	0.0	0.1	0.3	0.7	1.0	∞
31	240	5.58	5.59	5.59	5.59	5.59	5.95
32	402	5.58	5.59	5.58	5.58	5.58	5.95
33	420	5.58	5.59	5.59	5.59	5.59	5.95
34	061	5.81	5.81	5.81	5.81	5.81	6.21
35	601	5.81	5.81	5.81	5.81	5.81	6.21
36	222	5.99	5.99	5.99	5.99	5.99	6.18

+TABLE. 4.1 (Cont.)

TABLE. 4.2 THE SELF CORRELATION DIAGONAL ELEMENTS

(See Table. 4.1 $kr_o = \infty$ column)

kr_o	0.0	0.3	0.7	1.0	2.0	4.0
$\frac{1}{2}$ M(lmn/000)	0.0	0.0	0.0	0.0	0.0	0.0
$\frac{1}{2}$ M(001/001)	0.0	0.063	0.33	0.66	2.2	4.11
$\frac{1}{2}$ {M(002/002) + M(002/020) + M(002/200)}	0.0	0.063	0.34	0.67	2.2	4.12

+TABLE. 4.3 VARIATION OF SOME "CONSERVATION" ELEMENTS WITH kr_o

+ units of $n r_o^2 v_o$

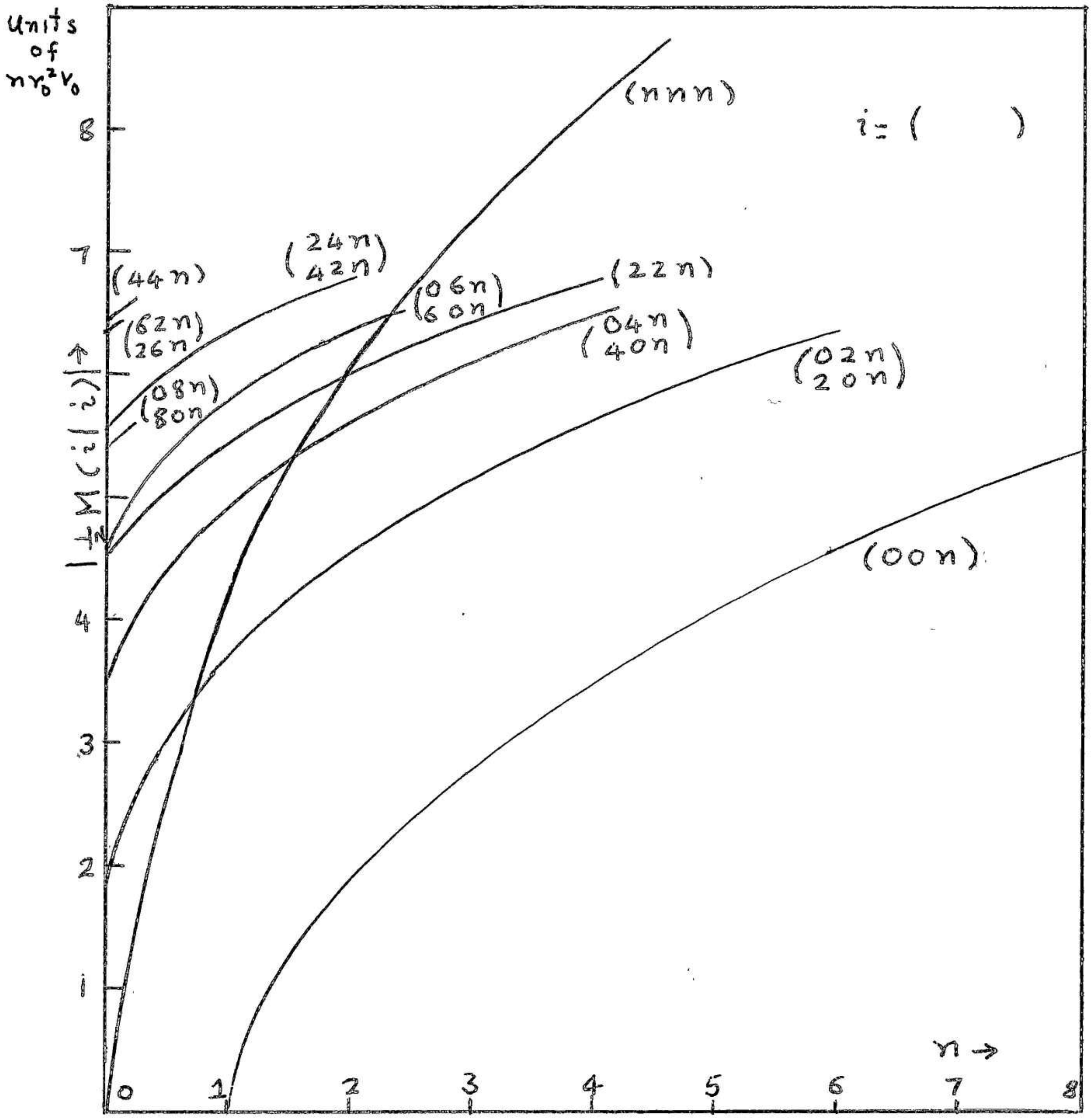

FIG. 4.2 DEPENDENCE OF THE DIAGONAL MATRIX ELEMENTS ON THE INDICES

of kr_0 only the M(lmn/000) element still remains zero. The deviation from zero of the other elements gets larger as kr_0 is increased. One possible physical interpretation of this behaviour is that with constant diameter of the particles increase in kr_0 corresponds to an increase in the wave number k. This means that we are looking at a smaller and smaller volume of space. Eventually the volume we are looking at becomes smaller than the interaction volume, in fact even smaller than the dimensions of the particles themselves. In this case we cannot expect momentum and energy to be conserved as we cannot keep track of both colliding particles. In fact the equation can only keep track of one particle or in other words we have gone over to the self-correlation case where only number density is conserved. As was mentioned earlier $\Sigma_s(\underline{\xi}\,\underline{\xi}')$ is indeed the large kr_0 limit of $\Sigma(\underline{k},\underline{\xi}\,\underline{\xi}',z)$. Table 4-3 illustrates this behaviour for the diagonal 'conservation' elements.

Finally we show groups of diagonal elements as a function of the index n in Figure 4-2. This is useful for extrapolation purposes as the 'Matrix' program computes elements along lines of constant l and constant m but varying n. This turned out to be more efficient in our case than computing by blocks.

The matrix elements corresponding to the truncated basis of Table 4-1 are available in λ-ordering for $kr_0=0$. For other values of kr_0 they are available but have not been organized into any particular order.

CHAPTER 5

Discussion of Numerical Results

5-1 Introduction

The relaxation process in a structureless monoatomic fluid is essentially characterized by two basic lengths and two basic times. This is said of course under the assumption that the mean energy is not high enough for electronic excitation to occur. The two basic lengths are the mean free path and a length characterizing the interatomic potential. In the case of a hard sphere gas this characteristic length would be the dimensions of the sphere. Corresponding to this length there is the time characterizing the duration of the collision and corresponding to the mean free path there is the intercollision time. The hard sphere gas, however, is a pathological case. Its collision duration is zero.

The linearized Boltzmann equation, as has been stated before, is only good for times and distances long compared to the collision duration and the particle size (18). This limitation is incorporated into the collision kernel as it describes the fluid in terms of point masses and instantaneous collisions.

So when this Kinetic equation is used to calculate $S(k,\omega)$ for gases only two parameters are needed to characterize the solution. The two parameters we choose to base this part of the discussion on, have a simple physical interpretation. One of these is, what we call the collision parameter y*. This relates the wavelength to the mean free path of the medium. The other parameter is y/x* and it measures the time in terms of the intercollision time. Other combinations of these parameters could be used. In fact Sugawara uses x and y (3).

Mazenko's equation, on the other hand, with its wavelength and frequency dependent generalized collision kernel is good for all times and distances and it describes the behaviour of the fluid in terms of all four characteristic lengths and times.

When the Fourier-Laplace transformed equation (3-30a) is examined for the hard sphere gas, it will be noticed that we have only three parameters x, y and kr_0. We are however, missing a parameter related to the collision duration. As has been mentioned before the hard sphere is a pathological case. The collision duration is zero and the fourth parameter is a constant. It is either zero or infinite depending on how we define the parameter.

5-2 Comparison with Sugawara#

Sugawara's spectrum calculations used the linearized

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*y and x are defined in chapter 3

Boltzmann equation (3). To compare Mazenko's equation in the Boltzmann region with Sugawara's results we have to take $kr_0=0$. This test will not only enable us to check our computation but it will also demonstrate that the generalized equation has the correct limiting behaviour. In the process of checking the computation we have also calculated the spectrum using the Wang Chang and Uhlenbeck method of polynomial expansion.

The major difficulty that the test ran into was the problem of convergence. As noted in section 3-3 there is the problem of truncating the basis. It is not at all certain that the convergence properties will be the same using the Sonine polynomial basis and the Hermite polynomial basis. There is no one to one correspondence. But it is certain that if the two truncated matrix representations of the collision operator contain the same information then we should obtain the same values for the spectrum. This is what was done and the results are tabulated in Table 5-1. On the basis of this comparison we confirm that the two approaches are indeed equivalent.

Going back to the question of convergence the elements were ordered according to two different schemes, poly-

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#Sugawara uses the dimensionless quantity $R(x,y) = kv_0 S(x,y)/\sqrt{2}\pi$ in his graphs. The $R(x,y)$ used in our plots is identical to his.

$y=1.2275$

$2R(x,y)$

x	Our Calculation N=14	Sugawara N=9
0.0	1.0710	1.068
0.4	0.8437	0.844
0.8	0.7775	0.775

TABLE. 5.1 COMPARISON OF SUGAWARA'S CALCULATION WITH OUR CALCULATION- POLYNOMIAL ORDERING SCHEME - EQUIVALENT KINETIC MODEL ORDER

$\frac{1}{2}$ M(001/001)

kr_0	Parabolic fit	Analytic result	%Error
0.01	0.0000707	0.00007	1.0
0.03	0.000623	0.000637	2.2
0.06	0.00269	0.0025	5.5
0.3	0.0617	0.0634	2.7
0.5	0.1714	0.1746	2.4
1.0	0.6854	0.67	2.23

TABLE. 5.2 MATRIX ELEMENT M(001/001) - ERROR INCURRED USING A PARABOLIC FIT THROUGH THE POINTS kr_0 =0.0,0.1 AND 0.7

nomial order and λ-order. In the polyonomial order scheme, as the name implies, one orders the set $\{\Psi_i\}$ according to the order of the polynomial Ψ_i, that is according to the sum of the three indices. Within each closed shell of polynomials of the same order one tries to arrange the basis functions such that inherent rotational symmetry groups are not broken. The idea behind the polynomial ordering lies in the empirical observation that the zeroth order polynomial corresponds to number conservation, the first order polynomial to momentum conservation, the next orders include the energy conservation, the heat flux vector and so on. Heuristically, as the order increases one seems to add in more physical processes of decreasing importance on the microscopic scale.

λ-ordering on the other hand is the ordering of the elements according to the magnitude of the corresponding diagonal elements. As noted in section 3-3 the reasoning behind this ordering is quite quantitative as the diagonal elements are indeed related to the decay constants of the eigen modes. Thus λ-ordering systematically brings in the transient modes on the basis of promptness of relaxation and would therefore gradually improve the microscopic description.

However we did not have a simple analytic expression for the magnitudes of the diagonal elements, so what we finally ended up doing was to compute all the diagonal elements upto and including a certain polynomial order and then reorder the basis according to the λ-ordering scheme. The success of this procedure is based upon the assumption that the diagonal element distribution is sufficiently monotonic in the indices that we leave out very few gaps. Figure 4-2 tends to substantiate our position.

The Kinetic model approximation, as we have noted in section (3-2), should be very good near the free particle limit, and from the argument above it should also be quite good in the hydrodynamical limit. This is because the hydrodynamical region is essentially that of long times and distances. This leaves us with the region between these two extrema of behaviour, which we would expect to be not so well described by our approximation. Given the restriction of limited computer time this is the region we should investigate with regard to the convergence and accuracy of our approximation. The y-value of 1.2275 which we finally used to examine the convergence properties of the approximation is slightly biased towards the hydrodynamical region. We chose that value because experimental data is available for that particular condition. The x-value was chosen to be 0.0 because from Sugawara's calculations it looked as though the approximation would be worst at this value.

Figure 5-1 shows the convergence behaviour for the two ordering schemes. As was expected the λ-order convergence is much smoother and more rapid. This behavior was also noted by Sugawara. In both his work and in ours it cannot be said that the polynomial scheme has converged. The orders of the respective Kinetic models used were simply not high enough for this scheme to converge.

On the other hand, his λ-ordering calculations converged around a Kinetic model order of 23 while ours converged around an order of 40. Our asymptotic value is of the order of a percent off from his. There are a number of possible reasons for this difference. One of them is the possibility that our λ-ordering has skipped a few elements. This was discussed above. More important is the possibility of computational round-off error as the Hermite polynomials basis in a certain sense is not a very efficient basis as it, unlike the Sonine polynomials, does not make direct use of the azimuthal symmetry in our system. For the same amount of information, the matrix obtained by using the Sonine polynomial representation is smaller than the one obtained by using the Hermite polynomials. The computer had to, essentially, compress this data and in the numerical inversion of matrices the larger the inverted matrix the larger the round-off error. For a 60x60 matrix this error could

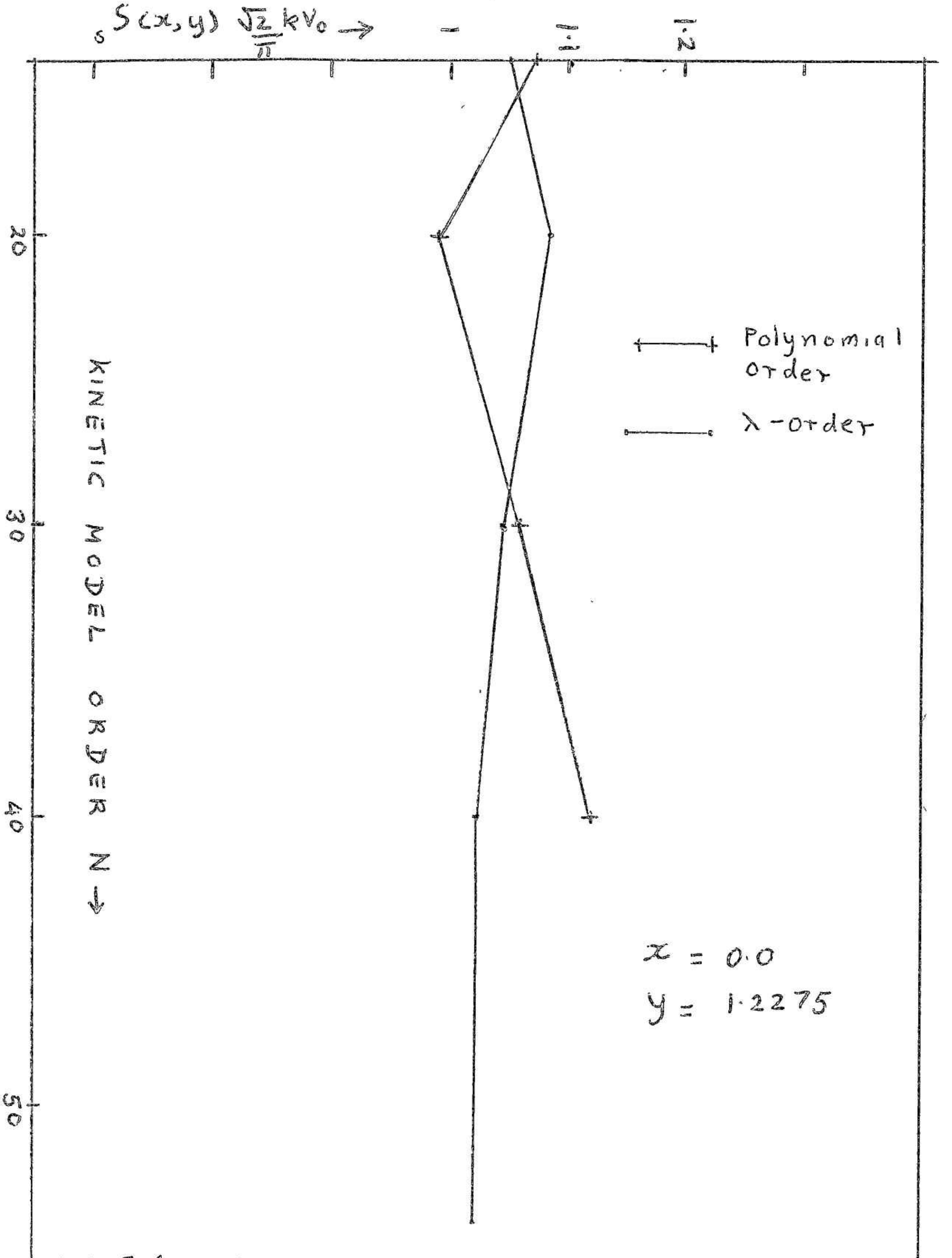


FIG. 5.1 COMPARISON OF λ-ORDER CONVERGENCE WITH POLYNOMIAL ORDER CONVERGENCE

possibly be of the order of a percent.

The main emphasis of our work is on the effect of finite kr_0 on the spectrum. This will enable us to delineate the region of validity for the Boltzmann equation and obtain quantitative corrections for wavelengths outside this region. From Mazenko's preliminary computations we know that the effects we will be examining will lead to differences of around thirty percent between Sugawara's analysis and our calculations for finite values of kr_0. With this in mind we decided that a Kinetic model of order 35 would be sufficiently accurate for all our subsequent work.

5-3 The spectrum of density fluctuations at finite kr_0

If we integrate the two particle spectrum over all ω we find that

$$\frac{1}{2\pi}\int d\omega \; {}_M S(k,\omega) = {}_M S(k) = 1 + n\,h(k) \tag{5-1}$$

With this result in hand we can immediately obtain an estimate of the range of validity of our equation by noting that ${}_M S(k)$, on physical grounds, can never be negative. Thus,

$$1 \geq n\,h(k) \tag{5-2}$$

where

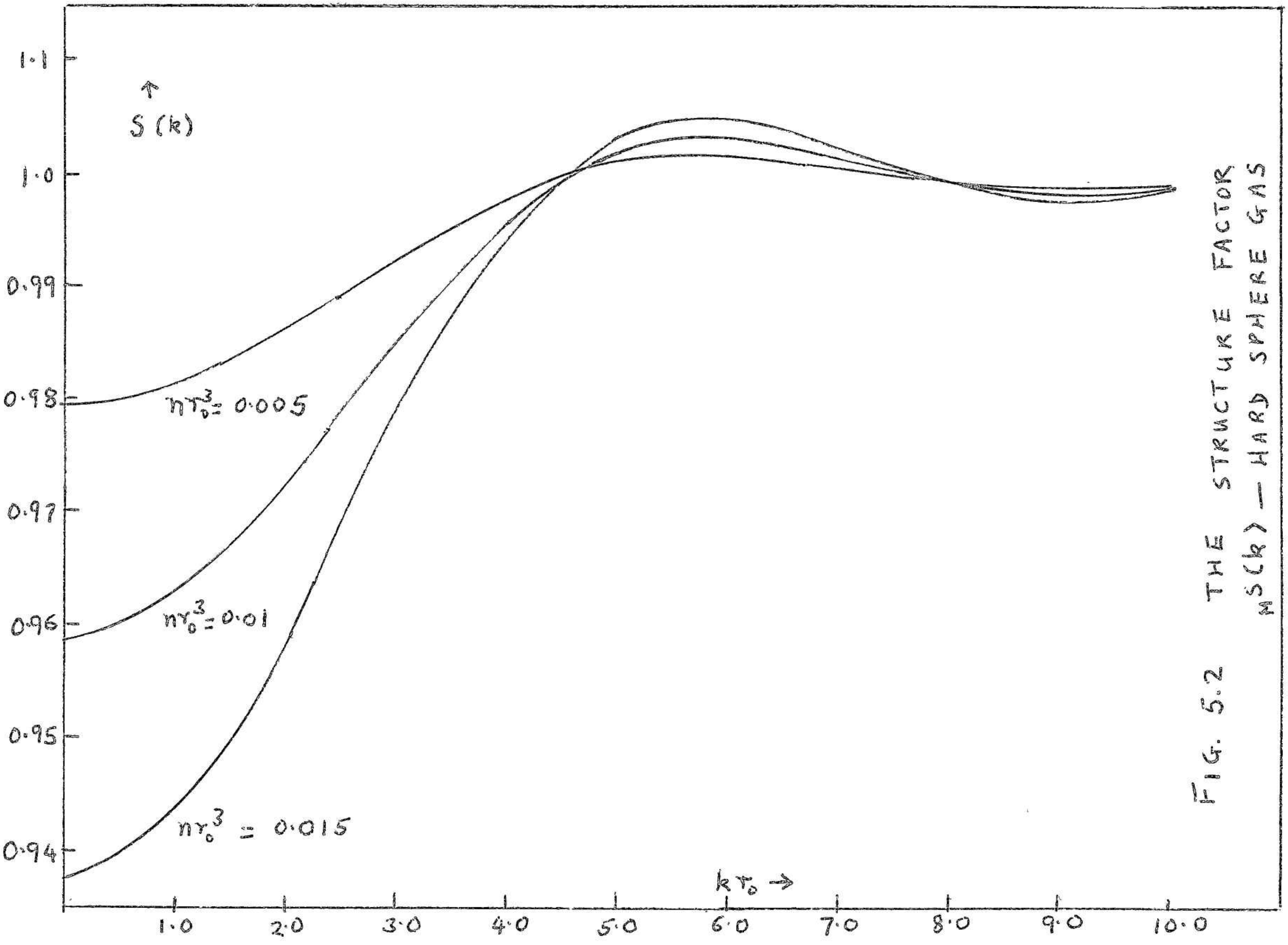


FIG. 5.2 THE STRUCTURE FACTOR ${}_{M}S(k)$ — HARD SPHERE GAS

$$h(k) = \int d^3r \, e^{-i\underline{k}\cdot\underline{r}} \left[g(r) - 1 \right] \tag{5-3}$$

For our low density approximation h(k) reduces to

$$h(k) = -\frac{4\pi r_0^3}{kr_0} j_1(kr_0) \tag{5-4}$$

If we approximate the spherical Bessel function $j_1(kr_0)$ by the leading term of its expansion in kr_0, (5-2) leads to

$$1 > \frac{4}{3}\pi n r_0^3 \tag{5-5}$$

This bound is definitly not the least upper bound as significant error in our first order approximation for y(r) already sets in at densities much lower than the limit given by equation (5-5). This can be shown by using the solution of the Percus-Yevick equation for hard spheres (20). This Percus-Yevick results also enables us to put a quantitative value on the error involved as the density increases. Egelstaff (20) has shown that the Percus-Yevick equation is quite good for $nr_0^3 < 0.25$. If that equation is used to obtain an equation of state we find

$$\frac{P}{\rho kT} = 1 + 4\left(\frac{\pi}{48} n r_0^3\right) + 10\left(\frac{\pi}{48} n r_0^3\right)^2 + \cdots \tag{5-6}$$

So the error, ε , we are interested in is of the order

$$\varepsilon \sim \frac{10}{4} \cdot \frac{\pi}{48} \cdot n r_0^3 \qquad (5\text{-}7)$$

For nr =0.01 this is around 0.5%. It would be more realistic to say that the error is of the order a percent.

Figure 5-3 provides a graphic illustration of the region we are restricted to. From our experience with the Boltzmann equation we use the parameter y to roughly divide the figure into hydrodynamic and free particle regions. A word of caution is necessary here as in the case of finite kr_0 the terms hydrodynamic and free particle may convey physical interpretations quite different from those associated with the Boltzmann equation. However we do expect that for kr_0 small enough we will obtain the same qualitative behaviour. It should be remembered that the limits taken ($kr_0 \to 0$ and $kr_0 \to \infty$) to obtain the Boltzmann equation and the equation for the self correlation are only taken for the collision operator. They are not taken for the entire spectrum equation; or there would be questions regarding the continuity of the solution at those limits.

If we examine our calculation again we see that it differs from Sugawara's calculation (3) in three respects.

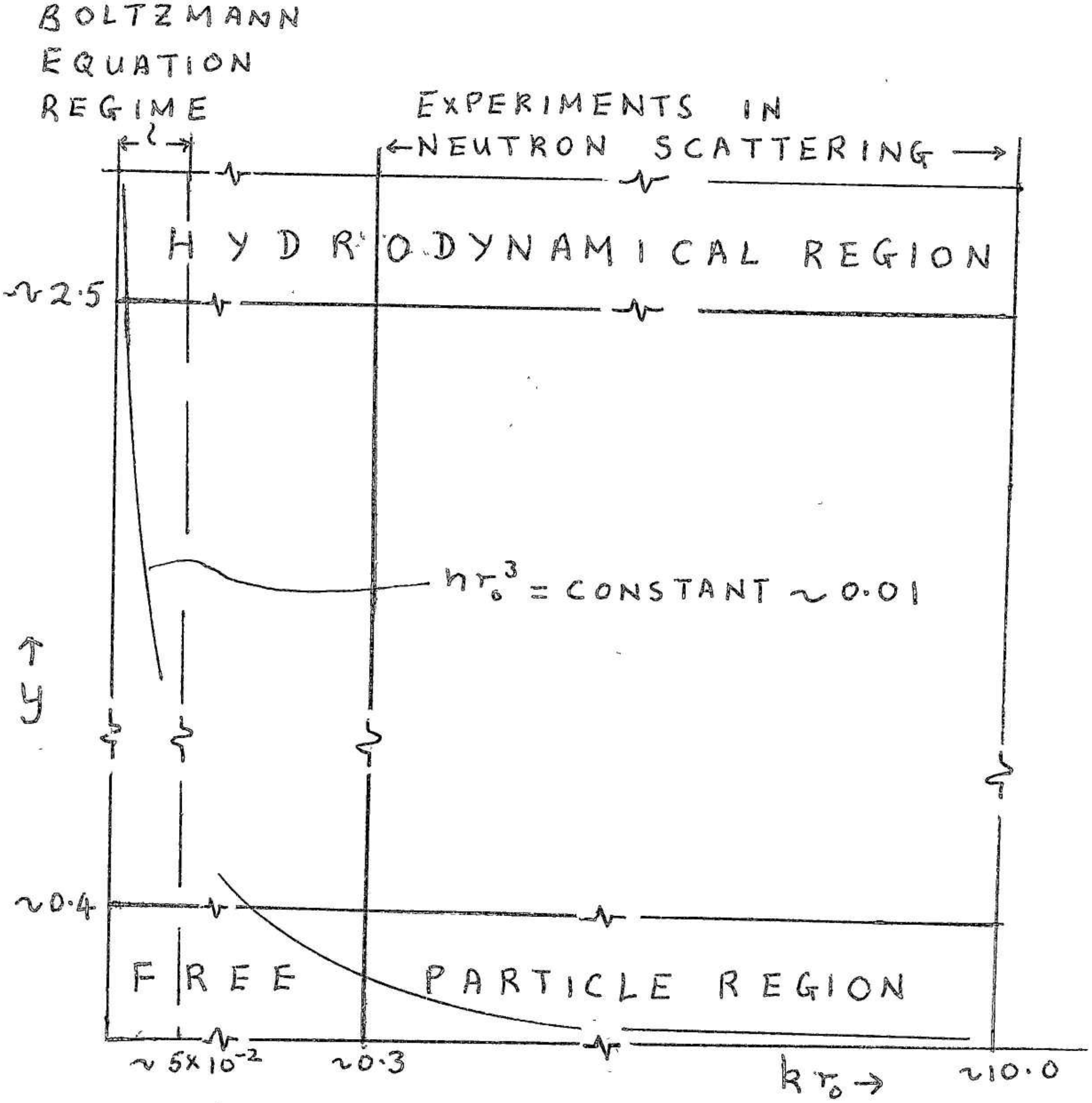


FIG. 5.3 SCHEMATIC REPRESENTATION OF REGION OF INTEREST

Mazenko's equation has a static term which the Boltzmann equation does not have. The collision matrix elements now have a kr_0 dependence. Aside from these major differences, there is the matter of the initial condition. Sugawara's initial condition does not contain the term involving the direct correlation as ours does.

Before we move on to discuss our results it must be noted that we have used a three point parabolic fit to calculate our matrix elements for a general kr_0. As most of our points of interest fell in the region $0 \leq kr_0 \leq 1.0$, we calculated explicitly the elements at the points $kr_0=0$, 0.1, 0.3, 0.7. The $kr_0=0$, 0.1 and 0.7 results were then used to obtain the co-efficients of the parabola. To check the goodness of fit we compared our parabolic fit numbers with the analytic results for the element M(001/001). As can be seen from Table 5-2, the accuracy is quite good. As a final check, the sensitivity of the spectrum calculation to variation in the values of the matrix elements was examined. The elements have been observed to exhibit two general characteristics. They are either almost constant in kr_0 or they start from zero and increase somewhat parabolically in our region of interest.

We first calculated the spectrum using a linear interpolation for the matrix elements. Then we changed the parabolically increasing elements by 10% and recalculated

M (i/j) :- $kr_0=0.068$ Matrix elements obtained by linear interpolation between $kr_0=0.0$ and $kr_0=0.3$

Case I :- M (i/j) used without any change

Case II:- All M (i/001) elements and all purely imaginary elements multiplied by factor of 0.9

Case III:- All the elements multiplied by factor of 0.9

$y=1.17$

x	Case I	Case II	Case III
0.0	0.90286	0.90629	0.90453
1.0	0.47844	0.47612	0.46372

TABLE. 5.3 SENSITIVITY OF 2R(x,y) TO VARIATION IN THE VALUE OF THE MATRIX ELEMENTS

nr_0^3 y	0.00997 0.04		0.00997 0.5	
x	Our Calculation	†Sugawara's	Our Calculation	Sugawara's
0.0	1.06476	1.1286	1.00421	1.0487
0.2	0.976679	1.0844	0.910398	1.0103
0.4	0.843499	0.96178	0.799935	0.93811
0.6	0.700791	0.7874	0.718141	0.84143
0.8	0.547915	0.5951	0.605648	0.67183
1.0	0.393627	0.4153	0.439335	0.45964
1.2	0.263125	0.2674	0.278856	0.27599
1.4	0.166173	0.15898	0.161009	0.14663
1.6	0.0976929	0.0872	0.085265	
1.8	0.0528238	0.0442	0.0429029	
2.0	0.0269757	0.0207	0.0217578	

†We have used the Free particle result for this comparison

TABLE. 5.4 2R(x,y) - COMPARISON OF OUR RESULTS WITH SUGAWARA's (cont.)

TABLE. 5.4 (cont.)

nr_o^3	0.01		0.01	
y	1.17		3.0	
x	Our Calculation	Sugawara's	Our Calculation	Sugawara's
0.0	0.974874	1.0326	1.21195	1.3347
0.2	0.866804	0.96731	0.810106	0.90579
0.4	0.752976	0.86968	0.549495	0.61051
0.6	0.707924	0.82529	0.558026	0.63790
0.8	0.671646	0.77015	0.811539	1.0067
1.0	0.524565	0.55586	0.789593	0.82178
1.2	0.298314	0.27820	0.273169	0.21353
1.4	0.141506	0.11823	0.950314	0.06646
1.6	0.0661308		0.0413453	
1.8	0.0326984		0.0212016	
2.0	0.0174123		0.0121779	

the spectrum. Finally, we computed the spectrum for a change of 10% in all the matrix elements. The y and kr_o values were of course fixed throughout this calculation. The results are presented in Table 5-3. They show that at the most a 1/2% change in the spectrum value will result from a 10% change in the matrix elements.

Figures (5-4) to (5-7) are comparisions of our results with Sugawara's (3). In our work we first fix the density nr_o^3 and examine the spectrum for various values of y and the corresponding values of kr_o . We then vary the density for a fixed y.

What is noticed immediately is that the central peak has been lowered. This can be attributed to the difference in initial conditions discussed above.

Aside from the lowering of the central peak there is a difference in shape. For y=0.0 we still obtain the Gaussian as we should, but as we increase the value of y the fall off is linear (for x less than 1.0) though we are still in the so-called free particle region.

At a y-value of around 0.133 we begin to move into a transition region as a shoulder starts appearing. In Sugawara's calculation even at y=0.5 the spectrum shape is still roughly Gaussian. It is almost as though our value of y has been somehow transformed to a higher value. Mathematically this can probably be explained by the fact

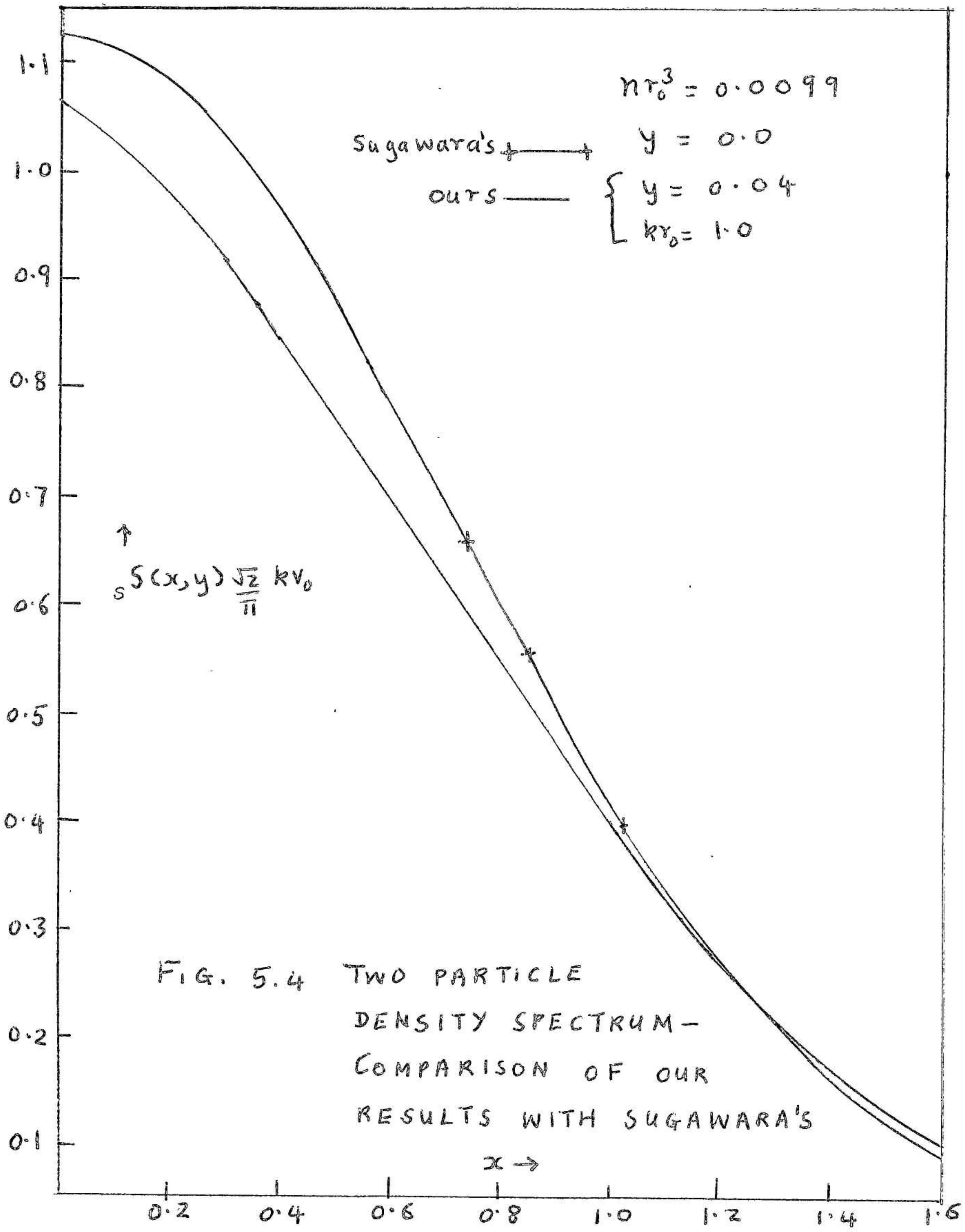


FIG. 5.4 TWO PARTICLE DENSITY SPECTRUM- COMPARISON OF OUR RESULTS WITH SUGAWARA'S

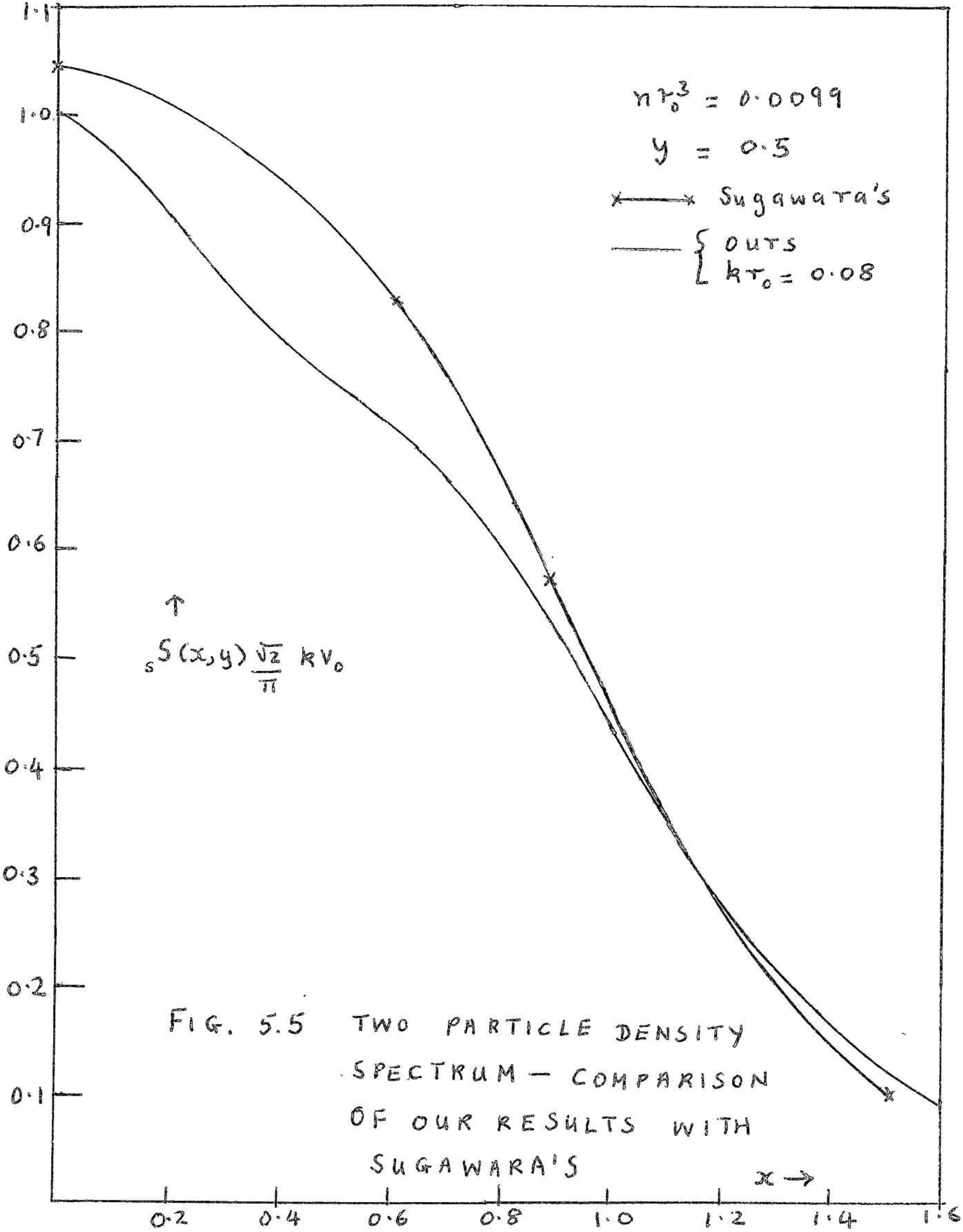


FIG. 5.5 TWO PARTICLE DENSITY SPECTRUM — COMPARISON OF OUR RESULTS WITH SUGAWARA'S

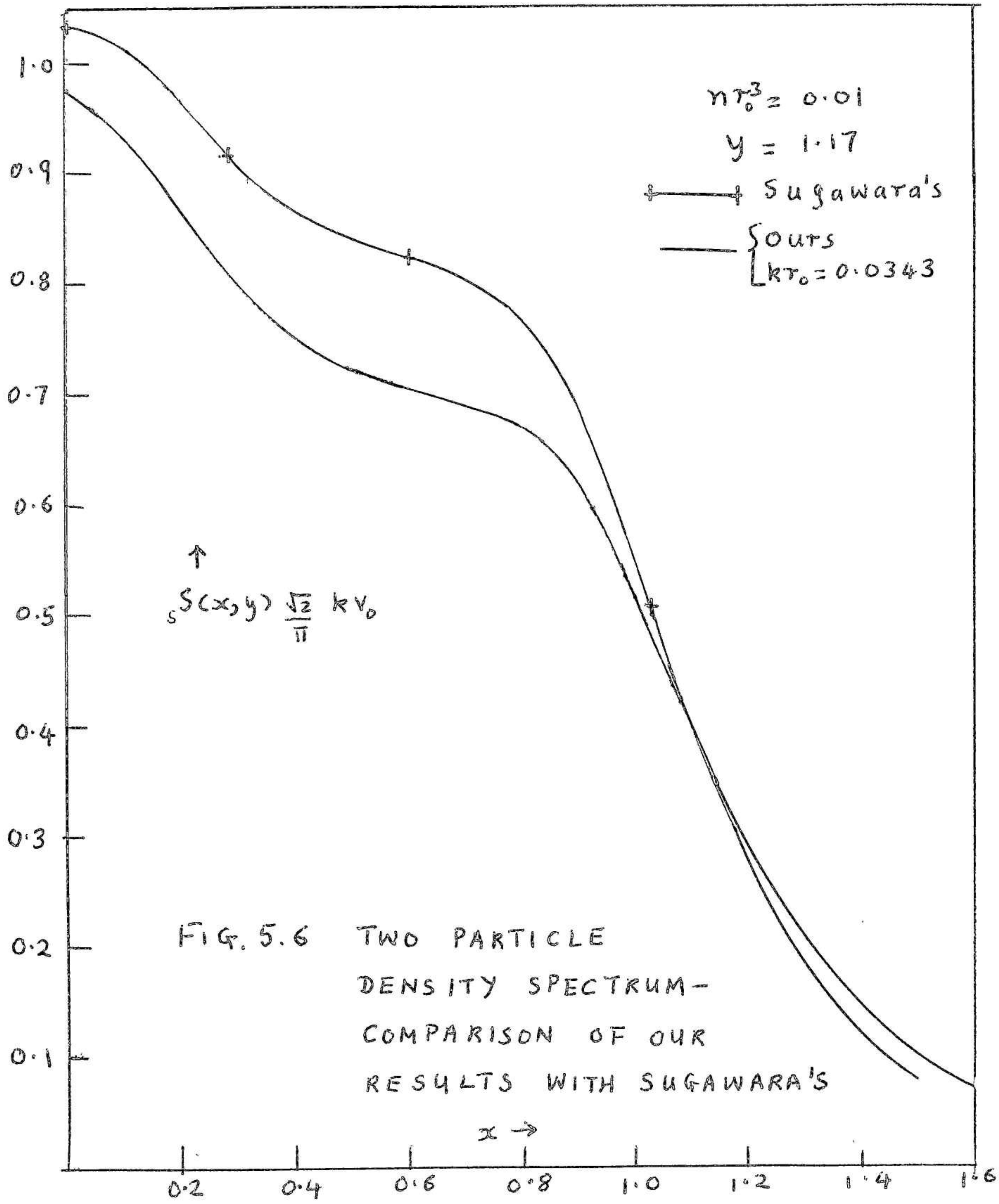


FIG. 5.6 TWO PARTICLE DENSITY SPECTRUM- COMPARISON OF OUR RESULTS WITH SUGAWARA'S

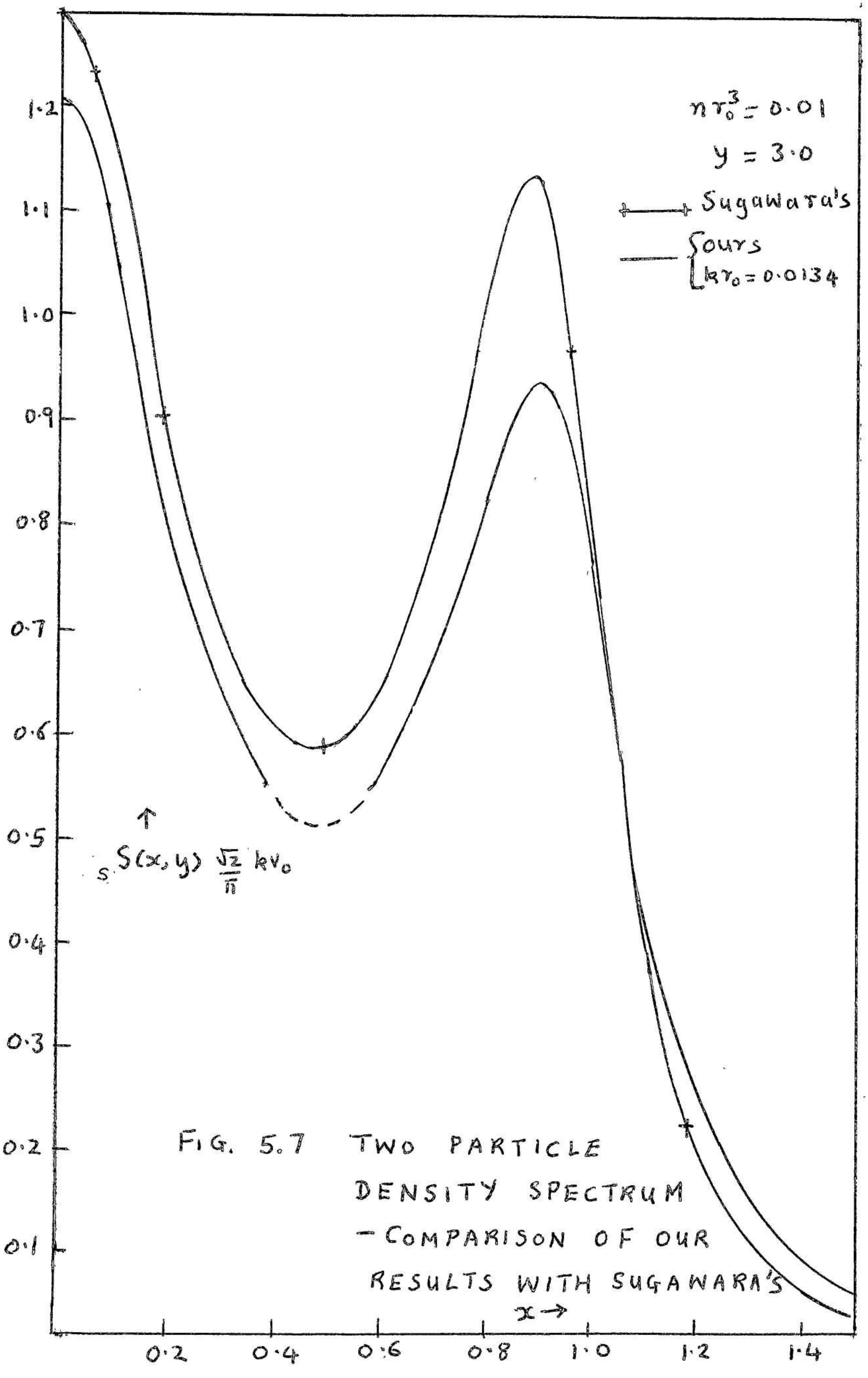


FIG. 5.7 TWO PARTICLE DENSITY SPECTRUM – COMPARISON OF OUR RESULTS WITH SUGAWARA'S

that our final equation (3-30a) has a term involving the product of y and the matrix elements M(i/j). Since these elements are increasing with kr_o in the region we are examining the effect is similar to increasing the value of y. There is this competition between y and kr_o . This is of course an oversimplified picture as an increase in kr_o destroys two of the three conservation laws and we could never obtain the familiar 3-peak hydrodynamic spectrum just by increasing kr_o .

Figure (5-7) shows that the sound peak moves out as we increase the kr_o value. On the whole the spectrum shape is definitely broader than Sugawara's. To see this from the graphs one has to examine the width to peak ratio as we do have this difference in initial condition.

At y=3.0 we still obtain the familiar three peak spectrum. This is not suprising as we have fixed the density at $nr_o^3=0.01$ and at this value the corresponding kr_o value is just 0.0134. Apparently this deviation in kr_o from the zero value is not enough to produce startling changes in the line shape. However, numerically absolute deviations of around 10-20% can be found. This is true even for kr_o as small as 0.0134. It would seem that the Boltzmann equation would be valid for kr_o around 0.005. This rough estimate is arrived at by using the results presented in Table 5-3 and Figure 4-3.

If we examine the ratio of the central peak to the spectrum value at x=0.8, differences of around 15% can be found between our calculation and Sugawara's. This indicates that if line shapes are measured experimentally it should be possible to detect the deviations between the Boltzmann equation and Mazenko's equation.

As to thedirect effect of kr_0, that is keeping y fixed and varying kr_0, we only have limited data. Figure (5-8) shows that at y=0.067, aside from the lowering of the spectrum, there is no noticeable change. The shapes are essentially identical. Apparently a 60% change in kr_0 has very little effect on the shape at this low value of y.

The above results seem to suggest that the general behaviour of the spectrum can basically be characterized by the two parameters kr_0 and y. Working along these lines we note that we can think of the neutron beam in terms of a probing volume of dimensions characterized by the wave number transfer. For a rough physical idea of the processes taking place consider Figure (5-10) for a fixed r_0.

In region I, we would expect something similar to the Gaussian spectrum as the particle radius is small enough so that the region examined by the probe can contain at most a single particle. Region III would give us a

† y=0.067

nr_o^3	0.01	0.0167
kr_o / x	0.6	1.0
0.0	1.0568	1.0178
0.2	0.963981	0.9087
0.4	0.8314	0.7741
0.6	0.69722	0.6479
0.8	0.5504	0.5164
1.0	0.3954	0.3783
1.2	0.2637	0.2587
1.4	0.1668	0.1689
1.6	0.09816	0.05802
1.8	0.05281	0.05802
2.0	0.02688	0.03097

† For the Free particle result see Table. 5.4

TABLE. 5.5 TWO PARTICLE DENSITY SPECTRUM - 2R(x,y)
DEPENDENCE ON kr at y=0.067

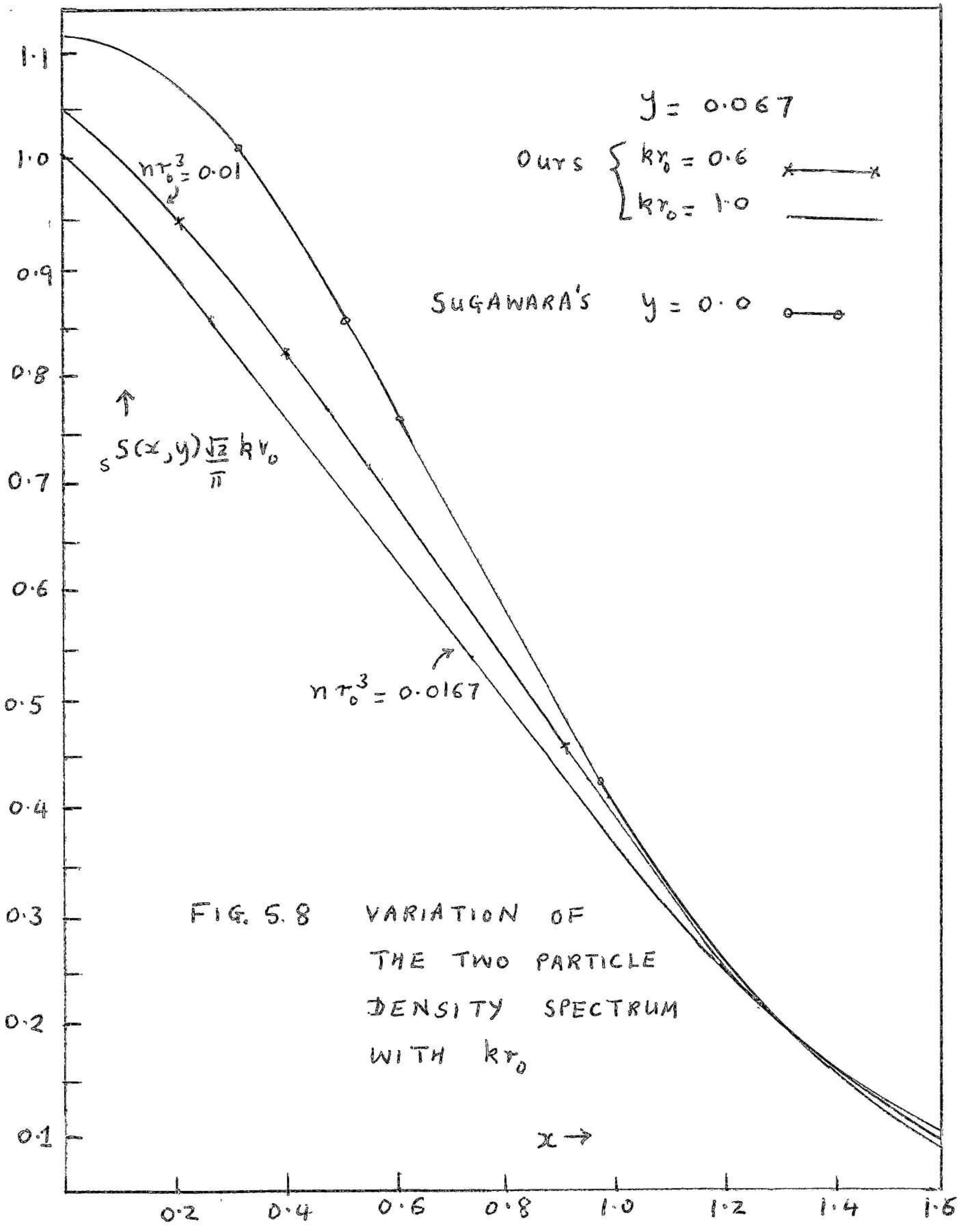


FIG. 5.8 VARIATION OF THE TWO PARTICLE DENSITY SPECTRUM WITH kr_0

$y=0.133$

$nr_0^3=0.00995$

$kr_0=0.3$

x	2R(x,y)
0.0	1.04898
0.2	0.951719
0.4	0.821489
0.6	0.700551
0.8	0.561560
1.0	0.402143
1.2	0.265259
1.4	0.166675
1.6	0.0970209
1.8	0.0513484
2.0	0.025898

TABLE. 5.6 TWO PARTICLE DENSITY SPECTRUM
$y=0.133, nr_0^3=0.00995, kr_0=0.3$

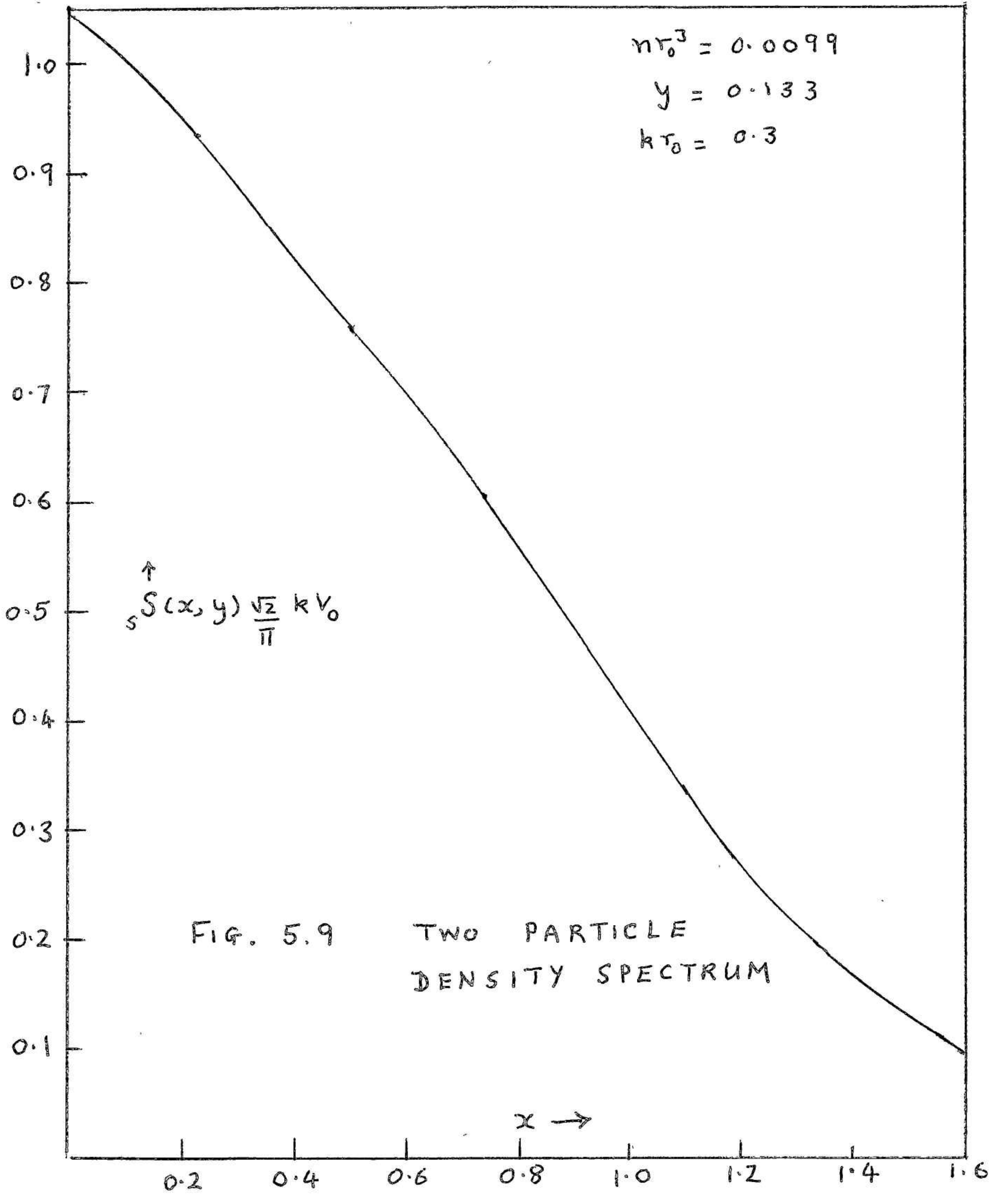


FIG. 5.9 TWO PARTICLE DENSITY SPECTRUM

spectrum characteristic of a continuum of particles. As the probe's wavelength is still large compared to the dimensions of the particles, a spectrum similar to the familiar 3-particle spectrum would be expected. Region II would be the transition between region I and region III. This is a spectrum with a protruding shoulder. Speculating further, we note that in region VII the parameter kr_o is such that the probing volume is completely taken up by a particle. As far as the probe is concerned there is no structure at all. It is just one rigid continuum. So the effect would be like probing a vacuum. The spectrum would therefore be a constant close to zero. In a sense it is a very broad curve.

The probing volume for region IX on the other hand, aside from the behaviour described for region VII, can also contain a small number of particles simultaneously. We would therefore expect a spectrum composed of a mixture of the spectra associated with regions II and VII; a lower broader spectrum with a central peak and a shoulder. As the speed of sound does increase to a certain extent with density, we would expect the shoulder to have moved out as region IV is the range of quite high densities. The spectrum of the other regions would be expected to be transitions between their adjoining extremes.

This is of course a very crude picture and it is

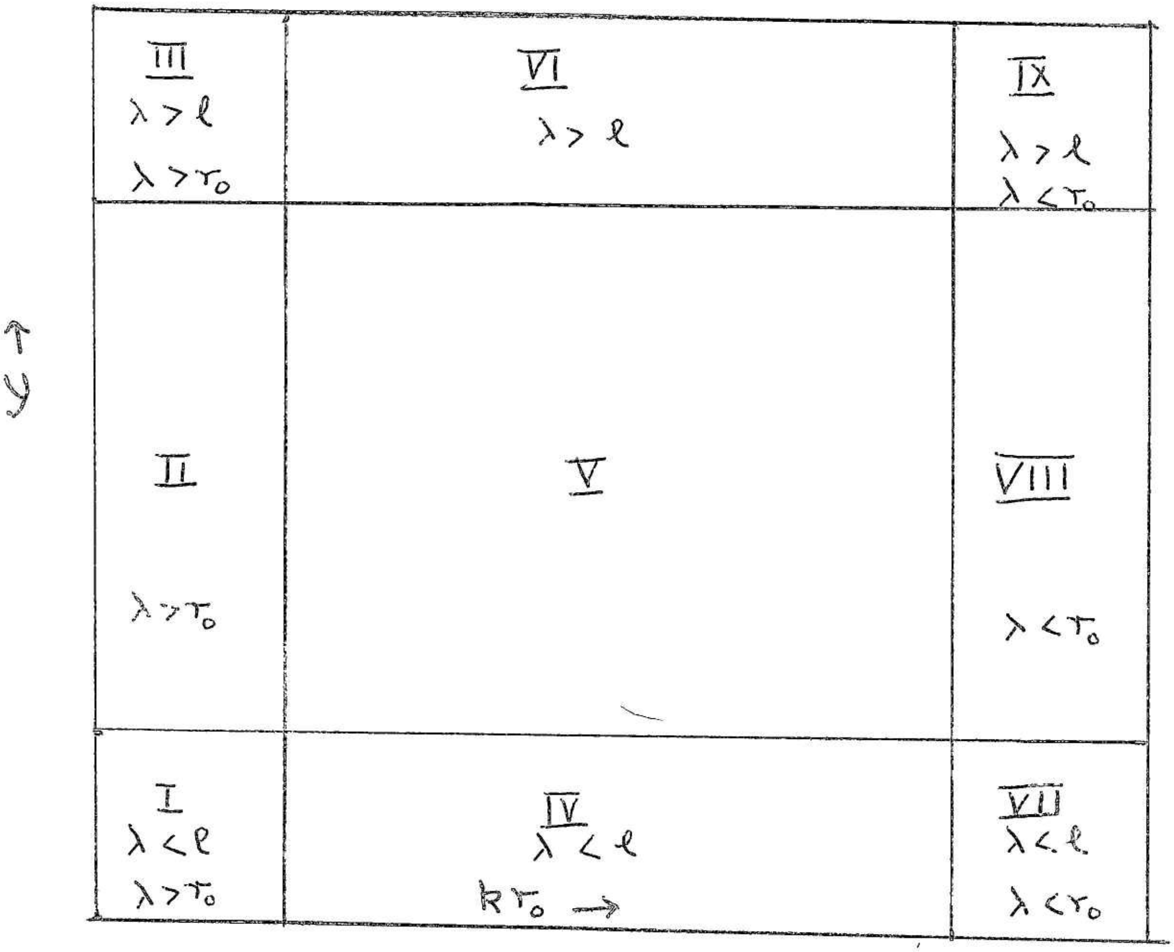


FIG. 5.10 SCHEMATIC DIVISION OF $y - kr_0$ PLANE

even cruder than it appears at first glance as some of the regions may be physically unreal. For example with rigid spheres there is a limiting density and it is questionable at least, whether or not region IX is physically attainable.

5-4 Self-Correlation Spectrum

As can be seen from the discussions presented in chapters 3 and 4 the calculation of the self-correlation function for the hard sphere gas involves a generalized Kinetic equation which is not essentially different from the Boltzmann equation. Thus the results presented in this section could also be obtained by solving the Boltzmann equation. Work has been done along these lines for hydrogen gas using the single relaxation time approximation proposed by Nelkin and Ghatak (15,30). This approximation corresponds to a Kinetic model of the lowest order. Our calculations are for a converged Kinetic model and so our results are more accurate. However it is expected that the two calculations will give comparable results in the free particle and hydrodynamic regimes. It is in the transition region between these two extreme regions that we expect significant differences to occur.

Figures (5-11) and (5-12) illustrate the dependence of the self-correlation function on the value of y. As

x	Converged Kinetic Model, y=2.62	Self Diffusion limit Analytic Result
0.0	3.0469	3.0469
0.2	1.7231	1.7363
0.4	0.73518	0.7581
0.6	0.36529	0.391
0.8	0.20717	0.233
1.0	0.12842	0.1533
1.2	0.0846	0.108
1.4	0.0582	0.080
	Converged Kinetic Model, y=0.247	Free particle limit Analytic Result
0.0	1.2624	1.2624
0.2	1.1716	1.2129
0.4	0.9805	1.0757
0.6	0.7716	0.8807
0.8	0.5555	0.6656
1.0	0.3609	0.4644
1.2	0.2210	0.299
1.4	0.1318	0.1778

TABLE. 5.7 [†]SELF CORRELATION SPECTRUM - VALUES OF 2R(x,y) IN THE FREE PARTICLE AND SELF DIFFUSION LIMITS

[†] It must be noted that the analytic curves have been normalized so that their peaks match those of the kinetic model curves

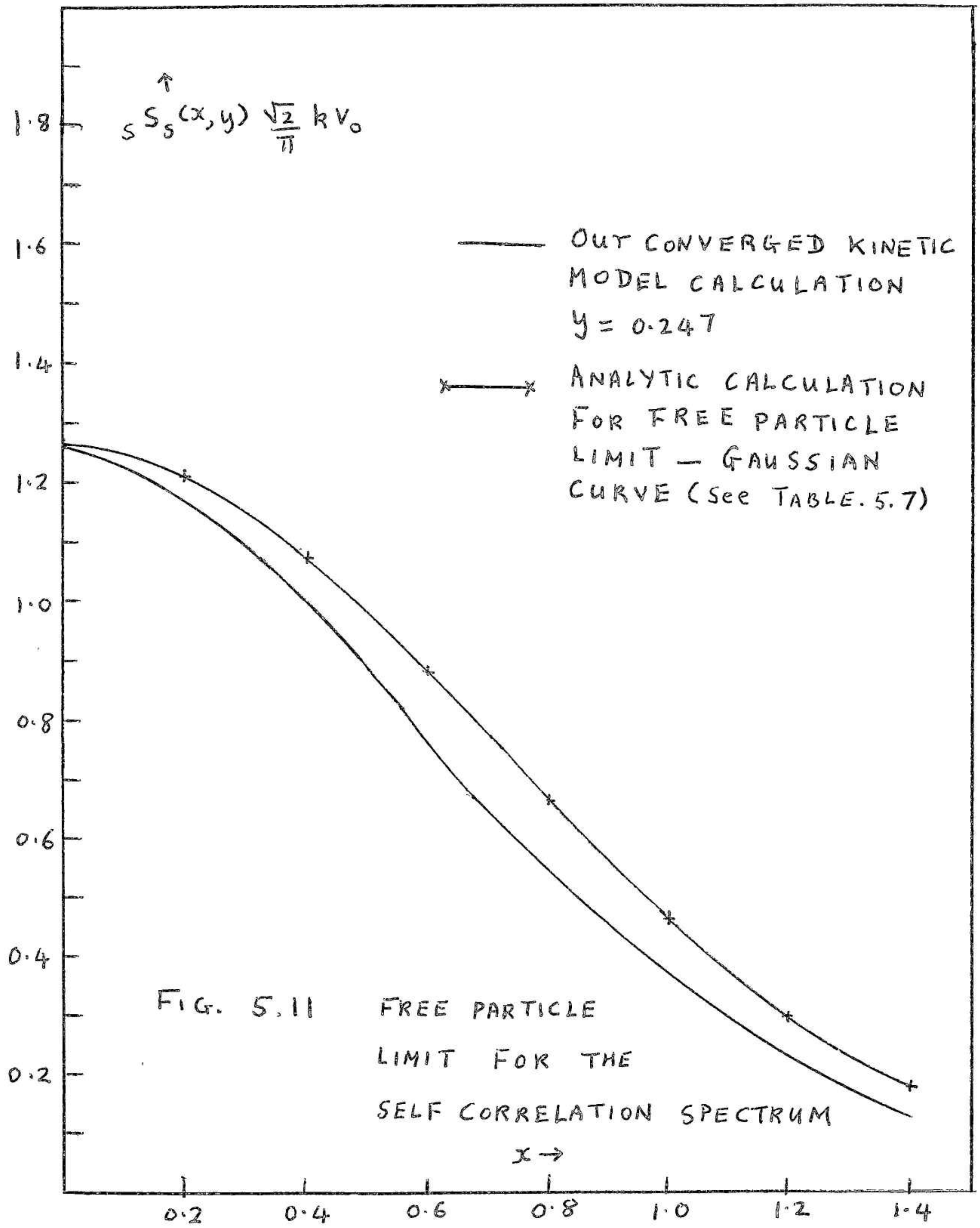


FIG. 5.11 FREE PARTICLE LIMIT FOR THE SELF CORRELATION SPECTRUM

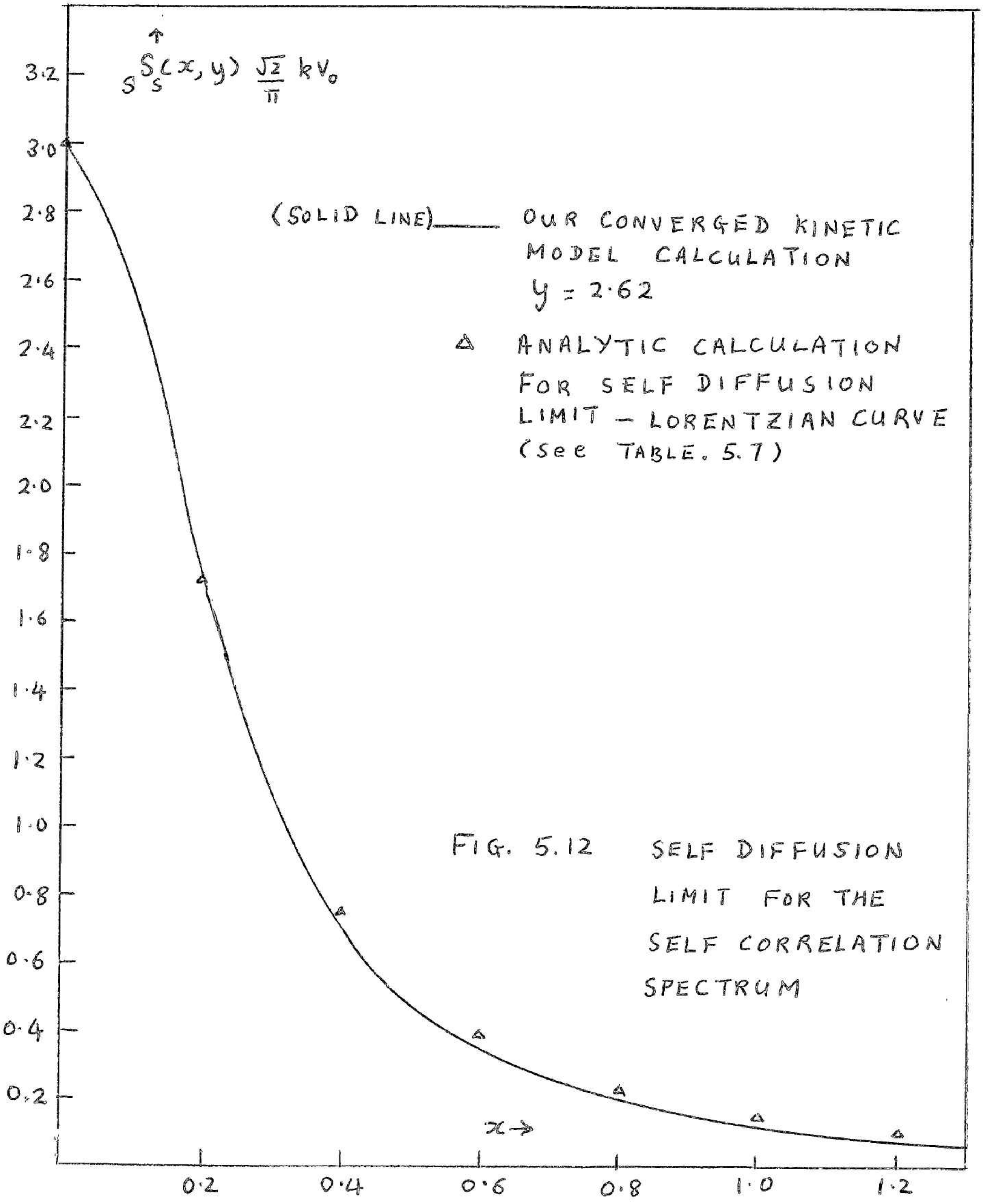


FIG. 5.12 SELF DIFFUSION LIMIT FOR THE SELF CORRELATION SPECTRUM

y	Nelkin - Ghatak Model	y	Converged Kinetic Model
0.1735	1.45	0.247	1.45
0.342	1.27	0.487	1.27
0.348	1.28	0.975	0.95
0.685	1.0	1.46	0.74
1.02	0.82	2.62	0.46
1.3	0.72		Self Diffusion Limit Analytic Result
1.85	0.57		
2.2	0.482		
2.62	0.436	2.0	0.608
3.0	0.39	2.5	0.487
		3.0	0.405
			Free Particle Limit Analytic Result
		0.0	1.66

TABLE. 5.8 FWHM OF THE SELF CORRELATION DENSITY SPECTRUM

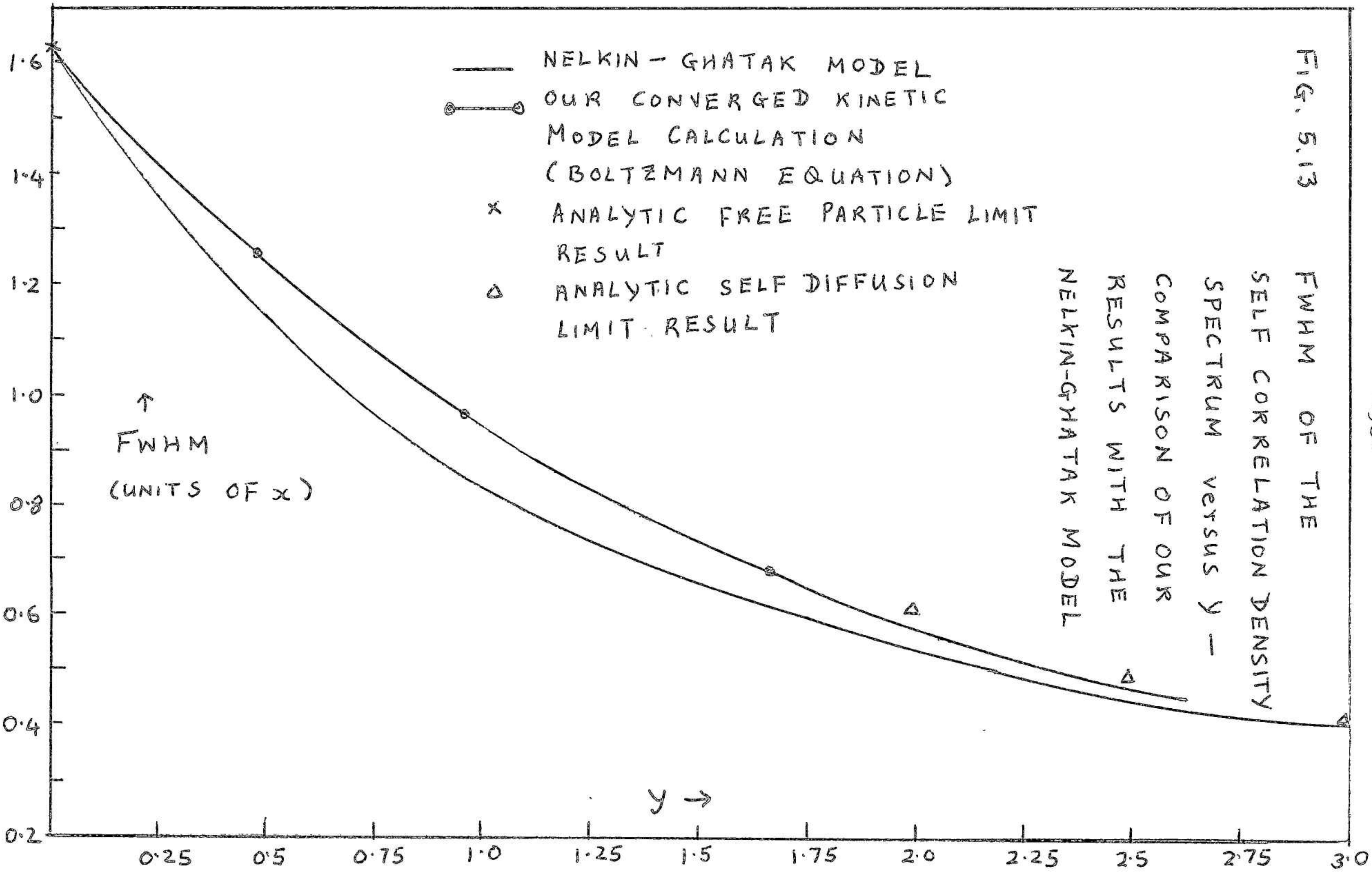


FIG. 5.13

FWHM OF THE SELF CORRELATION DENSITY SPECTRUM versus y — COMPARISON OF OUR RESULTS WITH THE NELKIN-GHATAK MODEL is expected the line shape goes from a Gaussian in the free particle limit to a narrower Lorenztian in the hydrodynamic limit. The central peak increase in height with y.

What is more interesting is the variation of the full width at half maximum (FWHM) with y. This is plotted in Figure (5-13). The FWHM obtained for hydrogen gas using the single relaxation time model is also plotted on the same graph. It can be seen that our calculations definitely lead to a broader curve. As was expected the numerical difference between the two calculations is smallest at the two extremes. It is this behaviour which, at least qualitatively, brings the theoretical calculations into closer agreement with the experimental results of Lefreve et al (30).

CHAPTER 6

Conclusion

We have shown that the generalized Kinetic equation derived by Mazenko leads to results which are significantly different from those of the linearized Boltzmann equation for the spectrum of density fluctuations. For kr_0 even as small as 0.0134, absolute differences of around 20% have been obtained for $y=3.0$. In terms of differencesof ratios of intensities our work shows that differences of around 15% can occur. It seems that it should be possible to experimentally detect such differences. The one difficulty that may be encountered is that kr_0 around 0.1 may lie in the region between those covered by light scattering and neutron scattering. For larger kr_0 one will have to go to lower y as we do have the restriction of low density. As of now the largest value of kr_0 we have gone to is 1.0, but results for higher values of kr_0 can be obtained.

Experiments for the self-correlation spectrum have been done using hydrogen gas and our calculations for the self-correlation spectrum are in general agreement with the experimental results.

It may be interesting to redo Sugawara's calculation with the direct correlation term in the initial condition and adding the static term to the Boltzmann equation.

This would allow us to numerically evaluate the contribution of these terms to the spectrum of the density fluctuations. It would also help us to isolate the effect of the r_0k dependence of the homogeneous matrix elements. However, it would be very hard to obtain a clear physical idea of the relative contribution of the various physical processes with this approach as dealing with thirty five different modes is inherently very complex. It would perhaps be more valuable to restrict ourselves to a generalized B.G.K model based on the Mazenko equation. In terms of the Kinetic model it would mean investigating a Kinetic model of order three with a k-dependent mode. This would lead to a better physical understanding of the importance of the various parameters such as y and kr_0.

We intend to see if it is possible to calculate other correlation functions, such as the current-current correlation, as a by-product of our calculation for the density correlation.

We will then go on to calculate the density spectrum using square well potential in Mazenko's equation.

APPENDICES

APPENDIX A

Mathematical derivation of results quoted in Chapter 2

(i) Equation (2-16):-

To prove this equation we write

$$\left(\frac{\partial}{\partial t} + \frac{\underline{p}\cdot\nabla}{m}\right)\left(\frac{\partial}{\partial t} + \frac{\underline{p}'}{m}\cdot\nabla\right) S_2(\underline{r}, \underline{p}\, \underline{p}', t) =$$

$$\frac{1}{2!}\int d1\, d2\ \phi(p_1)\,\phi(p_2)\, e^{-\beta V(r_1 - r_2)} \left(\frac{\partial}{\partial t} + \frac{\underline{p}\cdot\nabla}{m}\right)$$

$$\left(\frac{\partial}{\partial t} + \frac{\underline{p}'\cdot\nabla}{m}\right)\left\{\left[e^{itL(12)} \sum_{i=1}^{2} \delta(x - x_i)\right]\right.$$

$$\left.\sum_{j=1}^{2} \delta(x' - x_j) - \sum_{i=1}^{2}\left[e^{itL_0(12)} \delta(x - x_i)\right]\right\}$$

$$= \frac{1}{2!}\int d1\, d2\, \phi(p_1)\,\phi(p_2)\, e^{-\beta V(r_1 - r_2)} \left[I_1 - I_2\right] \tag{A-1}$$

We now examine I_1 and I_2 separately

$$I_2 = \left(\frac{\partial}{\partial t} + \frac{\underline{p}\cdot\nabla}{m}\right)\left(\frac{\partial}{\partial t} + \frac{\underline{p}'\cdot\nabla}{m}\right)\sum_{i=1}^{2}\left[e^{itL_0(12)}\delta(x - x_j)\right]$$

$$= \sum_{i=1}^{2} e^{itL_0(12)}\left[iL_0(12) + \underline{p}\cdot\nabla/m\right]\left[iL_0(12) + \frac{\underline{p}'\cdot\nabla}{m}\right]\delta(x - x_j) \tag{A-2}$$

where we have used

$$e^{itL_0(12)} L_0(12) = L_0(12)\, e^{itL_0(12)} \tag{A-3}$$

Using the property of delta functions we interchange ∇ with ∇_1, for particle 1 and ∇ with ∇_2 for particle 2.

Then,

$$I_2 = [iL_0(12) + \underline{p}'\cdot\nabla/m]\,[\underline{p}_1\cdot\frac{\nabla_1}{m} - p\cdot\frac{\nabla_1}{m}]\,\delta(x-x_1)$$
$$+ [iL_0(12) + \underline{p}'\cdot\nabla/m]\,[\underline{p}_2\cdot\frac{\nabla_2}{m} - \underline{p}_2\cdot\frac{\nabla_2}{m}]\,\delta(x-x_2)$$
$$= 0 \qquad \text{(A-4)}$$

Now for I_1,

$$I_1 = (\partial/\partial t + \underline{p}\cdot\nabla/m)(\partial/\partial t + \underline{p}'\cdot\nabla/m)\Big[e^{itL(12)}$$
$$\sum_{i=1}^{2}\delta(x-x_i)\Big]\sum_{j=1}^{2}\delta(x'-x_i) \qquad \text{(A-5)}$$

By using Commutative properties

$$I_1 = \Big(\sum_{j=1}^{2}\delta(x'-x_i)\Big)e^{itL(12)}(iL(12) + p'\cdot\nabla/m)\,[iL_0(12)$$
$$+ p\cdot\nabla/m + iL_1(12)]\sum_{i=1}^{2}\delta(x-x_i) \qquad \text{(A-6)}$$

Using the technique applied in the case of I_2, we see

$$I_1 = \Big(\sum_{j=1}^{2}\delta(x'-x_j)\Big)e^{itL(12)}(iL(12) + p'\cdot\nabla/m)$$
$$iL_1(12)\sum_{i=1}^{2}\delta(x-x_i) \qquad \text{(A-7)}$$
$$= \Big(\sum_{j=1}^{2}\delta(x'-x_j)\Big)(iL(12) + \underline{p}'\cdot\nabla/m)\,e^{itL(12)}$$
$$iL_1(12)\sum_{i=1}^{2}\delta(x-x_i)$$
$$= -\Big[(iL(12) + \underline{p}'\cdot\nabla/m)\sum_{j=1}^{2}\delta(x'-x_j)\Big]$$
$$\Big[e^{itL(12)}iL_1(12)\sum_{i=1}^{2}\delta(x-x_i)\Big] + \Big[(iL(12) + \underline{p}'\cdot\nabla/m)\Big]$$
$$\Big[\sum_{j=1}^{2}\delta(x'-x_j)\,e^{itL(12)}\,iL_1(12)\sum_{i=1}^{2}\delta(x-x_i)\Big] \qquad \text{(A-8)}$$

Now we take advantage of the fact that I is actually integrated and drop out those terms in (A-8) evaluated at the limits. This leaves us with

$$I_1 = -\left[iL(12) \sum_{j=1}^{2} \delta(x'-x_j) \right] \left[e^{itL(12)} iL_1(12) \sum_{i=1}^{2} \delta(x-x_i) \right] + \left(\underline{p}' \cdot \frac{\underline{\nabla}}{m}\right) \left[\sum_{j=1}^{2} \delta(x'-x_j)\, e^{itL(12)} iL_1(12) \sum_{i=1}^{2} \delta(x-x_i) \right] \tag{A-9}$$

We are really interested in the integral

$$\frac{1}{2!} \int d1\, d2\, \phi(p_1)\, \phi(p_2)\, e^{-\beta V(r_1-r_2)}\, I_1 = W_B + R_B \tag{A-10}$$

where

W_B = Boley's result

and

$$R_B = 1/2! \int d1\, d2\, \phi(p_1)\, \phi(p_2)\, e^{-\beta V(r_1-r_2)} \left[-iL_0(12) \sum_{j=1}^{2} \delta(x'-x_j) + \sum_{j=1}^{2} \delta(x'-x_j)\, \underline{p}' \cdot \nabla/m \right] \left[e^{itL(12)} iL_1(12) \sum_{i=1}^{2} \delta(x-x_i) \right] \tag{A-11}$$

However final result is the same as Boley's as

$$\mathcal{F}(R_B) = \int d^3r\, e^{-i\underline{k}\cdot\underline{r}} R_B = \frac{1}{2!} \int d1\, d2\, \phi(p_1)\, \phi(p_2) \left[-iL_0(12) \sum_{j=1}^{2} \delta(x'-x_j) + i\underline{k}\cdot\underline{p}'/m \sum_{j=1}^{2} \delta(x'-x_j) \right] \left[\sum_{i=1}^{2} e^{-ikr_i}\, e^{-itp_i k/m}\, e^{itL_1}\, \delta(\underline{p}-\underline{p}_i) \right] \tag{A-12a}$$

Integrating the L_0 term by parts and using the properties of the delta function we see

$$\mathcal{F}(R_B) = \frac{1}{2!} \int d1\, d2\, \phi(p_1)\phi(p_2) \left[\sum_{j=1}^{2} \delta(x'-x_j)\, (iL_0 + i\underline{k}\cdot\underline{p}'/m) \right] \left[\sum_{i=1}^{2} e^{-ikr_i}\, e^{-itp_i k/m}\, e^{itL_1}\, \delta(\underline{p}-\underline{p}_i) \right] = 0 \tag{A-12b}$$

(ii) Static Part:-

$$\Sigma_1^{(s)}(\underline{k}, \underline{p}\,\underline{p}')\,\phi(p') = \Big[i\,(\partial/\partial t + i\,\underline{p}\cdot\underline{k}/m)\, S_2(\underline{k},$$

$$\underline{p}\,\underline{p}', t)\Big]_{t=0}$$

$$= 1/2!\int d1\, d2\, \phi(p_1)\,\phi(p_2)\,\Big\{ e^{-\beta V(r_1 - r_2)} \int d^3r\, e^{-i\underline{k}\cdot\underline{r}}$$

$$\Big[(i L(12) + i\,\underline{p}\cdot\underline{k}/m) \sum_{i=1}^{2} \delta(x - x_i)\Big] \sum_{j=1}^{2} \delta(x' - x_j)$$

$$- \sum_{i=1}^{3} \int d^3r\, e^{-i\underline{k}\cdot\underline{r}} \big[(i L_0(12) + i\underline{p}\cdot\underline{k}/m)\, \delta(x - x_i\big]\, \delta(x' - x_i)\Big\}$$

$$- i\,\underline{p}\cdot\underline{k}/m\, \phi(p)\,\phi(p')\,(2\pi)^3\,\delta(k) \qquad \text{(A-13)}$$

Note that since

$$f(r) = \exp[-\beta V(r)] - 1 \qquad \text{(A-14)}$$

we have

$$f(k) = \int d^3r\, e^{-i\underline{k}\cdot\underline{r}} \exp[-\beta V(r)] - (2\pi)^3\,\delta(k). \qquad \text{(A-15)}$$

Equation (A-13) can be simplified to

$$\Sigma_1^{(s)}(\underline{k}, \underline{p}\,\underline{p}', z)\,\phi(\underline{p}') = \underline{p}\cdot\underline{k}/m\, \phi(p)\,\phi(p')\,(2\pi)^3\,\delta(k)$$

$$+ \frac{i}{2!}\int d^3r_1\, d^3r_2\, d^3p_1\, d^3p_2\, \phi(p_1)\,\phi(p_2)\, e^{-\beta V(r_1 - r_2)}$$

$$\Big[i L_1(12) \int d^3r\, e^{-i\underline{k}\cdot\underline{r}} \sum_{i=1}^{2} \delta(x - x_i)\Big] \sum_{j=1}^{2} \delta(x' - x_j) \qquad \text{(A-16)}$$

For notational convenience denote the integral term by A_1. If we perform the change of co-ordinates on A_1

$$\underline{r}_1 - \underline{r}_2 = \bar{\underline{r}}$$

$$\underline{r}_1 + \underline{r}_2 = 2\bar{R} \qquad \text{(A-17)}$$

integrate over $\bar{R}$ first and then over $\bar{r}$ by parts we can show that

$$A_1 = -\underline{k}\cdot\underline{p}\ \phi(p')\ \phi(p) \int d^3\bar{r}\ e^{-\beta V(\bar{r})}\ e^{-i\underline{k}\cdot\underline{\bar{r}}} \tag{A-18}$$

This gives us

$$\Sigma_1^{(s)}(\underline{k}\ \underline{p}) = -\underline{p}\cdot\underline{k}/m\ f(k)\ \phi(p) \tag{A-19}$$

(iii) Collision Part:-

$$\Sigma_1^{(c)}(\underline{k}, \underline{p}\,\underline{p}', z)\,\phi(p') = i\int_0^\infty dt\ e^{izt}\int d^3r\ e^{-i\underline{k}\cdot\underline{r}}\Big[\left(-\tfrac{1}{2!}\right)\int d1\,d2\ \phi(p_1)\ \phi(p_2)\ e^{-\beta V(r_1-r_2)}\Big[e^{itL(12)}\ iL_1(12)\sum_{i=1}^{2}\delta(x-x_i)\Big]\ iL_1(12)\sum_{j=1}^{2}\delta(x'-x_j)\Big] \tag{A-20}$$

Asides from the transformation (A-17) we also apply the transformation

$$\begin{aligned} \underline{p}_1 + \underline{p}_2 &= 2\,\underline{\alpha} \\ \underline{p}_1 - \underline{p}_2 &= 2\,\underline{p} \end{aligned} \tag{A-21}$$

We then carry out the integration in turn to obtain

$$\Sigma_1^{(c)}(\underline{k}, \underline{p}\,\underline{p}', z)\,\phi(p') = -i\int d^3\alpha\, d^3\bar{p}\, d^3\bar{r}\ d^3R\ \phi(\alpha)\,\phi(\bar{p})\ e^{-\beta V(\bar{r})}\Big(iL_1(12)\sum_{j=1}^{2}\delta(\alpha'-x_j)\Big) \Big\{\ \Big[\frac{z+L(12)}{-i}\Big]^{-1}\int d^3r\ e^{-i\underline{k}\cdot\underline{r}}\ iL_1(12)\sum_{i=1}^{2}\delta(x-x_i)\Big\} \tag{A-22}$$

where the differential operators are

$$i L_0(12) = \underline{\alpha}\cdot\nabla_R/m + 2\underline{\bar{p}}\cdot\nabla_{\bar{r}}/m \qquad \text{(A-23)}$$

$$i L_1(12) = \nabla_{\bar{r}} V(\bar{r}) \;\partial/\partial \bar{p} \qquad \text{(A-24)}$$

Let us consider the r-integration first.

$$\begin{aligned} B_1 &= \int d^3r\, e^{-i\underline{k}\cdot\underline{r}}\, iL_1(12) \sum_{i=1}^{2} \delta(x - x_i) \\ &= \frac{\partial}{\partial p} \nabla_{\bar{r}} V(\bar{r}) \int d^3r\, e^{-i\underline{k}\cdot\underline{r}} \Big[-\delta(\underline{p} - \underline{\alpha} - \underline{\bar{P}})\, \delta\Big(\\ &\qquad \underline{r} - \Big(\frac{\underline{\bar{r}} + \underline{R}2}{2}\Big)\Big) - \delta(\underline{p} - \underline{\alpha} + \underline{\bar{P}})\, \delta\Big(\underline{r} - \Big(2\,\frac{\underline{R} - \underline{\bar{r}}}{2}\Big)\Big)\Big] \end{aligned}$$

(A-25)

We then transform $\underline{\bar{P}} \to -\underline{\bar{P}}$

$\underline{\bar{r}} \to -\underline{\bar{r}}$ (A-26)

in the second product in (A-25)

This gives

$$B_1 = \frac{\partial}{\partial p} \nabla_{\bar{r}} V(\bar{r})\, 2 e^{-ik\left(\frac{\bar{r} + 2R}{2}\right)} \delta(\underline{p} - \underline{\alpha} - \underline{\bar{P}})$$

(A-27)

Now consider the R-integration

$$\begin{aligned} &\int d^3R\; \partial/\partial\bar{p} \sum_{j=1}^{2} \delta(x' - x_j)\, e^{-i\underline{k}\cdot\underline{R}} \\ &\qquad = -\partial/\partial p' \Big[\delta(\underline{p}' - \underline{\alpha} - \underline{\bar{p}})\, e^{i\frac{k\cdot\bar{r}}{2}} - \delta(p' - \alpha + \bar{p})\, e^{-ik\cdot\bar{r}/2} \Big] \end{aligned}$$

(A-28)

Using (A-27) and (A-28) in (A-22) we find

$$\Sigma_1^{(c)}(\underline{k}, \underline{p}\underline{p}', z)\, \phi(p') = \partial/\partial p_i\; \partial/\partial p'_j \int d^3\alpha\, d^3\bar{p}\, d^3\bar{r}\; \phi(\alpha)$$

$$\phi(\bar{p})\, e^{-\beta V(\bar{r})}\, \nabla_{\bar{r}}^{j} V(\bar{r})\, [\delta(\underline{p}' - \underline{\alpha} - \bar{\underline{p}})\, e^{ik\bar{r}/2}$$
$$- \delta(\underline{p}' - \underline{\alpha} + \bar{\underline{p}})\, e^{-i\underline{k}\cdot\bar{r}/2}]\, [z + i \nabla_{\bar{r}} V(\bar{r})\, \partial/\partial\bar{p} - \underline{\alpha}\cdot\underline{k}/m$$
$$- 2i\bar{p}\nabla_{\bar{r}}/m]^{-1}\, \nabla_{\bar{r}}^{i} V(\bar{r})\, e^{-ik\bar{r}/2}\, \delta(\underline{p} - \underline{\alpha} - \bar{\underline{p}}) \qquad \text{(A-29)}$$

(iv) The Limit $z \rightarrow i0^+$

To reduce the collision memory operator to the linearized Boltzmann operator we have to take the limit $z \rightarrow i0^+$.

Employing Boltzmann's idea of an action sphere, we assume that the relative momentum of the interacting particles, after some large time T, approaches arbitrarily close to some asymptotic value. This limits us to 'short range' potentials.

With this assumption we have

$$\underline{p}(t) = \underline{p}^{*} \qquad \text{for } t > \tau_c \qquad \text{(A-30)}$$

Therefore

$$f(\underline{p}(t)) = f^{*}(\underline{p}^{*}) \qquad \text{for } t > \tau_c \qquad \text{(A-31)}$$

So

$$\lim_{z \rightarrow i0^+} iz \int_0^{\infty} dt\, e^{izt} f(\underline{p}(t)) = \lim_{z \rightarrow i0^+} iz \left[\int_0^{\tau_c} + \int_{\tau_c}^{\infty}\right] dt\; e^{izt} f(\underline{p}(t))$$

$$= \lim_{z \to i0^+} iz \left[\int_0^{\tau_c} dt\, e^{izt} f(\underline{p}(t)) - \frac{f^*(\underline{p}^*)}{iz} - \int_0^{\tau_c} dt\, e^{izt} f^*(\underline{p}^*) \right]$$

$$= -f^*(\underline{p}^*) + \lim_{z \to i0^+} iz \int_0^{\tau_c} dt\, e^{izt} \left(f(\underline{p}(t)) - f^*(\underline{p}^*) \right)$$

(A-32)

Since $(f(\underline{p}(t)) - \overset{*}{f}(\overset{*}{\underline{p}}))$ is bounded,

$$\lim_{z \to i0^+} iz \int_0^{\tau_c} dt\, e^{izt} \left(f(\underline{p}(t)) - f^*(\underline{p}^*) \right) = 0$$

(A-33)

So we have

$$\lim_{z \to i0^+} iz \int_0^{\infty} dt\, e^{izt} f(\underline{p}(t)) = -f^*(\underline{p}^*)$$

(A-34)

APPENDIX B

Mathematical derivations of results quoted in Chapter 4

This Appendix is devoted to derivations of some of the analytic results used in Chapter 4. To be more specific they pertain to the reduction of the general Memory operator to the Hard Sphere case.

(i)

$$
\begin{aligned}
g(r)\,\nabla_r V(r) &= e^{-\beta V(r)}\,\nabla_r V(r) \\
&= -1/\beta\,\nabla_r e^{-\beta V(r)} \\
&= -1/\beta\,\nabla_r \left(e^{-\beta V(r)} - 1\right) \qquad \text{(B-1)}
\end{aligned}
$$

For the hard sphere (B-1) becomes

$$
\begin{aligned}
g(r)\,\nabla_r V(r) &= 1/\beta\,\nabla_r \left(1 - e^{-\beta V(r)}\right) \\
&= \hat{r}/\beta\,\partial/\partial r\left(1 - \theta\,(r - r_0)\right) \\
&= -\hat{r}/\beta\,\delta(r - r_0) \qquad \text{(B-2)}
\end{aligned}
$$

Notation used:

$\delta(x) =$ Delta function

$\theta_-(x) = 1 - \theta(x)$

$\wedge$ signifies unit vector

(ii)

To simplify matters slightly let us write

$$\Omega = z - \underline{k}\cdot\underline{\alpha}/m \qquad \text{(B-3)}$$

then we have that:-

$$A(\underline{r}, \alpha, \underline{p}\,\underline{\bar{p}}) = \nabla_r V(r)\, \nabla_{\bar{p}} \frac{e^{-i\underline{k}\cdot\underline{r}/2}}{(\Omega + L(\underline{r}, \underline{\bar{p}}))}\, \delta(\underline{p} - \underline{\alpha} - \underline{\bar{p}})$$

$$= (-i)\left[-\frac{1}{\Omega + L} + \frac{1}{\Omega + L_0} \right] \left[\Omega - \frac{\underline{k}\cdot\underline{\bar{p}}}{m} \right] e^{-i\underline{k}\cdot\underline{r}/2}\, \delta(\underline{p} - \alpha - \underline{\bar{p}})$$

(B-4)

But

$$\frac{1}{(\Omega + L)} = -i \int_0^\infty dt\, e^{i(\Omega + L)t} \qquad \text{for } \operatorname{Im}(z) > 0$$

(B-5)

and

$$e^{iL_0 t} e^{-i\underline{k}\cdot\underline{r}/2} \delta(\underline{p} - \underline{\alpha} - \underline{\bar{p}}) = \delta(\underline{p} - \underline{\alpha} - \underline{\bar{p}})\, e^{-i\underline{k}\cdot[\underline{r} + 2\underline{\bar{p}}t/m]/2}$$

(B-6)

Using the results (B-5) and (B-6) in our equation (B-4) we see that

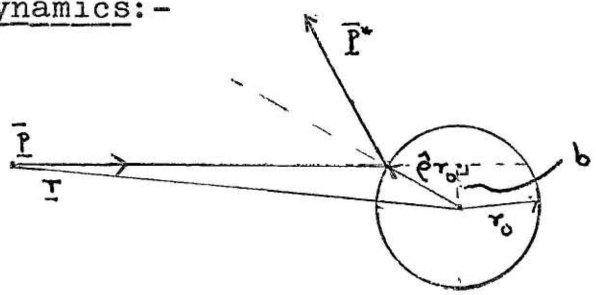
$$A(\underline{r}, \underline{\alpha}, \underline{p}\,\underline{\bar{p}}) = \int_0^\infty dt \left\{ e^{i(\Omega + L)t} - e^{i(\Omega + L_0)t} \right\} \left(e^{-i\underline{k}\cdot\underline{r}/2} (\Omega - \underline{k}\cdot\underline{\bar{p}}/m)\, \delta(\underline{p} - \underline{\alpha} - \underline{\bar{p}}) \right)$$

$$= \left(\Omega - \frac{\underline{k}}{m}\cdot(\underline{p} - \alpha) \right) \int_0^\infty dt\, e^{i\Omega t} \Big\{ e^{-i\underline{k}\cdot\underline{r}(t)/2}\, \delta(\underline{p} - \underline{\alpha} - \underline{\bar{p}}(t)) - e^{-i\frac{\underline{k}}{2}\cdot[\underline{r} + 2\underline{\bar{p}}t/m]}\, \delta(\underline{p} - \underline{\alpha} - \underline{\bar{p}}) \Big\}$$

(B-7)

$$= (\Lambda - \underline{k}\cdot(\underline{p} - \underline{\alpha})/m) \int_0^\infty dt\, e^{i\Lambda t} \{ e^{-i\underline{k}\cdot\underline{r}(t)/2} \delta(\underline{p} - \underline{\alpha} - \overline{\underline{p}}(t))\} + e^{-i\underline{k}\cdot\underline{r}/2} \delta(\underline{p} - \underline{\alpha} - \overline{\underline{p}}) \tag{B-8}$$

<u>(iii) Collision dynamics:-</u>



It can be seen that there will only be a collision if $\underline{r}\cdot\overline{\underline{p}} < 0$ and $r_0 \gtrless b$

$\overline{\underline{p}}$ = momentum initially

$\overline{\underline{p}}^*$ = momentum after collision

$= \overline{\underline{p}} - 2\hat{e}(\hat{e}\cdot\overline{\underline{p}})$

Given that there will be a collision it occurs time τ later

$$\tau = |\underline{r}\cdot\hat{\overline{p}}| - [r_0^2 - b^2]^{1/2} \tag{B-9}$$

We now obtain an expression for $\hat{e}$ in terms of the initial values.

$$r_0 \hat{e} = -\hat{e}[r_0^2 - b^2]^{1/2} + \underline{r} - (\underline{r}\cdot\hat{\overline{p}})\hat{\overline{p}} \tag{B-10}$$

where

$$b^2 = r^2 - (\underline{r}\cdot\hat{\overline{p}})^2 \tag{B-11}$$

Combining all these results we have

$$\delta(\underline{\rho}-\underline{\alpha}-\underline{\bar{p}}(t)) = \theta(r_0^2-b^2)\,\theta_-(\hat{r}\cdot\hat{\bar{p}})\,[\theta(\tau-t)\,\delta(\underline{\rho}-\underline{\alpha}-\underline{\bar{p}})$$
$$+\,\theta(t-\tau)\,\delta(\underline{\rho}_1-\underline{\alpha}-\underline{\bar{p}}^*)]$$
$$+\,[\theta(b^2-r_0^2)\,\theta_-(\hat{r}\cdot\bar{p})+\theta(\hat{r}\cdot\hat{\bar{p}})]\,\delta(\underline{\rho}_1-\underline{\alpha}-\underline{\bar{\rho}}) \tag{B-12}$$

where $\Theta(x)$ is the unit step function. We therefore have

$$\frac{d}{dt}\theta(\pm t\mp\tau) = \pm\,\delta(t-\tau) \tag{B-13}$$

<u>(iv)</u> In this part we will examine the effect of $\mathbf{L}_0$ operating on $\{ g(r)\, e^{i(z-\underline{k}\cdot\underline{\alpha})\tau}\, e^{-i\underline{k}\cdot\hat{e}r_0/2}\,\theta(r_0^2-b^2)$ $\theta_-(\hat{r}\cdot\underline{\bar{p}})\,[\,\delta(\underline{\rho}'-\underline{\alpha}-\underline{\bar{p}})-\delta(\underline{\rho}'-\underline{\alpha}-\underline{\bar{\rho}}^*)\,]\}$

We first note that for any function f,

$$\underline{\bar{p}}\cdot\nabla_r f(b^2) = \frac{\partial}{\partial b^2}f(b^2)\,\underline{\bar{p}}\cdot\nabla_r b^2 = 0 \tag{B-14}$$

This means that

$$L_0(\underline{r},\underline{\bar{p}})\,\theta(r_0^2-b^2) = 0 \tag{B-15}$$

We also have

$$L_0(\underline{r},\underline{\bar{p}})\,\hat{e}r_0 = 0 \tag{B-16}$$

$$L_0(\underline{r},\underline{\bar{p}})\,\underline{p}^* = 0 \tag{B-17}$$

Then we note that

$$L_0\theta_-(\hat{r}\cdot\underline{\bar{p}}) = \delta(\hat{r}\cdot\hat{\underline{\bar{p}}}) \tag{B-18}$$

This gives us

$$b^2 = r^2$$

Thus the condition $\Theta(r_0^2-b^2)$ becomes $\Theta(r_0^2-r^2)$. However

$$g(r) = e^{-\beta V(r)} = \begin{cases} 0 & r<r_0 \\ 1 & r>r_0 \end{cases}$$

$$= \theta(r - r_0) \qquad \text{(B-19)}$$

So therefore we only have to worry about the $L_0(\underline{r}\underline{\bar{p}})$ $(g(r)\, e^{i(z-\underline{k}\cdot\underline{\alpha}/m)t}$) part of the derivative.

Since we have the $\theta_-(\hat{r}\cdot\underline{\bar{p}})$ factor,

$$L_0(\underline{r}\,\underline{\bar{p}})\tau = -i\frac{2}{m}\cdot\nabla_r(-1)\left(\frac{\underline{r}\cdot\underline{\bar{p}}}{\bar{p}^2}\right)\frac{m}{2} = i \qquad \text{(B-20)}$$

These results enable us to write

$$\left[z - \underline{k}\cdot\underline{\alpha}/m + L_0(\underline{r},\underline{\bar{p}})\right]\left[g(r)\, e^{i(z-k\cdot\frac{\alpha}{m})\tau}\right]$$

$$= e^{i(z-\underline{k}\cdot\underline{\alpha}/m)\tau} L_0(\underline{r},\underline{\bar{p}})g(r) + (z-\underline{k}\cdot\underline{\alpha}/m)g(r)\big(e^{i(z-\underline{k}\cdot\underline{\alpha}/m)\tau}\big) + i\,g(r)\,(z-\underline{k}\cdot\underline{\alpha}/m)e^{i(z-\underline{k}\cdot\underline{\alpha}/m)\tau}\big(L_0(\underline{r},\underline{\bar{p}})\tau\big)$$

$$= e^{i(z-\underline{k}\cdot\underline{\alpha}/m)\tau} L_0(\underline{r},\underline{\bar{p}})\, g(r). \qquad \text{(B-21)}$$

Thus

$$\mathcal{E}_H^{(c)}(\underline{k},\underline{p}\,\underline{p}',z)\,\phi(p') = -n^2(\beta/\pi m)^3\int d^3\alpha\, d^3r\, d^3\bar{p}$$
$$\left[e^{i\underline{k}\cdot\underline{r}/2}\,\delta(\underline{\alpha}-\underline{p}+\underline{\bar{p}}) + e^{-i\underline{k}\cdot\underline{r}/2}\,\delta(\underline{\alpha}-\underline{p}-\underline{\bar{p}})\right]$$
$$e^{-\beta(\alpha^2+\bar{p}^2)/m}\, e^{i(z-\underline{k}\cdot\underline{\alpha}/m)\tau}\, e^{-i\underline{k}\cdot\hat{\rho}r_0/2}\,\theta(r_0^2-b^2)$$
$$\theta_-(\hat{r}\cdot\underline{\bar{p}})\left[\delta(\underline{p}'-\underline{\alpha}-\underline{\bar{p}}) - \delta(\underline{p}'-\underline{\alpha}-\underline{\bar{p}}^*)\right]L_0(\underline{r},\underline{\bar{p}})\,g(r)$$
$$\text{(B-22)}$$

APPENDIX C

Transformation from Sonine polynomials to modified Hermite polynomials

As has been mentioned earlier the modified Hermite polynomial tends to be a less efficient basis as far as numerical computation goes as it does not take direct advantage, as the Sonine polynomial does, of azimuthal symmetry. A reduction in the size of the inversion matrix would decrease the round off error. It was with this in mind that a transformation between the two bases was sought.

$$\Psi_{lmn}(\vec{\xi}) = A_{lmn}\bar{H}_l(\xi_1)\bar{H}_m(\xi_2)\bar{H}_n(\xi_3). \qquad (c-1)$$

This is our orthonormal modified Hermite polyonomial basis with the weighting factor

$$R(\xi) = e^{-\xi^2/2}/(2\pi)^{3/2} \qquad (c-2)$$

The orthonormal Sonine polynomial basis as generally used is:-

$$\Phi_{\alpha\beta\gamma}(\vec{\xi}) = C_{\alpha\beta\gamma}\,\xi^{\alpha}\,Y_{\alpha}^{\gamma}(\theta,\varphi)\,L_{\beta}^{\alpha+1/2}(\xi^2/2). \qquad (c-3)$$

where $L_{\beta}^{\alpha+1/2}(\xi^2/2)$ are the Laguerre polynomials and $Y_{\alpha}^{\gamma}(\theta,\varphi)$ are the spherical harmonics as used in Wang Chang and Uhllenbeck. By using azimuthal symmetry, as in Sugawara, we reduce the number of free indices by one and the basis now becomes

$$\Phi_{\alpha\beta}(\vec{\xi}) = \Phi_{\alpha\beta 0}(\vec{\xi}) = C_{\alpha\beta}\,\xi^{\alpha}\,P_{\alpha}(\cos\theta)\,L_{\beta}^{\alpha+1/2}(\xi^2/2) \qquad (c-4)$$

$P_\alpha(\cos\theta)$ is the Legendre polynomial. The normalization factors are:-

$$A_{\ell mn} = 1 \Big/ (\ell!\, m!\, n!)^{1/2} \qquad (c\text{-}5)$$

$$C_{\alpha\beta} = \left[\beta! \frac{(2\alpha+1)\, \pi^{1/2}}{2^{\alpha+1}\, \Gamma(\alpha+\beta+3/2)} \right]^{1/2} \qquad (c\text{-}6)$$

Let us naively expand

$$\Phi_{\alpha\beta}(\vec{\zeta}) =. \sum_{\ell mn=0}^{\infty} B(\ell mn/\alpha\beta)\, \psi_{\ell mn}(\vec{\zeta}) \qquad (c\text{-}7)$$

Using orthonormality we then have

$$B(\ell mn/\alpha\beta) = \int d^3\zeta \; \Phi_{\alpha\beta}(\vec{\zeta})\, \psi_{\ell mn}(\vec{\zeta})\, R(\vec{\zeta})$$

$$= \int d^3\zeta \; A_{\ell mn} C_{\alpha\beta}\, \zeta^{\alpha} L_{\beta}^{\alpha+1/2}(\zeta^2/2)\, P_\alpha(\cos\theta)\, \bar{H}_\ell(\zeta_1)$$

$$\bar{H}_m(\zeta_2)\, \bar{H}_n(\zeta_3)\, e^{-\zeta^2/2} \Big/ (2\pi)^{3/2} \qquad (c\text{-}8)$$

We now use the polynomial expansion of our modified Hermite polynomials to put equation (c-8) in the form of three sums:-

$$B(\ell mn|\alpha\beta) = \frac{A_{\ell mn} C_{\alpha\beta}}{(2\pi)^3} \left(\frac{1}{2^{\frac{\ell+m+n}{2}}} \right) \sum_{j=0}^{\ell} \sum_{i=0}^{m} \sum_{k=0}^{n}$$

$$\frac{\gamma(\ell,j)\, \gamma(m,i)}{2^{\frac{i+j+k}{2}}}\, \gamma(n,k) \left[\int d\zeta \; \zeta^2 L_{\beta}^{\alpha+1/2}(\zeta^2/2)\, \zeta^{\alpha+i+j+k} e^{-\zeta^2/2} \right]$$

$$\left[\int_0^{2\pi} d\phi\, (\sin\phi)^i (\cos\phi)^j \right] \left[\int_0^{\pi} d\theta\, (\sin\theta)^{i+j+1} (\cos\theta)^k P_\alpha(\cos\theta) \right] (c\text{-}9)$$

where

$$\gamma(\ell,j) = \frac{2^\ell}{(\pi)^{1/2}} \frac{\ell!}{j!\,(\ell-j)!} (i)^{\ell-j}\, \Gamma\left(\frac{\ell-j+1}{2}\right) \left[\frac{1+(-1)^{\ell-j}}{2} \right]$$

(c-10)

After carrying out the various integration one arrives at the following formula

$$B(\ell m n|\alpha\beta) = A_{\ell m n}\frac{c_{\alpha\beta}}{(2\pi)^{3/2}}\Bigg[\sum_{j=0}^{\ell}\sum_{i=0}^{m}\sum_{k=0}^{n}\gamma(\ell,j)\,\gamma(m,i)$$

$$\frac{\gamma(n,k)}{(\sqrt{2})^{\ell+m+n+i+j+k}}\,[(-1)^{i}+1]\,\frac{[1+(-1)^{j}]}{2\,\Gamma(\frac{i+j}{2}+1)}\,\Gamma(i+\tfrac{1}{2})\,\Gamma(j+\tfrac{1}{2})$$

$$\Bigg(\sum_{r=0}^{\frac{i+j}{2}}\ \sum_{p=0}^{(\frac{2r+k-1}{2},\ \frac{2r+k}{2})}\ {}^{i+j/2}C_{r}\,(-1)^{r}\,W^{2r+k}_{2r+k-2p}\,\frac{2}{(2\alpha+1)}$$

$$\delta_{(2r+k-2p)\alpha}\Bigg)\,\Big(2^{\frac{\alpha+i+j+k}{2}}\Big)$$

$$\left\{\begin{matrix}\dfrac{t!}{(t-\beta)!} & \dfrac{\Gamma(\alpha+\frac{1}{2}+t+1)}{\Gamma(\beta+1)}\,(-1)^{\beta} & \text{for } \beta\le t \\ 0 & & \text{for } \beta>t\end{matrix}\right\}\Bigg] \qquad \text{(c-11)}$$

where

${}^{N}C_{r}$ = binomial co-efficient

$(\frac{2r+k-1}{2},\ \frac{2r+k}{2})$ = the integer is used (c-12)

$$W_m^n = \frac{(2m+1)\,2^{m}\,n!}{(\frac{1}{2}n-\frac{1}{2}m)!}\ \frac{(\frac{1}{2}n+\frac{1}{2}m)!}{(n+m+1)!}$$

The mathematics also gives the following rules for the indices (l,m,n)

(i) l and m must be even

(ii) l + m + n = $2\beta + \alpha$

As we never had to resort to the transformation there is unfortunately no computer program for the co-efficient $\beta(lmn/\alpha\beta)$.

APPENDIX D

Description of the Programs

The three major programs used in the course of this work are Matrix, Dispersion and Polynomial. Versions of each with slight variations were also written but in this Appendix we will only describe the version most frequently used. However one point has to be stressed. One version of Matrix punches out the diagonal elements as positive numbers. This version has to be used with those versions of Dispersion and Polynomial which reads these elements into core with the signs reversed. The other version of Matrix punches out the diagonal elements as negative numbers. This version has to be used with the corresponding versions of Dispersion and Polynomial which read the elements back into core without changing the signs.

(i) MATRIX.-

Matrix, as is implied by its name, computes the matrix elements given by equation (4-32) that is the elements of the homogeneous collision operator. As a by-product it also computes the matrix elements for the self-collision operator.

The homogeneous collision matrix element given by equation (4-32) can be reduced to a series of finite sums.

$$M_H^{(c)}(\ell m n \mid \ell' m' n') = \frac{2 i N \pi^{7/2}}{(2)^{\ell_1+\ell'_i}} (\ell_i!\,\ell'_i!)^{1/2}$$

$$\delta(\ell+\ell')\,\delta(m+m')\,\delta(n+n')\,(-1)^{n+n'}\Big[<\ell_i|A_0(0)|\ell'_i>$$

$$+ (-1)^{\ell'_T} <\ell_i|\tilde{A}_0(k)|\ell'_i> \Big]$$

(D-1)

where ℓ_i is short hand for (lmn)

$$<\ell_i|A_0(0)|\ell'_i> = \sum_{\bar{\ell}_i=0}^{\mathrm{Min}(\ell_i,\ell'_i)} \frac{(-2)^{\bar{\ell}_T}}{\bar{\ell}_i!} <\ell_i-\bar{\ell}_i|A_1(0)|\ell'_i-\bar{\ell}_i>$$

(D-2)

$$<\ell_i|\tilde{A}_0(k)|\ell'_i> = \sum_{\bar{\ell}_i=0}^{\mathrm{Min}(\ell_i,\ell'_i)} \frac{(2)^{\ell_T}}{\bar{\ell}_i!} <\ell_i-\bar{\ell}_i|A_1(k)|\ell'_i-\bar{\ell}_i>$$

(D-3)

$$<\ell_i|A_1|\ell'_i> = \sum_{L_i=0}^{(\ell_i/2)} \sum_{L'_i=0}^{(\ell'_i/2)} (2)^{L_T+L'_T}\,\bar{\gamma}(\ell_i,L_i)$$

$$R(L'_i) <\ell_i-2L_i|A_2|\ell'_i-2L'_i>$$

(D-4)

$$<\ell_i|A_2|\ell'_i> = \sum_{\bar{\ell}_i=0}^{\ell'_i} \left(\frac{1}{\bar{\ell}_i!}\right) \frac{(\ell_i+\ell'_i-\bar{\ell}_i)}{(\ell'_i-\bar{\ell}_i)!} (4)^{\bar{\ell}_T}$$

$$(\bar{\ell}_T+1)! <\ell_i+\ell'-\bar{\ell}_i|A_3|\bar{\ell}_i> \Delta_{\bar{\ell}_i}$$

(D-5)

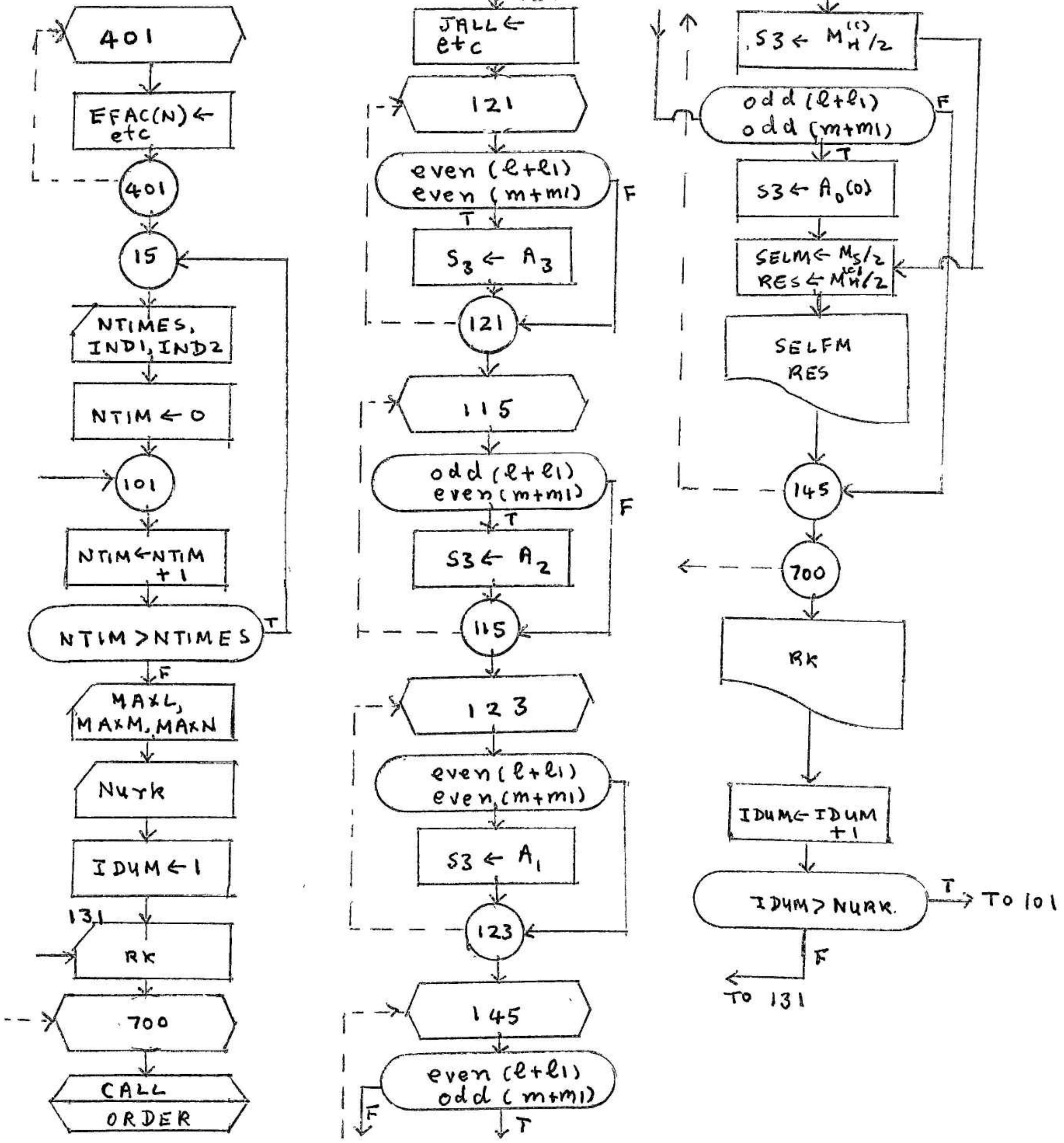


Fig. D.1 FLOW CHART FOR MATRIX (It must be noted that this is only intended to give a very rough idea of the basic logic of the program)

$$\langle \ell_i | A_3 | \ell'_i \rangle = \sum_{L_i=0}^{(\ell i/2)} (-2)^{L_T} \bar{\gamma}(\ell_i, L_i) E\left(\frac{\ell'+\ell-2L}{2}\right)$$

$$E\left(\frac{m'+m-2M}{2}\right) \langle \ell_i - 2L_i | A_4 | \ell'_i \rangle \qquad \text{(D-6)}$$

$$\langle \ell_i | A_4 | \ell'_i \rangle = \begin{pmatrix} RF(\ell+\ell'+m'+m, n+n') \, RW3(\ell'_T - \ell_T/2) \\ IF(\ell+\ell'+m'+m, n+n') \, IW3(\ell'_T + 1 - \ell_T/2) \end{pmatrix}$$

(D-7)

$$\frac{\pi}{2}(1+(-1)^{\ell})(1+(-1)^{m}) E(\ell/2) E(m/2) \left[(1+(-1)^{n})\right.$$

$$\left. RF(\ell+m, n) + i\, IF(\ell+m, n)(1-(-1)^{n})\right]$$

$$= \int d\Omega_r \, r_i^{\ell_i+\ell'_i} e^{i\underline{k}\cdot\underline{r}}$$

(D-8)

$$\frac{\ell!}{2\sqrt{\pi}}\left[\left(\frac{1-(-1)^{\ell-m}}{2}\right) RW3\left(\frac{\ell-m-1}{2}\right) + i\left(1+\frac{(-1)}{2}^{\ell-m}\right) IW\left(\frac{\ell-m}{2}\right)\right]$$

$$= \int \frac{d\omega}{2\pi} \frac{1}{(\omega - i\epsilon)} \frac{\partial^{\ell}}{\partial \omega^{\ell}} \left(\omega^m e^{-\omega^2/4}\right) \qquad \text{(D-9)}$$

$$\gamma(n, j) = \frac{2^n}{\sqrt{\pi}} \frac{n!}{(n-j)!\, j!} (i)^{n-j} \Gamma\left(\frac{n-j}{2}+1\right)\left(\frac{1+(-1)^{n-j}}{2}\right)$$

(D-10)

$$\bar{\gamma}\,(\ell_i, L_i)\cdot(\ell_i - 2L_i)! = E(L_i)/2L_i! = R(L_i) \qquad \text{(D-11)}$$

$$E(L_i) = \frac{\Gamma}{\sqrt{\pi}}\left(\frac{2L_i+1}{2}\right) 2^{L} \qquad \text{(D-12)}$$

$$\varsigma(\ell) = (-1)^{\ell/2}\,(1+(-1)^{\ell}) \qquad \text{(D-13)}$$

$$\Delta\bar{\ell}_i = (\delta_{\bar{n}0}\,\delta_{\bar{m}0}\,\delta_{\bar{\ell}0} - 1) \qquad \text{(D-14)}$$

$$\xi(\ell) = \left[(-1)^{\ell/2}(1+(-1)^{\ell}) \quad i(-1)^{\frac{\ell+1}{2}}(1-(-1)^{\ell}\right] \text{a row vector} \qquad \text{(D-15)}$$

Matrix calculates each of the sums (D-4) through (D-6) in a Do-loop, stores it temporarily (or in the case of (D-2) permanently) in an array and passes it on to the next do-loop for the next summation. The self-correlation matrix element proportional to the $\langle \ell_i | A_0(0) | \ell_i' \rangle$ term and is punched out along with two-particle matrix elements. This term is common to the calculations for any value of kr_0 and is stored during the $kr_0 = 0$ run for further use.

To save core space the elements are calculated along lines instead of by blocks, that is in the do-loops only the n-index is allowed to vary. One tries to group the elements together so that the dimensions (l m n indices) are about the same. The order subrountine brings in the ket vector $\langle l'm'n'|$ in the order desired to form the dot product and by varying n and n' all the desired matrix elements are obtained. Once we have the desired grouping of the basis, all the possible combinations of (lmn) and ($l'm'n'$) have to be run. It is basically a combinational problem.

Language used:- FortranIV

Precision:- Single as it was(in this program)numerically proved that double precision had a negligible effect on the spectrum calculation.

Main Program:- Main

Subroutines used:-	ORDER	RW	RAT
	CW	RF	
	CF	SF	

Dimensions:-

The array S3(JJ1, JJ2, JJ3, JJ4+1, IJ3+1, IJ6) used is a six-dimensional one. To arrive at the minimum dimensions use the formula

JJi = Maximum ($l_i + l'_i + 1$)
IJi = Maximum ($l'_i + 1$)

where ($l_1 l_2 l_3$) is used interchangeably with (lmn) and l' is synonymous with the program variable $\ell 1$.

Input Data

Card #	Data	Format
1	Ntimes = number of runs with different values of (MAXL, MAXM MAXN) for these values of	I5
	IND 1 =	I5
	IND 2 =	I5

Card #	Data	Format
	The subroutine ORDER compresses the indices $(l'm'n')$ into one index (i). (i) is varied in increments of unity between IND1 and IND2 (inclusive) to give the desired values of $(l'm'n')$.	
† 2	MAXL = MAXM = MAXN = } Correspond to the indices (lmn) with n being the maximum value for the given line	I5 I5 I5
3	NURK: the number of varying kr_o runs to be made with the preceding values on cards 1 and 2.	I5
*4	RK - this is the parameter kr_o. The first RK value must be 0.0.	I5

The self-correlation cards will be every second card. The IBM 082 sorter can be used to sort the cards.

(ii) DISPERSION:-

DISPERSION is the program which uses the matrix elements from MATRIX to calculate the spectrum by the method of Kinetic modelling described in chapter 3. It

---

[+] (i) Ntimes sets of data

[*] (ii) NURK sets of data

essentially solves the sets of equation (3-30a), (3-30b), (3-34b). One important point to remember is that it calculates $2R(x,y)$ directly and not $_{M}S(x,y)$.

Language used:- Fortran IV

Precision:- Double Precision

Main Program:- MAIN

Subroutines:- SKW HN BETA
BETAM CROSS W
SPHB1 I ORDER

The subroutine W is the subroutine W used by Sugawara to calculate the Plasma dispersion integral. ORDER as in MATRIX orders the basis and essentially compresses the three indices (lmn) into one index(i). The matrix inversion has been incorporated into SKW.

Dimensions:- Before running the program check the following variables for possible dimensional incompatibility with the data variable NMAX. The minimum requirements are

Subroutine	Variables
(a) MAIN	BHDSPH, GAMMA both NMAX by NMAX matrices
(b) SKW	A, GAMMA, BHDSPH, C, B, D

GAMMA, BHDSPH as in (a)
A =2KMX by 2KMX matrix B =2KMX dimensional vector
D =KMX by KMX matrix C =KMX dimensional vector

(c) BETAM	BHDSPH as in (a)

Input Data:-

Data Sequence:	Data	Format
1	NMAX = number of MATRIX cards read in for each kr_0 spectrum calculation	I5
2	RK = the parameter kr_0	E16.5
	KMDUMX = number of different KMX runs with the preceding values of RK and NMAX	I5
	N.B for the self-correlation input RK =0.0	
3	(I1I2I3I4I5I6)	6I5
	BMAX1	2E16.5
	the MATRIX element $\lambda_q/2$ (that is the one related to the shear viscosity).	
4	set of matrix cards from MATRIX for one kr_0 value	6I5 2E16.5
5	TITLE - comments	18A4
6	KMX = order of Kinetic model	I5
	MAXY = number of different nr_0^3 runs with the preceding infomation	2E16.5
7	(I1I2I3I4I5I6)	6I5
	BMAXN	2E16.5

Data Sequence:		Data	Format
KMDUMX sets		the matrix element corresponding to $\frac{1}{2}\lambda_N$ of the Kinetic model	
8	MAXY sets	XMIN XMAX DX The spectrum is calculated for x between XMIN and XMAX(inclusive) in increments of DX	3D16.6
		Y - the parameter y	D16.6

(iii) POLYNOMIAL:-

POLYNOMIAL performs the same functions as DISPERSION except that the calculation is performed by, essentially, the Wang Chang Uhlenbeck method as explained in 5.2

This program was not in any sense intended to be a production program. It was merely used to check the results of DISPERSION and so it will not be discussed any further.

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