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Approach to Equilibrium in Statistical Mechanics

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Abstract

TWe start with a time evolution equation in nonequilibrium statistical mechanics and study the conditions under which an approach to equilibrium results. This study supplements the H-theorem approach from the Boltzmann equation.

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Introduction

PHYSH classification: kinetic theory

Review of Time Evolution of the Single Particle Distribution Function

We follow definitions and conventions in [1,2] and review them for clarity and consistency with previous results.

Let f(r,p,t) be the single-particle distribution function of a many-body system. It represents the probability that at a particle in location r possesses the momentum p at time t. We use the phase space variables $r=(x,y,z),p=(p_x,p_z,p_z)$ in keeping with kinetic theory. Later, we will replace the average momentum divided by the particle mass m with velocity. Using factored initial distributions for the initial data, that is, $f_2(r,r')=f_1(r)$ f₁(r'), etc., we start with the equation derived in [1,2]:

$$\begin{split} f(r,p,t) &= f \bigg(r - \frac{pt}{m}, 0 \bigg) \, \phi(p) \\ &+ n_o \int_0^t \mathrm{d}s_1 \, e^{-s_1 L_0} \int \mathrm{d}r' \, \bigg[V(r-r') \frac{\partial}{\partial r_j'} f(r',0) \bigg] \frac{\partial}{\partial p_j} \bigg(\frac{p_i}{m} \frac{\partial}{\partial r_i} f(r,0) \phi(p) \bigg) \\ &+ n_o \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 e^{-s_2 L_0} \int \mathrm{d}r' \, \bigg[V(r-r') \frac{\partial}{\partial r_j'} f(r',0) \bigg] \frac{\partial}{\partial p_j} \bigg(\frac{p_i}{m} \frac{\partial}{\partial r_i} f(r,0) \phi(p) \bigg) \\ &- n_o \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 e^{-s_2 L_0} \int \mathrm{d}r' V(r-r') \frac{\partial}{\partial r_j'} f(r',0) \bigg(\frac{\partial}{\partial r_i} f(r,0) \frac{\partial}{\partial p_j} \phi(p,0) \bigg) \int \mathrm{d}p' \frac{p_i'}{m} \phi(p') \\ &+ \frac{n_o^2}{2} \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 e^{-s_2 L_0} f(r) \int \mathrm{d}r' V(r-r') \frac{\partial f(r')}{\partial r_j'} \int \mathrm{d}r'' \, V(r-r'') \frac{\partial}{\partial r_j'} \frac{\partial}{\partial r_i'} f(r') \frac{\partial}{\partial p_j} \frac{\partial}{\partial p_j} \phi(p) \bigg) \\ &+ \frac{n_o^2}{2} \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 e^{-s_2 L_0} f(r) \int \mathrm{d}r' \, V(r-r') \bigg)^2 \frac{\partial}{\partial r_j'} \frac{\partial}{\partial r_i'} f(r') \frac{\partial}{\partial p_j} \frac{\partial}{\partial p_j} \phi(p) \\ &\qquad \qquad (1) \end{split}$$

the contribution of an infinite number of terms in addition to above is zero, effectively truncating the series to six terms due to the vanishing of the momentum distribution at the boundary of the momentum space. We use the operator $L_0 = \frac{p}{m} \frac{\partial}{\partial r}$. n_0 is the average particle density. $V(r-r^{"})$ is a general form of the pair-potential

of two particles located at r,r". We follow Cartesian dot product conventions. Anticipating results presented in Section 2, we remark this early that the first term of Eq. (1) describes an ideal gas. We analyze each of the six terms in Eq. (1):

$$f1 = f\left(x - \frac{p_x t}{m}, y - \frac{p_y t}{m}, z - \frac{p_z t}{m}\right) \phi(p_x, p_y, p_z)$$
(2)

$$\begin{split} f2 &= \int_0^t \! ds_1 \, e^{-s_1 L_0} S1 \\ S1 &= \int dr^{'} \bigg[V(r-r^{'}) \frac{\partial}{\partial x^{'}} f(r^{'},0) \bigg] \frac{\partial}{\partial p_x} \bigg(\frac{p_x}{m} \frac{\partial}{\partial x} f(r) \phi(p) \bigg) \\ &+ \int dr^{'} \bigg[V(r-r^{'}) \frac{\partial}{\partial x^{'}} f(r^{'}) \bigg] \frac{\partial}{\partial p_x} \bigg(\frac{p_y}{m} \frac{\partial}{\partial y} f(r) \phi(p) \bigg) \\ &+ \int dr^{'} \bigg[V(r-r^{'}) \frac{\partial}{\partial x^{'}} f(r^{'}) \bigg] \frac{\partial}{\partial p_x} \bigg(\frac{p_z}{m} \frac{\partial}{\partial z} f(r) \phi(p) \bigg) \\ &+ \int dr^{'} \bigg[V(r-r^{'}) \frac{\partial}{\partial y^{'}} f(r^{'}) \bigg] \frac{\partial}{\partial p_x} \bigg(\frac{p_x}{m} \frac{\partial}{\partial x} f(r) \phi(p) \bigg) \end{split}$$

f2,f3 differ only in the time integrals

$$f4 = -n_o \int_0^t ds_1 \int_0^{s_1} ds_2 e^{-s_2 L_0} S3$$
(5)

$$\begin{split} &\mathrm{S3} = \int d\mathbf{r}' \left[V(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial \mathbf{x}'} f(\mathbf{r}') \right] \frac{\partial}{\partial p_x} \left(\frac{p_x}{m} \frac{\partial}{\partial \mathbf{x}} f(\mathbf{r}) \phi(\mathbf{p}, \mathbf{0}) \right) \int d\mathbf{p}' \frac{p_x'}{m} \phi(\mathbf{p}') \\ &+ \int d\mathbf{r}' \left[V(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial \mathbf{x}'} f(\mathbf{r}') \right] \frac{\partial}{\partial p_x} \left(\frac{p_y}{m} \frac{\partial}{\partial \mathbf{y}} f(\mathbf{r}) \phi(\mathbf{p}, \mathbf{0}) \right) \int d\mathbf{p}' \frac{p_y'}{m} \phi(\mathbf{p}') \\ &+ \int d\mathbf{r}' \left[V(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial \mathbf{x}'} f(\mathbf{r}') \right] \frac{\partial}{\partial p_x} \left(\frac{p_z}{m} \frac{\partial}{\partial \mathbf{z}} f(\mathbf{r}) \phi(\mathbf{p}) \right) \int d\mathbf{p}' \frac{p_z'}{m} \phi(\mathbf{p}') \\ &+ \int d\mathbf{r}' \left[V(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial \mathbf{y}'} f(\mathbf{r}') \right] \frac{\partial}{\partial p_y} \left(\frac{p_x}{m} \frac{\partial}{\partial \mathbf{x}} f(\mathbf{r}) \phi(\mathbf{p}, \mathbf{0}) \right) \int d\mathbf{p}' \frac{p_x'}{m} \phi(\mathbf{p}') \\ &+ \int d\mathbf{r}' \left[V(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial \mathbf{y}'} f(\mathbf{r}') \right] \frac{\partial}{\partial p_y} \left(\frac{p_x}{m} \frac{\partial}{\partial \mathbf{y}} f(\mathbf{r}) \phi(\mathbf{p}, \mathbf{0}) \right) \int d\mathbf{p}' \frac{p_x'}{m} \phi(\mathbf{p}') \end{split}$$

$$\begin{split} &+\int dr' \left[V(r-r') \frac{\partial}{\partial y'} f(r') \right] \frac{\partial}{\partial p_y} \left(\frac{p_z}{m} \frac{\partial}{\partial z} f(r) \phi(p) \right) \int dp' \frac{p_z'}{m} \phi(p') \\ &-\int dr' \left[V(r-r') \frac{\partial}{\partial z'} f(r') \right] \frac{\partial}{\partial p_z} \left(\frac{p_x}{m} \frac{\partial}{\partial x} f(r) \phi(p) \right) \int dp' \frac{p_x'}{m} \phi(p') \\ &+\int dr' \left[V(r-r') \frac{\partial}{\partial z'} f(r') \right] \frac{\partial}{\partial p_z} \left(\frac{p_z}{m} \frac{\partial}{\partial y} f(r) \phi(p) \right) \int dp' \frac{p_y'}{m} \phi(p') \\ &+\int dr' \left[V(r-r') \frac{\partial}{\partial z'} f(r') \right] \frac{\partial}{\partial p_z} \left(\frac{p_z}{m} \frac{\partial}{\partial z} f(r) \phi(p) \right) \int dp' \frac{p_z'}{m} \phi(p') \\ &+\int dr' \left[V(r-r') \frac{\partial}{\partial z'} f(r') \right] \frac{\partial}{\partial p_z} \left(\frac{p_z}{m} \frac{\partial}{\partial z} f(r) \phi(p) \right) \int dp' \frac{p_z'}{m} \phi(p') \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial x''} \left(\frac{\partial}{\partial p_x} \frac{\partial}{\partial p_x} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial z'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial x''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial y''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial y''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_y} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial z'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial y''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_y} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial y''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_y} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial y''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_y} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial z''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial z''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial z''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial z''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial z''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial z''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \int dr'' V(r-r') \frac{\partial f(r'')}{\partial z''} \left(\frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \right) \\ &+\int dr' V(r-r') \frac{\partial f(r')}$$

$$\begin{split} f6 &= + \frac{n_o^2}{2} \int_0^t ds_1 \int_0^{s_1} ds_2 e^{-s_2 L_0} \, f(r) S5 \\ S5 &= \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial x'} \frac{\partial}{\partial x'} \, f(r') \frac{\partial}{\partial p_x} \frac{\partial}{\partial p_x} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial y'} \frac{\partial}{\partial x'} \, f(r') \frac{\partial}{\partial p_y} \frac{\partial}{\partial p_x} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial x'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_x} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial x'} \frac{\partial}{\partial y'} \, f(r') \frac{\partial}{\partial p_x} \frac{\partial}{\partial p_y} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial y'} \, f(r') \frac{\partial}{\partial p_x} \frac{\partial}{\partial p_y} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial y'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_y} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial x'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_x} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial x'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_y} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_y} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, \frac{\partial}{\partial z'} \, f(r') \frac{\partial}{\partial p_z} \frac{\partial}{\partial p_z} \phi(p) \\ &+ \int dr' \left(V(r-r') \right)^2 \frac{\partial}{\partial z'} \frac{\partial}{\partial z'} \, \frac{\partial}$$

For an initially uniform system, only the first and sixth terms are non-zero. The most general initial data activates the second, third, fourth and fifth terms of Eq. (1)

Further Analysis for General Pair Potential

Our analysis depends on the assumption of product forms of the initial data: f(r,r')=f(r)f(r'); f(r)=f(x)f(y)f(z); $\phi(p,p')=\phi(p)\phi(p')$; $\phi(p)=\phi(p_x)\phi(p_y)\phi(p_z)$, $\phi(p_y)\phi(p_z)\phi(p_z)$. From a physical standpoint, these product or factored forms for the initial data and pair potential are not unduly restrictive.

We further introduce the definitions

$$W(x,X) = \int_{-x}^{x} dx' V(x - x') \frac{\partial f(x')}{\partial x'}$$
(10)

$$Z(y,Y) = \int_{-Y}^{Y} \! dy' V(y-y') f(y')$$

to rewrite the time evolution of the single-particle distribution function. The volume of the system is 8XYZ. The definitions will help us determine the conditions necessary to study the approach to steady state of the one particle distribution function and hydrodynamic variables.

The six terms of the distribution function are rewritten as

$$f1 = f\left(x - \frac{p_x t}{m}, y - \frac{p_y t}{m}, z - \frac{p_z t}{m}\right) \phi(p_x, p_y, p_z)$$

$$f2 = \int_0^t ds_1 e^{-s_1 L_0} S1$$

$$(12)$$

$$S1 =$$

$$+W(x,X)Z(y,Y)Z(z,Z)\begin{bmatrix} \frac{\partial}{\partial p_x} \left(\frac{p_x}{m} \frac{\partial}{\partial x}\right) \\ +\frac{\partial}{\partial p_y} \left(\frac{p_y}{m} \frac{\partial}{\partial y}\right) \\ +\frac{\partial}{\partial p_z} \left(\frac{p_z}{m} \frac{\partial}{\partial z}\right) \end{bmatrix} f(r)\phi(p)$$

$$+ Z(x,X)W(y,Y)Z(z,Z) \begin{bmatrix} \frac{\partial}{\partial p_x} \left(\frac{p_x}{m} \frac{\partial}{\partial x}\right) \\ + \frac{\partial}{\partial p_y} \left(\frac{p_y}{m} \frac{\partial}{\partial y}\right) \\ + \frac{\partial}{\partial p_z} \left(\frac{p_z}{m} \frac{\partial}{\partial z}\right) \end{bmatrix} f(r)\phi(p)$$

$$+Z(x,X)Z(y,Y)W(z,Z)\begin{bmatrix} \frac{\partial}{\partial p_{z}} \left(\frac{p_{x}}{m} \frac{\partial}{\partial x}\right) \\ +\frac{\partial}{\partial p_{z}} \left(\frac{p_{y}}{m} \frac{\partial}{\partial y}\right) \\ +\frac{\partial}{\partial p_{z}} \left(\frac{p_{z}}{m} \frac{\partial}{\partial z}\right) \end{bmatrix} f(r)\phi(p)$$

$$(13)$$

In all equations, the large brackets enclose sums, not matrix elements.

$$f3 = n_o \int_0^t ds_1 \int_0^{s_1} ds_2 e^{-s_2 L_0} S1$$
(14)

f2,f3 differ only in the time integrals.

$$f4 = -n_o \int_0^t ds_1 \int_0^{s_1} ds_2 e^{-s_2 L_o} S3$$

$$S3 = \begin{bmatrix} W(x, X)Z(y, Y)Z(z, Z) \frac{\partial}{\partial p_x} \left(\frac{p_x}{m} \frac{\partial}{\partial x} + \frac{p_y}{m} \frac{\partial}{\partial y} + \frac{p_z}{m} \frac{\partial}{\partial z} \right) \\ + W(y, Y)Z(x, Z)Z(z, Z) \frac{\partial}{\partial p_y} \left(\frac{p_x}{m} \frac{\partial}{\partial x} + \frac{p_y}{m} \frac{\partial}{\partial y} + \frac{p_z}{m} \frac{\partial}{\partial z} \right) \\ + W(z, Z)Z(x, Z)Z(y, Y) \frac{\partial}{\partial p_z} \left(\frac{p_x}{m} \frac{\partial}{\partial x} + \frac{p_y}{m} \frac{\partial}{\partial y} + \frac{p_z}{m} \frac{\partial}{\partial z} \right) \end{bmatrix} f(r)\phi(p)$$

$$(15)$$

 $f5 = \frac{n_o^2}{2} \int_0^t ds_1 \int_0^{s_1} ds_2 e^{-s_2 L_0} f(\mathbf{r}) S4$

(16)

$$\begin{bmatrix} W(x,X)Z(y,Y)Z(z,Z)\frac{\partial}{\partial p_x} \bigg(W(x,X)Z(y,Y)Z(z,Z)\frac{\partial \phi(p)}{\partial p_x} + W(y,Y)Z(x,X)Z(z,Z)\frac{\partial \phi(p)}{\partial p_y} + W(z,Z)Z(x,X)Z(y,Y)\frac{\partial \phi(p)}{\partial p_z} \bigg) \\ + W(y,Y)Z(x,X)Z(z,Z)\frac{\partial}{\partial p_y} \bigg(W(x,X)Z(y,Y)Z(z,Z)\frac{\partial \phi(p)}{\partial p_x} + W(y,Y)Z(x,X)Z(z,Z)\frac{\partial \phi(p)}{\partial p_y} + W(z,Z)Z(x,X)Z(y,Y)\frac{\partial \phi(p)}{\partial p_z} \bigg) \\ + W(z,Z)Z(x,X)Z(y,Y)\frac{\partial}{\partial p_z} \bigg(W(x,X)Z(y,Y)Z(z,Z)\frac{\partial \phi(p)}{\partial p_x} + W(y,Y)Z(x,X)Z(z,Z)\frac{\partial \phi(p)}{\partial p_y} + W(z,Z)Z(x,X)Z(y,Y)\frac{\partial \phi(p)}{\partial p_z} \bigg) \bigg] \\ (17)$$

$$f6 = \frac{n_0^2}{2} \int_0^t ds_1 \int_0^{s_1} ds_2 e^{-s_2 L_0} f(r) S5$$
(18)

$$S5 = \begin{cases} \int d\mathbf{r}' \left(\frac{\partial V(\mathbf{r} - \mathbf{r}')}{\partial \mathbf{x}'} \right)^2 f(\mathbf{x}') Z(\mathbf{y}, \mathbf{Y}) Z(\mathbf{z}, \mathbf{Z}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{x}}^2} \\ + W(\mathbf{x}, \mathbf{X}) W(\mathbf{y}, \mathbf{Y}) Z(\mathbf{z}, \mathbf{Z}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{x}} \partial \mathbf{p}_{\mathbf{y}}} \\ + W(\mathbf{x}, \mathbf{X}) W(\mathbf{z}, \mathbf{Z}) Z(\mathbf{y}, \mathbf{Y}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{x}} \partial \mathbf{p}_{\mathbf{z}}} \\ + W(\mathbf{y}, \mathbf{Y}) W(\mathbf{x}, \mathbf{X}) Z(\mathbf{z}, \mathbf{Z}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{y}} \partial \mathbf{p}_{\mathbf{x}}} \end{cases}$$

$$S5 = \begin{cases} + \int d\mathbf{r}' \left(\frac{\partial V(\mathbf{r} - \mathbf{r}')}{\partial \mathbf{y}'} \right)^2 f(\mathbf{y}') Z(\mathbf{x}, \mathbf{X}) Z(\mathbf{z}, \mathbf{Z}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{y}} \partial \mathbf{p}_{\mathbf{z}}} \\ + W(\mathbf{y}, \mathbf{Y}) W(\mathbf{z}, \mathbf{Z}) Z(\mathbf{x}, \mathbf{X}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{y}} \partial \mathbf{p}_{\mathbf{x}}} \\ + W(\mathbf{z}, \mathbf{Z}) W(\mathbf{x}, \mathbf{X}) Z(\mathbf{y}, \mathbf{Y}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{z}} \partial \mathbf{p}_{\mathbf{y}}} \\ + W(\mathbf{z}, \mathbf{Z}) W(\mathbf{y}, \mathbf{Y}) Z(\mathbf{x}, \mathbf{X}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{z}} \partial \mathbf{p}_{\mathbf{y}}} \\ + \int d\mathbf{r}' \left(\frac{\partial V(\mathbf{r} - \mathbf{r}')}{\partial \mathbf{z}'} \right)^2 f(\mathbf{z}') Z(\mathbf{x}, \mathbf{X}) Z(\mathbf{y}, \mathbf{Y}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{z}}^2} \right] \end{cases}$$

$$(19)$$

The above rewrite of older work [1,2] facilitates further analysis of our results.

Symmetry Arguments from Initial Data

When the initial data is symmetric in x,y,z, we find that

$$W(x,X) = \int_{-X}^{X} dx' V(x - x') \frac{\partial f(x')}{\partial x'} = \int_{-X}^{X} dx' \frac{\partial}{\partial x'} (V(x - x') f(x')) - \frac{\partial V(x - x')}{\partial x'} f(x') = 0$$
(20)

and we get S1=S2=S3=S4=0.

$$f6 = \frac{n_0^2}{2} \int_0^t ds_1 \int_0^{s_1} ds_2 e^{-s_2 L_0} f(r) S5$$
(21)

$$f(r, p, t) = f(r)\phi(p) + \frac{n_0^2}{2} \int_0^t ds_1 \int_0^{s_1} ds_2 e^{-s_2 L_0} f(r) S5$$
(22)

$$\begin{split} S5 = \begin{bmatrix} \int dr' \bigg(\frac{\partial V(r-r')}{\partial x'} \bigg)^2 \, f(x') Z(y,Y) Z(z,Z) \, \frac{\partial^2 \phi(p)}{\partial p_x^2} \\ + \int dr' \bigg(\frac{\partial V(r-r')}{\partial y'} \bigg)^2 \, f(y') Z(x,X) Z(z,Z) \, \frac{\partial^2 \phi(p)}{\partial p_y^2} \\ + \int dr' \bigg(\frac{\partial V(r-r')}{\partial z'} \bigg)^2 \, f(z') Z(x,X) Z(y,Y) \, \frac{\partial^2 \phi(p)}{\partial p_z^2} \end{bmatrix} \end{split}$$

where

$$Z(y,Y) = \int_{-Y}^{Y} dy' V(y - y') f(y')$$
(23)

Eq. (22) is a general result for any reasonable pair potential and initial data symmetric in x,y,z.

Finding complete solutions of the time evolution becomes an implementable analytic or numeric procedure consisting of these steps: (1) choose the initial data; (2) perform space integrations over x',y',z', (3) apply the

free particle shift operator $e^{-\frac{p_x s}{m} \frac{\partial}{\partial x} - \frac{p_y s}{m} \frac{\partial}{\partial z}}$; (3) perform the time integrals; (4) followed by momentum integrals. Steps 3 and 4 may be reversed. We thus have a prescription for generating solutions of the single particle distribution function. The result of the above steps still requires work, dictated by chosen physical applications, of which there will be many. In another paper, we will model a one-dimensional shock wave. We invite readers to generate solutions using our initial value approach.

Approach to Steady State

The time derivative of each of the six terms of our time evolution equation are:

$$\frac{\partial}{\partial t} f 1 = \frac{\partial}{\partial t} f \left(r - \frac{pt}{m}, p \right)$$
(24)

If the system is bound, the ballistic term eventually hits the boundary and goes to zero under the limit $t \rightarrow \infty$, a limit that we will take for all the terms that follow.

$$\frac{\partial f^{2}}{\partial t} = e^{-tL_{0}}f(r) \begin{bmatrix} \int dr' V(r-r') \frac{\partial f(r')}{\partial x'} \frac{\partial \varphi(p)}{\partial p_{x}} \\ + \int dr' V(r-r') \frac{\partial f(r')}{\partial y'} \frac{\partial \varphi(p)}{\partial p_{y}} \\ + \int dr' V(r-r') \frac{\partial f(r')}{\partial z'} \frac{\partial \varphi(p)}{\partial p_{z}} \end{bmatrix}$$
(25)

Eq. (25) will be zero for a uniform system.

Note that $L_o = \frac{p}{m} \frac{\partial}{\partial r}$

The second term also goes to zero for a uniform system.

Next, the third term also goes to zero for a uniform system:

$$\frac{\partial f3}{\partial t} = -n_o \int_0^t ds_2 e^{-s_2 L_o} S3$$

$$S3 = \begin{bmatrix}
W(x, X)Z(y, Y)Z(z, Z) \frac{\partial}{\partial p_x} \left(\frac{p_x}{m} \frac{\partial}{\partial x} + \frac{p_y}{m} \frac{\partial}{\partial y} + \frac{p_z}{m} \frac{\partial}{\partial z} \right) \\
+W(y, Y)Z(x, Z)Z(z, Z) \frac{\partial}{\partial p_y} \left(\frac{p_x}{m} \frac{\partial}{\partial x} + \frac{p_y}{m} \frac{\partial}{\partial y} + \frac{p_z}{m} \frac{\partial}{\partial z} \right) \\
+W(z, Z)Z(x, Z)Z(y, Y) \frac{\partial}{\partial p_z} \left(\frac{p_x}{m} \frac{\partial}{\partial x} + \frac{p_y}{m} \frac{\partial}{\partial y} + \frac{p_z}{m} \frac{\partial}{\partial z} \right) \end{bmatrix} f(r)\varphi(p)$$
(26)

where again

$$W(x,X) = \int_{-X}^{X} dx' V(x - x') \frac{\partial f(x')}{\partial x'} = 0$$

$$(27)$$

$$Z(y,Y) = \int_{-Y}^{Y} dy' V(y - y') f(y')$$

$$(28)$$

The fourth term

$$\frac{\partial f4}{\partial t} = -n_o g \int_0^\infty ds e^{-sL_o} \left[W(x,X)Z(y,Y)Z(z,Z) \frac{\partial}{\partial p_x} \left(\frac{p_x}{m} \frac{\partial f(r)}{\partial x} + \frac{p_y}{m} \frac{\partial f(r)}{\partial y} + \frac{p_z}{m} \frac{\partial f(r)}{\partial z} \right) \varphi(p) \right] \\ + W(y,Y)Z(x,Z)Z(z,Z) \frac{\partial}{\partial p_y} \left(\frac{p_x}{m} \frac{\partial f(r)}{\partial x} + \frac{p_y}{m} \frac{\partial f(r)}{\partial y} + \frac{p_z}{m} \frac{\partial f(r)}{\partial z} \right) \varphi(p) \\ + W(z,Z)Z(x,Z)Z(y,Y) \frac{\partial}{\partial p_z} \left(\frac{p_x}{m} \frac{\partial f(r)}{\partial x} + \frac{p_y}{m} \frac{\partial f(r)}{\partial y} + \frac{p_z}{m} \frac{\partial f(r)}{\partial z} \right) \varphi(p) \right]$$

$$(29)$$

is also zero. Finally,

$$\frac{\partial f5}{\partial t} = +\frac{n_0^2}{2} \int_0^t ds_2 e^{-s_2 L_0} f(r) S5$$
(30)

$$S5 = \begin{cases} \int d\mathbf{r}' \left(\frac{\partial V(\mathbf{r} - \mathbf{r}')}{\partial \mathbf{x}'} \right)^2 f(\mathbf{x}') Z(\mathbf{y}, \mathbf{Y}) Z(\mathbf{z}, \mathbf{Z}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{x}}^2} \\ + W(\mathbf{x}, \mathbf{X}) W(\mathbf{y}, \mathbf{Y}) Z(\mathbf{z}, \mathbf{Z}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{x}} \partial \mathbf{p}_{\mathbf{y}}} \\ + W(\mathbf{x}, \mathbf{X}) W(\mathbf{z}, \mathbf{Z}) Z(\mathbf{y}, \mathbf{Y}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{x}} \partial \mathbf{p}_{\mathbf{z}}} \\ + W(\mathbf{y}, \mathbf{Y}) W(\mathbf{x}, \mathbf{X}) Z(\mathbf{z}, \mathbf{Z}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{y}} \partial \mathbf{p}_{\mathbf{x}}} \end{cases}$$

$$S5 = \begin{cases} + \int d\mathbf{r}' \left(\frac{\partial V(\mathbf{r} - \mathbf{r}')}{\partial \mathbf{y}'} \right)^2 f(\mathbf{y}') Z(\mathbf{x}, \mathbf{X}) Z(\mathbf{z}, \mathbf{Z}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{y}} \partial \mathbf{p}_{\mathbf{z}}} \\ + W(\mathbf{y}, \mathbf{Y}) W(\mathbf{z}, \mathbf{Z}) Z(\mathbf{x}, \mathbf{X}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{y}} \partial \mathbf{p}_{\mathbf{x}}} \\ + W(\mathbf{z}, \mathbf{Z}) W(\mathbf{x}, \mathbf{X}) Z(\mathbf{y}, \mathbf{Y}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{z}} \partial \mathbf{p}_{\mathbf{y}}} \\ + W(\mathbf{z}, \mathbf{Z}) W(\mathbf{y}, \mathbf{Y}) Z(\mathbf{x}, \mathbf{X}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{z}} \partial \mathbf{p}_{\mathbf{y}}} \\ + \int d\mathbf{r}' \left(\frac{\partial V(\mathbf{r} - \mathbf{r}')}{\partial \mathbf{z}'} \right)^2 f(\mathbf{z}') Z(\mathbf{x}, \mathbf{X}) Z(\mathbf{y}, \mathbf{Y}) \frac{\partial^2 \phi(\mathbf{p})}{\partial \mathbf{p}_{\mathbf{z}}^2} \end{cases}$$

$$(31)$$

again not necessarily zero at this point unless Z(x,X)=Z(y,Y)=Z(x,X)=0.

If both W=Z=0 the first two terms of time derivative of the distribution function sum up to

$$\frac{\partial f(\mathbf{r}, \mathbf{p}, \mathbf{t})}{\partial \mathbf{t}} = \frac{\partial f\left(\mathbf{r} - \frac{\mathbf{p}\mathbf{t}}{\mathbf{m}}, \mathbf{p}\right)}{\partial \mathbf{t}} + e^{-t\mathbf{L}_0} f(\mathbf{r}) \begin{bmatrix} \int d\mathbf{r}' \, V(\mathbf{r} - \mathbf{r}') \frac{\partial f(\mathbf{r}')}{\partial \mathbf{x}'} \frac{\partial \phi(\mathbf{p})}{\partial \mathbf{p}_x} \\ + \int d\mathbf{r}' \, V(\mathbf{r} - \mathbf{r}') \frac{\partial f(\mathbf{r}')}{\partial \mathbf{y}'} \frac{\partial \phi(\mathbf{p})}{\partial \mathbf{p}_y} \\ + \int d\mathbf{r}' \, V(\mathbf{r} - \mathbf{r}') \frac{\partial f(\mathbf{r}')}{\partial \mathbf{z}'} \frac{\partial \phi(\mathbf{p})}{\partial \mathbf{p}_z} \end{bmatrix}$$

$$(32)$$

which, for an initially uniform system goes to zero as $t\to\infty$. A steady state is reached. This is a rigorous result when W=Z=0. It would be desirable to generalize the result without this condition and prove the equivalent of true ergodic behavior.

References

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