Chapter 2

Numerical Methods

2.1 Introduction

This chapter provides the details of the discrete Boltzmann equation discrete velocity model. The problem is to solve an adequate approximation to the Boltzmann equation (1.5). The most basic properties of a solution are that the distribution should become Maxwellian (since there are no external forces), and that particle density, momentum and energy should be conserved. The first is guaranteed by an $H$ theorem$^6$ and the others should be apparent from the description of the model. A full solution will give the temporal evolution of the distribution function, but the interesting result will be the relaxation of the temperature ratios.

The discrete velocity method simplifies the Boltzmann equation by restricting the domain of definition of the distribution functions to a finite set of velocity vectors. The integro-differential equation is reduced to a large set of coupled ordinary differential equations. The problem is now to find values of $N_i(t) \equiv f(v_i, t)$ given the initial values. An outline of the algorithm is given in table 2.1, and this chapter describes the details of the various steps.

2.2 The Discrete Boltzmann Equation

The difficult part in computing the solution to the Boltzmann equation for the problems in this thesis is the evaluation of the collision integral. The time integration is
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```
Set initial parameters
\( r, \Delta t \)

Set initial distribution function
Maxwellian or bi-Maxwellian

Compute time-saving look-up tables
possible collision outcomes
and symmetry tables

\hspace{1cm} \textbf{TIME ITERATION}

\hspace{1cm} For each particle \( i \)

\hspace{1cm} Add gain term \( \sum_{kl} A_{ij}^{kl} N_k N_l \)
\hspace{1cm} using collision tables

\hspace{1cm} Compute loss term \( A_{ij}^{kl} N_i N_j \)
\hspace{1cm} for each \( j \)

\hspace{1cm} Advance in time using second order differencing scheme

\hspace{1cm} Compute macroscopic quantities
\hspace{1cm} Check conservation of particles,
\hspace{1cm} momentum and temperature

\hspace{1cm} Output results for this time step

\hspace{1cm} If the distribution function is
\hspace{1cm} not close enough to equilibrium
\hspace{1cm} repeat iteration
```

Table 2.1: Flowchart for the DBE numerical algorithm.
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straightforward. The essence of this method is that the domain of the distribution function, the velocity space, is discrete. Specifically the velocities, \( \mathbf{v} \), used form a uniform lattice as shown in figure 2.1. The absolute scales are irrelevant and reduced units are used throughout. A discussion of the units accompanies the results in chapter 3. The DBE approximation to the Boltzmann equation is

\[
\frac{\partial N_i}{\partial t} = \sum_{j,k,l=1}^{p} A_{ij}^{kl} (N_k N_l - N_i N_j), \quad i = 1, ..., p = (2r)^3 \tag{2.1}
\]

\[
= \sum_j \left[ \left( \sum_{k,l} A_{ij}^{kl} N_k N_l \right) - \left( \sum_{k,l} A_{ij}^{kl} \right) N_i N_j \right], \tag{2.2}
\]

where the \( N_i \) are values of the distribution function on the box centered on velocity \( i \), and

\[ A_{ij}^{kl} = a_{ij}^{kl} = |\mathbf{v}_i - \mathbf{v}_j| a_{ij}^{kl}. \]

Here \( A_{ij}^{kl} \) is the transition probability for the collision pair with initial velocities \( \mathbf{v}_i, \mathbf{v}_j \) resulting in \( \mathbf{v}_k, \mathbf{v}_l \) velocities. The effect of the cross-section is given by \( a_{ij}^{kl} \), the probability of choosing the \( k, l \) outcome from a \( i, j \) collision. The resolution of the velocity grid is specified by, \( r \), the number of speeds on one half-axis.

2.3 Numerical Integration

The time evolution of the Boltzmann equation for the problems in this thesis should be smooth. A ‘predictor-corrector’ integration method should be able to follow the evolution without falling into any pathological, e.g., oscillatory or discontinuous, behaviour of \( f(t) \). The computational bottleneck in the integration is the evaluation of the collision integral. Although the goal of the discrete velocity approximation is to make the collision term as simple as possible to evaluate the dimensionality suggests that a method which requires very few evaluations of the collision terms desirable. This rules out high-order Runge-Kutta or Richardson extrapolation methods.\(^{91}\)
Figure 2.1: The discrete velocities lie on nodes in the grid. The picture in three dimensions is similar.
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The following is a standard derivation of differencing schemes, accurate to second order in time. The discrete Boltzmann equation can be written

$$\frac{d}{dt} N(t) = L(N) = C(N) - D(N), \quad (2.3)$$

where \( N(t) = (N_1(t), N_2(t), \ldots, N_p(t)) \) is the discrete representation of the distribution function, and \( C(N) \) is the first set of sums in equation (2.2) and \( D(N) \) is the second part of the collision sum. A Taylor expansion of \( N(t) \) in \( t \) is

$$N^{i+1} = N^i + \Delta t \frac{dN^i}{dt} \bigg|_i + \frac{1}{2} (\Delta t)^2 \frac{d^2N^i}{dt^2} \bigg|_i + O[(\Delta t)^3], \quad (2.4)$$

where the abbreviation \( N^i = N(t_i) \) has been used and \( N^{i+1} = N(t_i + \Delta t) \). The derivative terms can be rewritten another way:

$$\frac{dN^i}{dt} \bigg|_i = L^i \quad (2.5)$$

$$\frac{d^2N^i}{dt^2} \bigg|_i = \frac{dL}{dt} \bigg|_i$$

$$= \frac{L^i - L^{i-1}}{\Delta t}, \quad (2.6)$$

where \( L^i = L(N^i) \). This gives a second order (in \( \Delta t \)) explicit scheme for \( N \):

$$N^{i+1} = N^i + \frac{\Delta t}{2} (3L^i - L^{i-1}) + O[(\Delta t)^3] \quad (2.7)$$

An implicit scheme can also be worked out. Forward and backward time steps give

$$N^{i+1/2} = N^i + \frac{\Delta t}{2} \frac{dN}{dt} \bigg|_{i+1} + \frac{1}{2} \left( \frac{\Delta t}{2} \right)^2 \frac{d^2N}{dt^2} \bigg|_{i+1} + O[(\Delta t)^3], \quad (2.8)$$

$$= N^{i+1} - \frac{\Delta t}{2} \frac{dN}{dt} \bigg|_{i+1} + \frac{1}{2} \left( \frac{-\Delta t}{2} \right)^2 \frac{d^2N}{dt^2} \bigg|_{i+1} + O[(\Delta t)^3]. \quad (2.9)$$

Rearranging these equations yields

$$N^{i+1} = N^i + \frac{\Delta t}{2} (L^{i+1} + L^i) + O[(\Delta t)^3], \quad (2.10)$$
which is a second order implicit scheme. Computationally the $C$ term appears to handled adequately by the explicit method, but the $D$ term requires the implicit scheme to be stable. Approximate values for $D^{i+1}$ are computed with an iteration. The estimate $D^{i+1} = D^i$ is used to compute provisional values for $N^{i+1}$. Then better estimates for $D^{i+1}$ are computed and $N^{i+1}$ is re-evaluated. In the linear test particle problem the same scheme is used but no iteration is needed for the $D$ term.

2.4 Distribution Function Considerations

The initial distribution functions used – Maxwellian and bi-Maxwellian – have rotational symmetry about the $z$ axis. The effects of collisions can’t change this because the forces result from a radial potential; there is no azimuthal dependence in the cross-section. This means that a simplification in the collision sum, equation (2.2), can be made. The discrete velocity grid breaks the rotational symmetry so instead of getting an exact reduction in the dimension of the problem, only a large fraction of the terms are repeated and need to be calculated only once. The condition $f(v_a) = f(v_b)$ is

\begin{align}
|v_{ax}| &= |v_{bx}| \\
v_{ax}^2 + v_{ay}^2 &= v_{bx}^2 + v_{by}^2
\end{align}

(2.11)

(2.12)

Computationally this is achieved by checking the symmetry and using a recorded value of the collision sum for each $N_i$.

The representation of test particles with high (or low) energies relative to the bath particles or the representation of a bi-Maxwellian with $\alpha$ not near 1 causes some problems. Figure 3.1 illustrates this problem – either the distribution function is not zero on the boundary of the grid or the distribution function is non-zero only on a small region of the velocity grid. A possible solution to this problem is to increase the resolution in an effort to have a better representation of the ‘narrow’ distribution functions. This is undesirable
Figure 2.2: Collision sphere (represented by a circle) for particles with velocities $v_1, v_2$. Antipodal pairs of dots on the surface indicate the allowed resultant velocities.

because the objective is to use as few velocities as possible. Another solution is to change the velocity units while keeping the energy ratio constant.

2.5 Discrete Cross Sections

Since the collision integral is evaluated on a discrete set of velocities, the cross-section is also discretized. This is quite straightforward for cross-sections which depend only on $g$, but difficulties arise for angle dependent interactions. A typical collision relative velocity might only have 4 or 8 permissible outcomes, resulting in a very coarse sampling of $\sigma(\chi)$. Figure 2.3 shows a typical situation. The most obvious problem is the zero deflection
collisions; the cross-section diverges and must be replaced with a finite approximation.

Previous computations with the discrete velocity method have used hard sphere cross-
sections. This is easy to implement: a normalization \( \sum_{kl} a_{ij}^{kl} = 1 \) is used and in the
source term the \( k,l \) dependence of \( a_{ij}^{kl} \) is determined by weighting all possible collisions
equally. The relative velocity factor \( g_{ij} \) is simple to include in the sum on \( j \). The other
isotropic models used (e.g. Maxwell molecules) are a simple change which is accomplished
by changing the velocity weighting factor in the \( j \) sum. The anisotropic models are
implemented by changing the weightings in the \( \sum_{kl} a_{ij}^{kl} \) term. A complication arises for
the divergent cross-sections. For every collision there is a head on \( (\chi = 0) \) collision.
There is no obviously correct way to weight these terms which have an ‘infinite’ weight.

It is necessary to verify that some properties of the Boltzmann equation are pre-
served in the discrete Boltzmann equation approximation. The conservation of some
macroscopic quantities will be checked here, following the calculation done by Gatignol.\(^3\)
One concern is that the discretization of the cross-section into \( A_{ij}^{kl} \) weights could result
in errors due to coarse sampling between the gain and loss terms, or worse, due to some
asymmetry in the approximation. This possibility can be eliminated by checking some
velocity dependent averaged quantities. Consider a function \( \phi(v_i) = \phi_i \) which may de-
pend on \( v \) but not on \( t \). Then \( \langle \phi \rangle = \sum_i \phi_i N_i \). If \( \langle \phi \rangle \) is conserved then the collision sum
should be zero:

\[
0 = \frac{\partial}{\partial t} \sum_i \phi_i N_i = \sum_i \phi_i \left( \sum_{jkl} A_{ij}^{kl} (N_k N_l - N_i N_j) \right) \\
= \frac{1}{2} \sum_{ijkl} \left( \phi_i A_{ij}^{kl} N_k N_l + \phi_j A_{ij}^{kl} N_k N_l - \phi_i A_{ij}^{kl} N_i N_j - \phi_j A_{ij}^{kl} N_i N_j \right) \\
= \frac{1}{2} \sum_{ijkl} \left( \phi_i A_{ij}^{kl} N_k N_l + \phi_j A_{ij}^{kl} N_k N_l - \phi_k A_{ij}^{kl} N_k N_l - \phi_j A_{ij}^{kl} N_k N_l \right) \\
= \frac{1}{2} \sum_{ijkl} \left( \phi_i A_{ij}^{kl} N_k N_l + \phi_j A_{ij}^{kl} N_k N_l - \phi_k A_{ij}^{kl} N_k N_l - \phi_l A_{ij}^{kl} N_k N_l \right)
\]
Figure 2.3: Angular part of Rutherford cross-section, $\sigma(\chi) = 1/\sin^4(\chi/2)$. The solid line is the analytic form, symbols show typical sample points used in the discrete velocity computation.
\[
\frac{1}{2} \sum_{ijkl} A_{ij}^{kl} (\phi_i + \phi_j - \phi_k - \phi_l) N_k N_l
\]

The first step requires microreversibility, \( A_{ij}^{kl} = A_{kj}^{li} \). Subsequent manipulations involve the interchange of dummy summation variables and the symmetry condition \( A_{ij}^{kl} = A_{ji}^{lk} \). If these constraints are satisfied then \( \phi_i = 1, \phi_i = \nu_i \) and \( \phi_i = |\nu_i|^2 \) are conserved. This means that particle density, momentum and energy are all conserved. Each conserved \( \phi_i \) gives a transport equation for a macroscopic quantity.

Previous applications of the discrete velocity model to the Boltzmann equation have only used the isotropic hard sphere cross-section. For problems involving elastic collisions of neutral particles this is fine, but it is not satisfactory for collisions in a plasma. The Rutherford cross-section is very different; it is anisotropic and depends on the relative velocity in a collision. Five cross-sections are used in this thesis to test the expression of the different interactions within the coarse discretization. A list of the models used is in Table 2.2. The hard sphere, Maxwell molecule and Rutherford cross-sections are commonly used and implemented here to show the versatility of the DBE. The isotropic Rutherford and simple anisotropic cross-sections are included because they are two factors of the Rutherford cross-section which are implemented in different ways in the DBE. Modifying the program to use a different cross-section is much easier with the DBE than with other standard methods. For example, changing the cross-section in a polynomial expansion method requires a difficult computation of matrix elements (see section 3.3). This is one of the main advantages of the DBE, and is a consequence of the simplicity of the model.
<table>
<thead>
<tr>
<th>Cross-section</th>
<th>$\sigma$</th>
<th>$a_{ij}^{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hard Spheres</td>
<td>1</td>
<td>$\frac{1}{\sqrt{(v_j - v_i) \cdot (v_j - v_i)}}$</td>
</tr>
<tr>
<td>Maxwell Molecules</td>
<td>$g$</td>
<td>$\frac{1}{1/</td>
</tr>
<tr>
<td>Isotropic ‘Rutherford’</td>
<td>$1/g^4$</td>
<td>$\frac{g \cdot g}{(g \cdot g - g \cdot g')^2}$</td>
</tr>
<tr>
<td>Anisotropic ‘Rutherford’</td>
<td>$1/\sin^4(\chi/2)$</td>
<td>$\frac{1}{g \cdot g - g \cdot g'}^2$</td>
</tr>
<tr>
<td>Rutherford</td>
<td>$1/g^4 \sin^4(\chi/2)$</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.2: Cross-sections used in the DBE. The normalization constants have been omitted for clarity.
Chapter 3

Calculations and Results

3.1 Introduction

In this chapter the calculations performed and the results of the calculations are described. The details of the computations and the FORTRAN program used for the linear and the non-linear problems are very similar and so the description of both problems has been integrated. The DBE is very versatile and a variety of calculations are possible for different cross-sections. However, the nature of the five cross-sections affects the usefulness of the method as shall be seen from the calculations. The DBE is shown to be inefficient in the solution of the linear test particle problem, but this benchmark program serves as a test of the computer program's integrity.

Results were generated for five different cross-sections with several different temperature ratios for each cross-section. For each case several runs with different time step sizes and velocity grids were computed to verify that an accurate representation of the evolution of the distribution function was achieved. About 400 time steps were required to allow a typical distribution to relax. Each time iteration requires the computation of many terms in the collision integral. On our Silicon Graphics 4D/340S machine about 180 000 collisions can be evaluated each second. Table 3.1 gives timings for a single time step. These figures are from versions of the code that assume azimuthal symmetry of the distribution function about the z-axis. A listing of the program is provided in the Appendix.
Table 3.1: Timings for one iteration at various grid sizes. The times are directly related to the number of collision terms; the time to compute collision tables and start-up information is not included.

\begin{tabular}{|c|c|c|}
\hline
r & \# of collision terms & time for iteration \\
\hline
4 & 362,740 & < 2 s \\
5 & 1,762,500 & 8 s \\
6 & 6,048,050 & 32 s \\
7 & 17,344,886 & 90 s \\
8 & 43,507,108 & 230 s \\
9 & 96,156,270 & 9.2 min \\
10 & 197,351,718 & 17 min \\
11 & 379,343,580 & 37 min \\
12 & 835,730,228 & 77 min \\
\hline
\end{tabular}

3.2 Definitions of computational quantities

Reduced units for time and velocity were used for all the computations. This means that time, $t$, is scaled to a new time, $\tau$. This scaling depends on the units of the cross-section used and full details will be given with a description of each cross-section. This section describes the various units and computational simplifications made.

The first problem is concerned with the relaxation of a test particle distribution, initially Maxwellian at temperature $T_1(0)$, owing to elastic collisions with a second species of the same mass. This second species is in large extent and the distribution function is Maxwellian at temperature $T_2$. The precise details of the representation of the distribution function and the factors that will influence the computation are now established. A normalized Maxwellian distribution function for a particle density $n_0$ is

$$f(v) = n_0 \left( \frac{m}{2\pi k T} \right)^{3/2} e^{-mv^2/2kT}.$$  \hspace{1cm} (3.1)
The dimensions in cgs units are

\[
[n_0] = \text{particles/cm}^3 \\
m = 9.1096 \cdot 10^{-28} \text{ g} \\
k = 1.3806 \cdot 10^{-16} \text{ erg/°K} \\
[T] = \circ \text{K} \\
[v] = \text{cm/s}.
\]

A check shows that the exponential factor is dimensionless and that the normalization constant has dimensions of

\[
\left(\frac{g}{\text{erg}}\right)^{3/2} = \left(\frac{g}{g \text{ cm}^2/\text{s}^2}\right)^{3/2} = \left(\frac{\text{cm}}{\text{s}}\right)^{-3}.
\]

The choice of temperature then prescribes the velocity units (\(v'\) is the dimensionless computational velocity),

\[
v = v'\sqrt{2kT/m} \text{ cm/s}
\]

\[
= v' \cdot 5.5055 \cdot 10^5 \sqrt{T} \text{ cm/s}.
\]

The particle density factor can be factored out of the Boltzmann equation and included in the redefinition of time.

For a normalized equilibrium (Maxwellian) distribution the temperature is defined by

\[
\frac{3}{2}kT = \left(\frac{1}{2}m v^2\right) = \int \frac{1}{2}mv^2f(v)dv,
\]

and in the discrete velocity approximation is computed as

\[
\frac{3}{2}T = \sum_i N_i(v_x^2 + v_y^2 + v_z^2).
\]

The expression for the bi-Maxwellian (BM) anisotropic initial distribution function used in the second problem is given by

\[
f^{BM} = \left(\frac{m}{2\pi kT_\parallel(0)\alpha^2(0)}\right)^{3/2} e^{-m(v_x^2 + \alpha(0)v_z^2)/(2kT_\parallel(0))},
\]
where $\alpha(0) = T_{||}(0)/T_{\perp}(0)$ and

$$T(0) = T_{\perp}(0) \left( \frac{2\alpha(0) + 1}{3} \right).$$  \hspace{1cm} (3.8)

The temperature ratio at time $t$ is denoted by $\alpha(t)$. It is dimensionless and needs no conversion.

During the relaxation the distribution function does not necessarily remain Maxwellian. The evolution of $\alpha(t)$ is used as a measure of the relaxation of the distribution function.

The parallel and perpendicular temperatures for the anisotropic distributions used in the second problem are given by the following moments with the distribution function. Recall that the equipartition theorem indicates that each degree of freedom has $\frac{1}{2}kT$ of energy, thus the kinetic energy in the perpendicular plane is $2 \cdot \frac{1}{2}kT_{\perp}$.

$$\frac{1}{2}kT_{||} = \langle \frac{1}{2}mv_{||}^2 \rangle$$

$$= \frac{1}{2} m \sum_{i} N_i v_x^2$$

$$kT_{\perp} = \langle \frac{1}{2}mv_{\perp}^2 \rangle$$

$$= \frac{1}{2} m \sum_{i} N_i (v_x^2 + v_y^2).$$

This gives an expression to relate the parallel and perpendicular temperatures to the predicted equilibrium temperature,

$$\frac{3}{2}T = T_{\perp} + \frac{1}{2}T_{||}$$

$$T = \frac{2T_{\perp} + T_{||}}{3}.$$  \hspace{1cm} (3.9)

These definitions illustrate the problem with trying to represent distribution functions (or components of distribution functions) with significantly different temperatures: the sums are only computed over the range of discrete velocities used and not over all velocity space. If the distribution function differs much from zero for velocities beyond the range
of the velocity grid the computed temperatures will be wrong. The broader distribution function can be used to determine the velocity scaling to make it ‘fit’ the grid. This places a lower limit on the thinness of the cooler distribution; if it is too steep the temperature sum may be a poor approximation to the integral. The collision integral is similarly affected. Figure 3.1 illustrates this difficulty for anisotropic distributions with temperature ratios of $\alpha = 1/5$ and 5. For $r = 1$, the distribution function is very poorly represented – in fact, it is constant regardless of temperature. For $r = 2$, the 64 $N_i$ take on four different values. With $r = 4$ the temperature represented by a Maxwellian is only 98% of the temperature of a Maxwellian described by a velocity grid with $r = 5$. For higher resolutions, the numerical temperature deviates by less that 0.1% from the expected temperature, assuming that the distribution function is close enough to zero on the boundary of the velocity grid.

3.2.1 Cross-sections

As noted in the introduction, five different cross-sections (listed in table 2.2) are used with the DBE. The program is very easily modified for different cross-sections. The changes required involve changing a simple weighting function. By contrast, the description of an expansion method in section 3.3 makes it clear that changing the cross-section can be a very difficult task with the expansion method.

The first two cross-sections are important models. The hard-sphere cross-section is often used to describe non-reactive collisions in neutral fluids. It is the only cross-section which has been previously used with discrete velocity models. The Maxwell molecule cross-section arises from a potential function, $V(r) \propto 1/r^5$, and is important in kinetic theory because some calculations of transport properties simplify when it is used. The next two cross-sections are the isotropic and anisotropic factors of the Rutherford cross-section and are included as stages towards the implementation of the fifth cross-section,
Figure 3.1: Representation of a bi-Maxwellian distribution for two different temperature ratios showing computational resolution, \( r = 8 \). \( x \) and \( z \) are the \( v_x \) and \( v_z \) components of the reduced velocity. The distribution function has been integrated over \( v_y \); the function plotted is \( f = \int f^{BM} \, dv_y \).
the full Rutherford cross-section.

The hard sphere cross-section is

\[ \sigma(g, \chi) = \frac{d^2}{4} \]  \hspace{1cm} (3.10)

where \( d \) is the diameter of the colliding particle. The total cross-section is \( 4\pi \sigma = \pi d^2 \).

An examination of the Boltzmann equation determines the scaling of time in the computation. Recall that

\[ \frac{\partial f}{\partial t}(v_1, t) = \int [f(v'_1)f(v'_2) - f(v_1)f(v_2)] g \sigma(g, \chi) d\Omega dv_2. \]  \hspace{1cm} (3.11)

The dimensions on the right hand side are

\[ [f^2 dv_2] = [n_0^2 f] = (\text{cm})^{-6}(\text{cm/s})^{-3} \]

\[ [g] = \text{cm/s} \]

\[ [\sigma(g, \chi) d\Omega] = \text{cm}^2 \]

and the left hand side has units of \([f] = \text{cm}^{-3}(\text{cm/s})^{-3} \).

In the computation, \( n_0 = 1 \), the velocity is scaled as described above and the total cross-section is scaled to 1. A change of variables,

\[ t = n_0 \sqrt{m/2kT} \pi d^2 \tau \]  \hspace{1cm} (3.12)

\[ = 5.70 \cdot 10^{-6} n_0 d^2 T^{-1/2} \tau \]  \hspace{1cm} (3.13)

transforms the reduced time in the computation, \( \tau \), to real time, \( t \). Different cross-sections have different normalizations, but they can all be written as \( \sigma(\chi, g) = \sigma_0 \cdot \sigma_d(\chi, g) \) where \( \sigma_d \) is the dimensionless cross-section and \( \sigma_0 \) has units of \( \text{cm}^2 \), so the scaling of time for other cross-sections has the same form with \( \pi d^2 \) replaced with different constants.

The isotropic Maxwell molecule cross-section is

\[ \sigma(\chi, g) = \frac{d^2}{\pi} \left( \frac{2 V_0}{\mu} \right) \frac{1}{g} \]  \hspace{1cm} (3.14)
where $d$ and $V_0$ are related to the polarizability and are taken from the potential function,

$$V(r) = V_0 \left( \frac{d}{r} \right)^4.$$  \hspace{1cm} (3.15)

For the DBE calculations I have set $\frac{2V_0d^2}{\mu} \sqrt{\frac{m}{2kT}} = 1$. The time scaling for this cross-section is adjusted accordingly to $t = n_0 \frac{m}{2kT} \frac{4V_0d^2}{m} \tau = \frac{2n_0V_0d^2}{kT} \tau$.

### 3.2.2 Sample results

In this section some sample results are given. The purpose is to introduce the kinds of plots drawn and to give a few examples of the calculations done to test the convergence of the results.

Figure 3.2 shows how the temperature relaxation for the linear problem converges with increasing velocity resolution. A large temperature ratio, $T_1(0)/T_2 = 4$, was used but the curves are still nearly indistinguishable except at very short times. Figure 3.3 illustrates an example of an anisotropic distribution function at various times during the relaxation. Figure 3.4 shows the relaxation of $T_{||}$ and $T_{\perp}$ for several different velocity resolutions for the second problem with the hard sphere cross-section and $\alpha(0) = 5$.

Three different types of plot are used to show the results of the computations. The first is a plot of the temperature relaxation computed from the distribution functions. For the linear problem the relaxation of the test particle temperature to the bath temperature is shown, e.g., figure 3.2. For the relaxation of an anisotropic distribution, two curves, $T_{\perp}(t)$ and $T_{||}(t)$, are shown relaxing from initial temperatures to the effective temperature of the whole distribution function, equation 3.9 and figure 3.4. A second plot illustrates the relaxation of the anisotropy by plotting $\alpha(t) = T_{||}(t)/T_{\perp}(t)$ versus time. The third plot, a log-linear plot of the temperature deviation from equilibrium versus time which indicates the degree to which the decay to an equilibrium temperature is exponential, is used for both problems.
Figure 3.2: Temperature relaxation for the linear problem with the hard sphere cross-section at different velocity resolutions, $r = 5, 6, \text{ and } 7$. At short times the curves do not overlap. The uppermost curve corresponds to $r = 5$. 
Figure 3.3: The relaxation of an anisotropic distribution function, initially bi-Maxwellian with $\alpha(0) = 5$. 
Figure 3.4: The evolution of $T_{||}$ and $T_{\perp}$ for different velocity grid resolutions, $r = 6$, 7, and 8, with $\alpha(0) = 5$, using the hard sphere cross-section.