## Chapter 3

# COLLISIONS

## 3.1 Background

The foundational Boltzmann transport equation (BTE), which describes how a gas evolves by molecular collisions, normally appears early in a non-equilibrium statistical physics course. Some basic consequences of the BTE include the Maxwell-Boltzmann velocity distribution, the determination of transport coefficients, and the derivation of the Navier-Stokes equations of hydrodynamics. The latter two items involve the formidable and subtle Chapman-Enskog expansion, and the complexity of this approach makes kinetic theory an intimidating subject with which to begin studying non-equilibrium statistical physics. We think it is more useful pedagogically to focus on simpler and explicitly solvable models, such as the Lorentz gas, where a test particle interacts with a fixed scattering background, and the Maxwell model, where the collision rate is independent of the velocities of collision partners. The solutions of these models help illustrate the master equation methodology that we use throughout this book, as well as provide intuition about how to deal with more realistic collisional dynamics.

#### The Maxwell-Boltzmann Distribution

As a preliminary, let's derive the Maxwell-Boltzmann (MB) velocity distribution for a classical gas of identical molecules. The gas is in equilibrium at temperature T and two molecules scatter elastically when they are sufficiently close due to a short-range repulsive intermolecular potential. Let  $P(\mathbf{v}) d\mathbf{v}$  be the probability to find a molecule within a range  $d\mathbf{v}$  about  $\mathbf{v}$  when the temperature is T. The MB distribution is based on two fundamental assumptions:

1. Spatial symmetry, which implies that the MB distribution is isotropic:

$$P(\mathbf{v}) = P(v^2); \tag{3.1}$$

*i.e.*, the distribution depends only on the magnitude v and not on the direction of  $\mathbf{v}$ .

2. Molecular chaos, which implies that different velocity components are uncorrelated. Together with symmetry, this assumption allows the velocity distribution to be factorized as

$$P(v^2) = p(v_x^2) \, p(v_y^2) \, p(v_z^2), \tag{3.2}$$

where  $p(v_i^2, T) dv_i$  is the probability that the *i*<sup>th</sup> velocity component is in a range  $dv_i$  about  $v_i$ .

Let us now derive the MB distribution using Maxwell's original approach. First, take the logarithm of (3.2) and then differentiate with respect to one velocity component to give

$$\frac{\partial \ln P(v^2)}{\partial v_i^2} = \frac{\partial \ln P}{\partial v^2} \frac{\partial v^2}{\partial v_i^2} = \frac{\partial \ln P}{\partial v^2} = \frac{\partial \ln p(v_i^2)}{\partial v_i^2}$$

Since this equation holds for any component, the right-hand side must be constant. Thus we conclude that  $\ln P = a + bv^2$ . The unknown constants in  $P = A e^{bv^2}$  can then be found by normalization and equipartition (each degree of freedom contributes an average energy per particle<sup>1</sup> of  $\frac{1}{2}m\langle v_x^2 \rangle = \frac{1}{2}T$ ) to give

$$P(\mathbf{v}) = \left(\frac{m}{2\pi T}\right)^{3/2} e^{-m\mathbf{v}^2/2T} .$$
(3.3)

Notice that almost nothing about the interparticle potential enters into this argument. We only require that there exists some scattering mechanism that conserves mass, momentum, and energy in each collision, so that a steady state actually exists. With these modest requirements, the steady-state velocity distribution is the Maxwell-Boltzmann form, independent of the intermolecular interaction. After this derivation, a cynical physics student might ask: isn't it simpler still to "derive" by MB distribution from the Boltzmann factor,  $e^{-E/T}$  of equilibrium statistical mechanics? While it is true that there is no work involved in writing  $P \propto e^{-E/T}$ , considerable effort is involved in developing the entire apparatus of equilibrium statistical mechanics, upon which the Boltzmann factor is based.

#### The Boltzmann Transport Equation (BTE)

It is instructive present some of the basic features of the BTE as a prelude for discussing the collisional processes of this chapter. In classical kinetic theory, the fundamental quantity is the space- and velocity-dependent distribution,  $P(\mathbf{r}, \mathbf{v}; t) d\mathbf{r} d\mathbf{v}$ , defined as the probability that a particle is within a range  $d\mathbf{r} d\mathbf{v}$  about  $\mathbf{r}, \mathbf{v}$  at temperature T. This distribution evolves according to the BTE, which we write in the slightly symbolic form:

$$\left(\frac{\partial}{\partial t} + v_i \frac{\partial}{\partial r_i} + F_i \frac{\partial}{\partial v_i}\right) P(\mathbf{r}, \mathbf{v}; t) = 
= \int |\mathbf{v} - \mathbf{v}'| \frac{d\sigma}{d\Omega} \left[ P_2(\mathbf{r}, \mathbf{v}; \mathbf{r}, \mathbf{v}') - P_2(\mathbf{r}, \mathbf{v}''; \mathbf{r}, \mathbf{v}''') \right] \delta(\mathbf{p}^{(i)} - \mathbf{p}^{(f)}) \delta(E^{(i)} - E^{(f)}) d\mathbf{v}' d\mathbf{v}' d\mathbf{v}'' \quad (3.4)$$



Figure 3.1: Binary collision with pre-collision velocities  $u_1$  and  $u_2$  and post-collision velocities  $v_1$  and  $v_2$ .

The terms on the left-hand side represent the change in  $P(\mathbf{r}, \mathbf{v}; t)$  due to particle motion in the absence of collisions; these terms simply comprise the total time derivative. We use the Einstein summation convention that repeated Cartesian indices are summed. The right-hand side represents the change in  $P(\mathbf{r}, \mathbf{v}; t)$  due to collisions. The second term represents the loss of particles with phase space coordinates  $\mathbf{r}, \mathbf{v}$  due to collisions with particles whose coordinates are  $\mathbf{r}, \mathbf{v}'$ . The total collision rate involves the product of the relative speeds of the two particles, the cross section for their scattering into any outgoing state, and the probability that the collision partners are at the same spatial point. This latter probability is expressed by the *two-body* correlation function  $P_2$ . The first term represents a gain in which particles with coordinates  $\mathbf{r}, \mathbf{v}''$  and  $\mathbf{r}, \mathbf{v}'''$  collide, with one of the outgoing particles having coordinates  $\mathbf{r}, \mathbf{v}$  and the other  $\mathbf{r}, \mathbf{v}'$  By time reversal invariance, both the collision cross-section and the relative velocity of the gain term are the same as that of the loss term. Finally, the delta functions impose overall momentum and energy conservation; here the superscripts denote the total momentum and energy in the initial and final states.

As written, the BTE is not closed: the equation of motion of the first single-particle distribution involves a two-body distribution. However, the equation for the two-body distribution involves the three-body

<sup>&</sup>lt;sup>1</sup>In this chapter, we set Boltzmann's constant  $k_B = 1$ 

distribution, etc. To make this infinite equation hierarchy closed, it is necessary to break the hierarchy at some level by replacing n-body distributions as products of lower-order distributions. For the BTE, the conventional approach is to replace two-body distributions by the product of single-body distributions; that is,

$$P_2(\mathbf{r}, \mathbf{v}; \mathbf{r}, \mathbf{v}') \rightarrow P(\mathbf{r}, \mathbf{v}) P(\mathbf{r}, \mathbf{v}').$$

This is the *molecular chaos* assumption, which is crucial for making further progress in solving the BTE.

At this point, it is worthwhile to highlight the assumptions underlying the BTE and some of their implications:

- 1. The gas is sufficiently dilute that the one-body distribution  $P(\mathbf{r}, \mathbf{v}; t)$  describes the state of the gas accurately.
- 2. The gas is sufficiently dilute that only binary collisions are important.
- 3. Particles move with constant velocity between collisions and undergo scattering events according to classical mechanics when two molecules are in physical contact. We can therefore view molecules as *hard spheres*.
- 4. We decompose a two-body distribution as a product of one-body distributions; that is, the states of two particles are uncorrelated. This is the *mean-field*, or the *molecular chaos* assumption. This decomposition may be regarded as a truncation at second order of an infinite hierarchy of equations that describe the evolution of *n*-body correlation functions in terms of (n + 1)-body correlations. For the BTE, the decomposition of the two-particle correlation function also leads to the crucial feature of the breaking of time-reversal symmetry.

The solution of the equation hierarchy for multi-particle correlation functions has not been obtained for any finite level of truncation, even for the simplest second-order truncation of the BTE. To make progress for this second-order truncation, one normally resorts to the perturbative Chapman-Enskog expansion in which the small parameter is the ratio of the mean-free path to a characteristic system size and the distribution is expressed as a local Maxwell-Boltzmann distribution plus correction terms.

It is at this stage that we terminate our discussion of the BTE because of its technical complications and instead turn to idealized and simpler descriptions of kinetic theory to avoid the daunting calculations needed to deal the BTE. While these idealizations contain some element of fantasy, they are still sufficiently grounded in the underlying kinetics that they provide useful insights about physical reality. An especially useful simplification in this spirit is the *Maxwell model*. The basic feature of this model is the replace the relative velocity inside the collision integral by a constant, a device that greatly facilitates further analysis.

This seemingly drastic approximation can also be justified physically, as a collision rate that is independent of the relative velocity arises for a specific form of the interaction potential between molecules. Suppose that this potential has the form  $U(r) = \frac{A}{r^n}$ . We may then estimate the closest approach of two molecules in equilibrium at temperature T by equating their interaction energy with the kinetic energy,  $\frac{A}{r^n} = \frac{1}{2}mv^2 = T$ . Thus  $r \propto v^{-2/n}$ ; we may view this distance as the scattering radius of each molecule. Then the overall collision rate has the following dependence on the relative velocity:

$$u \frac{d\sigma}{d\Omega} \propto u r^{d-1} \sim u^{1-2(d-1)/n}$$

Thus the collision rate is *independent* of the relative velocity when n = 1/[2(d-1)]. In the physical case of d = 3, the Maxwell model corresponds to an  $r^{-4}$  interaction potential between molecules.

Another description is that of very hard particles in which the overall collision rate is written as the square of the relative velocity between two molecules. Because of this quadratic interaction, the interaction is "harder" than the hard-sphere interaction of classical kinetic theory. On the other hand, the Maxwell model is a "softer" interaction because of the velocity-independent interaction. In fact, the Maxwell model and very hard particles can be viewed bounds on classical kinetic theory.

## 3.2 The Lorentz Gas

## 3.3 Inelastic Gases

While kinetic theory traditionally deals with gases whose molecules interact via elastic collisions, many new and unexpected phenomena arise when collisions are *inelastic*. Perhaps the most spectacular is the large-scale clustering and the *inelastic collapse* of a freely-evolving inelastic gas. At a more microscopic but still fundamental level, the velocity distribution of inelastic gases is generally not Gaussian. We now discuss these and related basic kinetic features of inelastic gases.



Figure 3.2: Example of inelstic clustering. The resitution coefficient is 0.6 and there are on average 500 collisions per particle. The number of particles is 40000 and the area fraction is 0.05.

#### where to put the statement of the origin of non-Gaussianity

### Haff's Law

Because of inelastic collisions, the mean kinetic energy, and correspondingly, the temperature decreases with time. What is the time dependence of this cooling? Using simple ideas from kinetic theory, we can determine this time dependence under the assumption that the gas remains spatially homogeneous. As we shall see, homogeneity is a reasonable approximation at early times, but this naive assumption is quite wrong in the long-time limit because large-scale density heterogeneities arise.

We estimate the cooling rate of an inelastic gas from the outcome of a typical collision. The kinetic energy lost in an inelastic collision is  $\Delta T = -\epsilon(1-\epsilon)(\Delta v)^2 \approx -\epsilon(\Delta v)^2$ , with  $\Delta v$  the relative velocity between colliding particles. We consider the quasi-elastic limit  $\epsilon \to 0$ , where the spatial homogeneity assumption is a reasonable approximation over a non-negligible time range. The typical time  $\Delta t$  between collisions is roughly  $\ell/\Delta v$ , with  $\ell$  the mean-free path. We assume that a single scale characterizes all velocities so that  $\Delta v \sim v \sim \sqrt{T}$ . Putting these elements together, the temperature cooling rate therefore is  $\frac{dT}{dt} \approx -\frac{\Delta T}{\Delta t} \propto -\epsilon T^{3/2}$ . From this rate equation, the temperature decays as

$$T(t) = T_0 (1 + c\epsilon t)^{-2}, (3.5)$$

with the constant c of the order of one. Notice that the gas remains effectively elastic  $T(t) \approx T(0)$  for  $t \ll \epsilon^{-1}$ . This time range can be substantial if the dissipation by collisions is sufficiently small. Beyond this time range, the temperature decays algebraically in time,  $T(t) \sim (\epsilon t)^{-2}$ .

#### Inelastic Collapse in One Dimension

In one dimension, many aspects of inelastic collapse can be quite simply understood and it is therefore instructive to first focus on this case. In one dimension, the post-collision velocities  $(v_1, v_2)$  are related to the pre-collision velocities  $(u_1, u_2)$  of two approaching equal-mass particles by momentum conservation:

$$v_{1} = \frac{1}{2}(1-r)u_{1} + \frac{1}{2}(1+r)u_{2} \equiv \epsilon u_{1} + (1-\epsilon)u_{2}$$

$$v_{2} = \frac{1}{2}(1+r)u_{1} + \frac{1}{2}(1+r)u_{2} \equiv (1-\epsilon)u_{1} + \epsilon u_{2},$$
(3.6)

where  $0 \le r \le 1$  is the restitution coefficient and, for later convenience, we define the collision parameter  $\epsilon \equiv \frac{1}{2}(1-r)$ . The restitution coefficient is defined by the incoming momenta  $\pm p$  in the center-of-mass reference frame becoming  $\mp rp$  after the collision. Setting the particle mass to one, the energy loss in a collision is

$$\Delta E = (u_1^2 + u_2^2)/2 - (v_1^2 + v_2^2)/2 = -\epsilon(1-\epsilon)(u_1 - u_2)^2.$$

The energy loss is maximal for a completely inelastic collision  $(r = 0, \epsilon = 1/2)$  and vanishes for elastic collisions  $(r = 1, \epsilon = 0)$ .

Consider now N particles that are initially at  $x_i = i, i = 2, 3, ..., N$ . Particle 1 is incident on particle 2 with velocity +1, leading to a subsequent series of inelastic collisions according to (3.6). How does this deterministic system evolve with time?



Figure 3.3: Illustration of the collision sequence for 3 unit-mass particles in one dimension. Particle 1 initially moves at velocity +1, while particles 2 & 3 are at rest. Shown are the particle worldlines in the center-of-mass reference frame that moves at velocity +1/3 for restitution coefficient  $r = 0.11 > r_c(3)$ . The trajectories initially converge, but after the last collision between particles 1 & 2 at  $t \approx 10.164$ , the trajectories diverge.

When there are two particles, they collide at most once. The first non-trivial case is N = 3, where a sequence of alternating 12 and 23 collisions occurs (Fig. 3.3). Without loss of generality, let us assume that the first collision is 12. The total number of collisions and the ultimate fate of the particles — either collapse or diverging — depends on the restitution coefficient. It is convenient to represent the collision outcome in matrix notation. Then after the pair of collisions 12 and 23, the post-collision velocities  $v_i$  are related to the pre-collision velocities  $u_i$  by Eq. (3.6),

$$\begin{pmatrix} v_1\\v_2\\v_3 \end{pmatrix} = M_{23}M_{12} \begin{pmatrix} u_1\\u_2\\u_3 \end{pmatrix} \quad \text{with} \quad M_{12} = \begin{pmatrix} \epsilon & 1-\epsilon & 0\\1-\epsilon & \epsilon & 0\\0 & 0 & 1 \end{pmatrix} \quad M_{23} = \begin{pmatrix} 1 & 0 & 0\\0 & \epsilon & 1-\epsilon\\0 & 1-\epsilon & \epsilon \end{pmatrix}.$$
(3.7)

After 2n collisions, the particle velocities are given by  $\mathbf{v} = M^n \mathbf{u}_0$ , where  $M = M_{23}M_{12}$  and  $\mathbf{u}_0$  is the initial velocity vector, while after 2n + 1 collisions, the velocities are given by  $\mathbf{v} = M_{12}M^n\mathbf{u}_0$ . The nature of the collisions follows from the eigenvalues of the matrix M whose values are

$$\lambda_{1,2} = \frac{1}{2} \left[ (\epsilon^2 + 2\epsilon - 1) \pm \sqrt{(1 - 2\epsilon - \epsilon^2)^2 - 4(2\epsilon - 1)^2} \right], \quad \lambda_3 = 1$$



Figure 3.4: "Bending" of a test particle as it collides inelastically to penetrate a static particle array. Particle labels are exchanged in each collision so that particle 1 is decelerated by collisions.

When  $\epsilon > \epsilon_c = 2\sqrt{3}-3$ , corresponding to restitution coefficient  $r < r_c = 7-4\sqrt{3}$ , then  $\lambda_{1,2}$  are both real with absolute values less than 1. Consequently the particle velocities asymptotically decay as  $[\max(|\lambda_1|, |\lambda_2|)]^n$ . Conversely for  $r > r_c$ , the collision sequence terminates after a finite number as the particles ultimate diverge.

When N > 3, the collision sequence is not necessarily periodic and the matrix formulation no longer provides the exact value of the critical restitution coefficient for collapse. However, we can give a simple heuristic argument for the dependence of the critical restitution coefficient  $r_c$  on N for large N. Consider a test particle with speed 1 that is incident on an array of static, equally-spaced particles when the restitution coefficient is nearly 1. After the first collision, the target particle moves with a slightly smaller speed, while the incident particle comes nearly to rest.

It is now helpful to exchange the identities of the two particles when they collide, so that the worldline of particle 1 is merely deflected slightly as it "passes through" particle 2. This same pattern continues in subsequent collisions so that the initial particle worldline gradually bends as it penetrates the array (Fig. 3.4). Let v(n) be the velocity of the initial trajectory after n collisions. From the collision rule (3.6) and accounting for the change in particle labeling,  $v(1) = 1 - \epsilon$ . Similarly, to first order in  $\epsilon$ ,  $v(n) = (1 - \epsilon)^n \approx 1 - n\epsilon$ . If n is sufficiently large, then the initial particle momentum is eventually exhausted and inelastic collapse has occurred. Setting v(N) = 0 then yields the critical collision parameter  $\epsilon_c(N) \sim N^{-1}$  or critical restitution coefficient

$$r_c(N) \sim 1 - \frac{2}{N}$$
 (3.8)

Thus collapse occurs even for nearly elastic particles as N becomes sufficiently large — inelastic collapse becomes inevitable in the thermodynamic limit!

#### Maxwell Model for Free Cooling in One dimension

Because it is not feasible to solve the inelastic collision dynamics of a gas analytically, we turn to the simpler Maxwell model in which the collision rate is *independent* of particle velocities and positions — a particularly simple version of mean-field theory. Operationally, we pick two particles at random and define them to collide according to Eq. (3.6). Because of the simplicity of this collision dynamics, it is possible to solve the underlying Boltzmann transport equation and determine the velocity distribution analytically.

The Boltzmann transport equation for this Maxwell model model is

$$\frac{\partial P(v,t)}{\partial t} + P(v,t) = \int \int P(u_1,t)P(u_2,t)\delta\left[v - \epsilon u_1 - (1-\epsilon)u_2\right] du_1 du_2.$$
(3.9)

This BTE conserves both the total number of particles,  $\int P(v,t) dv = 1$ , and the total momentum,  $\int v P(v,t) dv = 0$ . Because the time between every collision is the same, the elapsed time is proportional to the average number collisions that any particle experiences up to time t.

As an instructive starting point, we study low-order moments of the velocity distribution. Multiplying Eq. (3.9) by  $v^n$ , integrating over v, and performing some straightforward algebra, the rate equations for the

moments  $M_n(t) = \int v^n P(v, t) dv$  are:

$$\dot{M}_n + a_n M_n = \sum_{m=2}^{n-2} \binom{n}{m} \epsilon^m (1-\epsilon)^{n-m} M_m M_{n-m}$$
(3.10)

for  $n \ge 1$ , with the coefficients  $a_n(\epsilon) = 1 - \epsilon^n - (1 - \epsilon)^n$ . These equations may be solved recursively, starting with  $M_0 = 1$  and  $M_1 = 0$ , and the first few non-trivial moments are:

$$M_{2}(t) = M_{2}(0)e^{-a_{2}t},$$
  

$$M_{3}(t) = M_{3}(0)e^{-a_{3}t},$$
  

$$M_{4}(t) = \left[M_{4}(0) + 3M_{2}^{2}(0)\right]e^{-a_{4}t} - 3M_{2}^{2}(t).$$
(3.11)

The second moment quantifies velocity fluctuations through  $M_2 \equiv T$ , where this equivalence defines the effective temperature of the gas T. Since  $M_2$  decays exponentially with time, the particles continuously slow down and eventually come to rest, with  $P(v) \rightarrow \delta(v)$ .

In stark contrast to equilibrium statistical mechanics, however, the temperature does not characterize the entire velocity distribution. The crucial point is that moments  $M_n$  with  $n \leq 3$  obey scaling, but higher moments do not. For example, the leading asymptotic behavior of  $M_3$  is  $M_3 \sim e^{-a_3 t}$ . Since  $a_n(\epsilon) =$  $1 - \epsilon^n - (1 - \epsilon)^n$ , with  $a_3 = 3a_2/2$ , one can also write  $M_3 \sim e^{-3a_2/2} \sim M_2^{3/2}$ . Consequently, the second moment characterizes the scaling behavior of the third moment. However,  $a_4 < 2a_2$  so that the ratio  $M_4/M_2^2$ diverges as  $t \to \infty$ . In general, the moments scale as

$$M_n \sim \begin{cases} e^{-na_2/2} & n \le n^* \\ e^{-a_n t} & n \ge n^*, \end{cases}$$
(3.12)

with  $n^* = 3$ .

This change in scaling behavior is a sign that the velocity distribution has a power-law tail, rather than a Gaussian form. To determine the velocity distribution, we exploit the fact that the collision term in the Boltzmann equation is a convolution, so that the Fourier transform of this term is just a product. We thereby find that why F? also give a derivation step  $F(k,t) = \int P(v,t) e^{ikv} dv$  evolves according to following derivation is too rushed

$$\frac{\partial F(k,t)}{\partial t} + F(k,t) = F((1-\epsilon)k,t) F(\epsilon k,t).$$
(3.13)

We seek a scaling solution of the form  $P(v,t) = T^{-1/2}\mathcal{P}(w)$ , with the scaling variable  $w = vT^{-1/2}$  to account for the velocity distribution approaching its final state in a self-similar fashion. The equivalent scaling of the Fourier transform is F(k,t) = f(z) with  $z = |k|T^{1/2}$ , and the two scaling functions are related  $f(z) = \int \mathcal{P}(w) e^{izw} dw$ . Substituting the scaling ansatz into Eq. (3.13) and using the temperature decay rate  $\frac{d}{dt}T = -\epsilon(1-\epsilon)T$ , the scaling function f(z) satisfies the ordinary differential equation

$$\epsilon(1-\epsilon)zf'(z) + f(z) = f(z-\epsilon z)f(\epsilon z).$$
(3.14)

This equation is subject to the boundary conditions  $f(z) \cong 1 - \frac{1}{2}z^2$ , that follows from  $F(k) \cong 1 - \frac{1}{2}k^2T$ .

The solution to (3.14) is **explain!!** 

$$f(z) = (1+z)e^{-z}.$$
(3.15)

Inverting this Fourier transform, the scaled velocity distribution is<sup>2</sup>

$$\mathcal{P}(w) = \frac{2}{\pi} \frac{1}{(1+w^2)^2}.$$
(3.16)

Thus the velocity distribution of the inelastic Maxwell model gas has a power-law tail,  $\mathcal{P}(w) \sim w^{-4}$  for  $w \gg 1$ , whose exponent is independent of the collision parameter  $\epsilon$ .

The same general approach can be pursued in spatial dimension d > 1 but the details are much more complicated. The main point, however, is that the velocity distribution again has a power-law tail, but with the exponent now dependent on d and the collision parameter  $\epsilon$ . the

<sup>&</sup>lt;sup>2</sup>The inverse Fourier transform of  $e^{-\kappa z}$  is  $\frac{1}{\pi} \frac{\kappa}{\kappa^2 + w^2}$ ; the inverse transforms of  $z^n e^{-\kappa z}$  can be obtained using successive differentiation with respect to  $\kappa$ .

#### **External Forcing**

When energy is continuously injected into an inelastic gas, a steady state is reached as the energy input balances the energy loss in the inelastic collisions. The most natural way to realize such an energy input is by putting an inelastic gas in a closed container and shaking it. Experiments on this type of system indicate that the velocity distribution generically has a non-Maxwellian tail for a host of geometries and energy injection mechanisms. Here we discuss how to obtain this tail in the framework of the Maxwell model of random collisions.

We model the effect of the energy input by white-noise forcing in which each particle experiences an acceleration

$$\frac{dv_j}{dt} = \xi_j$$

due to random noise amplitude that has zero mean,  $\langle \xi_j \rangle = 0$ , and no correlations in time,  $\langle \xi_i(t)\xi_j(t') \rangle = D\delta_{ij}\delta(t-t')$ . This white-noise forcing is equivalent to diffusion in velocity space with diffusion coefficient D. To account for the external forcing, the Boltzmann equation (3.9) should be augmented by a diffusion term in velocity space; that is

$$rac{\partial P(v,t)}{\partial t} 
ightarrow rac{\partial P(v,t)}{\partial t} - D rac{\partial^2 P(v,t)}{\partial v^2} \; .$$

With this additional term, the steady state velocity distribution  $P(v) \equiv P(v, t = \infty)$  now satisfies:

$$\left(1 - D\frac{\partial^2}{\partial v^2}\right)P(v,t) = \int \int P(u_1)P(u_2)\delta\left[v - \epsilon u_1 + (1 - \epsilon)u_2\right] du_1 du_2.$$
(3.17)

The temperature changes according to  $dT/dt + 2p(1-\epsilon)T = 2D$  where does this come from? so the steady state temperature is  $T = D/[\epsilon(1-\epsilon)]$  and the relaxation toward the steady state is exponential,  $|T - T_{\infty}| \sim \exp(-\text{const.} \times t)$ . In the steady state, the Fourier transform  $F(k) \equiv F(k, t = \infty)$  satisfies, following (3.13):

$$F(k) = (1 + Dk^2)^{-1} F((1 - \epsilon)k) F(\epsilon k).$$
(3.18)

To determine the large-velocity tail of the distribution, we solve (3.18) iteratively by repeatedly substituting the left-hand-side into the right-hand-side. Using the boundary conditions F(0) = 1 and F'(0) = 0imposed by the conservation of the total particle number and the total momentum, the solution is

$$F(k) = \prod_{l=0}^{\infty} \prod_{m=0}^{l} \left[ 1 + \epsilon^{2m} (1-\epsilon)^{2(l-m)} Dk^2 \right]^{-\binom{l}{m}} .$$
(3.19)

To extract the form of the high-velocity tail, we use the fact that the Fourier transform has an infinite series of poles located at  $\pm i \left[p^{2m}(1-\epsilon)^{2(l-m)}D\right]^{-1/2}$ . The simple poles at  $\pm i/\sqrt{D}$  closest to the origin imply an exponential decay of the velocity distribution

$$P(v) \simeq \frac{A(\epsilon)}{v_*} e^{-|v|/v_*}$$
(3.20)

with  $v_* = \sqrt{D}$  when  $|v| \to \infty$  in which the dependence on the dissipation parameter appears only in the prefactor. In the quasi-elastic limit  $\epsilon \to 1/2$ ,  $A(\epsilon) \propto \exp[\pi^2/(12\epsilon)]$ .

The leading behavior of the high-energy tail can be alternatively obtained using a useful and generic heuristic argument. For sufficiently large velocities, the gain term in the collision integral in Eq. (3.17) is negligible. The resulting equation for the steady state distribution

$$D \frac{d^2}{dv^2} P(v) = -P(v)$$
 (3.21)

yields the exponential high-energy tail (3.20). This argument applies to arbitrary collision rates. For example, if  $K(u_1, u_2) \propto |u_1 - u_2|^{\delta}$  for  $|u_1 - u_2| \rightarrow \infty$ , then the right-hand side in (3.21) becomes  $-|v|^{\delta}P_{\infty}$  implying that  $P_{\infty}(v) \propto \exp(-|v|^{\gamma})$  with  $\gamma = 1 + \delta/2$ . For hard spheres Boltzmann equation ( $\delta = 1$ ) one finds  $\gamma = 3/2$ .

#### 3.4. AGGLOMERATION

Another important observation is that in the quasi-elastic limit, the velocity has a substantial Maxwellian core. In this limit, the Fourier transform (cumulant-1d) reads  $F(k) \sim \exp[-Dk^2/\epsilon]$ , so the velocity distribution is Gaussian. Comparing with the universal, dissipation-independent, tail behavior (3.20) shows that there is a cross-over velocity  $v \sim \epsilon^{-1}$  marking the transition from the core to the tail. In summary,

$$P(v) \sim \begin{cases} \exp(-\epsilon v^2) & |v| \ll \epsilon^{-1};\\ \exp(-|v|) & |v| \gg \epsilon^{-1}. \end{cases}$$
(3.22)



Figure 3.5: The steady state distribution versus the Maxwell-Boltzmann distribution. Shown is P(v) versus  $v \equiv v_x$  in the forced case for d = 2 and r = 0 (solid line). Also shown is the Maxwell-Boltzmann distribution (3.3) (dashed line). Both distributions are normalized such that  $\langle v^2 \rangle = 1$ . The distribution was obtained using a Monte-Carlo simulation of the inelastic collision process with white noise forcing.

## 3.4 Agglomeration

A simple and beautiful model is *ballistic agglomeration* in which particles move in straight-line trajectories and irreversibly stick together whenever a collision occurs. Such a model provides an idealized description of the large-scale agglomeration of matter in the universe to form planets and stars. We start with a gas of compact spherical objects that are randomly distributed in space, with masses  $m_i$  and radii proportional to  $m_i^{1/3}$ , and initial velocities  $\mathbf{v}_i$ . The initial values of  $m_i$  and  $v_i$  are drawn from some prescribed distributions. When the separation between two aggregates is less than the sum of their radii, they are defined to collide to form a larger aggregate, with the mass and the momentum conserved in the collision. That is

$$(m_1, \mathbf{p}_1) + (m_2, \mathbf{p}_2) \to (m_1 + m_2, \mathbf{p}_1 + \mathbf{p}_2).$$
 (3.23)

The resulting aggregate is also assumed to maintain a spherical shape with a volume proportional to its mass.



Figure 3.6: Illustration of ballistic agglomeration. The state of the system is illustrated at an early stage (left) and a late stage (right).

We anticipate that the aggregate growth proceeds in a self-similar manner, as illustrated in Fig. 3.6. There are several heuristic arguments one can formulate to determine the time dependence of the process. We give an argument that is based on elementary kinetic theory. A key assumption is that the momenta of aggregates remain uncorrelated throughout the process. Consequently the momentum of an aggregate of mass m is just the sum of m uncorrelated momenta. Thus  $p \sim m \sim m^{1/2}$  and the aggregate velocity is  $v \sim p/m \sim m^{-1/2}$ . If there exists a typical aggregate mass, then after one collision time  $\tau$ , two aggregates of approximately the same mass will meet, so that the typical mass should grow by of the order of itself. Thus the growth of aggregates is described by the rate equation

$$\frac{dm}{dt} \sim \frac{m}{\tau} \ . \tag{3.24}$$

We estimate  $\tau$  from the elementary kinetic theory criterion that a collision occurs when the density times the volume of the collision tube swept out by the trajectory of an aggregate equals one:  $n\ell R^{d-1} = 1$ , where *n* is the aggregate density,  $\ell \sim v\tau$  is the mean-free length, and *R* is the aggregate radius. Rewriting all these quantities in terms of the typical aggregate mass we have

$$\tau \sim \frac{1}{nvR^{d-1}} \sim m \times m^{1/2} \times m^{-(d-1)/d} \sim m^{(d+2)/2d}$$

Finally, using this dependence for  $\tau$  in the rate equation (3.24), we obtain

$$m \sim t^{2d/(d+2)}, \qquad v \sim t^{-d/(d+2)}, \qquad n \sim t^{-2d/(d+2)}.$$
 (3.25)

Is the heuristic argument correct? Numerical simulations unambiguously support the result  $\alpha = 2/3$  in one dimension. In this case, the theoretical argument stands on a firm ground: as agglomerates grow, they encompass a growing linear segment of the initial conditions. The corresponding region in space is indeed compact, so the constituent particles must be uncorrelated. In higher-dimensions the situation is less clear. The exponent  $\alpha = 1$  certainly is close to the numerical results but recent simulations may be indicating a departure from this law. Such a departure may be due to the blobs acquiring a nontrivial non-compact geometry.

## 3.5 Jamming Traffic

An amusing application of kinetic theory is to traffic on rural highways, where often there is a single lane in each direction with no passing allowed. As many of us have experienced, faster cars accumulate behind slower-moving vehicles and significant clustering can arise. Each cluster is led by a slow vehicle that will ultimate catch up to a still-slower cluster if the road is sufficiently long. We can view traffic as a onedimensional gas that evolves from a homogeneous to a clustered state because of the no-passing constraint.

We describe the traffic clustering phenomenon by the following idealized model. Each car has its own intrinsic speed at which it would move on an empty road. When a faster car catches up to a slower car, both cars subsequently move with speed the of the slower car (Fig. 3.7). Generally, when a cluster of  $m_2$  cars, all moving at speed  $v_2$ , catches up to a cluster of  $m_1$  cars moving at speed  $v_1 < v_2$ , the resulting "collision" leads to a cluster of  $m_1 + m_2$  cars that moves at speed  $v_1$ . This clustering is described by the collision rule

$$(m_1, v_1) + (m_2, v_2) \to (m_1 + m_2, v_1).$$
 (3.26)

For simplicity, we assume: (i) instantaneous collisions, (ii) sizeless cars, (iii) the initial car speeds that are drawn from an intrinsic distribution P(v, t = 0), and (iv) initial car spacings are drawn from an independent exponential distribution with mean spacing equal to 1. Once the initial car speeds and positions are specified, traffic evolves deterministically according to the collision rule (3.26). The only source of randomness is the initial conditions. We are interested in the properties of the traffic, averaged over all initial configurations, or alternatively, in an infinite-size system.

Let's begin by giving a heuristic argument to obtain the basic characteristics of clustered traffic, namely, the time dependence of the typical cluster mass m, the typical separation between clusters  $\ell$ , and the



Figure 3.7: Traffic with no passing. Shown are the world lines of position x versus time t for initially unclustered traffic.

typical cluster speed v. As we shall see, these quantities are determined by the behavior of the initial speed distribution of the slowest cars. As a general example, let us assume the initial distribution of speeds<sup>3</sup>

$$P(v,0) \sim a v^{\mu} \tag{3.27}$$

as  $v \to 0$ .

On dimensional grounds, the quantities  $\ell$  and v are related by  $\ell \sim vt$ . Because the separation between clusters should scale as the inverse of the concentration of clusters, which, in turn, is proportional to their inverse mass, we also have  $\ell \sim m^{-1}$ . Now let's relate the mass and speed of a cluster. Consider a car with speed v. The probability that a cluster of size k forms behind this car is given by  $P_{\leq}P_{\geq}^{k}$ , where  $P_{\leq} = \int_{0}^{v} P(v', 0) dv'$  and  $P_{\geq} = 1 - P_{\leq}$  are the respective probabilities to find a car with speed less than or greater than v. Then the average size  $\langle m(v) \rangle$  of the cluster behind a car of speed v is

$$\langle m(v)\rangle = \sum_{k=1}^{\infty} k P_{<} P_{>}^{k} = \frac{P_{>}}{P_{<}}$$

For the power-law initial speed distribution  $P(v,0) \sim av^{\mu}$  as  $v \to 0$ , we then find  $\langle m(v) \rangle \sim v^{-1-\mu}$ . Finally, we combine this relation with  $m \sim vt$  to find

$$m \sim t^{\alpha} \qquad \alpha = \frac{\mu + 1}{\mu + 2}$$
$$v \sim t^{-\beta} \qquad \beta = \frac{1}{\mu + 2}.$$
(3.28)

The decay exponents satisfy the scaling relation  $\alpha + \beta = 1$  which merely reflects the dimensions of the basic relations  $\ell \sim vt$  and  $\ell \sim m^{-1}$ .

Now let's turn to the speed distribution of clusters. For simplicity, consider first the special case where cars have only 2 possible speeds,  $v_1$  and  $v_2$ , with respective probabilities  $P_1(0)$  and  $P_2(0)$ . Slow cars never catch any other vehicle, so their density is conserved,  $P_1(t) = P_1(0)$ . Fast cars move at their intrinsic speed  $v_2$  before colliding a slower car. To avoid a collision up to time t, a fast car must have a segment of length  $(v_2 - v_1)t$  ahead of its initial position that is free of slow cars. Since the initial spatial distribution of cars is random, this exclusion probability decays exponentially with the interval length  $\exp[-P_1(0)(v_2 - v_1)t]$ . Therefore, the density of the faster cars is

$$P_2(t) = P_2(0) \exp\left[-P_1(0)(v_2 - v_1)t\right].$$
(3.29)

Now consider traffic with cars that move at three distinct intrinsic speeds  $v_1 < v_2 < v_3$ . Clusters with speeds  $v_1$  and  $v_2$  are simply unaffected by the presence of faster cars so the previous conclusions for their densities  $P_1(t)$  and  $P_2(t)$  hold! On the other hand, for a fast car to maintain a speed  $v_3$ , it must avoid colliding with both clusters of speeds  $v_1$  and  $v_2$ . The probability for these two independent events is given by a product of the two "exclusion probabilities"

$$P_3(t) = P_3(0) \exp[-P_1(0)(v_3 - v_1)t] \exp[-P_2(0)(v_3 - v_2)t].$$
(3.30)

 $<sup>^{3}</sup>$ Without loss of generality, we subtract the speed of the slowest car from all speeds so that the minimum speed is 0.

We may now generalize the cluster speed distribution for an arbitrary initial speed distribution:

$$P_n(t) = P_n(0) \exp\left[-t \sum_{i=1}^{n-1} P_i(0)(v_n - v_i)\right],$$
(3.31)

where  $P_n(0)$  is the probability that a car has an initial speed  $v_n$  for a discrete set of speeds  $\{v_n\}$ , with  $v_1 < v_2 < v_3 < \ldots$  In the continuum limit, Eq. (3.31) now becomes

$$P(v,t) = P(v,0) \exp\left[-t \int_0^v dv' \, (v-v') P(v',0)\right].$$
(3.32)

Thus the density of cars of any positive speed decays exponentially in time, with a decay rate that is a growing function of v — the faster the intrinsic speed of a car, the more likely it will become stuck behind a bus.

We can express Eq. (3.32) in a Boltzmann-like form by differentiating the logarithm of this equation with respect to time to give the *linear* evolution equation

$$\frac{\partial P(v,t)}{\partial t} = -P(v,t) \int_0^v dv'(v-v') P(v',0).$$
(3.33)

As in the classic Boltzmann equation (3.4), there is an integration over all possible collision partners with speeds v' < v in which the collision rate is proportional to the relative speed |v - v'|. There does not exist, however, a gain term because a cluster of a given speed cannot be created if it doesn't already exist. However, traffic theory has a fundamental difference with classical kinetic theory. The evolution equations of traffic, Eqs. (3.32) of (3.33) are *non-local* in time because of the perpetual memory of the initial conditions: the speed distribution at time t is expressed in terms of the initial speed distribution. **paragraph incomplete** 

Substituting the initial distribution of speeds  $P(v,0) \sim a v^{\mu}$  as  $v \to 0$ . in Eq. (3.32), we find, in the long-time limit,

$$P(v,t) \sim a v^{\mu} \exp(-btv^{\mu+2}),$$
 (3.34)

with  $b = a/[(\mu + 1)(\mu + 2)]$ . Notice that the speed distribution can be written in the scaling form

$$P(v,t) \simeq t^{\beta-\alpha} \Phi(vt^{\beta}). \tag{3.35}$$

However, the speed distribution near v = 0 is an invariant of the dynamics. No matter how long the time, a small number of cars have yet to encounter still slower cars and  $P(v,t) \sim P_0(v)$  for these slow cars. From this speed distribution, the leading asymptotic behaviors of the concentration,  $c(t) = \int P(v,t) dv$ , and the average speed,  $\langle v(t) \rangle = c^{-1} \int v P(v,t) dv$ , are simply

$$c(t) \sim A t^{-\alpha} \quad \text{with} \quad A = (\mu + 1)b^{\beta}\Gamma(\alpha), \quad \alpha = \frac{\mu + 1}{\mu + 2}$$
$$\langle v(t) \rangle \sim B t^{-\beta} \quad \text{with} \quad B = \frac{b^{-\beta}}{\Gamma(\alpha)}, \qquad \beta = \frac{1}{\mu + 2}.$$
(3.36)

The asymptotic behavior reflects the initial conditions very strongly. The exponents are non-universal and are dictated by a particular aspect of the initial conditions, namely, the form of the distribution of the slowest cars. This of course reflects the nature of the collision rule as the slowest cars (unfortunately) govern the congestion.

I don't know how to derive the correlation function. Moreover, the joint probability density  $P_2(v, v'; t)$ , the probability of finding two particles of speed v and speed v' at time t, can be read immediately from the integrand

$$P(v, v'; t) = P(v_{>}, t)P(v_{<}, 0)$$
(3.37)

with  $v_{>} = \max(v, v')$  and  $v_{<} = \min(v, v')$ . This joint density differs from the traditional mean-field theory (the stossansatz) where P(v, v'; t) = P(v, t)P(v', t). Such factorization does not hold because spatial correlations build-up dynamically. Even though the initial state contains no correlations between the speeds of the particles and their positions, such correlations do eventually develop. Intuitively, space-speed correlations may reflect regions where particles have very close speeds and thus experience very few collisions due to this "shielding" effect.

#### Problems

- 1. Verify the general behavior of the moments quote in Eq. (3.12) for the one-dimensional inelastic gas by exploiting the inequality  $a_n < a_m + a_{n-m}$  for all 1 < m < n 1. inelastic.
- 2. Large moment as a characteristic of the tails of the distribution. Show that the for the 1D freely cooling inelastic Maxwell model, kinetics of large moments  $\lim_{n\to\infty} M_n(t)$  coincide with the behavior of the tail of the distribution  $\lim_{v\to\infty} P(v, t)$ .
- 3. The quasi-elastic limit as a singular perturbation. Expand the rate equation (3.13) to first order in  $\epsilon$  and then solve it. Show that the emerging solution remembers the initial conditions forever.
- 4. Development of singularities in compact velocity distributions. Express the Fourier transform F(k,t) explicitly in terms of the initial distribution  $F_0(k)$ . Introducing the transformations  $G(k,t) = e^t F(k,t)$  and  $\tau = 1 - e^{-t}$ , reduce the evolution equation (3.13) to  $G_{\tau}(k) = G(\epsilon k)G(k - \epsilon k)$  and express then, express the solution as a formal Taylor series in powers of  $\tau^n$ .
- 5. Estimating the large-velocity tail  $\sigma$ . Find the leading asymptotic behavior of the exponent  $\sigma$  as  $d \to \infty$ . To perform this asymptotic analysis, note that for large dimensions, the integral  $\langle \eta^{(\sigma-d)/2} \rangle$  vanishes exponentially with the dimension d and then write  $\sigma/d = f(\epsilon)$ .
- 6. Obtain the solution (cumulant-1d) from the solution (3.19).

#### Solutions

- 1. The large moments decay universally as  $M_n \sim \exp(-t)$  because  $a_n \to 1$  as  $n \to \infty$ . For the tail of the velocity distribution, the gain term is negligible in the rate equation (3.9) (Intuitively, large velocities can only shrink due to collisions). Thus,  $\frac{d}{dt}P(v,t) = -P(v,t)$  and the large-v tail of the velocity distribution also decays as  $P(v,t) \sim P(v,0) \exp(-t)$ .
- 2. The equation is  $F_t + pkF_k = 0$  and using the method of characteristics, the solution is  $F(k,t) = F_0(ke^{-pt})$ . It remembers the initial conditions forever, in contradiction with the similarity solution (3.16).
- 3. The formal Fourier expansion reads  $F(k,t) = e^{-t} \sum_{n=0}^{\infty} \frac{(1-e^{-t})^n}{n!} F_n(k)$ . The expansion functions  $F_n(k)$  are obtained from the recursion relation  $F_{n+1}(k) = \sum_{m=0}^{n} {n \choose m} F_m(k \epsilon k) F_{n-m}(\epsilon k)$  and  $F_0(k) \equiv F(k,t=0)$ . The expansion functions are products of  $F_0$  with stretched arguments of the form  $k\epsilon^l(1-\epsilon)^m$ . This implies that starting from a compact initial distribution P(v,0), the velocity distribution P(v,t) develops a set of singularities. For instance, a distribution with support in  $[-v_0, v_0]$  becomes non-analytic at an infinite set of points  $v_{l,m} = \pm \epsilon^l (1-\epsilon)^m v_0$ .

4. 
$$f(\epsilon) = \frac{1+\frac{3}{2}\epsilon - \epsilon^3 - \epsilon^{1/2} \left(1+\frac{5}{4}\epsilon\right)^{1/2}}{\epsilon(1-\epsilon^2)}$$

- 5. Assume that the restitution coefficient is randomly chosen according to the distribution  $f(\epsilon)$ . Generalize Eq. (refroot).
- 1. Heuristic derivation of extremal statistics. Evaluate the limiting behaviors of the scaling function  $\Phi(z)$  in Eq. (3.35) when  $z \to 0$  and  $z \to \infty$ . This scaling form is consistent with the exact solution (3.32) with the scaling function (problem 2)

$$\Phi(z) = az^{\mu} \exp\left[-bz^{\mu}\right].$$
(3.38)

- 2. Evaluate the cluster size distribution P(v, t) and the cumulative distribution  $Q_m(v, t)$  for the special case  $P_0(v) = e^{-v}$ . Show that the result is consistent with the general scaling behavior.
- 3. Uniform final distribution. Obtain the initial speed distribution  $P_0(v)$  and the flux for the final speed distribution P(v) = c for 0 < v < 1. What is the corresponding  $\mu$ ?
- 4. What is the scaling distribution in the ballistic aggregation model. Evaluate the tail of the speed distribution using the Lifshitz tail argument.

#### Solutions

1. The limit  $z \to 0$  is discussed in the text,  $P(v,t) \simeq P_0(v)$ . The limit  $z \to \infty$  is obtained from the Lifshitz tail argument (see matters of technique and freely cooling inelastic gases) by noting that  $P(v,t) \sim \exp(-Ct)$  for fast particles. An interval of the length t has to be empty ahead in the initial configuration.

2. The cluster size distribution is  $P(v,t) = \exp[-v - t(e^{-v} + v - 1)]$ . The cumulative distribution is

$$Q_m(v,t) = P(v,t)e^{-(m-1)v}t^{n-1}\frac{\Gamma(t+1)}{\Gamma(t+m)}$$

These solutions are consistent with the scaling behavior for the case a = 1 and  $\mu = 1$ .

- 3. The initial speed distribution is  $P_0(v) = R^{-1} + \frac{1}{2}cv^2$ . The flux is  $J = [(3 + \lambda)\sqrt{\lambda}\tan^{-1}\sqrt{\lambda} + \lambda \ln(1 + \lambda)]/R$ with  $\lambda = \frac{1}{2}Rc = \frac{3}{2}[\sqrt{1 + 2R/2} - 1]$ . The corresponding  $\mu = 2$  and  $J \sim R^{-1/4}$ .
- 4. The speed distribution has the scaling form  $P(v,t) \simeq t^{-\alpha+d\beta} \Phi(vt^{\beta})$ . The tail of the speed distributing is  $\Phi(z) \sim \exp(-z^{\gamma})$  with  $\gamma = \frac{d+2}{d}$ .