2

Plasma dynamics and equilibrium

One way to model the dynamics of the plasma contained in a reactor would be to calculate rigorously the trajectory of each of the charged particles using Newton's laws. This is not feasible for many reasons: (i) the number of charged particles is too large given the typical densities (10^{16}–10^{18} m^{-3}) and the reactor volume (a few litres); (ii) charged particles move in response to the electromagnetic (Lorentz) force associated with electromagnetic fields, which in this case are generated by the presence and motion of all the other charged particles – that is, by local space charge and currents; the problem is non-linear and should be solved self-consistently; (iii) particles experience collisions that modify their velocities and energies on very short time scales.

Q (i) How many ions are there in a cubic millimetre ($V = 10^{-9}$ m^3) of plasma of charged particle density $n = 10^{16}$ m^{-3}?
(ii) How far will an electron travel in $t = 0.1$ μs when accelerated in vacuum from rest by an electric field of $E = 10^2$ $\mathrm{V\,m}^{-1}$?
(iii) In a typical low-pressure, electrical discharge plasma a large fraction of electrons have speeds around $v = 10^6$ $\mathrm{m\,s}^{-1}$ and collide with gas atoms typically every $\lambda \sim 10^{-1}$ m, depending on the pressure; what is the average time between successive collisions?

A (i) $N = n \times V = 10^7$.
(ii) $s = \frac{1}{2}(eE/m)t^2 \approx 10^{-1}$ m.
(iii) $\tau = \lambda/v \sim 10^{-7}$ s.

The first level of simplification of the above problem is achieved in particle-in-cell (PIC) computer simulations. The basic idea behind the PIC method is indeed to solve Newton's law and the electromagnetic fields simultaneously, including collisions between particles. However, the difference between a simulated plasma and a real plasma lies in the representation of the charges, the fields and the space-time in which the phenomena occur. In a PIC simulation a large number of neighbouring charged particles are represented by a ‘super-particle’; it is always multiply charged and has the same charge-to-mass ratio as that of the actual particles. The large number of charges in a plasma are thus replaced by a much smaller number of these super-particles. Time and space are discretized and the calculations of electromagnetic fields and super-particle motions are done iteratively until a steady state is reached. PIC simulations are useful to understand subtle kinetic phenomena, but the computational time required is often too long to model the general macroscopic behaviour using purely numerical schemes.

From an analytical point of view, there are two approaches to the modelling of the plasma dynamics: one based on kinetic theory and the other based on fluid theory. The first is a microscopic approach and relies on statistical physics. Velocity (or energy) distribution functions are introduced, $f(\mathbf{r}, \mathbf{v}, t)$, and the evolution of these distributions is solved using conservation laws. Kinetic theory is useful to model non-linear wave–particle interactions and collisionless phenomena such as stochastic heating. Knowledge of the velocity distribution function is also important in detailed calculations of transport and reaction coefficients. However, kinetic calculations are too complicated to describe the macroscopic behaviour of a plasma reactor. Most of the fundamental properties described in this text do not require a kinetic treatment and will be addressed by a macroscopic fluid theory (hydrodynamics). For this, macroscopic quantities such as the fluid density n, the fluid velocity, $\mathbf{u}$, etc. are obtained from integrations over velocity of the distribution function $f(\mathbf{r}, \mathbf{v}, t)$.

In the following the basic ideas of kinetic theory will be introduced along with definitions of distribution functions, thermal equilibrium distributions, and various averages over these distributions. Some basic concepts of collisions and reactions will also be presented. The fluid equations will then be introduced – the exact derivation of these equations, starting from kinetic equations, is beyond the scope of this text (details can be found in many plasma physics textbooks such as [23]). The fluid equations will then be combined to obtain particle and energy balance equations that are the building blocks of the physics described in this book. Finally, the fluid equations will be linearized to examine the propagation of electromagnetic and electrostatic perturbations.

2.1 The microscopic perspective

2.1.1 Distribution functions and Boltzmann equation

The kinetic theory of gases is a useful starting point from which to appreciate the microscopic view of plasmas. Consider N particles with a random distribution of positions ($\mathbf{r}$) and velocities ($\mathbf{v}$). The velocity distribution function $f(\mathbf{r}, \mathbf{v}, t)$ defines the number of particles being at a given time t inside the six-dimensional elementary volume of phase space $\mathrm{d}x\mathrm{d}y\mathrm{d}z \times \mathrm{d}v_\mathrm{x}\mathrm{d}v_\mathrm{y}\mathrm{d}v_\mathrm{z}$. It is sometimes convenient to express this elementary volume in a more compact notation, namely $\mathrm{d}^3\mathbf{r}\ \mathrm{d}^3\mathbf{v}$. The number of particles $\mathrm{d}N$ in the volume $\mathrm{d}^3\mathbf{r}\mathrm{d}^3\mathbf{v}$ in the neighbourhood of the position $\mathbf{r}$, with velocity around $\mathbf{v}$, is thus

$$\mathrm{d}N = f(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{v}. \tag{2.1}$$

Having defined the velocity distribution function, one can then calculate macroscopic quantities by averaging over the velocity coordinates. These macroscopic quantities are determined by taking the velocity moments of the distribution function. They are the basic variables of the fluid theory presented in Section 2.2. The first of these is the particle density defined as

$$n(\mathbf{r}, t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}^3\mathbf{v}. \tag{2.2}$$

The average value of any quantity in a distribution of particles is found in statistical mechanics by integrating over the distribution weighted by that quantity, divided by the total number of particles in the distribution. It is usual to denote this process by angled brackets so for example the mean velocity, also called the drift velocity, is

$$< \mathbf{v}(\mathbf{r},t)) > = \frac{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathbf{v} f(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}^3\mathbf{v}}{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}^3\mathbf{v}};$$

the drift velocity is often given the more concise notation $\mathbf{u}(\mathbf{r}, t)$. The total particle flux can therefore be defined as

$$\Gamma(\mathbf{r}, t) = n(\mathbf{r}, t)\mathbf{u}(\mathbf{r}, t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathbf{v} f(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}^3\mathbf{v}. \tag{2.3}$$

Similarly, the total kinetic energy density in the distribution is given by

$$w = n(\mathbf{r}, t) < \frac{1}{2}mv^2 > = \frac{1}{2}m \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} v^2 f(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}^3\mathbf{v}, \tag{2.4}$$

where m is the particle mass. It turns out that the kinetic energy density can be divided into two components, one associated with the random motion of the particles and the other associated with the net drift:

$$w = \frac{3}{2}p(\mathbf{r}, t) + n(\mathbf{r}, t)\frac{1}{2}m\, \mathbf{u}(\mathbf{r}, t)^2; \tag{2.5}$$

the first term is identified with the internal energy density, so $p(\mathbf{r}, t)$ is the isotropic pressure, and the second term is due to the net flow of momentum. When the drift velocity is zero, that is for symmetrical distribution functions, the net momentum flow is zero and the kinetic energy density is just proportional to the pressure.

Distribution functions obey a conservation equation that has the form of a continuity equation. Particles enter and leave an elementary volume and can be produced by ionizating collisions, or destroyed by recombination, within this volume. The equation governing the evolution of the distribution is called the Boltzmann equation, and is given by (see for example [2])

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f + \frac{\mathbf{F}}{m} \cdot \nabla_v f = \left.\frac{\partial f}{\partial t}\right|_{\mathrm{c}}, \tag{2.6}$$

where the force acting on charged particles is $\mathbf{F} = q\,[\mathbf{E} + \mathbf{v} \times \mathbf{B}]$, with q the particle charge, and $\mathbf{E}$ and $\mathbf{B}$ the local electric and magnetic fields, respectively. The right-hand side of Eq. (2.6) is a symbolic representation of collision processes and in practice it can be difficult to set up a model for what this symbol represents (e.g., see [2]). The velocity moments of this equation allow one to construct the fluid equations, described in Section 2.2.

2.1.2 Thermal equilibrium distributions

Equation (2.6) effectively follows the continuous evolution of the distribution function in response to the electromagnetic forces acting on the charged particles and to the various relaxation processes including many types of collisions. Nevertheless, within a plasma, the distribution function of electrons in particular is often near a thermal equilibrium distribution called the Maxwellian distribution (also known as a Maxwell–Boltzmann distribution). The Maxwellian distribution conveniently relates a characteristic electron temperature to the average energy of electrons and to the mean speed of electrons. However, in the calculation of ionization or excitation coefficients, it is sometimes important to take account of the deviation of the actual distribution of electron energies from a Maxwellian.

In the remainder of this section the spatial and temporal dependence of the distribution function will not be written explicitly, so $f(\mathbf{r}, \mathbf{v}, t) \to f(\mathbf{v})$.

Q Distinguish between $\mathbf{v}$, v and v_{x}.

A $\mathbf{v}$ is the velocity vector, $v = (v_{\mathrm{x}}^2 + v_{\mathrm{y}}^2 + v_{\mathrm{z}}^2)^{1/2}$ is the magnitude of the velocity vector (also called the speed) and v_{x} is the x-component of the velocity vector (effectively the speed in the x-direction).

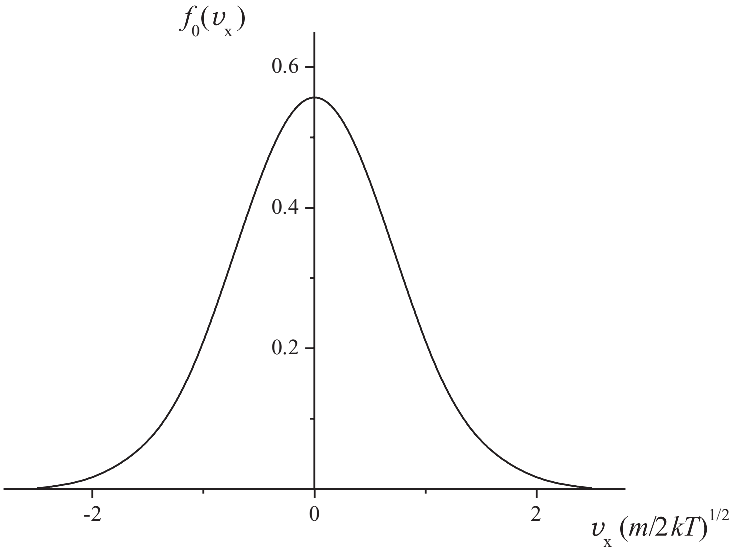

Figure 2.1 A one-dimensional Maxwellian velocity distribution normalized so that the area under the curve is unity: $f_0(v_x) = (m/2\pi kT)^{1/2} \exp\left(-mv_x^2/2kT\right)$.

The Maxwellian three-dimensional velocity distribution is given by

$$f(\mathbf{v}) = n\left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m\left(v_x^2+v_y^2+v_z^2\right)}{2kT}\right), \tag{2.7}$$

where n is the particle number density defined in Eq. (2.2). The distribution function $f(\mathbf{v})$ is proportional to the number of particles with velocities between $\mathbf{v}$ and $\mathbf{v} + \mathrm{d}\mathbf{v}$. Figure 2.1 shows the one-dimensional version, the component velocity distribution, that is obtained by integrating over v_y and v_z:

$$f(v_x) = n\left(\frac{m}{2\pi kT}\right)^{1/2} \exp\left(-\frac{mv_x^2}{2kT}\right).$$

Using Eqs (2.3) and (2.4), one can evaluate important averaged (mean) quantities. First note that the net particle flux, Eq. (2.3), in any particular direction must be zero, because the distribution is symmetrical and thus the drift velocity is zero. One can still evaluate a characteristic speed by averaging $|\mathbf{v}| = v$ over the distribution:

$$< v > = \left(\frac{m}{2\pi kT}\right)^{3/2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(v_x^2+v_y^2+v_z^2\right)^{1/2} \times \exp\left(-\frac{m\left(v_x^2+v_y^2+v_z^2\right)}{2kT}\right) \mathrm{d}v_x\mathrm{d}v_y\mathrm{d}v_z. \tag{2.8}$$

Q What does the condition of thermal equilibrium require of the mean of a distribution of particle velocities?

A The mean velocity must be zero otherwise there would be a net flow and therefore internal processes would not be in equilibrium.

Since the Maxwellian velocity distribution is isotropic (the same in all directions), the distribution can also be expressed entirely in terms of the scalar speed rather than the velocity vector, $\mathbf{v}$, and its components, v_x, v_y, v_z. This simplifies the integral in Eq. (2.8).

The speed distribution $f_s(v)$ gives the proportion of particles with speeds between v and $v + \mathrm{d}v$:

$$f_s(v) = n \left(\frac{m}{2\pi kT}\right)^{3/2} 4\pi v^2 \exp\left(-\frac{mv^2}{2kT}\right), \tag{2.9}$$

where the factor of 4π represents an integration over all the angles in which particle trajectories may point. The density is now recovered by integrating over all possible speeds,

$$n = \int_0^\infty f_s(v)\,\mathrm{d}v.$$

The mean speed of a particle is then defined by

$$< v > = \left(\frac{m}{2\pi kT}\right)^{3/2} 4\pi \int_0^\infty v^3 \exp\left(-\frac{mv^2}{2kT}\right) \mathrm{d}v. \tag{2.10}$$

This average (or mean) speed, $< v >$, is also often given the symbols $\overline{v}$ or $\overline{c}$; the former will be used here. Evaluating the integral in Eq. (2.10) gives

$$\overline{v} = \left(\frac{8kT}{\pi m}\right)^{1/2}. \tag{2.11}$$

Q According to Figure 2.2, what is the most probable speed for a particle in a Maxwellian distribution?

A The figure has a peak that corresponds with the most probable speed at $v\,(m/2kT)^{1/2} = 1$. This corresponds with $v = (2kT/m)^{1/2}$, which is clearly not the same as the mean speed $\overline{v}$ which is about 13% larger.

Electrons have a small mass and, in gas discharge plasmas, a high temperature. Using the typical value of $T \approx 30\,000$ K leads to $\overline{v}_e \approx 10^6$ m s^{-1}. This is much larger than the typical drift speeds observed in the plasma. By contrast, ions are heavy particles and are close to room temperature, typically $T \approx 500$ K, so that for

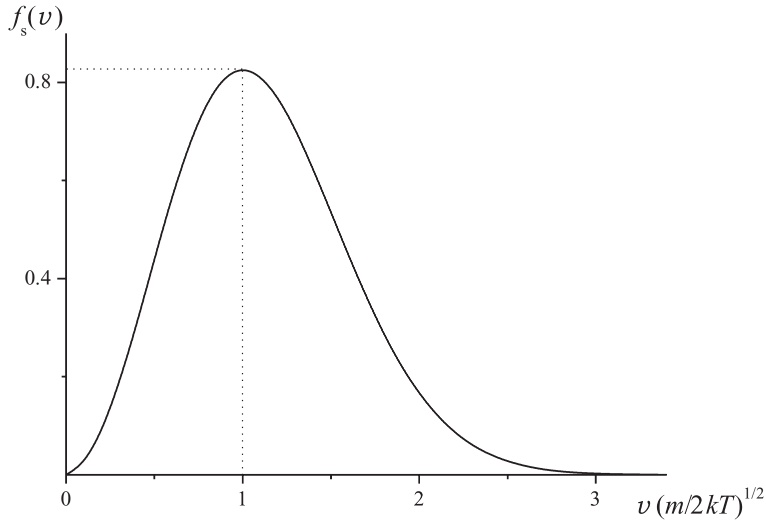

Figure 2.2 A Maxwellian speed distribution normalized so that the area under the curve is unity: $f_s(v) = (4/\sqrt{\pi})\left(mv^2/2kT\right)\exp(-mv^2/2kT)$.

argon ions $\overline{v}_i \approx 500\,\mathrm{m\,s^{-1}}$. In Chapter 3 it will be shown that ions leave the plasma with drift speeds significantly larger than $\overline{v}_i$. Therefore, except in the very central region of the plasma, ions are far from thermal equilibrium.

In a similar way, the isotropic distribution of particle speeds can be recast as a distribution in energy space with $f_e(\varepsilon)$ being the number of particles with kinetic energy between ε and $\varepsilon + \mathrm{d}\varepsilon$:

$$f_e(\varepsilon) = \frac{2n}{\sqrt{\pi}}\left(\frac{1}{kT}\right)^{3/2} \varepsilon^{1/2} \exp\left(-\frac{\varepsilon}{kT}\right). \tag{2.12}$$

Q What is the most probable energy for a particle in a Maxwellian distribution (Figure 2.3)?

A The most probable energy corresponds with the peak at $\varepsilon = kT/2$.

The kinetic energy density can be found from the velocity distribution by multiplying the energy distribution by $\varepsilon = mv^2/2$ and integrating over all energies:

$$w = \frac{2n}{\sqrt{\pi}}\left(\frac{1}{kT}\right)^{3/2} \int_0^\infty \varepsilon^{3/2} \exp\left(-\frac{\varepsilon}{kT}\right) \mathrm{d}\varepsilon = \frac{3}{2}nkT. \tag{2.13}$$

Since $w \equiv n < \varepsilon >$, the average kinetic energy of a particle is $3kT/2$. The distribution is isotropic and any particle is free to move in three independent directions,

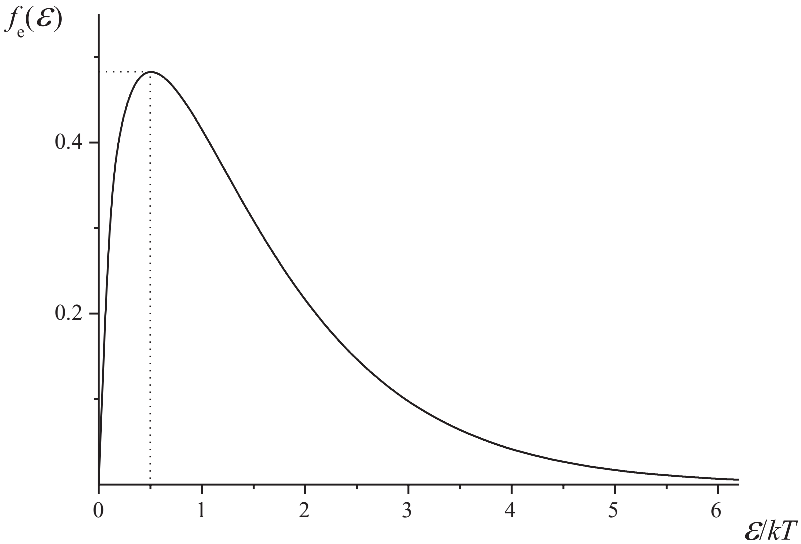

Figure 2.3 A Maxwellian energy distribution normalized so that the area under the curve is unity: $f_e(\varepsilon) = (2/\sqrt{\pi})(\varepsilon/kT)^{1/2}\exp(-\varepsilon/kT)$.

suggesting that the average energy corresponds with $kT/2$ in each of the three translational degrees of freedom.

Q How can the mean kinetic energy per particle of a Maxwellian distribution be obtained, considering only energy associated with its motion in the x-direction?

A Multiply the velocity distribution by $mv_x^2/2$ and integrate over all velocities to get the total kinetic energy associated with the x components of motion and then divide by n to get the average energy per particle:

$$< \frac{mv_x^2}{2} > = \left(\frac{m}{2\pi kT}\right)^{3/2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{mv_x^2}{2} \times \exp\left(-\frac{m(v_x^2+v_y^2+v_z^2)}{2kT}\right) dv_x dv_y dv_z.$$

The integrals are standard ones and the result confirms the suggestion that each degree of freedom has a mean thermal energy of $kT/2$ associated with it. Note that the characteristic temperature T of a Maxwellian distribution gives a measure of thermal energy.

Although the random thermal flux of particles is zero for a Maxwellian distribution, it is useful to have a local measure of the flux crossing any particular plane at any time as a consequence of the thermal motion of particles. For the particles crossing the $x-y$ plane in the positive z-direction, this is determined by an integral over all x and y components of velocity, but only positive z components:

$$\Gamma_{\text{random}} = n\left(\frac{m}{2\pi kT}\right)^{3/2}\int_{-\infty}^{\infty} \mathrm{d}v_{\mathrm{x}} \int_{-\infty}^{\infty} \mathrm{d}v_{\mathrm{y}} \int_{0}^{\infty} v_{\mathrm{z}} \exp\left(-\frac{mv^2}{2kT}\right)\mathrm{d}v_{\mathrm{z}}. \quad (2.14)$$

Evaluating this integral yields

$$\Gamma_{\text{random}} = n\left(\frac{kT}{2\pi m}\right)^{1/2}.$$

Using the expression for the random speed in Eq. (2.11), this can also be written

$$\Gamma_{\text{random}} = \frac{n\bar{v}}{4}. \quad (2.15)$$

Given the very large difference between the electron average speed and the ion average speed, the thermal flux of electrons heading towards the plasma boundaries is very large compared to the thermal flux of ions leaving the plasma. Ions and electrons are created at the same rate within the plasma volume and the main loss mechanism is often recombination at the walls. So, to maintain the flux balance at the wall in the steady state, as will be seen later, the potential in the plasma must be higher than the potential at the wall. In effect, close to the wall the potential falls by $\Delta\phi$ with respect to the plasma. In that case only electrons with sufficient perpendicular velocity, $v_{\mathrm{z}} > \sqrt{2e\Delta\phi/m}$, can reach the wall. The *particle* flux leaving the plasma is the same as that reaching the wall; that is,

$$\Gamma_{\text{wall}} = n\left(\frac{m}{2\pi kT}\right)^{3/2}\int_{-\infty}^{\infty} \mathrm{d}v_{\mathrm{x}} \int_{-\infty}^{\infty} \mathrm{d}v_{\mathrm{y}} \int_{\sqrt{2e\Delta\phi/m}}^{\infty} v_{\mathrm{z}} \exp\left(-\frac{mv^2}{2kT}\right)\mathrm{d}v_{\mathrm{z}}. \quad (2.16)$$

Evaluating the integral Eq. (2.16) yields

$$\Gamma_{\text{wall}} = \frac{n\bar{v}}{4}\exp\left(-\frac{e\Delta\phi}{kT}\right). \quad (2.17)$$

The *energy* flux leaving the plasma can also be calculated in a similar manner:

$$Q = n\left(\frac{m}{2\pi kT}\right)^{3/2}\frac{m}{2}\int_{-\infty}^{\infty} \mathrm{d}v_{\mathrm{x}} \int_{-\infty}^{\infty} \mathrm{d}v_{\mathrm{y}} \int_{\sqrt{2e\Delta\phi/m}}^{\infty} v^2 v_{\mathrm{z}} \exp\left(-\frac{mv^2}{2kT}\right)\mathrm{d}v_{\mathrm{z}}. \quad (2.18)$$

This can be shown to give

$$Q = \left[\frac{n\bar{v}}{4}\exp\left(-\frac{e\Delta\phi}{kT}\right)\right](2kT + e\Delta\phi)\,. \tag{2.19}$$

The energy flux leaving the plasma is not equal to the energy flux reaching the wall because some of the energy is deposited in the electrostatic field at the plasma boundary. The amount of energy flux reaching the wall is only

$$Q_\mathrm{w} = \left[\frac{n\bar{v}}{4}\exp\left(-\frac{e\Delta\phi}{kT}\right)\right] 2kT\,. \tag{2.20}$$

The term in square brackets is just the number of particles lost to the wall per square metre per second. The average kinetic energy carried out by each particle that escapes therefore is $2kT$.

Q The SI unit for energy is the joule (J); in atomic, molecular and plasma physics an alternative energy unit, the electron volt (eV), is formed by dividing the quantity in joules by the magnitude of the electronic charge, e, so that 1 eV $\equiv 1.602 \times 10^{-19}$ J. What is the equivalent temperature in eV of a distribution with $kT = 3.2 \times 10^{-19}$ J?

A The temperature is said to be "2 eV" because $kT/e = (3.2 \times 10^{-19}/e)\,\mathrm{V} \approx 2\,\mathrm{V}$.

Exercise 2.1: Electron energy flux to a wall For a Maxwellian electron population of $10^{16}\,\mathrm{m}^{-3}$ with mean energy 2 eV, calculate the rate of energy transfer to a wall that is at -10 V with respect to the plasma.

2.1.3 Collisions and reactions

The different types of particle in a plasma (electrons, ions, atoms, free radicals, molecules) interact in the volume via collision processes that occur on very short time scales. These collisions can be *elastic* (without loss of total kinetic energy) or *inelastic* (with transfer between the kinetic energy and the internal energy of the colliding particles).

In the simple situation of weakly ionized plasmas in noble gases, the most frequent collisions involving charged particles are elastic encounters with neutral atoms.

Collisions between charged particles (electron–electron, electron–ion and ion–ion) are not frequent and direct electron–ion recombination is usually negligible in the volume of low and medium-density plasmas at low pressure. Consequently, the charged particles tend to be generated in the plasma volume by ionization