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Plasma and Atomic Physics

A plasma is created by adding energy to a gas so that electrons are removed from atoms, producing free electrons and ions. Electric and magnetic fields interact strongly with the charged electrons and ions in plasmas (unlike solids, liquids and gases) and, consequently, plasmas behave differently to imposed electric and magnetic fields and modify electromagnetic waves in different ways to solids, liquids and gases. The different behaviour of plasmas has caused them to be regarded as a fourth fundamental state of matter in addition to solids, liquids and gases.

More than 99% of the observable universe is plasma. For example, the Sun is a plasma and has mass comprising 99.85% of the solar system, so the fraction of plasma in the solar system is slightly higher once interplanetary plasma is included. Present understanding of the universe has been enabled by the detection of electromagnetic radiation emitted by or passing through plasma material. To understand the universe, we need to understand plasmas, and, in particular, we need to understand the processes of light emission and propagation in plasmas.[1]

Plasmas have many realised and potential applications. The fusion of isotopes of hydrogen in plasmas confined using magnetic fields or confined by inertia before a dense plasma can expand should provide a new source of energy production to replace the burning of fossil fuels, though the exact physics and many technical issues are not yet resolved [35]. The fuel for a fusion reactor (the deuterium isotope of hydrogen) is abundant in seawater (at concentration 33 mg/litre). Large-scale experiments are under way to make fusion reactors because of the enormous potential impact of the development of a fusion power plant [79, 67].

Plasmas are used in many technological applications, including semiconductor etching and thin-film coating [15]. Plasma is created during the welding of

[1] In astrophysics, plasma material is sometimes referred to as an ‘ionised gas’, while in laboratory plasma work involving partial ionisation of atoms, the term ‘gaseous electronics’ has been employed to denote the physics of ‘low-temperature’ plasmas. The use of the word ‘plasma’ to describe both ‘ionised gases’ and ‘gaseous electronics’, however, is now almost ubiquitous.

solid material and is under study for biological and medical applications such as bacterial sterilisation. The emission of light from plasmas has many applications, ranging from fluorescent tubes to the use of extreme ultra-violet light emitted from laser plasmas for the lithography of semiconductors [105]. Many different lasers utilising plasmas have been developed, including argon ion lasers and an extensive array of plasma lasers designed to operate at short wavelengths [108, 91], with the record for saturated lasing achieved at wavelength 5.9 nm [125, 100]. A road map for plasma applications shows the range of applicability of plasmas in technology [97].

A plasma can be defined as a collection of ions and free electrons where the charged ions and electrons produce collective responses to electric and magnetic fields, but the net charge density averages to zero over longer-length scales. Similar definitions have often been used to define material in the plasma state (see [17, 35, 5]). Our given definition of plasma leads to the concept of the plasma frequency, which is a minimum frequency for an oscillating field to exist in a plasma, and to the concept of the Debye length, which is the distance over which electron and ion charges average to zero. We start our examination of plasmas by considering the plasma frequency and Debye length in Section 1.1. The plasma frequency is particularly important for the physics of the propagation of electromagnetic radiation in a plasma.

To ionise material so that free electrons and ions are present to form a plasma, elevated temperatures are required, causing plasmas to emit electromagnetic radiation, depending on the temperature of the plasma, in, typically, the infra-red to X-ray spectral range, though the spectrum of emission can extend to longer wavelength microwaves and radio waves, and to high-photon-energy gamma rays. In plasmas, electrons often occupy the excited bound quantum states of the ions and the free unbound quantum states. Such excitation and ionisation lead to radiation emission. The atomic physics producing electromagnetic waves in plasmas, and the subsequent propagation and absorption of electromagnetic radiation in plasmas, are the main subjects of this book.

For the relatively low-density but hot plasmas found in the laboratory, atoms and ions can be regarded as having an atomic physics structure close to that of an isolated atom or ion, but with quantum-state populations far from equilibrium. Free electrons, photons, ions and atoms have ‘collisions’ with the ions, causing excitation and ionisation. Astrophysical and space plasmas span energy-density ranges from extremely low (interstellar space) to extremely high (e.g. dwarf stars), and are associated with long timescales, often with equilibrium population and radiation fields.

The atomic and radiation physics of plasmas covers a wide range of modern physics understanding involving electricity and magnetism, relativity, atomic structure, quantum mechanics, particle collision theory, statistical physics and more. The analysis of light emission and collisional processes relevant to plasmas has provided much of the experimental evidence for quantum mechanics.

Analysis of the emission and absorption of light is an effective and non-invasive method to measure plasma conditions, such as density and temperature. Analysing spectral emission and absorption is the sole diagnostic technique applicable to astrophysical plasmas and is essential for diagnosing conditions in magnetic and inertial fusion plasmas. To determine plasma conditions, light probing involving scattering, absorption and radiation phase measurements (interferometry) can be used in laboratory plasmas. An understanding of radiation interaction in plasmas allows the interpretation of such probing.

There are books which concentrate on the diagnosis of plasma conditions using radiation emission – a subject known as plasma spectroscopy [51, 38]. Comprehensive research-level treatments of the atomic [95] and radiation [93] physics of plasmas, as well as an introduction to astronomical spectroscopy [111] and a graduate-level text emphasising atomic physics of relevance to astrophysics [86] are available. Codes and databases relevant to the atomic physics of plasmas include the Atomic Data and Analysis Structure (ADAS), (see, for example, Guzman et al. [41]) the FLYCHK code [18], the Astrophysical Plasma Emission Code (APEC) [101], and the National Institute of Standards and Technology (NIST) Atomic Spectra [63].

An understanding of the atomic physics of plasmas is needed for plasma simulation. The emission and absorption of light in a plasma can affect the plasma dynamics by, for example, transporting energy. However, as well as affecting plasma dynamics, the atomic and radiation physics of plasmas enables simulations of plasma density to be 'closed'. Fluid codes require a relationship between material density and pressure which, in turn, requires a knowledge of the degree of ionisation. Simulation particle codes similarly need a measure of the degree of ionisation for closure. This requirement for closure is explored in Section 1.1. We also show how atomic physics affects the velocity of sound in a plasma. This first chapter then presents an introduction to some radiation and atomic physics which is important in plasmas. The equilibrium relationship for ionisation (the Saha–Boltzmann equation), the distribution of speeds and energies of the particles (the Maxwellian distribution) and the Bohr model for atomic and ionic energy levels are introduced.

1.1 Plasma Physics

Some fundamental aspects of plasma physics are encapsulated in the definition of a plasma given above: 'A plasma is a collection of ions and free electrons where the charged ions and electrons produce collective responses to electric and magnetic fields with the net charge density over longer-length scales averaging to zero.' The concept of a collective response and the idea of the charge density averaging to zero lead to the concept of the plasma frequency and Debye length.

Plasma Frequency

Consider a uniform plasma of free electrons and ions which is neutrally charged and occupying a defined space. An imposed electric field can cause the centre of mass of the lighter electrons to be displaced by a distance x relative to the more massive ions. To deduce the necessary electric field, we can use the integral form of Gauss' law (see Appendix A.2) given by

$$\int_S \mathbf{E} \cdot d\mathbf{A} = \frac{1}{\epsilon_0} \int_V \rho_c dV.$$

Assume a cubic volume V extends into the plasma with one surface of area A perpendicular to the electric field and parallel to the plane of the plasma edge. The total charge enclosed by the volume is $-n_e e Ax$, where n_e is the electron number density and $-e$ is the charge of the electron. The electric field across the area is then

$$E = -\frac{n_e e\, x}{\epsilon_0} \tag{1.1}$$

after cancelling the area A from both sides of the expression for Gauss's law. If the imposed electric field is switched off, there is a force eE on the electrons in the opposite direction to the force arising from the imposed electric field and an equation of motion of the electrons such that

$$m_0 \frac{d^2 x}{dt^2} = eE = -\frac{n_e e^2}{\epsilon_0} x \tag{1.2}$$

where m_0 is the mass of an electron. Solutions of this equation are of form

$$x(t) = x(0) \exp(-i\omega_p t)$$

where, upon substitution into Equation 1.2, we have

$$\omega_p^2 = \frac{n_e e^2}{m_0 \epsilon_0}. \tag{1.3}$$

The frequency ω_p is known as the plasma frequency. It represents the natural, collective oscillation frequency of the electrons relative to the ions and, we shall later see, defines a minimum frequency of light that can propagate in a plasma in the absence of a magnetic field.

The Debye Length

The characteristic distance for charge neutrality in a plasma can be found by considering a situation with two parallel plates separated in the x-direction by a distance $2a$. The plates are assumed to be at earth potential with electrons of density n_e filling the space between the plates. The electrostatic potential V_P is related to charge density ρ at positions x by Poisson's equation (see Appendix A.2). We have

$$\nabla^2 V_P = \frac{d^2 V_P}{dx^2} = -\frac{\rho_e}{\epsilon_0} = \frac{n_e e}{\epsilon_0}.$$

At the midway point between the plates (distance $x = a$), the potential is given by

$$V_P = \frac{n_e e a^2}{2\epsilon_0}$$

and the energy required to move another electron to the midway point between the plates is $V_P e = n_e e^2 a^2/(2\epsilon_0)$. In one direction, the average kinetic energy of an electron at temperature T_e is $(1/2)k_B T_e$ (see Exercise 1.2). We can equate this kinetic energy to the energy required to move an electron to the midway distance between the two plates:

$$\frac{1}{2}k_B T_e = \frac{n_e e^2 a^2}{2\epsilon_0}.$$

The distance a, where the electron kinetic energy is equal to the energy required to move an electron to the midway points between the plates, is the distance over which the ground potential of the plates stops influencing the 'average' electron. The distance is given by

$$a = \lambda_D = \left(\frac{\epsilon_0 k_B T_e}{n_e e^2}\right)^{1/2}. \tag{1.4}$$

This distance is known as the Debye length λ_D.

The number of electrons in a sphere of radius λ_D reflects the number of electrons likely to move 'collectively' together during, for example, light scattering from a plasma. We can write for the number of electrons in a Debye sphere

$$N_D = n_e \frac{4}{3}\pi \lambda_D^3 = \left(\frac{4}{3}\right)\pi \left(\frac{\epsilon_0 k_B T}{n_e e^2}\right)^{3/2} n_e. \tag{1.5}$$

Plasma Pressure and the Speed of Sound in a Plasma

In a plasma, pressure P is related to the mass density ρ and temperature T by adding up the electron, ion and atom pressure given by Boyle's law. We can write for a plasma where all particles have the same temperature and behave as ideal gases that

$$P = n_i k_B T_i + n_e k_B T_e = \frac{\rho(1 + Z_{av})k_B T}{A m_p} \tag{1.6}$$

where A is the average atomic mass, m_p is the mass of the proton and the average degree of ionisation $Z_{av} = n_e/n_i$, where n_e is the electron density and n_i is the ion-plus-atom density. The electron temperature T_e and ion temperature T_i are assumed equal to T for the last equality. Equation 1.6 is an example of an equation of state relationship between state variables in thermodynamic equilibrium.

Changes of mass density ρ and the velocity $\mathbf{u}$ of a plasma fluid can be related by the continuity equation (representing conservation of mass) and the equation of motion (representing a fluid version of Newton's law that force is equal to mass times acceleration). The equation of motion for a fluid is also known as the Navier-Stokes equation. We can use standard fluid treatments (e.g. [84]) and write for these two equations respectively

$$\frac{\partial \rho}{\partial t} + \nabla.\rho\mathbf{u} = 0, \tag{1.7}$$

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}.\nabla)\mathbf{u}\right) = -\nabla P. \tag{1.8}$$

The fluid equation of continuity and the equation of motion can be used to simulate plasmas if the pressure P and the density ρ can be related to each other by a known closure relationship, for example, Equation 1.6. This is not always straightforward. For example, the pressure/density relationship is affected strongly by the value of the degree of ionisation Z_{av} and it is often necessary to evaluate separate temperatures for the different ion, atomic and electron components of the plasma.

For variations in mass density, velocity and pressure in one dimension z, the continuity equation and equation of motion can be written such that

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial z} = 0,$$

$$\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial z}\right) = -\frac{\partial P}{\partial z}.$$

Assuming a small time-varying deviation of density $\rho = \rho_0 + \rho_1$, velocity $u = u_0 + u_1$ and pressure $P = P_0 + P_1$ from steady-state values ρ_0, u_0 and P_0, it is possible to show that to a good approximation the one-dimensional continuity equations combine to give an equation for the propagation of the deviation of density such that

$$\frac{\partial^2 \rho_1}{\partial z^2} + \frac{1}{(\partial P/\partial \rho)}\frac{\partial^2 \rho_1}{\partial t^2} = 0.$$

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This equation has the form of a wave equation where the speed c_s of the wave is given by

$$c_s^2 = \left(\frac{\partial P}{\partial \rho}\right). \tag{1.9}$$

The propagation of a disturbance in density is usually known as a sound wave, so this equation shows that the sound speed is given by the square root of the rate of change of pressure with density changes. (The partial derivative here means that other parameters such as entropy and energy density are held constant.) The sound speed determines the rate of expansion of a freely expanding plasma and the speed of shock waves and other disturbances propagating in plasmas.

Statistical mechanics tells us that for a gas (or other system) characterised by a temperature T, the average energy per degree of freedom per particle is equal to $(1/2)k_BT$ (see Exercise 1.2). A degree of freedom can be represented by translational motion in one direction (giving three degrees of freedom for a monatomic gas or a plasma species such as the electrons), but can also include, for example, vibrational degrees of freedom for polyatomic gases.

Rather than consider degrees of freedom in a plasma, it is often more convenient to define a parameter γ_{eos} using the relationship between pressure and energy density. We introduce the energy density per unit mass (ϵ_m) and write for the energy density per unit volume $U = \rho\epsilon_m$ that

$$U = \rho\epsilon_m = \frac{P}{\gamma_{eos} - 1} \tag{1.10}$$

which then defines γ_{eos}. Equation 1.10 illustrates that the pressure P and energy density per unit volume U are essentially the same thing, as for an ideal gas with n_d degrees of freedom, we can write that

$$\gamma_{eos} = 1 + \frac{2}{n_d}. \tag{1.11}$$

The energy density per unit volume of the electrons or ions is then given by

$$U_{e,i} = \frac{n_d}{2} n_{e,i} k_B T \tag{1.12}$$

where $n_{e,i}$ represents the electron or ion number density. The energy density per unit mass is consequently given by

$$\epsilon_m = \frac{3}{4}\frac{(1 + Z_{av})k_BT}{Am_p} \tag{1.13}$$

upon substituting into Equation 1.10 using our Boyle's law expression for the pressure (Equation 1.6) and setting $n_d = 3$. A particle such as an electron or ion has $n_d = 3$ degrees of freedom as there are three directions for the components of velocity. This energy per unit mass expression is equivalent to the one that can be obtained by counting $(1/2)k_BT$ energy per degree of freedom assuming that there are three degrees of freedom for both the electrons and ions.

Differentiating the equation that defines γ_{eos} (Equation 1.10), we get

$$\frac{\partial P}{\partial \rho} = (\gamma_{eos} - 1)\left(\epsilon + \rho\frac{\partial \epsilon_m}{\partial \rho}\right). \tag{1.14}$$

The change of energy content $\Delta\epsilon_m$ per unit mass of a gas is given by the summation of energy added (Δq), minus the work done by the gas due to volume changes ($-P\Delta V$), a statement often known as the first law of thermodynamics. We can write that

$$\Delta\epsilon = \Delta q - P\Delta\left(\frac{1}{\rho}\right) \tag{1.15}$$

as the volume change ΔV is equal to the change of $1/\rho$. As

$$\frac{d(1/\rho)}{d\rho} = -\frac{1}{\rho^2},$$

the partial derivative of the energy content per unit mass with respect to density can now be evaluated from Equation 1.15. We use a partial derivative, which means that quantities other than density are held constant (so the heat flow $\Delta q = 0$) and obtain

$$\frac{\partial \epsilon_m}{\partial \rho} = \frac{P}{\rho^2}.$$

Substituting into Equation 1.14 and using Equation 1.10 gives another expression for the sound speed

$$c_s^2 = \frac{\partial P}{\partial \rho} = \frac{\gamma_{eos}P}{\rho}. \tag{1.16}$$

Interestingly, we see that any factor that affects the relationship between energy density and pressure (Equation 1.10) will affect the speed of sound in the plasma. For example, the degree of ionisation in a plasma affects this relationship, so we have the seemingly perverse result that different ionisation can cause changes in the speed of sound in a plasma. The speed of sound determines the velocity of propagation of shock waves and rarefaction waves and the speed of expansion of an unconstrained plasma [5].

1.1.1 Adiabatic Condition

An adiabatic process is one that occurs without transfer of heat or matter between a thermodynamic system and its surroundings. The adiabatic condition for a plasma element means that no external energy is added so that any change in the internal energy per unit volume $dU_{e,i}$ of the electrons or ions is balanced by the work $P_{e,i}dV$ associated with a volume change dV. As the electron or ion pressure $P_{e,i} = n_{e,i}k_BT$ (see Equation 1.6), using Equation 1.12 we have

$$dU_{e,i} = \frac{n_d}{2}(P_{e,i}dV + VdP_{e,i}). \tag{1.17}$$

Equating $dU_{e,i}$ and $-PdV$ gives

$$\frac{n_d}{2}(P_{e,i}dV + VdP_{e,i}) = -P_{e,i}dV.$$

Rearranging, we have

$$\frac{dP_{e,i}}{P_{e,i}} = -\left(1 + \frac{2}{n_d}\right)\frac{dV}{V} = -\gamma_{eos}\frac{dV}{V}$$

using Equation 1.11. Integrating the pressure from P_0 to $P_{e,i}$ and volume from V_0 to V gives

$$\ln\left(\frac{P_{e,i}}{P_0}\right) = -\gamma_{eos}\ln\left(\frac{V}{V_0}\right).$$

We can write that

$$P_{e,i}V^{\gamma_{eos}} = P_0V_0^{\gamma_{eos}}. \tag{1.18}$$

Equation 1.18 means that for an adiabatic element of plasma, $P_{e,i}V^{\gamma_{eos}}$ is constant.

Another way of stating this adiabatic condition for a plasma is found by recognising that the volume V of a plasma element is proportional to the inverse of the number density $1/n_{e,i}$ and that $P_{e,i} = n_{e,i}k_BT$. For a perfect gas, $\gamma_{eos} = 5/3$, so that the constant $P_{e,i}V^{\gamma_{eos}}$ is equivalent to a constant $n_{e,i}/(k_BT)^{3/2}$. A freely expanding plasma volume element is often adiabatic with constant value of $n_{e,i}/(k_BT)^{3/2}$.

1.2 Free Electron Speed and Energy Distributions

We discuss the division of particles into fermions and bosons in Section 8.1, but we can utilise here the main result of that discussion: that only one fermion can occupy a quantum state. For particles in a thermodynamic equilbrium, the probability $P(E)$ of occupancy by a particle of a quantum state of energy E is given by the proportionality

$$P(E) \propto \exp\left(\frac{N(\mu - E)}{k_BT}\right) \tag{1.19}$$

where N is the number of particles occupying the state with energy E, μ is the chemical potential and T is the temperature. The chemical potential is the energy required to add one more particle to the 'gas' of particles. If the state is not occupied by a particle $P(E) \propto 1$ as $N = 0$. As electrons are fermions, a state can only be occupied by one electron, or it can be unoccupied. If occupied, the probability relationship is $P(E) \propto \exp((\mu - E)/k_B T)$. The proportionality constants to turn the probabilities into absolute probabilities are the same for both occupied and not-occupied states, so the average occupancy $n(E)$ of a state of energy E is given by the ratio of the probabilities here for $P_{occupied}/(P_{occupied} + P_{notoccupied})$ giving

$$n(E) = \frac{\exp\left((\mu - E)/k_B T\right)}{\exp\left((\mu - E)/k_B T\right) + 1} = \frac{1}{1 + \exp\left((E - \mu)/k_B T\right)}. \tag{1.20}$$

This average occupancy of a quantum state can be immediately utilised to obtain an expression for the distribution of speeds of electrons. The number of electrons per unit volume $f_v(v)dv$ with speeds between v and $v + dv$ is given by the proportionality

$$f_v(v)dv \propto 4\pi v^2 n(E) dv$$

where $E = (1/2)m_0 v^2$ is the electron energy for electron mass m_0. The factor $4\pi v^2 dv$ is the velocity space volume corresponding to the speed range v to $v + dv$ given by the volume of a shell of radius v and thickness dv. The expression for the electron distribution of speeds can then be written as

$$f_v(v)dv \propto 4\pi v^2 \frac{dv}{1 + \exp(((1/2)m_0 v^2 - \mu)/k_B T)}.$$

To convert the proportionality constant here to an absolute value of the distribution of speeds requires normalisation. We choose to require that integrating over all possible speeds gives the total electron number density n_e per unit volume. We then have that

$$\int_0^\infty f_v(v)dv = n_e.$$

The probability distribution function with this normalisation gives the number of electrons per unit volume with speeds between v and $v + dv$. An alternative normalisation with $\int_0^\infty \hat{f}_v(v)dv = 1$ would give the probability of finding an electron with a speed in the range v to $v + dv$ (not the number of electrons) and is used in Chapter 12. Unfortunately, the integrations to do the normalisation are not straightforward, except in the limiting case where the chemical potential is large and negative corresponding to the thermodynamic state of a lower-density electron gas where the electron quantum states are not close to being fully occupied. We consider the chemical potential in Chapter 13. In the case of a lower-density gas, we have the Maxwellian distribution of speeds with

$$f_v(v)dv = n_e \left(\frac{m_0}{2\pi k_B T}\right)^{3/2} 4\pi v^2 \exp\left(-\frac{m_0 v^2}{2k_B T}\right) dv. \tag{1.21}$$