

Appendix A

Physics Equations, Units, and Constants

This appendix provides a summary of the fundamental physical laws from other areas of physics, as they are commonly used in plasma physics. Key equations, units and physical constants are given for mechanics, electrodynamics, statistical mechanics, kinetic theory of gases, stochastic diffusion processes, fluid mechanics and quantum mechanical effects. While the procedures for deriving these equations are given in outline form, details are omitted. Readers should consult the textbook references listed at the end of each section for more detailed explanations and theoretical developments. In some parts of this appendix extensive use is made of the vector algebra and calculus relations given in Appendix D. The International System of Units (*Système International d'Unités*), often called mks units, are used throughout this appendix, and the book. Physical constants and SI unit interrelationships are given in tables in Section A.8 at the end of this Appendix.

A.1 Mechanics

Newton's second law states that the mass m times the acceleration \mathbf{a} of a particle is given by the force \mathbf{F} (in units of newtons or $\text{kg} \cdot \text{m}/\text{s}^2$)

$$m\mathbf{a} = \mathbf{F}, \quad \text{Newton's second law.} \quad (\text{A.1})$$

A conservative force is one that is derivable from the gradient of a potential that is independent of time:

$$\mathbf{F} = -\nabla V(\mathbf{x}), \quad \text{conservative force.} \quad (\text{A.2})$$

Since the acceleration in (A.1) is just the time derivative of the particle velocity, $\mathbf{a} \equiv d\mathbf{v}/dt$, taking the dot product of the velocity \mathbf{v} with Newton's second law

for a conservative force yields:

$$\frac{d}{dt} \left[\frac{mv^2}{2} + V(\mathbf{x}) \right] = 0 \quad \Longrightarrow \quad \varepsilon = \frac{mv^2}{2} + V(\mathbf{x}) = \text{constant},$$

energy conservation, (A.3)

where $mv^2/2 \equiv m(\mathbf{v} \cdot \mathbf{v})/2 \equiv T$ is the particle kinetic energy and $V(\mathbf{x})$ is the potential energy. The SI unit of energy is the joule (J), which is equal to a newton·meter (N·m). In plasma physics particle energies are usually quoted in electron volts (eV), which is the energy in joules divided by the elementary charge [eV \equiv J/e = J/(1.602 \times 10⁻¹⁹)].

The force on a particle of charge q subjected to an electric field $\mathbf{E}(\mathbf{x}, t)$ and a magnetic induction field $\mathbf{B}(\mathbf{x}, t)$ is

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \quad \text{Lorentz force.} \quad (\text{A.4})$$

For electrostatic situations with no magnetic field, the electric field can be written in terms of the electrostatic potential $\phi(\mathbf{x})$: $\mathbf{E} = -\nabla\phi$. Then, the Lorentz force becomes conservative [see (A.2)] with $V(\mathbf{x}) = -q\phi(\mathbf{x})$, and the energy conservation relation (A.3) is applicable.

When only a magnetic field is present, the combination of Newton's second law and the Lorentz force becomes

$$m \frac{d\mathbf{v}}{dt} = q\mathbf{v} \times \mathbf{B} \quad \Longrightarrow \quad \frac{d\mathbf{v}}{dt} = \boldsymbol{\omega}_c \times \mathbf{v}, \quad (\text{A.5})$$

where

$$\boldsymbol{\omega}_c \equiv -q\mathbf{B}/m, \quad \text{the angular velocity,} \quad (\text{A.6})$$

for gyromotion of the charged particle in the magnetic field. The negative sign is needed in this vectorial definition so that charged particles gyrate according to the right-hand rule with the thumb pointing in the direction of $\boldsymbol{\omega}_c$. The magnitude of $\boldsymbol{\omega}_c$ gives the radian frequency (rad/s) for the gyromotion:

$$\omega_c = qB/m, \quad \text{gyrofrequency,} \quad (\text{A.7})$$

which is also called the cyclotron (the source of the subscript c) or Larmor¹ frequency. This formula is unchanged for relativistic particles except for the fact that then the mass becomes the relativistic mass: $m \rightarrow m/\sqrt{1 - v^2/c^2}$. Since the dot product of (A.5) with the velocity \mathbf{v} vanishes, the particle kinetic energy is constant — a magnetic field does no work on a charged particle in its gyromotion. In gyromotion a charged particle executes a circular motion about the magnetic field \mathbf{B} with a radius of

$$\varrho \equiv v_{\perp}/\omega_c, \quad \text{gyroradius,} \quad (\text{A.8})$$

in which v_{\perp} is the magnitude of the velocity component perpendicular to the magnetic field direction [$\mathbf{v}_{\perp} \equiv -\mathbf{B} \times (\mathbf{B} \times \mathbf{v})/B^2$].

¹Actually, the Larmor frequency is defined to be half the cyclotron frequency.

For situations where both electric and magnetic fields are present, it is convenient to write them in terms of the scalar potential $\phi(\mathbf{x}, t)$ and vector potential $\mathbf{A}(\mathbf{x}, t)$: $\mathbf{E} = -\nabla\phi - \partial\mathbf{A}/\partial t$, $\mathbf{B} = \nabla \times \mathbf{A}$ — see (A.55). Then, Newton's second law (A.1) for a nonrelativistic charged particle subjected to the Lorentz force (A.4) can be written as

$$m \frac{d\mathbf{v}}{dt} = -\frac{\partial U}{\partial \mathbf{x}} + \frac{d}{dt} \left(\frac{\partial U}{\partial \mathbf{v}} \right), \quad U = q\phi - q(\mathbf{v} \cdot \mathbf{A}) \quad (\text{A.9})$$

in which U is a generalized potential energy, $\partial U/\partial \mathbf{x} \equiv \nabla U$, $\partial U/\partial \mathbf{v} \equiv \nabla_{\mathbf{v}} U$, where $\nabla_{\mathbf{v}}$ is the gradient in velocity space. The single particle Lagrangian, which has units of energy and is given by the kinetic energy minus the generalized potential energy, is defined by

$$L(\mathbf{x}, \mathbf{v}, t) \equiv T - U = \frac{mv^2}{2} - q\phi + q(\mathbf{v} \cdot \mathbf{A}), \quad \text{Lagrangian}, \quad (\text{A.10})$$

where again $T = mv^2/2$ is the particle kinetic energy. The vector equation of motion for a charged particle (i.e., Newton's second law with the Lorentz force) can be written in terms of the Lagrangian as

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \mathbf{v}} \Big|_{t, \mathbf{x}} \right) - \frac{\partial L}{\partial \mathbf{x}} \Big|_{t, \mathbf{v}} = \mathbf{0}, \quad \text{Lagrangian equations of motion.} \quad (\text{A.11})$$

For an orthogonal coordinate system with unit base vectors $\hat{\mathbf{e}}_k$, the orthogonal projections of this vector equation yield

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_k} \right) - \frac{\partial L}{\partial q_k} = 0, \quad k = 1, 2, 3 \quad \text{Lagrange's equations.} \quad (\text{A.12})$$

Here, the spatial coordinates are $q_k \equiv \hat{\mathbf{e}}_k \cdot \mathbf{x}$ and the velocity coordinates are $\dot{q}_k \equiv \hat{\mathbf{e}}_k \cdot \mathbf{v} = \hat{\mathbf{e}}_k \cdot d\mathbf{x}/dt$. Note that, like Newton's second law, Lagrange's equations are in general second order ordinary differential equations in time.

It is often convenient to change the charged particle equation of motion into two coupled first order differential equations. To effect this change one first defines

$$\mathbf{p} \equiv \frac{\partial L}{\partial \mathbf{v}} = m\mathbf{v} + q\mathbf{A}, \quad \text{canonical momentum}, \quad (\text{A.13})$$

in which $\mathbf{v} \equiv d\mathbf{q}/dt$. Next, the single particle Hamiltonian function H , which also has units of energy, is defined through the Legendre transformation:

$$H(\mathbf{x}, \mathbf{p}, t) \equiv \mathbf{p} \cdot \frac{d\mathbf{x}}{dt} - L = \frac{|\mathbf{p} - q\mathbf{A}|^2}{2m} + q\phi \equiv T + V, \quad \text{Hamiltonian.} \quad (\text{A.14})$$

It is the sum of the kinetic energy ($T = |\mathbf{p} - q\mathbf{A}|^2/2m = mv^2/2$) and the potential energy ($V = q\phi$), and by construction is independent of velocity: $\partial H/\partial \mathbf{v}|_{\mathbf{x}, \mathbf{p}, t} = \mathbf{0}$. The equation of motion for a charged particle can be written

(for both orthogonal and nonorthogonal coordinate systems) in terms of the Hamiltonian function H , as two coupled first order vector differential equations in time:

$$\frac{d\mathbf{p}}{dt} = - \left. \frac{\partial H}{\partial \mathbf{x}} \right|_{t,\mathbf{p}}, \quad \frac{d\mathbf{x}}{dt} = \left. \frac{\partial H}{\partial \mathbf{p}} \right|_{t,\mathbf{x}}, \quad \text{Hamilton's equations of motion.} \quad (\text{A.15})$$

The total time derivative of the Hamiltonian is given via chain-rule partial differentiation by

$$\frac{dH}{dt} = \left. \frac{\partial H}{\partial t} \right|_{\mathbf{x},\mathbf{p}} + \frac{d\mathbf{x}}{dt} \cdot \left. \frac{\partial H}{\partial \mathbf{x}} \right|_{t,\mathbf{p}} + \frac{d\mathbf{p}}{dt} \cdot \left. \frac{\partial H}{\partial \mathbf{p}} \right|_{t,\mathbf{x}}.$$

Using Hamilton's equations of motion, the sum of all terms except the explicit partial time derivative vanish — because the Hamiltonian does not vary along the charged particle's motion in the relevant (\mathbf{x}, \mathbf{p}) six-dimensional phase space: $d\mathbf{x}/dt \cdot \partial H/\partial \mathbf{x} + d\mathbf{p}/dt \cdot \partial H/\partial \mathbf{p} = 0$. Thus, the total time derivative of the Hamiltonian is simply

$$\frac{dH}{dt} = \left. \frac{\partial H}{\partial t} \right|_{\mathbf{x},\mathbf{p}} = - \left. \frac{\partial L}{\partial t} \right|_{\mathbf{x},\mathbf{v}} = q \left(\frac{\partial \phi}{\partial t} - \mathbf{v} \cdot \frac{\partial \mathbf{A}}{\partial t} \right), \quad (\text{A.16})$$

which indicates the increase in energy due to a temporally increasing potential ϕ and due to the work $\mathbf{v} \cdot q\mathbf{E}$ done by the inductive component $-\partial \mathbf{A}/\partial t$ of the electric field.

Projecting out the geometrical components of the Hamiltonian form of the equations of motion (A.15) for a charged particle in the orthogonal directions $\hat{\mathbf{e}}_k$ yields

$$\frac{dp_k}{dt} = - \frac{\partial H}{\partial q_k}, \quad \frac{dq_k}{dt} = \frac{\partial H}{\partial p_k}, \quad k = 1, 2, 3, \quad \text{Hamilton's equations,} \quad (\text{A.17})$$

in which $p_k \equiv \hat{\mathbf{e}}_k \cdot \mathbf{p}$ are the canonical momentum coordinates and $q_k \equiv \hat{\mathbf{e}}_k \cdot \mathbf{x}$ are the conjugate spatial coordinates.

The various equations of motion have been written in forms that are independent of the coordinate system and they are valid in the initial coordinate system as well as transformed ones. Also, the equations are valid for non-relativistic particles ($v \ll c$) and are all Galilean invariant. That is, they are unchanged upon transformation to another inertial (non-accelerating) frame according to $\mathbf{v}' = \mathbf{v} + \mathbf{V}_f$ and $\mathbf{E}' = \mathbf{E} + \mathbf{V}_f \times \mathbf{B}$, where \mathbf{V}_f is the velocity of the second inertial frame (subscript f) relative to the first.

When the potential ϕ and vector potential \mathbf{A} do not depend explicitly on time, (A.16) shows that the Hamiltonian is a constant of the motion:

$$H = \frac{|\mathbf{p} - q\mathbf{A}|^2}{2m} + q\phi = \frac{mv^2}{2} + q\phi = \varepsilon = \text{constant},$$

$$\text{for } \frac{\partial \phi}{\partial t} = 0, \quad \frac{\partial \mathbf{A}}{\partial t} = 0, \quad \text{energy conservation.} \quad (\text{A.18})$$

In such conservative systems the particle energy and time are canonical conjugate Hamiltonian coordinates: $p = \varepsilon$ and $q = t$.

When the gradient of the Hamiltonian vanishes in a particular direction \mathbf{e}_k , (A.15) shows that the conjugate canonical momentum in the same direction is a constant of the motion:

$$p_k \equiv \mathbf{e}_k \cdot \mathbf{p} = \mathbf{e}_k \cdot (m\mathbf{v} + q\mathbf{A}) = \text{constant for } \mathbf{e}_k \cdot \frac{\partial H}{\partial \mathbf{x}} = 0, \quad \text{canonical momentum conservation.} \quad (\text{A.19})$$

In an orthogonal coordinate system the base vector \mathbf{e}_k becomes the unit vector $\hat{\mathbf{e}}_k$; then, the criterion for canonical momentum conservation in the $\hat{\mathbf{e}}_k$ direction becomes simply $\partial H / \partial q_k = 0$ (i.e., H independent of the coordinate q_k , which implies symmetry in the $\hat{\mathbf{e}}_k$ direction).

Lagrange's or Hamilton's equations of motion can be derived (by considering variations with \mathbf{x} and $\mathbf{v} \equiv d\mathbf{x}/dt$ or \mathbf{p} as the independent variables, respectively) from Hamilton's variational principle of least action (time integral of difference between kinetic and potential energy): $\delta \int L dt = 0$. It can also be shown using (A.14) that for a conservative system where the Hamiltonian is a constant of the motion [see (A.18)], the action $\int \mathbf{p} \cdot d\mathbf{q}$ is a variational quantity along a particle trajectory.

For *periodic motion* in a given coordinate \mathbf{q}_i it is convenient to introduce as a variable the action integral over a cycle:

$$J_i = \frac{1}{2\pi} \oint \mathbf{p}_i \cdot d\mathbf{q}_i = \frac{1}{2\pi} \int_0^{2\pi} d\theta_i \mathbf{p}_i \cdot \frac{\partial \mathbf{q}_i}{\partial \theta_i}, \quad \text{action variable.} \quad (\text{A.20})$$

The action variable, which is a momentum-like quantity, is the “area” in p_i, q_i phase space encompassed by the periodic motion. The canonically conjugate action-angle θ_i is the angular or cyclic variable corresponding to periodic motion around the perimeter of this area. Hamilton-Jacobi theory (see references at end of this section) can usually be used to determine the action angle coordinate $q_i \equiv \theta_i$. Writing the Hamiltonian in terms of the action variable J_i , the Hamilton equation $dq_i/dt = \partial H / \partial p_i$ [see (A.17)] becomes:

$$\frac{d\theta_i}{dt} = \frac{\partial H}{\partial J_i} \equiv \omega_i, \quad \text{action angle evolution equation.} \quad (\text{A.21})$$

The period of the oscillatory motion can be determined in general from

$$\tau_i \equiv \oint dt = \oint \frac{dq_i}{dq_i/dt} = \oint \frac{dq_i}{\partial H / \partial p_i}, \quad \text{oscillation period.} \quad (\text{A.22})$$

The radian frequency for the periodic motion is

$$\omega_i(J_i) = 2\pi/\tau_i, \quad \text{oscillation frequency.} \quad (\text{A.23})$$

The Hamiltonian for a periodic system in action-angle variables is thus simply

$$H_i = \omega_i J_i, \quad \text{action-angle Hamiltonian.} \quad (\text{A.24})$$

For *nearly periodic motion* in situations where the generalized potential U in (A.9) varies slowly and aperiodically in space and time (compared to the oscillations), the action in (A.20) is nearly constant and given by the ratio of the oscillation energy to the oscillation frequency:

$$J_i \simeq \frac{H_i}{\omega_i} = \frac{\varepsilon_i}{\omega_i}, \quad \text{action for nearly periodic motion.} \quad (\text{A.25})$$

For slow, temporal changes that are characterized by a parameter $a(t)$ and are not themselves periodic, it can be shown that, while the slow variations cause “linearly small,” oscillatory [$\sim (\dot{a}/\omega_i a) \sin \omega_i t \ll 1$] changes in J , the average of dJ/dt over an oscillation period τ is “quadratically small” in the rate of temporal change:

$$\left\langle \frac{dJ_i}{dt} \right\rangle_{\theta_i} \equiv \frac{1}{\tau} \oint \frac{d\theta_i}{\dot{\theta}_i} \frac{dJ_i}{dt} = 0 + \mathcal{O} \left\{ \left(\frac{\dot{a}}{\omega_i a} \right)^2, \frac{\ddot{a}}{\omega_i^2 a} \right\} \frac{J_i}{\tau}, \quad (\text{A.26})$$

where the dots over quantities indicate their time derivatives. For such situations the action J_i is called an adiabatic invariant; it is often a very useful approximate constant of the motion. When the small variations in the potential oscillate at a slow frequency $\omega_i \gg \omega_a \equiv \sqrt{-(1/a) \partial^2 a / \partial t^2}$, harmonics of this slower oscillation that are resonant with the fundamental oscillations (i.e., $\omega_i = n \omega_a$, $n \equiv$ an integer) can lead to secular changes in the action J_i that grow slowly in time. Hence they can break the constancy of the adiabatic invariant over a long time period. This usually occurs when the slow oscillations exceed a small critical amplitude (typically ~ 0.1 of the main oscillations). The relevant multiple time scale analysis and conditions for such breakdowns of adiabaticity are discussed in E.6.

As an example of the use of mechanics theory, consider the “central-force” problem of determining the scattering angle ϑ and elastic cross-section σ for a Coulomb collision of two non-relativistic, charged particles. Assume a charged particle of species s with charge q_s , mass m_s and initial velocity \mathbf{v} experiences a Coulomb collision (i.e., interaction via the Coulomb electric field force) with another charged particle of species s' with parameters $q_{s'}$, $m_{s'}$ and \mathbf{v}' . Multiplying the force balance equations obtained from (A.1) and (A.4) for each particle by the mass of the other particle and subtracting, taking account of the equal and oppositely directed electric field forces on the two particles due to the Coulomb potential [$q\mathbf{E} = -q\nabla\phi$, $\phi = q/(\{4\pi\epsilon_0\}|\mathbf{x}|)$ — see (A.33)], yields the equation of motion for the two-particle system in the center-of-momentum coordinate system:

$$m_{ss'} \frac{d}{dt} (\mathbf{v} - \mathbf{v}') = - \frac{q_s q_{s'}}{\{4\pi\epsilon_0\}} \nabla \frac{1}{|\mathbf{x} - \mathbf{x}'|} \quad (\text{A.27})$$

in which $m_{ss'} = m_s m_{s'} / (m_s + m_{s'})$ is the “reduced” mass for the two particle system.

Initially, when the particles are very far apart, one can define the impact speed as $u = |\mathbf{v} - \mathbf{v}'|$ and the collision impact parameter as b (distance of closest

approach if the Coulomb electric field did not deflect the particles). Further, one defines the classical (i.e., not quantum mechanical) minimum distance of closest approach as

$$b_{\min}^{\text{cl}} \equiv \frac{q_s q_{s'}}{\{4\pi\epsilon_0\} m_{ss'} u^2}, \quad \text{classical minimum impact parameter} \quad (\text{A.28})$$

at which the center-of-momentum kinetic energy is half the Coulomb potential energy [$q_s q_{s'} / (\{4\pi\epsilon_0\} b_{\min}^{\text{cl}})$] and below which large-angle deflections ($> 90^\circ$) can be expected to occur.

Since the collision takes place in a plane defined by the vectors $\mathbf{x} - \mathbf{x}'$ and $\mathbf{v} - \mathbf{v}'$, it is convenient to define instantaneous radial and angular coordinates in the center-of-momentum frame by the radial separation of the particles $r \equiv |\mathbf{x} - \mathbf{x}'|$ and by the angle θ that the line $\mathbf{x} - \mathbf{x}'$ makes with the line $|\mathbf{x} - \mathbf{x}'|$ when the particles were initially very far apart. In these coordinates the angular momentum p_θ [constant because of symmetry of the Coulomb potential in the θ direction — see (A.19)] and total energy ε [constant because the potential ϕ does not depend explicitly on time — see (A.18)] can be written as

$$\begin{aligned} p_\theta &= m_{ss'} r^2 \dot{\theta} = m_{ss'} b u, \\ \varepsilon &= T + V = \frac{1}{2} m_{ss'} (\dot{r}^2 + r^2 \dot{\theta}^2) + \frac{q_s q_{s'}}{\{4\pi\epsilon_0\} r} = \frac{1}{2} m_{ss'} u^2. \end{aligned}$$

Solving the second (energy conservation) equation for \dot{r} and dividing by the $\dot{\theta}$ obtained from the first equation yields

$$\frac{dr}{d\theta} = \pm \frac{r}{b} \sqrt{r^2 - 2r b_{\min}^{\text{cl}} - b^2},$$

where the sign is negative when the particles are approaching each other and positive as they recede.

At the minimum or closest approach distance r_m , $dr/d\theta = 0$. The angle θ_m at this point is given by

$$\theta_m = \int_{r_m}^{\infty} \frac{dr}{dr/d\theta} = -\arctan\left(\frac{b_{\min}^{\text{cl}}}{b}\right) + \frac{\pi}{2}.$$

In the center-of-momentum frame the angular deflection ϑ caused by the collision is given by $\pi - 2\theta_m$ and hence

$$\tan \frac{\vartheta}{2} = \frac{b_{\min}^{\text{cl}}}{b} = \frac{q_s q_{s'}}{\{4\pi\epsilon_0\} m_{ss'} u^2 b}, \quad \text{scattering angle.} \quad (\text{A.29})$$

Thus, $b > b_{\min}^{\text{cl}}$ causes Coulomb scattering by less than 90° ($\vartheta < \pi/2$), while $b < b_{\min}^{\text{cl}}$ induces more than 90° scattering.

The differential cross-section $d\sigma$ (measured in meters² or barns $\equiv 10^{-28}$ m²) by which Coulomb collisions of incoming charged particles of species s with impact parameter b and azimuthal angle φ scatter off of charged particles of

species s' into spherical angles ϑ, φ within the differential solid angle $d\Omega \equiv \sin \vartheta d\vartheta d\varphi$ is thus given [using (A.29) to write $b(\vartheta) = b_{\min}^{\text{cl}} / \tan(\vartheta/2)$] by

$$d\sigma = b db d\varphi = \frac{b}{\sin \vartheta} \left| \frac{db}{d\vartheta} \right| d\Omega = \left(\frac{b_{\min}^{\text{cl}}}{2 \sin^2 \vartheta/2} \right)^2 d\Omega$$

or,

$$\frac{d\sigma}{d\Omega} = \left(\frac{b_{\min}^{\text{cl}}}{2 \sin^2 \vartheta/2} \right)^2 = \left(\frac{q_s q_{s'}}{2 \{4\pi\epsilon_0\} m_{ss'} u^2 \sin^2 \vartheta/2} \right)^2, \quad \text{Rutherford differential scattering cross-section.} \quad (\text{A.30})$$

Standard intermediate level mechanics textbooks, which include extensions to relativistic systems, are:

Symon, *Mechanics* (1971) [?].

Barger and Olsson, *Classical Mechanics: A Modern Perspective* (1973) [?].

The standard advanced level mechanics textbook is:

Goldstein, *Classical Mechanics* (1950, 1980) [?].

A.2 Electrodynamics

An *electrostatic* theory is appropriate for time-independent charge density distributions $\rho_q(\mathbf{x})$, electric fields $\mathbf{E}(\mathbf{x})$, and magnetic induction fields $\mathbf{B}(\mathbf{x})$. In electrostatics the irrotational ($\nabla \times \mathbf{E} = \mathbf{0}$) electric field \mathbf{E} with units of volts/meter is written in terms of the scalar potential $\phi(\mathbf{x})$ with units of volts, $\mathbf{E} \equiv -\nabla\phi$, and related to the charge density distribution:

$$\nabla \cdot \mathbf{E} = \rho_q / \epsilon_0, \quad \text{Gauss' law,} \quad (\text{A.31})$$

$$-\nabla^2 \phi = \rho_q / \epsilon_0, \quad \text{Poisson's equation.} \quad (\text{A.32})$$

The charge density distribution has units of coulombs/meter³. For localized charge density distributions [$\lim_{|\mathbf{x}| \rightarrow \infty} \rho_q(\mathbf{x}) \rightarrow 0$] the general (Green-function-type) solution of Poisson's equation in an infinite medium is [see also (??)]

$$\phi(\mathbf{x}) = \int d^3x' \frac{\rho_q(\mathbf{x}')}{\{4\pi\epsilon_0\} |\mathbf{x}' - \mathbf{x}|}. \quad (\text{A.33})$$

For a point charge at $\mathbf{x} = \mathbf{x}_0$ the charge distribution is $\rho_q(\mathbf{x}) = q \delta(\mathbf{x} - \mathbf{x}_0)$ and the potential becomes

$$\phi(\mathbf{x}) = \frac{q}{\{4\pi\epsilon_0\} |\mathbf{x} - \mathbf{x}_0|}, \quad \text{Coulomb potential.} \quad (\text{A.34})$$

Here and throughout this book the mks factor $\{4\pi\epsilon_0\}$ is written in braces; eliminating this factor yields the corresponding cgs forms of these electrostatic response formulas.

In a dielectric (ponderable) medium the charge density ρ_q is composed of a part ρ_{free} due to “free” charges and a part due to a polarization charge density, $\rho_{\text{pol}} = -\nabla \cdot \mathbf{P}$ where $\mathbf{P} \equiv \epsilon_0 \chi_E \mathbf{E}$ is the presumed linear and isotropic polarization (units of coulomb/meter²) of the medium induced by the electric field \mathbf{E} and χ_E is the dimensionless electric susceptibility of the medium:

$$\rho_q = \rho_{\text{free}} + \rho_{\text{pol}} = \rho_{\text{free}} - \nabla \cdot \mathbf{P} = \rho_{\text{free}} - \nabla \cdot \epsilon_0 \chi_E \mathbf{E}. \quad (\text{A.35})$$

Thus, in an isotropic dielectric medium Gauss’ law becomes Coulomb’s law:

$$\nabla \cdot \mathbf{D} = \rho_{\text{free}}, \quad \mathbf{D} \equiv \epsilon_0 \mathbf{E} + \mathbf{P} = \epsilon_0 (1 + \chi_E) \mathbf{E} = \epsilon \mathbf{E} \quad (\text{A.36})$$

in which the medium’s dielectric constant $\epsilon \equiv \epsilon_0 (1 + \chi_E)$ is the constitutive relation between the displacement vector \mathbf{D} and the electric field \mathbf{E} .

A *magnetostatic* theory is appropriate for time-independent current density distributions $\mathbf{J}(\mathbf{x})$ and magnetic induction fields $\mathbf{B}(\mathbf{x})$. In magnetostatics the solenoidal (transverse, $\nabla \cdot \mathbf{B} = 0$) magnetic induction field \mathbf{B} which has units of weber/meter² or tesla can be written in terms of the vector potential \mathbf{A} , i.e., $\mathbf{B} = \nabla \times \mathbf{A}$, and related to the current density distribution \mathbf{J} which has units of ampere/meter²:

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} \quad \implies \quad -\nabla^2 \mathbf{A} = \mu_0 \mathbf{J}, \quad \text{static Ampere’s law} \quad (\text{A.37})$$

in which $\nabla \cdot \mathbf{A} = 0$ (the Coulomb gauge) has been assumed in the last form. For localized current density distributions [$\lim_{|\mathbf{x}| \rightarrow \infty} \mathbf{J}(\mathbf{x}) = \mathbf{0}$], the general (Green-function-type) solution for \mathbf{A} in an infinite medium is [see also (??)]

$$\mathbf{A}(\mathbf{x}) = \left\{ \frac{\mu_0}{4\pi} \right\} \int d^3x' \frac{\mathbf{J}(\mathbf{x}')}{|\mathbf{x}' - \mathbf{x}|}. \quad (\text{A.38})$$

The magnetic field around an infinite wire carrying a current I (amperes) along the z axis of a cylindrical coordinate system can be obtained from this equation using $\mathbf{B} = \nabla \times \mathbf{A}$ and a current density $\mathbf{J} = \hat{\mathbf{e}}_z (I/2\pi r) \lim_{a \rightarrow 0} \delta(r - a)$:

$$\mathbf{B} = \frac{\mu_0 I}{2\pi r} \hat{\mathbf{e}}_\theta, \quad \text{magnetic field around a current-carrying wire.} \quad (\text{A.39})$$

To obtain the corresponding cgs form of this and other magnetic field response equations, eliminate the $\{\mu_0/4\pi\}$ factor and replace \mathbf{J} by \mathbf{J}/c , or replace $\mu_0 \mathbf{J}$ by $4\pi \mathbf{J}/c$.

In a magnetizable medium the current density \mathbf{J} is composed of a part \mathbf{J}_{free} due to the current induced by “free” charges and a magnetization current density $\mathbf{J}_{\text{mag}} = \nabla \times \mathbf{M}$ where $\mathbf{M} \equiv \chi_M \mathbf{H}$ is the presumed linear and isotropic magnetization (units of ampere-turns/meter) of the medium induced by the magnetic field \mathbf{H} (units of ampere-turns/meter) and χ_M is the dimensionless magnetic susceptibility of the medium:

$$\mathbf{J} = \mathbf{J}_{\text{free}} + \mathbf{J}_{\text{mag}} = \mathbf{J}_{\text{free}} + \nabla \times \mathbf{M} = \mathbf{J}_{\text{free}} + \nabla \times (\chi_M \mathbf{H}). \quad (\text{A.40})$$

Thus, in an isotropic, magnetizable medium the static Ampere's law becomes

$$\nabla \times \mathbf{H} = \mu_0 \mathbf{J}, \quad \mathbf{H} = \mathbf{B}/\mu_0 - \mathbf{M}, \quad \mathbf{B} = \mu_0(1 + \chi_M) \mathbf{H} = \mu \mathbf{H} \quad (\text{A.41})$$

in which $\mu = \mu_0(1 + \chi_M)$ is the magnetic permeability of the medium and $\mathbf{B} = \mu \mathbf{H}$ is the constitutive relation between the magnetic induction \mathbf{B} and the magnetic field \mathbf{H} .

The *microscopic* Maxwell or electromagnetic (em) equations for determining time-varying electric and magnetic fields caused by charge and current density distributions $\rho_q(\mathbf{x}, t)$ and $\mathbf{J}(\mathbf{x}, t)$, respectively, in free space are

Maxwell Equations

name

differential form

integral form

Gauss' law

$$\nabla \cdot \mathbf{E} = \frac{\rho_q}{\epsilon_0} \quad \oiint_S d\mathbf{S} \cdot \mathbf{E} = \int_V d^3x \frac{\rho_q}{\epsilon_0} \quad (\text{A.41a})$$

Faraday's law

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad \oint_C d\boldsymbol{\ell} \cdot \mathbf{E} = -\frac{\partial}{\partial t} \iint_S d\mathbf{S} \cdot \mathbf{B} \quad (\text{A.41b})$$

no magnetic monopoles

$$\nabla \cdot \mathbf{B} = 0 \quad \oiint_S d\mathbf{S} \cdot \mathbf{B} = 0 \quad (\text{A.41c})$$

Ampere's law

$$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right) \quad \oint_C d\boldsymbol{\ell} \cdot \mathbf{B} = \mu_0 \iint_S d\mathbf{S} \cdot \left(\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right) \quad (\text{A.41d})$$

(A.42) ■

Here, ϵ_0 is the electric permittivity of free space which has units of farad/meter = coulomb/(volt · meter) = joule/(volt² · meter), μ_0 is the magnetic permeability of free space which has units of henry/meter = weber/(ampere · meter) = weber²/(joule · meter) and $\mu_0 \epsilon_0 = 1/c^2$ where c is the speed of light in free space. Taking the divergence of Ampere's law and making use of Gauss' law yields

$$\frac{\partial \rho_q}{\partial t} + \nabla \cdot \mathbf{J} = 0, \quad \text{continuity equation for charge and current.} \quad (\text{A.43})$$

In Ampere's law the displacement current $\epsilon_0 \partial \mathbf{E} / \partial t$ was introduced by Maxwell to make the electrodynamics equations consistent with the charge and current continuity equation (A.43).

The physical significance of the source terms on the right of the integral forms of the Maxwell equations are: $\int_V d^3x \rho_q \equiv Q$, net charge (in coulombs) within the volume V ; $\iint_S d\mathbf{S} \cdot \mathbf{B} \equiv \psi$, magnetic flux (in webers) penetrating the surface S ; $\iint_S d\mathbf{S} \cdot \mathbf{J} \equiv I$, the total electric current (in amperes) flowing through the surface S . The Maxwell equations are relativistically invariant; in particular, they are invariant under Lorentz transformations, which preserve the constancy of the speed of light, independent of the motion of the source, upon transformation to another inertial rest frame.

The corresponding *macroscopic* Maxwell equations in an isotropic, polarizable, magnetizable medium are written in terms of $\mathbf{D} \equiv \epsilon \mathbf{E} = \epsilon_0 \mathbf{E} + \mathbf{P}$ and the magnetic field $\mathbf{H} \equiv \mathbf{B}/\mu_0 - \mathbf{M}$, and free charge, current densities $\rho_{\text{free}}, \mathbf{J}_{\text{free}}$:

$$\nabla \cdot \mathbf{D} = \rho_{\text{free}}, \quad \nabla \times \mathbf{E} = -\partial \mathbf{B} / \partial t, \quad \nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{H} = \mathbf{J}_{\text{free}} + \partial \mathbf{D} / \partial t. \quad (\text{A.44})$$

The total rate at which the electromagnetic (em) fields do work on a medium in a finite volume V is $\int_V d^3x \mathbf{J}_{\text{free}} \cdot \mathbf{E}$ — the magnetic field does no work since the magnetic force $q\mathbf{v} \times \mathbf{B}$ on charged particles is perpendicular to the velocity. Using the macroscopic Maxwell equations to calculate the rate of doing work yields the energy conservation law for electromagnetic fields:

$$\frac{\partial w_{\text{em}}}{\partial t} + \nabla \cdot \mathbf{S}_{\text{em}} = -\mathbf{J}_{\text{free}} \cdot \mathbf{E}, \quad \text{em field energy conservation}, \quad (\text{A.45})$$

where

$$w_{\text{em}} \equiv w_E + w_B \equiv \frac{1}{2} (\mathbf{E} \cdot \mathbf{D} + \mathbf{B} \cdot \mathbf{H}), \quad \text{em energy density (J/m}^3\text{)}, \quad (\text{A.46})$$

$$\mathbf{S}_{\text{em}} = \mathbf{E} \times \mathbf{H}, \quad \text{Poynting vector (flux of em energy) (J/m}^2\text{ \cdot s)}, \quad (\text{A.47})$$

$$\mathbf{J}_{\text{free}} \cdot \mathbf{E} = \text{joule heating (W/m}^3 = \text{J/m}^3 \cdot \text{s} = \text{V} \cdot \text{A/m}^3\text{)}, \quad (\text{A.48})$$

in which the energy densities in the electric and magnetic fields are defined by

$$w_E \equiv \frac{1}{2} (\mathbf{E} \cdot \mathbf{D}), \quad \text{electric field energy density (J/m}^3\text{)}, \quad (\text{A.49})$$

$$w_B \equiv \frac{1}{2} (\mathbf{B} \cdot \mathbf{H}), \quad \text{magnetic field energy density (J/m}^3\text{)}. \quad (\text{A.50})$$

A corresponding momentum conservation equation for electromagnetic fields can be deduced, for situations where charge and current densities are present in free space, from the microscopic Maxwell equations:

$$\frac{\partial \mathbf{g}_{\text{em}}}{\partial t} + \nabla \cdot \mathbf{T}_{\text{em}} = \rho_q \mathbf{E} + \mathbf{J} \times \mathbf{B}, \quad \text{em field momentum conservation}, \quad (\text{A.51})$$

where

$$\mathbf{g}_{\text{em}} \equiv \frac{1}{c^2} \mathbf{E} \times \mathbf{B}, \quad \text{momentum density in em fields,} \quad (\text{A.52})$$

$$\mathbf{T}_{\text{em}} = \epsilon_0 \left[\frac{|\mathbf{E}|^2}{2} \mathbf{I} - \mathbf{E}\mathbf{E} \right] + \frac{1}{\mu_0} \left[\frac{|\mathbf{B}|^2}{2} \mathbf{I} - \mathbf{B}\mathbf{B} \right] \quad \text{em stress tensor,} \quad (\text{A.53})$$

$$\rho_q \mathbf{E} + \mathbf{J} \times \mathbf{B} = \text{momentum input to em fields from medium.} \quad (\text{A.54})$$

Here, the electromagnetic stress tensor is defined to be opposite in sign from the usual Maxwell stress tensor in electrodynamic theory [see Eq. (6.119) in Jackson, *Classical Electrodynamics*, 3rd Edition (1999)[?]] — so that the electromagnetic stress can be added to the pressure tensor \mathbf{P} to obtain the total force density in a plasma in the form $\mathbf{F} = -\nabla \cdot (\mathbf{P} + \mathbf{T}_{\text{em}})$. For a dielectric medium the conservation of momentum for electromagnetic fields depends somewhat on the medium considered because of the possible ambiguity as to which parts of $\rho_q \mathbf{E} + \mathbf{J} \times \mathbf{B}$ belong to the dielectric and which parts represent free charge and current densities.

Since the magnetic induction field \mathbf{B} is a solenoidal or transverse field ($\nabla \cdot \mathbf{B} = 0$), it can be represented in terms of a vector potential \mathbf{A} , i.e., $\mathbf{B} = \nabla \times \mathbf{A}$. Using this representation, Faraday's law can be written as $\nabla \times (\mathbf{E} + \partial \mathbf{A} / \partial t) = \mathbf{0}$, which indicates that $\mathbf{E} + \partial \mathbf{A} / \partial t$ can be represented in terms of the gradient of a scalar potential ϕ . Thus, the electromagnetic fields \mathbf{E} and \mathbf{B} can be represented in terms of the potentials ϕ (units of volts) and \mathbf{A} (units of weber · meter):

$$\mathbf{E} = -\nabla \phi - \partial \mathbf{A} / \partial t, \quad \mathbf{B} = \nabla \times \mathbf{A}, \quad \text{em fields in terms of potentials.} \quad (\text{A.55})$$

In terms of the potentials ϕ, \mathbf{A} the inhomogeneous, microscopic Maxwell equations (Gauss' and Ampere's laws) become ($\mu_0 \epsilon_0 = 1/c^2$)

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \phi = -\frac{\rho_q}{\epsilon_0}, \quad \left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \mathbf{A} = -\mu_0 \mathbf{J}, \quad (\text{A.56})$$

in which

$$\nabla \cdot \mathbf{A} + \frac{1}{c} \frac{\partial \phi}{\partial t} = 0, \quad \text{Lorentz gauge condition,} \quad (\text{A.57})$$

which provides a constraint relation between the potentials, has been used. [If the Coulomb gauge ($\nabla \cdot \mathbf{A} = 0$) is used, the equations (A.56) are different.]

For a dielectric medium [i.e., a medium that is polarizable ($\rho_q = -\nabla \cdot \mathbf{P}$) and magnetizable ($\mathbf{J} = \nabla \times \mathbf{M}$) but not significantly conducting which would imply $\mathbf{J} = \sigma \mathbf{E}$], equations (A.56) become scalar wave equations of the form

$$\left(\nabla^2 - \mu \epsilon \frac{\partial^2}{\partial t^2} \right) u(\mathbf{x}, t) = S(\mathbf{x}, t), \quad \text{dielectric medium wave equation.} \quad (\text{A.58})$$

Sinusoidal plane wave solutions of this equation are in general of the form

$$u(\mathbf{x}, t) = \hat{u}_{\mathbf{k}, \omega} e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} \equiv \hat{u} e^{i\varphi}, \quad \text{Fourier plane wave Ansatz,} \quad (\text{A.59})$$

where by convention \hat{u} is a complex constant for a given \mathbf{k}, ω and physical waves $u(\mathbf{x}, t)$ are obtained by taking the real part: $u(\mathbf{x}, t) \equiv \mathcal{R}e\{\hat{u} e^{i\varphi}\}$. Substituting this Ansatz into the sourceless ($S = 0$) wave equation yields the dispersion relation (relationship between ω and \mathbf{k}) for nontrivial (normal mode) solutions:

$$\omega^2 = \frac{k^2}{\mu\epsilon} = \frac{k^2 c^2}{n^2} \quad \Longrightarrow \quad \omega = \pm \frac{k c}{n}, \quad \text{light waves in a dielectric,} \quad (\text{A.60})$$

in which

$$n \equiv \frac{c k}{\omega}, \quad \text{index of refraction.} \quad (\text{A.61})$$

The index of refraction is the ratio of the speed of light in vacuum to that in the medium.

For a given \mathbf{k}, ω , a point of constant wave phase in $u(\mathbf{x}, t)$, which is defined by $0 = d\varphi/dt = \mathbf{k} \cdot d\mathbf{x}/dt - \omega \equiv \mathbf{k} \cdot \mathbf{V}_\varphi - \omega$, moves at

$$\mathbf{V}_\varphi \equiv \frac{\omega}{k} \hat{\mathbf{e}}_k, \quad \text{wave phase velocity,} \quad (\text{A.62})$$

in which $\hat{\mathbf{e}}_k \equiv \mathbf{k}/k$ is the unit vector along \mathbf{k} . The phase velocity for light waves in a dielectric medium is the speed of light in the medium in the direction of wave propagation (\mathbf{k}): $\mathbf{V}_\varphi = \pm (c/n) \hat{\mathbf{e}}_k$. Since a steady, monochromatic (single \mathbf{k}, ω) “carrier” wave carries no information, the wave phase speed can be greater than the speed of light. A wave packet, which results from superposing waves of different \mathbf{k}, ω , carries information at

$$\mathbf{V}_g \equiv \frac{\partial \omega}{\partial \mathbf{k}} = \nabla_{\mathbf{k}} \omega(\mathbf{k}), \quad \text{wave group velocity,} \quad (\text{A.63})$$

whose magnitude must, by causality, be less than or equal to the speed of light. For nondispersive media [$\partial n / \partial \mathbf{k} = \mathbf{0} \implies n = n(\omega)$], the group velocity is the same as the phase velocity. Thus, the group velocity of light waves in typical (nondispersive) dielectric media (e.g., water for visible light) is the same as their phase velocity. Since plasmas are typically dispersive media for ranges of \mathbf{k}, ω of interest, the group velocities of waves in plasmas are often different from their phase velocities.

The electric field for the most general homogeneous transverse ($\mathbf{k} \times \mathbf{E} = \mathbf{0}$) plane wave propagating in the direction \mathbf{k} can be represented by

$$\mathbf{E}(\mathbf{x}, t) = (\epsilon_1 E_1 + \epsilon_2 E_2) e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}, \quad \text{polarization representation.} \quad (\text{A.64})$$

Here, ϵ_1, ϵ_2 are mutually orthogonal “wave polarization” unit vectors in directions perpendicular to the direction of wave propagation ($\epsilon_1 \times \epsilon_2 \equiv \hat{\mathbf{e}}_k$) and E_1, E_2 are in general complex numbers. If E_1 and E_2 have the same complex phase, the wave is linearly polarized. If E_1 and E_2 have the same magnitude, but

differ in phase by 90 degrees the wave is circularly polarized. A representation that is useful for circularly and elliptically polarized waves is

$$\mathbf{E}(\mathbf{x}, t) = (E_+ \boldsymbol{\epsilon}_+ + E_- \boldsymbol{\epsilon}_-) e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}, \quad \text{alternative representation,} \quad (\text{A.65})$$

in which E_+ and E_- are complex amplitudes and

$$\boldsymbol{\epsilon}_\pm \equiv \frac{1}{\sqrt{2}} (\boldsymbol{\epsilon}_1 \pm i \boldsymbol{\epsilon}_2), \quad \text{rotating polarization unit vectors.} \quad (\text{A.66})$$

The $E_+ \equiv |E_+| e^{i\varphi_+}$ term represents a positive angular momentum and helicity (“left circularly polarized” in optics²) wave that rotates (for decreasing phase $\varphi \equiv \mathbf{k} \cdot \mathbf{x} - \omega t + \varphi_+$ at a fixed point in space) in the clockwise direction relative to the \mathbf{k} direction since $\mathcal{R}e\{\mathbf{E}(\mathbf{x}, t)_+\} = (|E_+|/\sqrt{2})(\boldsymbol{\epsilon}_1 \cos \varphi - \boldsymbol{\epsilon}_2 \sin \varphi)$. Conversely, the E_- term represents a negative angular momentum and helicity (“right circularly polarized”) wave that rotates in the opposite direction. Circularly polarized waves are represented by either E_+ or E_- , depending on whether they have positive or negative helicity. A wave is elliptically polarized if it has both E_+ and E_- components and they are dissimilar — when $E_+/E_- = \pm 1$, one reverts to a linearly polarized wave.

Standard intermediate level textbooks for electrodynamics, or electricity and magnetism as it has been called historically, are:

Reitz, Milford and Christy, *Foundations of Electromagnetic Theory* (1979) [?]

Lorrain, Corson and Lorrain, *Electromagnetic Fields and Waves* (??) [?]

Barger and Olsson, *Classical Electricity and Magnetism: A Contemporary Perspective* (1987) [?].

The standard advanced level textbooks are:

Jackson, *Classical Electrodynamics* (1962, 1975) [?]

Panofsky and Phillips, *Classical Electricity and Magnetism* (1962) [?].

A.3 Statistical Mechanics

A closed system of particles is in equilibrium in a statistical mechanics sense if for subsystems thereof all relevant macroscopic parameters are equal to their mean values to a high degree of accuracy. The particles in a system are weakly interacting and thus statistically independent if the total system Hamiltonian is approximately just the sum of the Hamiltonians for the individual particles. That is, the part of the total system Hamiltonian that represents interactions between particles must be small, or vanishing, except for infrequent collisions.

²In optics the rotation direction is determined by the direction of polarization rotation that would be seen by an observer facing into the oncoming wave. This direction of rotation is opposite to the modern physics definition which is determined by the direction of rotation relative to the wavevector \mathbf{k} .

Liouville's theorem, which follows from the incompressibility [see (A.79)] of the \mathbf{x}, \mathbf{p} Hamiltonian phase space for particle trajectories, states that the density of a system of N particles in their $6N$ -dimensional phase space is constant along the particle phase space trajectories. A consequence of Liouville's theorem is that the probability density in the $6N$ dimensional phase space must be expressible entirely in terms of constants of the motion. In the macroscopic rest frame (where the average momentum and angular momentum vanish) of a system of weakly interacting particles, the only relevant constant (or additive integral) of the motion is the single particle Hamiltonian.

Statistical mechanics predicts that the most probable distribution of a subsystem of a large number of weakly interacting, free (i.e., monoatomic gas or unbound) particles in equilibrium with an even larger system of such particles at a thermodynamic temperature³ T will have a probability density distribution in the macroscopic rest frame of the system that is given by

$$\rho(\mathbf{p}, \mathbf{q}) = \rho_0 e^{-H(\mathbf{p}, \mathbf{q})/T}, \quad \text{Gibb's distribution} \quad (\text{A.67})$$

in which ρ_0 is a constant and H is the Hamiltonian for a single particle. The constant ρ_0 is the density of particles in the six-dimensional phase space, which is obtained from the normalization $\int d^3p \int d^3q \rho(\mathbf{p}, \mathbf{q}) = 1$. Thus, for example, the most probable distribution function for weakly interacting charged particles in the presence of a potential ϕ that is constant in time or slowly varying (compared to the rate for thermal motion over a relevant scale length — for an adiabatic response, subscript A) is

$$f_A(\mathbf{x}, \mathbf{v}) = n_0 \left(\frac{m}{2\pi T} \right)^{3/2} e^{-H/T} = n_0 \left(\frac{m}{2\pi T} \right)^{3/2} e^{-mv^2/2T - q\phi/T}, \quad (\text{A.68})$$

in which n_0 is the equilibrium density (m^{-3}) of charged particles in the absence of the potential ϕ . The normalization here has been chosen such that integrating f over the three-dimensional velocity space yields the density distribution

$$n_A(\mathbf{x}) \equiv \int d^3v f(\mathbf{x}, \mathbf{v}) = n_0 e^{-q\phi(\mathbf{x})/T}, \quad \text{Boltzmann relation.} \quad (\text{A.69})$$

This result is applicable for adiabatic processes, i.e., ones that vary slowly compared to the reversible inertial or oscillatory time scales. As an example of an application of the Boltzmann relation, the gravitational potential near the earth's surface ($q\phi \rightarrow V = mgx$) confines neutral molecules in the atmosphere near the earth's surface according to the law of atmospheres — see (A.137).

In the absence of a potential, (A.68) becomes the Maxwell distribution function:

$$f_M(\mathbf{v}) = n_0 \left(\frac{m}{2\pi T} \right)^{3/2} e^{-mv^2/2T} = \frac{n_0 e^{-v^2/v_T^2}}{\pi^{3/2} v_T^3}, \quad \text{Maxwellian distribution,} \quad (\text{A.70})$$

³Temperatures (and particle energies) in plasma physics are usually quoted in electron volts, abbreviated eV, and the Boltzmann factor k_B that usually multiplies the temperature T in equations such as (A.67)–(A.75) is usually omitted for simplicity.

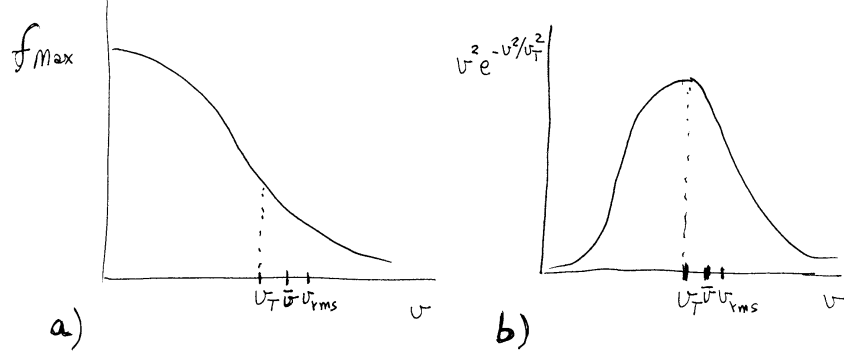


Figure A.1: Properties of a Maxwellian distribution function: a) speed dependence; b) number of particles per unit speed v .

in which $v_T \equiv \sqrt{2T/m}$. The dependence of the Maxwellian distribution on particle speed v is shown in Fig. A.1a. In spherical velocity-space coordinates the normalized (by density) integral of the Maxwellian distribution over all velocity space is [see (??)]

$$\int d^3v \frac{f_M(\mathbf{v})}{n_0} = \frac{4}{\sqrt{\pi}} \int_0^\infty \frac{dv}{v_T} \frac{v^2}{v_T^2} e^{-v^2/v_T^2} = \frac{4}{\sqrt{\pi}} \int_0^\infty dx x^2 e^{-x^2} = 1. \quad (\text{A.71})$$

Some of the characteristic speeds that can be deduced from the Maxwellian distribution are (see Fig. A.1b):

$$\begin{aligned} v_T = v_{\max} &\equiv \sqrt{2T/m}, & \text{thermal, most probable speed,} \\ \bar{v} &= \sqrt{8T/\pi m} = (2/\sqrt{\pi}) v_T, & \text{average speed,} \\ v_{\text{rms}} &= \sqrt{3T/m} = \sqrt{3/2} v_T, & \text{root mean square speed.} \end{aligned} \quad (\text{A.72})$$

It is customary in plasma physics to use v_T as the reference particle speed since this is the speed that appears naturally in the exponent of the Maxwellian. This is the most probable speed because in spherical velocity space the maximum in the number of particles with speeds between v and $v+dv$ ($\propto 4\pi v^2 e^{-v^2/v_T^2}$) occurs at this speed (cf., Fig. A.1b). The average speed \bar{v} (average of $v \equiv |\mathbf{v}|$ over the Maxwellian distribution) is relevant in calculations of the random particle flux to one side of a plane that is introduced into a medium whose particles have a Maxwellian distribution: $\int d^3v v \frac{1}{2} |\cos \vartheta| f_M = \pi \int_0^\infty dv v^3 f_M = n_0 \bar{v}/4$ [see (??)] where the z axis of the spherical velocity space coordinate system has been taken to be perpendicular to the plane being introduced. The root mean square speed v_{rms} (square root of average of v^2) is relevant in calculations of the average kinetic energy $m\bar{v}_x^2/2$ in a given direction x since all directions are equivalent for

an isotropic Maxwellian distribution ($\overline{v_x^2} = \overline{v_y^2} = \overline{v_z^2} = v_T^2/2 = \overline{v^2}/3 \equiv v_{\text{rms}}^2/3$):

$$\frac{\overline{mv_x^2}}{2} \equiv \frac{1}{n_0} \int d^3v \left(\frac{mv_x^2}{2} \right) f_M(\mathbf{v}) = \frac{mv_{\text{rms}}^2}{6} = \frac{T}{2},$$

one-dimensional particle thermal energy. (A.73)

The total thermal energy of a particle is given by

$$\frac{\overline{mv^2}}{2} \equiv \frac{1}{n_0} \int d^3v \left(\frac{mv^2}{2} \right) f_M(\mathbf{v}) = \frac{mv_{\text{rms}}^2}{2} = \frac{3T}{2},$$

three-dimensional particle thermal energy. (A.74)

Finally, the kinetic pressure embodied in the Maxwellian distribution is

$$p \equiv \int d^3v (mv_x^2) f_M(\mathbf{v}) = \int d^3v \left(\frac{mv^2}{3} \right) f_M(\mathbf{v}) = \frac{nv_{\text{rms}}^2}{3} = nT,$$

kinetic pressure. (A.75)

Entropy is the state of disorder of a closed system. It never decreases with time: it remains constant for reversible (e.g., Hamiltonian dynamics) processes, but increases for irreversible processes. Irreversible increases in the entropy of a system are caused by dissipative processes such as the cumulative effects of a large number of random collisions. For a system of weakly interacting, free particles the entropy is given by the logarithm of the average volume [$= 1/\rho_0$ — see (A.67)] of six-dimensional phase space occupied by a single particle, i.e., $s = \ln(1/\rho_0)$. [For quantum mechanical systems it is the logarithm of the number of statistically independent states, which is quantized to be the number of states that fit in the relevant phase space volume: $N^{\text{qm}} = \int d^3N_p d^3N_q e^{-H(\mathbf{p}, \mathbf{q})/T} / (N! h^{3N})$ in which h is Planck's constant and N is the number of degrees of freedom for the system being considered.] Thus, neglecting constants and using $\rho_0 = n_0(m/2\pi T)^{3/2} \sim n_0/v_T^3$ for an \mathbf{x}, \mathbf{v} phase space, for classical systems one has

$$s = \ln(1/\rho_0) = \ln(T^{3/2}/n_0) + \text{constant}, \quad \text{entropy.} \quad (\text{A.76})$$

For a volume V of uniform density (i.e., $n_0 = 1/V$) monotonic gas, the entropy is given by

$$s = \ln V + (3/2) \ln T + \text{constant},$$

which, when multiplied by the molar gas constant $R = k_B N_A$ is the conventional form of the entropy for an ideal gas. Alternatively, writing $T = p/n_0$ in (A.76) so that $s = (3/2) \ln(pV^{5/3}) + \text{constant}$, one obtains the constant entropy (isentropic) equation of state $pV^\Gamma = \text{constant}$ for an ideal gas in a three-dimensional system where $\Gamma = 5/3$.

Standard intermediate level textbooks for statistical mechanics are:

Kittel, *Elementary Statistical Physics* (1958) [?]

Reif, *Fundamentals of Statistical and Thermal Physics* (1965) [?]

Callen, *Thermodynamics* (1960) [?]

Kittel and Kroemer, *Thermal Physics* (1960). [?]

Some advanced level books on statistical mechanics are:

Huang, *Statistical Mechanics* (1963) [?]

Tolman, *The Principles of Statistical Mechanics* (1938) [?]

Landau and Lifshitz, *Statistical Physics* (1959) [?]

Prigogine, *Introduction to Thermodynamics of Irreversible Processes* (1961). [?]

A.4 Kinetic Theory of Gases

Kinetic theory is a rigorous formalism that is used to provide a description of the behavior of a large collection of neutral molecules (or atoms) in a gas, particularly when the assumptions of equilibrium statistical mechanics are not valid. In kinetic theory $d^3x d^3v f(\mathbf{x}, \mathbf{v}, t)$ is the (assumed large) number of molecules located in the six-dimensional (\mathbf{x}, \mathbf{v}) phase space with spatial positions lying between \mathbf{x} and $\mathbf{x} + d\mathbf{x}$ and velocity vectors lying between \mathbf{v} and $\mathbf{v} + d\mathbf{v}$, at time t . The quantity $f(\mathbf{x}, \mathbf{v}, t)$, which has units of $\#/(m^3 \cdot m^3/s^3)$, is called the distribution function. It is governed by the equation

$$\frac{df(\mathbf{x}, \mathbf{v}, t)}{dt} = \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{\mathbf{F}}{m} \cdot \nabla_v f = \left. \frac{\delta f}{\delta t} \right)_c, \quad \text{kinetic equation} \quad (\text{A.77})$$

in which \mathbf{F}/m is the acceleration of a molecule due to the force \mathbf{F} [e.g., the conservative force in (A.2)], $\nabla_v \equiv \partial/\partial \mathbf{v}|_{\mathbf{x}, t}$ is the gradient in velocity space, and $\delta f/\delta t)_c \sim -\nu f$ represents the effects of “abrupt,” binary (microscopic) collisions at rate ν that result from force fields not included in \mathbf{F} .

The (mathematical) characteristics of the first order differential operator (in the 7 variables $\mathbf{x}, \mathbf{v}, t$) on the left of (A.77) represent the trajectories of the molecules in the absence of collision effects. The first order differential equations governing the trajectories of the particles can be most generally written using Hamilton’s equations. Thus, the kinetic equation for $f(\mathbf{q}, \mathbf{p}, t)$, where \mathbf{p} is the canonical momentum defined in (A.13) and \mathbf{q} is the canonically conjugate position vector or for $f(\mathbf{z}, t)$ where $\mathbf{z} \equiv (\mathbf{q}, \mathbf{p}) = (\mathbf{x}, \mathbf{p})$ is a six-dimensional variable that represents all of phase space, can be written most generally in terms of the Hamiltonian variables:

$$\frac{df(\mathbf{q}, \mathbf{p}, t)}{dt} = \frac{\partial f}{\partial t} + \frac{d\mathbf{q}}{dt} \cdot \frac{\partial f}{\partial \mathbf{q}} + \frac{d\mathbf{p}}{dt} \cdot \frac{\partial f}{\partial \mathbf{p}} = \left. \frac{\delta f}{\delta t} + \frac{d\mathbf{z}}{dt} \cdot \frac{\partial f}{\partial \mathbf{z}} \right)_c = \left. \frac{\delta f}{\delta t} \right)_c,$$

or, using Hamilton’s equations [see (A.15)], as

$$\frac{df(\mathbf{q}, \mathbf{p}, t)}{dt} = \left. \frac{\delta f}{\delta t} + \frac{\partial H}{\partial \mathbf{p}} \cdot \frac{\partial f}{\partial \mathbf{q}} - \frac{\partial H}{\partial \mathbf{q}} \cdot \frac{\partial f}{\partial \mathbf{p}} \right)_c = \left. \frac{\delta f}{\delta t} \right)_c, \quad \text{kinetic equation}, \quad (\text{A.78})$$

Particle motion in the $\mathbf{z} \equiv (\mathbf{p}, \mathbf{q})$ six-dimensional Hamiltonian phase space is incompressible:

$$\frac{\partial}{\partial \mathbf{z}} \cdot \frac{d\mathbf{z}}{dt} = \frac{\partial}{\partial \mathbf{x}} \cdot \frac{d\mathbf{x}}{dt} + \frac{\partial}{\partial \mathbf{p}} \cdot \frac{d\mathbf{p}}{dt} = \frac{\partial}{\partial \mathbf{x}} \cdot \frac{\partial H}{\partial \mathbf{p}} - \frac{\partial}{\partial \mathbf{p}} \cdot \frac{\partial H}{\partial \mathbf{x}} = 0,$$

phase space incompressibility. (A.79)

Thus, the kinetic equation can also be written in the “conservative” form

$$\frac{df(\mathbf{q}, \mathbf{p}, t)}{dt} = \frac{\partial f}{\partial t} + \frac{\partial}{\partial \mathbf{q}} \cdot \left(\frac{d\mathbf{q}}{dt} f \right) + \frac{\partial}{\partial \mathbf{p}} \cdot \left(\frac{d\mathbf{p}}{dt} f \right) = \frac{\partial f}{\partial t} + \frac{\partial}{\partial \mathbf{z}} \cdot \left(\frac{d\mathbf{z}}{dt} f \right) = \left(\frac{\delta f}{\delta t} \right)_c. \quad (\text{A.80})$$

In the absence of collisions, or for time scales shorter than the collision time, the solution of (A.77) or (A.78) is that f must be a function of the constants of the motion — see (A.18), (A.19). For “collisionless” cases where the potentials ϕ, \mathbf{A} do not change in time and the Hamiltonian is the only constant of motion, the solution is $f = f[H(\mathbf{p}, \mathbf{q})] = f[H(\mathbf{z})]$. Assuming further that there are a large number of molecules which are interacting weakly (e.g., via collisions) with an even larger number of molecules that have a thermodynamic temperature T , and hence that the requirements for the validity of statistical mechanics are satisfied, the distributions given in (A.67) and (A.68) can be derived from the kinetic theory of gases.

The microscopic binary collision effects are most generally represented by

$$\begin{aligned} \left(\frac{\delta f}{\delta t} \right)_c &= \mathcal{C}_B \{ f(\mathbf{x}, \mathbf{v}, t) \} \\ &\equiv \int d^3v' \int d\Omega \frac{d\sigma}{d\Omega} |\mathbf{v} - \mathbf{v}'| [f(\mathbf{v}_1)f(\mathbf{v}'_1) - f(\mathbf{v})f(\mathbf{v}')], \end{aligned}$$

Boltzmann collision operator, (A.81)

in which \mathbf{v}, \mathbf{v}' and $\mathbf{v}_1, \mathbf{v}'_1$ are the velocities of the colliding particles before and after the collision and $d\sigma/d\Omega$ is the differential scattering cross-section for the collisions [cf., (A.30)]. Here, for simplicity $f(\mathbf{x}, \mathbf{v}, t)$ has been written as $f(\mathbf{v})$ inside the collision operator. In deriving the Boltzmann collision operator it is assumed that the force \mathbf{F} on the left of (A.77) is negligible during the collision process, that the gas is sufficiently dilute so that binary or two-body collision processes are predominant (i.e., three-body and many-body collisions or collective particle interactions are negligible), and that the collisions only change the velocity vectors of the particles (i.e., the collisions abruptly scatter the velocity vectors of the particles at a given “point” \mathbf{x}, t along a particle trajectory). The Boltzmann collision operator is a bilinear [because of $f(\mathbf{v})f(\mathbf{v}')$], integral operator in velocity space. In the absence of radiative effects, since binary collisions conserve particle number, momentum $m\mathbf{v}$ and energy $mv^2/2$, so does the Boltzmann collision operator:

$$\int d^3v \Psi(\mathbf{v}) \mathcal{C}_B(f) = 0 \quad \text{for} \quad \Psi(\mathbf{v}) = 1, m\mathbf{v}, mv^2/2. \quad (\text{A.82})$$

The functions $\Psi(\mathbf{v})$ are sometimes called summational invariants because linear combinations of them are also invariants of the collision operator.

For homogeneous ($\nabla f = \mathbf{0}$) gases in equilibrium ($\partial f / \partial t = 0$) with no external forces on the molecules ($\mathbf{F} = \mathbf{0}$), the kinetic equation (A.77) becomes

$$0 = \left. \frac{\delta f}{\delta t} \right|_c = \mathcal{C}_B(f_0), \quad (\text{A.83})$$

where the subscript zero on f indicates the equilibrium or lowest order solution. The general solution of this equation is

$$f_0 = f_M(\mathbf{v}) = n_0 \left(\frac{m}{2\pi T_0} \right)^{3/2} e^{-m|\mathbf{v}-\mathbf{V}_0|^2/2T_0} = \frac{n_0 e^{-|\mathbf{v}-\mathbf{V}_0|^2/v_T^2}}{\pi^{3/2} v_T^3},$$

Maxwellian distribution. (A.84)

This Maxwellian differs from the statistical mechanics result in (A.70) only by its explicit inclusion of the macroscopic flow velocity \mathbf{V}_0 of the gas ($\mathbf{V}_0 \equiv \int d^3v \mathbf{v} f_0 / n_0$), which is not present in (A.70) because that result is obtained in the rest frame of the gas (i.e., in the \mathbf{V}_0 rest frame). However, the result is arrived at by different methodologies in statistical mechanics and kinetic theory. Kinetic theory provides the more extendable framework for investigating more complicated situations that do not satisfy the assumptions used in deriving (A.70) and (A.84).

The Boltzmann collision operator also has the important property of irreversibility: entropy increases until the distribution function is given by (A.84). Specifically, taking the entropy functional to be $-f \ln f$ and defining $H_B \equiv \int d^3v f \ln f$, it can be shown that

$$\frac{dH_B}{dt} = \int d^3v \frac{\partial f}{\partial t} (1 + \ln f) = \int d^3v \mathcal{C}_B(f) \ln f \leq 0,$$

Boltzmann H -theorem, (A.85)

with the equal sign being applicable only when f becomes equal to the equilibrium, Maxwellian distribution given in (A.84).

In situations close to thermodynamic equilibrium the lowest order distribution is the Maxwellian given by (A.84) and the distortions of the distribution function are higher order and small. In order to understand the nature of these distortions and to obtain approximate solutions of the kinetic equation (A.77) for this situation, consider the expansion of the distribution in a combination of Laguerre and Legendre polynomials (see Appendix B), which are the complete orthogonal basis functions for speed (with the weighting function $v^2 e^{-v^2/v_T^2}$ that comes from the lowest order Maxwellian distribution in spherical velocity space)

and spherical angle dependence::

$$\begin{aligned}
 f = f_M & \left(1 + \left[\frac{\delta n}{n_0} L_0^{(1/2)} + \frac{\delta T}{T_0} L_1^{(1/2)} + \dots \right] P_0 \left(\frac{\mathbf{v}}{v_T} \right) \text{ moments} \right. \\
 & + \frac{2}{v_T^2} \mathbf{v} \cdot \left[\delta \mathbf{V} L_0^{(3/2)} + \mathbf{V}_1 L_1^{(3/2)} + \dots \right] P_1 \left(\frac{\mathbf{v}}{v_T} \right) \text{ moments} \\
 & + \frac{\mathbf{v}\mathbf{v} - (v^2/3)\mathbf{I}}{2mn_0v_T^4} : \left[\boldsymbol{\pi} L_0^{(5/2)} + \boldsymbol{\pi}_1 L_1^{(5/2)} + \dots \right] P_2 \left(\frac{\mathbf{v}}{v_T} \right) \text{ moments} \\
 & \left. + \dots \right) \quad \quad \quad \vdots \\
 & = \sum_{lmn} f_{lmn} Y_{lm}(\vartheta, \varphi) L_n^{(l+1/2)}(v^2/v_T^2) e^{-v^2/v_T^2}, \quad \text{moment expansion, (A.86)}
 \end{aligned}$$

in which the $P_l(\mathbf{v}/v_T)$ are Legendre polynomial (spherical velocity space angular) functionals [$\equiv 1, \mathbf{v}/v_T, (\mathbf{v}\mathbf{v} - (v^2/3)\mathbf{I})/(2v_T^2/3)$ for $l = 0, 1, 2$], the $L_n^{(l+1/2)}(x)$ are (energy functional) Laguerre polynomials with arguments $x \equiv mv^2/2T = v^2/v_T^2$, and $Y_{lm}(\vartheta, \varphi)$ are the usual spherical harmonics that are proportional to $P_l^m(\cos\vartheta) e^{im\varphi}$. Useful properties of these special functions are given in B.5 and B.6. The lowest order parameters of this expansion, which are the $\int d^3v P_l(\mathbf{v}/v) L_n^{(l+1/2)}$ moments of the distribution function, correspond physically to: the density (m^{-3}), flow velocity (m/s) and temperature (eV) distortions $\delta n, \delta \mathbf{V}$ and δT away from their equilibrium Maxwellian values of n_0, \mathbf{V}_0 and T_0 ; the heat flow vector \mathbf{q} (W/m^2), since $\mathbf{V}_1 \equiv -2\mathbf{q}/5nT$; and the traceless anisotropic part $\boldsymbol{\pi}$ (N/m^2) of the pressure tensor [see (A.95) below], which has 5 nonvanishing parameters and is sometimes called a kinetic stress tensor. An approximation in which the moments $\delta n, \delta \mathbf{V}, \delta T, \mathbf{q}$ and $\boldsymbol{\pi}$ ($= 1 + 3 + 1 + 3 + 5 = 13$ moments) are used to represent f is usually called a Grad 13 moment approximation.

Often one desires a reduced, fluid moment description which integrates the kinetic equation over velocity space to obtain equations for the physical quantities of density, flow velocity and temperature:

$$\text{density (m}^{-3}\text{):} \quad n(\mathbf{x}, t) = n_0 + \delta n \equiv \int d^3v f, \quad (\text{A.87})$$

$$\text{flow velocity (m/s):} \quad \mathbf{V}(\mathbf{x}, t) = \mathbf{V}_0 + \delta \mathbf{V} \equiv \int d^3v \mathbf{v} f/n, \quad (\text{A.88})$$

$$\text{temperature (eV):} \quad T(\mathbf{x}, t) = T_0 + \delta T \equiv \int d^3v [m(\mathbf{v} - \mathbf{V}^2)/3] f/n. \quad (\text{A.89})$$

The relevant fluid moment equations for these quantities are obtained by taking the relevant velocity-space moments [i.e., the $\Psi(\mathbf{v})$ in (A.82)] of the kinetic

equation in (A.77) using the Boltzmann collision operator in (A.81) and the conservation properties in (A.82), to obtain

$$\text{density equation: } \frac{\partial n}{\partial t} + \nabla \cdot n \mathbf{V} = 0, \quad (\text{A.90})$$

$$\text{momentum equation: } mn \frac{d\mathbf{V}}{dt} = n \bar{\mathbf{F}} - \nabla p - \nabla \cdot \boldsymbol{\pi}, \quad (\text{A.91})$$

$$\text{energy equation: } \frac{3}{2}n \frac{dT}{dt} + p \nabla \cdot \mathbf{V} = -\nabla \cdot \mathbf{q} - \boldsymbol{\pi} : \nabla \mathbf{V}, \quad (\text{A.92})$$

where

$$\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla, \quad \text{total time derivative,} \quad (\text{A.93})$$

is the total (partial plus flow-induced advection⁴) time derivative that is sometimes called the “material derivative,” and $\bar{\mathbf{F}}$ is the average of the single particle force \mathbf{F} over a Maxwellian distribution. The higher order moments needed for closure (complete specification) of these equations are

$$\text{pressure (N/m}^2\text{): } p \equiv \int d^3v \left(\frac{m}{3} |\mathbf{v}_r|^2 \right) f = nT, \quad (\text{A.94})$$

$$\text{conductive heat flux (W/m}^2\text{): } \mathbf{q} \equiv \int d^3v \mathbf{v}_r \left(\frac{m}{2} |\mathbf{v}_r|^2 - \frac{5T}{2} \right) f, \quad (\text{A.95})$$

$$\begin{aligned} \text{stress tensor (N/m}^2\text{): } \boldsymbol{\pi} &\equiv \int d^3v m \left(\mathbf{v}_r \mathbf{v}_r - \frac{1}{3} |\mathbf{v}_r|^2 \mathbf{I} \right) f, \quad (\text{A.96}) \\ &= \int d^3v m \mathbf{v}_r \mathbf{v}_r f - p \mathbf{I} \equiv \mathbf{P} - p \mathbf{I} \end{aligned}$$

in which $\mathbf{v}_r \equiv \mathbf{v} - \mathbf{V}(\mathbf{x}, t)$ is the relative velocity in the frame of reference moving at the macroscopic flow velocity \mathbf{V} . Note also that $\mathbf{q} = -T \int d^3v \mathbf{v}_r L_1^{(3/2)} f$. The total heat flux $\mathbf{Q} \equiv \int d^3v (m |\mathbf{v}_r|^2 / 2) \mathbf{v}_r f$ is the sum of the conductive heat flux and the convective heat flux: $\mathbf{Q} \equiv \mathbf{q} + (5/2)nT\mathbf{V}$.

The Chapman-Enskog procedure is used to obtain the needed closure relations for “collision-dominated” situations in which the gas density varies slowly in space (compared to the collision mean free path $\lambda \sim v/\nu$) and time (compared to the collision time $1/\nu$). Then, the lowest order kinetic equation that describes the distribution function is given by (A.83). Its solution is

$$f_0^{C-E} = f_M(\mathbf{x}, \mathbf{v}, t) \equiv n(\mathbf{x}, t) \left[\frac{m}{2\pi T(\mathbf{x}, t)} \right]^{3/2} \exp \left[-\frac{|\mathbf{v} - \mathbf{V}(\mathbf{x}, t)|^2}{2T(\mathbf{x}, t)} \right],$$

“dynamic” Maxwellian, (A.97)

which is the usual Maxwellian, but now parameterized in terms of the (total) spatially and temporally varying density, flow velocity and temperature. The

⁴In fluid mechanics advection means transport of any quantity by the fluid at its flow velocity \mathbf{V} ; convection refers only to the heat flow $\mathbf{q}_{\text{conv}} = (5/2)nT\mathbf{V}$ induced by \mathbf{V} .

conductive heat flux \mathbf{q} and anisotropic stress $\boldsymbol{\pi}$ vanish for f_0^{C-E} . Thus, in order to determine these needed closure relations, it is necessary to determine the first order distortion of the distribution function: $\delta f \equiv f - f_0^{C-E}$. (Note that, by construction, since the total density n flow velocity \mathbf{V} and temperature T are built into f_0^{C-E} , the density, momentum and energy moments of δf vanish:

$$\int d^3v \delta f = 0, \quad \int d^3v m \mathbf{v} \delta f = 0, \quad \int d^3v (mv^2/2) \delta f = 0, \quad \text{C-E constraints.} \quad (\text{A.98})$$

The kinetic equation for δf is obtained by substituting the definition $f = f_0^{C-E} + \delta f$ into (A.77), making use of the density, momentum and energy conservation equations to remove the dependences on $\partial n / \partial t$, $\partial \mathbf{V} / \partial t$ and $\partial T / \partial t$. Neglecting higher order corrections that are inversely proportional to the collision frequency, the result is

$$\mathcal{C}_B(\delta f) \simeq \left[\left(\frac{m |\mathbf{v}_r|^2}{2T} - \frac{5}{2} \right) \mathbf{v}_r \cdot \left(\frac{1}{T} \boldsymbol{\nabla} T \right) + \frac{m}{T} \mathbf{W} : \left(\mathbf{v}_r \mathbf{v}_r - \frac{|\mathbf{v}_r|^2}{3} \mathbf{I} \right) \right] f_0^{C-E}, \quad (\text{A.99})$$

in which, as above, $\mathbf{v}_r \equiv \mathbf{v} - \mathbf{V}(\mathbf{x}, t)$, and

$$\mathbf{W} \equiv \frac{1}{2} [\boldsymbol{\nabla} \mathbf{V} + (\boldsymbol{\nabla} \mathbf{V})^\top] - \frac{1}{3} \mathbf{I} (\boldsymbol{\nabla} \cdot \mathbf{V}), \quad \text{rate of strain tensor,} \quad (\text{A.100})$$

which is caused by gradients in the flow velocity \mathbf{V} and has units of per second. The normalized temperature gradient $\boldsymbol{\nabla} \ln T$ and rate-of-strain tensor \mathbf{W} are called thermodynamic forces — because they induce distortions δf of the distribution function away from a dynamic Maxwellian and hence away from thermodynamic equilibrium. Note that because of the invariants of the Boltzmann collision operator given in (A.82), a proper solution of (A.99) for δf will satisfy the Chapman-Enskog constraints in (A.98).

The Boltzmann collision operator needs to be specified in detail in order to properly solve (A.99). However, the nature of the solution for δf can be exhibited by using an approximate collision model:

$$\mathcal{C}_K(\delta f) = -\nu \delta f \equiv -\nu (f - f_0^{C-E}), \quad \text{Krook-type collision operator} \quad (\text{A.101})$$

in which

$$\nu \equiv n \overline{\sigma v}, \quad \text{collision frequency,} \quad (\text{A.102})$$

where the overbar indicates the “reaction rate” σv has been averaged over a Maxwellian distribution. Using this collision operator in (A.99), solving for δf and using the definitions in (A.95) and (A.96) yields the needed closure (constitutive) relations for the fluid moment equations (A.90)–(A.92):

$$\mathbf{q} = -\kappa^m \boldsymbol{\nabla} T, \quad \kappa^m \equiv n \chi^m, \quad \chi^m = \frac{5}{4} \frac{v_T^2}{\nu} = \frac{5}{4} \nu \lambda^2, \quad \text{conductive heat flux,} \quad (\text{A.103})$$

which is in the form of a Fourier law for the heat flux and

$$\boldsymbol{\pi} = -2\mu^m \mathbf{W}, \quad \mu^m = \frac{1}{2} nm \frac{v_T^2}{\nu} = \frac{1}{2} nm \nu \lambda^2, \quad \text{viscous stress,} \quad (\text{A.104})$$

in which

$$\lambda \equiv v_T/\nu, \quad \text{collision mean free path,} \quad (\text{A.105})$$

has been defined for thermal molecules. In these closure relations, κ^m is the heat conduction coefficient, χ^m is the heat diffusivity and μ^m is the viscosity coefficient. The superscript m on the various coefficients indicate that they arise from the microscopic (molecular) processes of discrete collisions in the gas. Equations (A.103) and (A.104) give the thermodynamic fluxes $\mathbf{q}, \boldsymbol{\pi}$ induced by the thermodynamic forces $\nabla T, \mathbf{W}$. If the appropriate Boltzmann collision operator is used instead of the approximate Krook-type model of (A.101), the scaling of the κ^m , χ^m , and μ^m “molecular diffusion” coefficients with collision frequency and thermal speed remains the same; however the numerical factors in (A.103) and (A.104) change slightly.

The reference cross section σ for atomic and molecular collisions is $\sigma_0 \equiv \pi a_0^2 \sim 10^{-20} \text{ m}^2$ in which a_0 is the Bohr (atomic) radius (A.154). For standard temperature and pressure (STP) air at the earth’s surface, the average cross section for molecular collisions is $\sigma \sim 40 \sigma_0 \sim 4 \times 10^{-19} \text{ m}^2$, the density is $n_n \sim 2.5 \times 10^{25} \text{ m}^{-3}$, and the thermal speed is $v_T \sim 300 \text{ m/s}$. Thus, for standard air $\nu \sim n\sigma v_T \sim 3 \times 10^9 \text{ s}^{-1}$, $\lambda \sim v_T/\nu \sim 10^{-7} \text{ m}$, and $\mu^m/nm \sim \nu \lambda^2/2 \sim 1.5 \times 10^{-5} \text{ m}^2/\text{s}$, $\chi^m \sim (5/2)(\mu^m/nm)$.

The Chapman-Enskog analysis is valid as long as the collision mean free path is short compared to the gradient scale lengths (i.e., $\lambda |\nabla \ln T| \ll 1$, $\lambda |\nabla \mathbf{V}|/|\mathbf{V}| \ll 1$) and temporal variations are slow compared to the collision time [e.g., $\nu^{-1}(\partial \ln n/\partial t) \ll 1$]. Substituting the closure relations given in (A.103) and (A.104) into the momentum and energy conservation equations yields (neglecting for simplicity the small effects due to gradients of the transport coefficients κ^m and μ^m):

$$mn \frac{d\mathbf{V}}{dt} = n\bar{\mathbf{F}} - \nabla \left(p - \frac{\mu^m}{3} \nabla \cdot \mathbf{V} \right) + \mu^m \nabla^2 \mathbf{V}, \quad (\text{A.106})$$

$$\frac{3}{2} \frac{dT}{dt} + T(\nabla \cdot \mathbf{V}) = \chi^m \nabla^2 T + 2 \frac{\mu^m}{n} |\mathbf{W}|^2. \quad (\text{A.107})$$

The diffusive components of these equations indicate that the “molecular” diffusion coefficients for momentum (viscous) and heat diffusion are μ^m/nm and χ^m , both of which scale as $\nu \lambda^2$ and have units of m^2/s . A physical interpretation of the processes and parametric scalings that underly these diffusion coefficients are given in the next section.

An equation can also be developed for the evolution of the collisional entropy s which is dimensionless and is defined in kinetic theory for $f \simeq f_0^{C-E}$ by

$$s \equiv -\frac{1}{n} \int d^3v f \ln f = \ln \left(\frac{T^{3/2}}{n} \right) + \text{constant}, \quad \text{collisional entropy.} \quad (\text{A.108})$$

Note that this entropy is the negative of the Boltzmann H_B function [see (A.85)] and yields the same result as that obtained from equilibrium statistical mechanics [see (A.76)]. Taking the total time derivative of this equation yields, upon substituting in (A.90) and (A.92),

$$\begin{aligned} nT \frac{ds}{dt} &= \frac{3}{2}n \frac{dT}{dt} - T \frac{dn}{dt} = T \left[\frac{\partial(ns)}{\partial t} + \nabla \cdot (ns\mathbf{V}) \right] \\ &= -\nabla \cdot \mathbf{q} - \boldsymbol{\pi} : \nabla \mathbf{V}, \quad \text{entropy evolution.} \end{aligned} \quad (\text{A.109})$$

Alternatively, since the flow of entropy density (entropy flux) is $ns\mathbf{V} + \mathbf{q}/T$, after using the density conservation relation (A.90) and the rate-of-strain tensor definition (A.100),

$$\partial(ns)/\partial t + \nabla \cdot (ns\mathbf{V} + \mathbf{q}/T) = \theta \equiv -(1/T) [\mathbf{q} \cdot \nabla \ln T + \boldsymbol{\pi} : \mathbf{W}] \quad (\text{A.110})$$

in which θ represents the rate of entropy production due to dissipative (irreversible) processes, which is positive definite and caused by the thermodynamic fluxes \mathbf{q} , $\boldsymbol{\pi}$ flowing in response to the thermodynamic forces $\nabla \ln T$, \mathbf{W} .

For the closure relations given in (A.103) and (A.104) the entropy production rate simplifies to (again neglecting gradients in the transport coefficients κ^m, μ^m):

$$\theta = n \chi^m |\nabla \ln T|^2 + 2 \mu^m |\mathbf{W}|^2, \quad \text{entropy production rate.} \quad (\text{A.111})$$

Thus, entropy is produced by the microscopic collisional processes that diffusively relax the gradients of the temperature and flow velocity in the gas. The entropy production rate is small under the Chapman-Enskog approximations (large ν , small $\lambda = v_T/\nu$): $ds/dt \sim \nu \lambda^2 |\nabla \ln T|^2 \ll \nu$ if heat conduction effects are dominant, or $ds/dt \sim \nu \lambda^2 |\nabla \mathbf{V}|^2 / v_T^2 \ll \nu$ if viscous flow damping is dominant. Hence, for processes that are rapid compared to the collisional entropy production rate and where the entropy flow induced by the conductive heat flux \mathbf{q} is negligible (e.g., in a constant temperature gas), it is sufficient to use the ‘‘adiabatic’’ or isentropic (i.e., non-dissipative, constant entropy) equation of state for an ideal gas obtained from setting $ds/dt = 0$:

$$\begin{aligned} \frac{d}{dt} \ln \left(\frac{T^{3/2}}{n} \right) = \frac{d}{dt} \ln \left(\frac{p^{3/2}}{n^{5/2}} \right) = 0 \quad \implies \quad \frac{p}{n^\Gamma} = \text{constant}, \\ \text{isentropic (‘‘adiabatic’’) equation of state,} \end{aligned} \quad (\text{A.112})$$

where Γ is 5/3 for the three-dimensional system being considered, but in general is given by $\Gamma = (N + 2)/N$ in which N is the number of degrees of freedom in the system. [In thermodynamics $\Gamma \equiv c_P/c_V$ is the ratio of the heat capacity ($\equiv \partial u/\partial T$) at constant pressure to that at constant volume.] Note that for a constant density gas of volume $V = 1/n$, (A.112) becomes the familiar equation of state for an ideal gas: $pV^\Gamma = \text{constant}$. The adiabatic or isentropic equation of state can be used in place of the energy balance equation (A.92) or (A.107) for studies of rapid, isentropic processes because there is no significant entropy production or heat flow for such processes.

Most of the previously noted standard textbooks on statistical mechanics provide intermediate level descriptions of the kinetic theory of gases. Advanced level textbooks and monographs that deal specifically with the kinetic theory of gases include:

Chapman and Cowling, *The Mathematical Theory of Non-Uniform Gases* (1952) [?]

H. Grad, "Principles of the Kinetic Theory of Gases," in *Handbuch der Physik*, Volume 12 (Springer-Verlag, Berlin, 1957) [?]

R. Herdan and B. S. Liley, "Dynamical Equations and Transport Relationships for a Thermal Plasma," *Rev. Mod. Phys.* **32**, 731 (1960). [?]

A.5 Stochastic Processes, Diffusion

The heat and momentum diffusion produced by the collision-induced random steps or motions of molecules in a gas can be understood in terms of a stochastic or random walk process. Such processes are often called Brownian motion (after a botanist Robert Brown who, in 1827, observed irregular motions of small colloidal size particles immersed in a fluid), or more formally a Markoff process (no memory of previous history or steps).

For a simple one-dimensional mathematical model of the random walk process, assume that between collisions (or another random process) a molecule moves a distance Δx in a random direction (to the right or left) in a time Δt . For such a process the position x_n of a molecule after the n^{th} step is related to the position x_{n-1} after the previous step by

$$x_n = x_{n-1} + R_n \Delta x \quad (\text{A.113})$$

in which R_n is randomly ± 1 . Using this mapping equation as a recursion relation, one finds that after N random steps the difference of the final position x_N from the initial position x_0 becomes

$$x_N = x_0 + \Delta x \sum_{n=1}^N R_n. \quad (\text{A.114})$$

In the limit of a large number N of random steps one obtains:

$$\lim_{N \rightarrow \infty} \left| \frac{x_N - x_0}{N \Delta x} \right| = \lim_{N \rightarrow \infty} \frac{|\sum_n R_n|}{N} = \lim_{N \rightarrow \infty} \frac{\mathcal{O}(1)}{N} = 0, \quad (\text{A.115})$$

because R_n is randomly ± 1 . Thus, after a large number N of random steps the average position of a molecule does not deviate much ($\ll N \Delta x$) from its initial position x_0 .

However, as illustrated in Fig. A.2, the random steps do have an effect: they cause such molecules to wander randomly in the x direction, to ever larger distances from x_0 as the number N of random steps increases. Thus, after a large number of random steps the position of a molecule is described by a probability

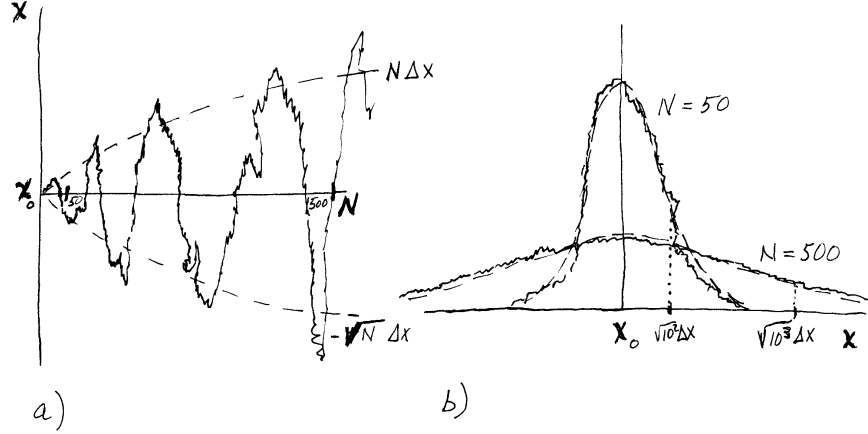


Figure A.2: Illustration of the random walk process of molecules stepping a distance Δx randomly to larger or smaller x for a total of $N = [t/\Delta t]$ steps: a) an example of a detailed particle trajectory; b) distribution of particle positions over the N steps. The smooth dashed curves represent the $N \rightarrow \infty$ analytic formulas given in (A.117) and (A.122) with $\Delta = 4Dt \rightarrow \Delta x\sqrt{2N}$.

distribution peaked at the initial position x_0 with a spatial spread that increases with N and a peak magnitude that decreases with N — see Fig. A.2.

To quantify the spatial spreading effect, and hence the width of the probability distribution, one uses the first form of (A.114) to calculate the square of the difference of the final from the initial spatial position:

$$(x_N - x_0)^2 = (\Delta x)^2 \left(\sum_{n=1}^N R_n \right)^2 = (\Delta x)^2 \left[\sum_{n=1}^N R_n^2 + \sum_{i=1}^N R_i \sum_{n \neq i}^N R_n \right]. \quad (\text{A.116})$$

In the limit of a large number N of random steps, the mean spread is given by

$$\lim_{N \rightarrow \infty} \frac{(x_N - x_0)^2}{N(\Delta x)^2} = \lim_{N \rightarrow \infty} \frac{1}{N} \left[\sum_{n=1}^N R_n^2 + \sum_{i=1}^N R_i \sum_{n \neq i}^N R_n \right] = \lim_{N \rightarrow \infty} \frac{N + \mathcal{O}(1)}{N} = 1, \quad (\text{A.117})$$

because $R_n^2 = (\pm 1)^2 = 1$. Hence, the average square of the spatial spreading after a large number N of random steps (or a time $t = N\Delta t$) will be given by

$$(x_N - x_0)^2 \simeq N(\Delta x)^2 = t \frac{(\Delta x)^2}{\Delta t}, \quad \text{or} \quad \frac{d(x_N - x_0)^2}{dt} \simeq \frac{(\Delta x)^2}{\Delta t}. \quad (\text{A.118})$$

In summary, a random walk process produces a spatial spreading, which is called stochastic diffusion or simply diffusion, of molecules about their initial position, but no net motion of the average position of the molecules.

However, in an *inhomogeneous* medium there is, on average, a net motion or flux of particles. The particle transport flux produced by a large number of molecules undergoing such random walk processes in a neutral gas with a spatially varying density $n = n(x)$ can be obtained as follows. In a time Δt the plane $x = x_0$ will be traversed by the half (on average) of the molecules that experience collisions in the layer between $x_0 - \Delta x$ and x_0 , and which are moving to the right (+). Thus, the flux ($\Gamma \equiv nV = n dx/dt$) of molecules moving to the right is

$$\Gamma_+ = \frac{1}{2} \int_{x_0 - \Delta x}^{x_0} n(x) \frac{dx}{\Delta t} = \frac{\Delta x}{2\Delta t} \left[n(x_0) - \frac{\Delta x}{2} \frac{dn}{dx} \Big|_{x_0} + \dots \right]$$

in which the density $n(x)$ has been expanded in a Taylor series about x_0 . Similarly, the flux of molecules moving through the $x = x_0$ plane to the left (−) is

$$\Gamma_- = \frac{1}{2} \int_{x_0}^{x_0 + \Delta x} n(x) \frac{dx}{\Delta t} = \frac{\Delta x}{2\Delta t} \left[n(x_0) + \frac{\Delta x}{2} \frac{dn}{dx} \Big|_{x_0} + \dots \right].$$

The net particle flux is the difference between these two fluxes:

$$\Gamma = \Gamma_+ - \Gamma_- = -D \frac{dn}{dx} \Big|_{x_0}, \quad \text{Fick's diffusion law.} \quad (\text{A.119})$$

For the simple model being considered D is given by

$$D = \frac{(\Delta x)^2}{2\Delta t}, \quad \text{diffusion coefficient,} \quad (\text{A.120})$$

which has units of m^2/s . Thus, the diffusion coefficient D is half the rate of spatial spreading for a random walk process — see (A.118).

The natural step size Δx for the motion of molecules between collisions in a neutral gas is λ , the collision mean free path. The characteristic time Δt between collisions of molecules is $1/\nu$. Thus, one infers from (A.120) that the scaling of diffusivities induced by molecular collisions should be $D \sim \nu\lambda^2$, which was what was obtained in (A.103) and (A.104) in the preceding section. In a monoatomic neutral gas there are heat and momentum diffusivities but there is no particle diffusivity (or particle flux Γ) because, while two colliding molecules exchange energy and momentum during the molecular collisions, the density of molecules is usually unchanged as a result of the collisions.

In more realistic situations different molecules may have different Δx and Δt values; then one must take an appropriate average and $D = \langle (\Delta x)^2 \rangle / (2\Delta t)$. Since the parametric scaling of the diffusion coefficient is quite general, but appropriate averages are often difficult to formulate or evaluate for various physical processes, the expression for D in (A.120) is mostly used to infer the scaling of the diffusion coefficient with physical parameters. Then, kinetic calculations are used to obtain the relevant numerical coefficients — the “headache factors.”

In the presence of this random walk process induced by molecular collisions, the equation for the density $n(x, t)$ [see (A.90)] becomes $\partial n/\partial t + \partial(nV_x)/\partial x = 0$. Using the Fick's diffusion law (A.116) for $nV_x = \Gamma$ yields a one-dimensional diffusion equation:

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x} D \frac{\partial n}{\partial x}, \quad \text{diffusion equation.} \quad (\text{A.121})$$

To illustrate the properties of solutions of this equation, imagine that a small number δN of molecules are added to the medium at the position x_0 : $n(x, 0) = \delta N \delta(x - x_0)$. After a short time, the appropriate (Green-function-type) solution of (A.121) is

$$n(x, t) = \delta N \frac{e^{-(x-x_0)^2/4Dt}}{\sqrt{\pi}\sqrt{4Dt}}, \quad \text{short-time diffusive distribution,} \quad (\text{A.122})$$

as can be verified by direct substitution. Note that this distribution of particles has the desired properties for a random walk process and represents it well in the $N \rightarrow \infty$ limit — see Fig. A.2b. In particular, it is peaked at $x = x_0$ and spreads spatially and decreases in magnitude as time progresses. In a time t (assumed $\gg \Delta t$) the average spreading of the molecules in the x direction is

$$\overline{(x - x_0)^2} \equiv \frac{\int_{-\infty}^{\infty} dx (x - x_0)^2 n(x, t)}{\int_{-\infty}^{\infty} dx n(x, t)} = 4Dt \frac{\int_0^{\infty} dy y^2 e^{-y^2}}{\int_0^{\infty} dy e^{-y^2}} = 2Dt = \frac{(\Delta x)^2}{\Delta t} t \quad (\text{A.123})$$

in which $y \equiv (x - x_0)/\sqrt{4Dt}$ and the integrals have been evaluated using (??). Note that this rate of spatial spreading of the density agrees with that inferred above for the random walk process of a molecule — (A.118).

The Gaussian character of this distribution can be emphasized by writing the short time diffusive density response in (A.122) in the form

$$n(x, t) = \delta N \frac{e^{-(x-x_0)^2/\Delta^2}}{\sqrt{\pi} \Delta}, \quad \Delta \equiv \sqrt{4Dt}. \quad (\text{A.124})$$

In this form one readily sees from (??) that in the $t \rightarrow 0$ limit the solution becomes a delta function (see Section B.2) at $x = x_0$: $\lim_{t \rightarrow 0} n(x, t) = \delta N \delta(x - x_0)$, which was the initial condition. Also, in terms of Δ the root mean square spatial spread becomes simply

$$\delta x_{\text{rms}} \equiv \left(\overline{(x - x_0)^2} \right)^{1/2} = \sqrt{2Dt} = \frac{\Delta}{\sqrt{2}} = \Delta x \sqrt{\frac{t}{\Delta t}} = \Delta x \sqrt{N},$$

root mean square spatial spread. (A.125)

The last result shows that, as indicated in Fig. A.2, the spatial spreading is proportional to the square root of the number of random walk steps.

Using these formulas, note also that the average time t required for molecules to diffuse a distance $\delta x \equiv x - x_0$ from the initial position x_0 is

$$t \sim \frac{(\delta x)^2}{2D} \sim \left(\frac{\delta x}{\Delta x} \right)^2 \Delta t, \quad \text{time to diffuse a distance } \delta x. \quad (\text{A.126})$$

Hence, the time t required to diffuse a short distance δx is the product of the basic random walk time Δt times $(\delta x/\Delta x)^2$ — the *square* of the number of random walk steps Δx in the distance δx to be traversed. This quadratic dependence of the spreading time on the spreading distance is an intrinsic property of diffusive processes. As a caveat on this analysis, note that the solution (A.122) is only valid for short times: $t < L_n^2/D \sim (L_n/\Delta x)^2 \Delta t$ — so the background medium density and diffusion coefficient are reasonably constant over the distance $\Delta/\sqrt{2} = \sqrt{2Dt} = \Delta x \sqrt{t/\Delta t}$ that typical particles spread over in the time t [i.e., $(\Delta/n)(dn/dx) \equiv \Delta/L_n \ll 1$ and $(\Delta/D)(dD/dx) \ll 1$].

In a finite box, as time progresses molecules eventually diffuse to the boundaries of the box where it will be assumed the molecules are absorbed. The question then becomes: what is the average confinement time for molecules in the box? Assume for simplicity that: the diffusion coefficient is constant in space; a one-dimensional treatment is sufficient; δN molecules are inserted at the center ($x = 0$) of a box of width $2L$ (assumed $\gg \Delta x = \lambda$) at time $t = 0$; and the density of molecules vanishes at the box boundaries ($x = \pm L$). Then, the solution of the diffusion equation (A.121) for this boundary value problem can be shown (by separation of variables, expansion in sinusoidal eigenfunctions) to be

$$n(x, t) = \frac{\delta N}{L} \sum_{j=0}^{\infty} e^{-t/\tau_j} \cos\left(\lambda_j \frac{x}{L}\right), \quad \text{with } \lambda_j \equiv \frac{(2j+1)\pi}{2}, \quad \tau_j \equiv \frac{L^2}{\lambda_j^2 D}. \quad (\text{A.127})$$

For short times ($t \ll \tau_0$) the box boundaries at $x = \pm L$ are unimportant and this solution reduces to (A.124), which is a more convenient form then. For intermediate times ($t \sim \tau_j$) the sinusoidal eigenfunctions (up to at least $2j$) must be summed to obtain the response. In the time asymptotic limit ($t > \tau_0 > \tau_1 > \tau_2 \dots$) the lowest order eigenmode solution dominates:

$$n(x, t) \stackrel{t \gg \tau_0}{\simeq} \frac{\delta N}{L} e^{-t/\tau_0} \cos\left(\frac{\pi x}{2L}\right). \quad (\text{A.128})$$

Thus, an average "confinement time" for molecules in the box can be identified as

$$\tau_0 \equiv \frac{L^2}{\lambda_0^2 D} = \frac{L^2}{(\pi/2)^2 D} \simeq \frac{L^2}{2.5D}, \quad \text{confinement time.} \quad (\text{A.129})$$

Note that upon using $D = (\Delta x)^2/2\Delta t$ one obtains $\tau_0 = (2/\lambda_0^2)(L/\Delta x)^2 \Delta t$, which quantifies (for this specific case where $\delta x \rightarrow L, t \rightarrow \tau_0$) the "headache factors" in the scaling relation (A.126). For cylindrical, spherical "boxes" the

eigenfunctions are Bessel, spherical Bessel functions and the lowest order eigenvalues are $\lambda_0 \simeq 2.405$, $\lambda_0 = \pi$, respectively. Then, using a as the radius of the “box,” one obtains confinement times of $\tau_0 \simeq a^2/6D$, $a^2/10D$ for cylindrical, spherical systems, respectively.

Many of the references noted at the end of the two preceding sections have discussions of random walk (Brownian motion) and stochastic diffusion processes. The classic and ageless reference for such processes is:

S. Chandrasekhar, “Stochastic Problems in Physics and Astronomy,” *Rev. Mod. Phys.* **15**, 1 (1943). [?]

A.6 Fluid Mechanics

The equations of “hydrodynamics” used to describe the behavior of a fluid are the fluid moment equations obtained from the kinetic theory of gases — (A.90), (A.91) and (A.112). However, they are usually modified by writing them in terms of the mass density $\rho_m \equiv n m$, which has units of kg/m^3 :

$$\text{mass continuity equation: } \frac{\partial \rho_m}{\partial t} + \nabla \cdot \rho_m \mathbf{V} = 0, \quad (\text{A.130})$$

$$\begin{aligned} \text{Navier-Stokes equation: } & \rho_m \frac{d\mathbf{V}}{dt} = \rho_m \frac{\bar{\mathbf{F}}}{m} - \nabla p' + \mu^m \nabla^2 \mathbf{V}, \quad (\text{A.131}) \\ & (\text{momentum balance}) \end{aligned}$$

$$\text{isentropic equation of state: } \frac{d}{dt} \ln \left(\frac{p}{\rho_m^{\bar{\Gamma}}} \right) = 0, \quad (\text{A.132})$$

in which $p' \equiv p - (\mu^m/3)\nabla \cdot \mathbf{V}$. (The equation of state is often called the “adiabatic” equation of state in hydrodynamics.) In these equations d/dt is the total time derivative taking account both of the direct temporal derivative and the effects of the advection by the flow velocity \mathbf{V} in the fluid:

$$\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla, \quad \text{total time derivative.} \quad (\text{A.133})$$

For gases or liquids in the earth’s atmosphere the relevant force on molecules is the gravitational force, which is a conservative force:

$$\bar{\mathbf{F}}_G = \mathbf{F}_G = -m \nabla V_G \simeq -mg \hat{\mathbf{e}}_x \equiv m \mathbf{g}, \quad \text{gravitational force,} \quad (\text{A.134})$$

where $V_G = -M_E G/R$ is the gravitational potential. In the last expression use has been made of the fact that near the earth’s surface ($x \equiv R - R_E \ll R_E$, radius of the earth) one has $V_G \simeq -(M_E G/R_E^2)(R_E - x + \dots)$. Also, here, $g \equiv (M_E G/R_E^2) \simeq 9.81 \text{ m/s}^2$ is the gravitational acceleration at the earth’s surface.

The velocity flow field \mathbf{V} can in general be decomposed into parts representable in terms of scalar, vector potentials ψ , \mathbf{C} (see Section D.5):

$$\mathbf{V} = -\nabla \psi + \nabla \times \mathbf{C}, \quad \text{potential representation of a flow field.} \quad (\text{A.135})$$

The scalar potential part represents the longitudinal, irrotational or compressible part of the flow since $\nabla \cdot \mathbf{V} = -\nabla \cdot \nabla \psi = -\nabla^2 \psi$. The vector potential part is incompressible since $\nabla \cdot \nabla \times \mathbf{C} = 0$. However, this component represents “rotation” or vorticity⁵ (units of s^{-1}) in the flow:

$$\boldsymbol{\omega} \equiv \nabla \times \mathbf{V} = \nabla \times (\nabla \times \mathbf{C}), \quad \text{vorticity.} \quad (\text{A.136})$$

The properties of sound waves in a fluid can be illustrated by considering compressible perturbations of air in the earth’s atmosphere. The equilibrium pressure distribution is determined from the “hydrostatic” force balance equilibrium, which is the equilibrium ($\partial/\partial t = 0$) and small viscosity limit of the Navier-Stokes equation that in the absence of equilibrium flows ($\mathbf{V}_0 = \mathbf{0}$) becomes simply:

$$\mathbf{0} = -\rho_{m0} \nabla V_G - \nabla p_0.$$

Assuming for simplicity that the temperature T is constant, taking x to be the vertical distance above the earth’s surface, and using $p = nT = \rho_{m0}T/m$ (Boyle’s law for this situation), the hydrostatic equilibrium becomes

$$0 = -\rho_{m0}g - \frac{T}{m} \frac{d\rho_{m0}}{dx} \quad \implies \quad \rho_{m0}(x) = \rho_{m0}(0) e^{-mgx/T},$$

law of atmospheres. (A.137)

Thus, in equilibrium the density of air decreases with distance above the surface of the earth on a scale length of $T/mg = v_T^2/2g \sim 10^4$ m.

To exhibit the properties of sound waves consider perturbations of the compressible air in this equilibrium:

$$\rho_m = \rho_{m0} + \tilde{\rho}_m, \quad \mathbf{V} = \tilde{\mathbf{V}}, \quad p = p_0 + \tilde{p}, \quad \text{perturbed equilibrium,} \quad (\text{A.138})$$

in which the tilde over a quantity indicates the perturbation in that quantity. Substituting these forms into the fluid equations (A.130)–(A.132) yields, upon neglecting the effect of gravity for simplicity and linearizing the equations (i.e., neglecting all quantities that are quadratic or higher order in the perturbations):

$$\frac{\partial \tilde{\rho}_m}{\partial t} + \rho_{m0} \nabla \cdot \tilde{\mathbf{V}} + \tilde{\mathbf{V}} \cdot \nabla \rho_{m0} = 0, \quad \rho_{m0} \frac{\partial \tilde{\mathbf{V}}}{\partial t} = -\nabla \tilde{p} + \mu^m \nabla^2 \tilde{\mathbf{V}}, \quad \tilde{p} = c_S^{H^2} \tilde{\rho}_m$$

where

$$c_S^H \equiv \sqrt{\Gamma p_0 / \rho_{m0}} = \sqrt{\Gamma T / m}, \quad \text{hydrodynamic sound speed,} \quad (\text{A.139})$$

which is typically about 340 m/s at the earth’s surface. Note that for a neutral gas $c_S^H = \sqrt{\Gamma/2} v_T$. For an equilibrium that is approximately homogeneous over the collision mean free path λ ($\lambda |\nabla \ln \rho_{m0}| \ll 1$), a perturbed density

⁵A physical example of vorticity is the circular flow of water around a drain in a bathtub as it is being emptied.

response $\tilde{\rho}_m$ exists only for compressible perturbations ($\nabla \cdot \tilde{\mathbf{V}} \neq 0$). For such perturbations these equations can be combined to yield

$$\frac{\partial^2 \tilde{\rho}_m}{\partial t^2} - \nabla \cdot \left(c_S^{H^2} \nabla \tilde{\rho}_m - \mu^m \nabla^2 \tilde{\mathbf{V}} \right) = 0.$$

Considering perturbations that are localized relative to the scale length of the equilibrium density gradient so that the $\nabla c_S^{H^2}$ and $\nabla \mu^m$ terms can be neglected, but longer scale than the collision mean free path (typically $\sim 10^{-7}$ m for air at the earth's surface) so the viscosity can be neglected (i.e., $c_S^{H^2}/g \sim 10^4$ m \gg perturbation scale length $\gg \lambda \sim 10^{-7}$ m), this equation becomes simply

$$\frac{\partial^2 \tilde{\rho}_m}{\partial t^2} - c_S^{H^2} \nabla^2 \tilde{\rho}_m = 0, \quad \text{sound wave equation.} \quad (\text{A.140})$$

Thus, density perturbations compress ($\nabla \cdot \tilde{\mathbf{V}} < 0$) and rarefy ($\nabla \cdot \tilde{\mathbf{V}} > 0$) the fluid as they propagate through it adiabatically (with negligible entropy production) at the sound speed c_S^H defined in (A.139).

To exhibit the properties of the most fundamental type of fluid instabilities, the Rayleigh-Taylor (R-T) instabilities, consider perturbations of nearly incompressible liquids, in a case where a heavy liquid is above a lighter liquid and the two fluids are immiscible. For incompressible ($\nabla \cdot \tilde{\mathbf{V}} \rightarrow 0$) perturbations the linearized continuity equation becomes

$$\frac{\partial \tilde{\rho}_m}{\partial t} = -\tilde{\mathbf{V}} \cdot \nabla \rho_{m0}, \quad \text{advective response,} \quad (\text{A.141})$$

which indicates the change in local mass density caused by a perturbed flow in the direction of the gradient in the equilibrium mass density. Combining this advective response with the partial time derivative of the linearized Navier-Stokes equation yields

$$\rho_{m0} \frac{\partial^2 \tilde{\mathbf{V}}}{\partial t^2} = \left(\tilde{\mathbf{V}} \cdot \nabla \rho_{m0} \right) \nabla V_G - \nabla \frac{\partial \tilde{p}}{\partial t}.$$

Taking the curl of this equation to eliminate the perturbed pressure gradient and hence the coupling to sound waves, and neglecting gradients in the equilibrium compared to those in the perturbations ($\rho_{m0} \nabla \times \tilde{\mathbf{V}} \gg \nabla \rho_{m0} \times \tilde{\mathbf{V}}$) and viscosity effects (valid for perturbation scale lengths long compared to the collision mean free path λ), yields for the perturbed flow vorticity $\tilde{\omega} \equiv \nabla \times \tilde{\mathbf{V}}$:

$$\rho_{m0} \frac{\partial^2 \tilde{\omega}}{\partial t^2} = \nabla \left(\tilde{\mathbf{V}} \cdot \nabla \rho_{m0} \right) \times \nabla V_G.$$

Considering a coordinate system where x is directed vertically upward and y, z are in a plane parallel to the earth's surface, and assuming wavelike perturbations of the type $\tilde{\mathbf{V}} = \nabla \times \tilde{\mathbf{C}} = -\hat{\mathbf{e}}_z \times \nabla \tilde{C}_z$, in which $\tilde{\mathbf{C}} = \tilde{C}_z \hat{\mathbf{e}}_z$, $\tilde{C}_z \sim \exp(i\mathbf{k} \cdot \mathbf{x} - i\omega t)$ with $k_x \ll k_y$ is a stream function [see (??,??)], so that $\tilde{\omega} = -\hat{\mathbf{e}}_z \nabla_{\perp}^2 \tilde{C}_z \simeq \hat{\mathbf{e}}_z k_y^2 \tilde{C}_z$, yields an equation for the perturbation frequency:

$$\omega^2 \simeq -\nabla V_G \cdot \nabla \ln \rho_{m0} = \mathbf{g} \cdot \nabla \rho_m. \quad (\text{A.142})$$

When $\nabla V_G \cdot \nabla \rho_{m0} < 0$ (light liquid above heavy liquid since $\nabla V_G \equiv -\mathbf{g}$ is upward), ω^2 is positive and two benign, oscillating waves occur. (Adding viscosity effects causes the waves to be damped.) However, when a heavy liquid is placed over a light liquid ($\nabla V_G \cdot \nabla \rho_{m0} = -\mathbf{g} \cdot \nabla \rho_{m0} > 0$) the $\omega^2 < 0$ indicates complex conjugate roots, one of which will be growing exponentially in time at rate:

$$\gamma \equiv \mathcal{I}m\{\omega\} \simeq (-\mathbf{g} \cdot \nabla \ln \rho_{m0})^{1/2}, \quad \text{R-T instability growth rate} \quad (\text{A.143})$$

This is the Rayleigh-Taylor (or interchange) instability by which the interface region between the upper heavy fluid and the lower lighter fluid develops growing undulations that lead ultimately to interchange of the positions of the heavy and light fluids.

The overall process of the interchange of the two fluids can be thought of as consisting of the following steps. First, thermal fluctuations excite a modest undulation of the boundary between the two liquids. If the heavy fluid is on top, this spontaneous perturbation grows exponentially in time at the rate indicated by (A.143). The undulations grow to a large amplitude where the linearization procedure used to derive (A.142) becomes invalid. Lagrangian coordinates (i.e., coordinates that follow particular fluid elements as they move rather than the usual fixed position Eulerian ones) can be used to explore the growth of the structures into the slightly nonlinear regime. However, ultimately the vortex-like collective motions of the fluids become highly nonlinear, very contorted and large enough to encounter adjacent vortices and/or the boundaries of the regions occupied by the fluids. Then, turbulence in the fluid develops and it cascades the large vortices into smaller ones, turbulently mixing the two fluids until the heavier one is on the bottom.

In order to describe the behavior of the vortices as they evolve nonlinearly toward the turbulent state, consider the total time derivative of the circulation $C_K \equiv \oint_C d\ell \cdot \mathbf{V}$ in the rotational part of the flow \mathbf{V} , which is responsible for the vortex, over the closed curve C within the fluid:

$$\begin{aligned} \frac{dC_K}{dt} &\equiv \frac{d}{dt} \oint_C d\ell \cdot \mathbf{V} = \frac{d}{dt} \iint_S d\mathbf{S} \cdot \nabla \times \mathbf{V} \\ &= \iint_S d\mathbf{S} \cdot [(\partial/\partial t + \mathbf{V} \cdot \nabla)(\nabla \times \mathbf{V})] + \iint_S (d\mathbf{S}/dt) \cdot \nabla \times \mathbf{V} \\ &= \iint_S d\mathbf{S} \cdot \{\nabla \times (\partial \mathbf{V}/\partial t) - \nabla \times [\mathbf{V} \times (\nabla \times \mathbf{V})]\} \\ &= \iint_S d\mathbf{S} \cdot [\partial \boldsymbol{\omega}/\partial t - \nabla \times (\mathbf{V} \times \boldsymbol{\omega})] \end{aligned} \quad (\text{A.144})$$

in which use has been made of Stokes' theorem (??), S is the open surface bounded by the closed curve C that moves with the encompassed fluid, $d\mathbf{S}/dt = (\nabla \cdot \mathbf{V})d\mathbf{S} - \nabla \mathbf{V} \cdot d\mathbf{S}$ [see (??)], and the vector identity in (??) has been used. Dividing the Navier-Stokes equation (A.131) with a conservative force \mathbf{F} by ρ_m

and taking its curl to obtain an equation for $\nabla \times \partial \mathbf{V} / \partial t$ yields, after making use of (??):

$$\frac{dC_K}{dt} = \iint_S d\mathbf{S} \cdot \left(\frac{1}{\rho_m^2} \nabla \rho_m \times \nabla \left[p - \frac{\mu^m}{3} (\nabla \cdot \mathbf{V}) \right] + \nabla \times \frac{\mu^m}{\rho_m} \nabla^2 \mathbf{V} \right). \quad (\text{A.145})$$

For an adiabatic equation of state (A.132), $p \propto \rho_m^\Gamma$ and hence $\nabla \rho_m \times \nabla p = \mathbf{0}$. Thus, the circulation C_K is constant in time, except for the dissipative effects due to viscosity that are small for all but very short scale lengths of the order of the collision mean free path λ because $\mu^m / \rho_m \sim \nu \lambda^2$. Thus, on most relevant scale lengths

$$\frac{dC_K}{dt} = 0 \text{ for } \mu^m \rightarrow 0, \quad \text{Kelvin's circulation theorem,} \quad (\text{A.146})$$

for inviscid (zero viscosity) fluids.

What this theorem shows is that a vortex tube moves with (or is “frozen into”) the fluid as it evolves, and that the amount of circulation C_K in the flow field \mathbf{V} remains constant — except for the effects of viscosity, which becomes important in boundary layers near the edge of the fluid or at the edge of vortices that come close to other vortices. However, the derivation relied on the use of Stokes’s theorem, which required that the topology of the closed curve C be continuous and that it remain so. Thus, the invariance of C_K could be broken by nonlinear interactions between vortex structures that break or reconnect the topology by causing the bounding curve C , which is expected to always move with the fluid and encompass the same vorticity flux $\iint_S d\mathbf{S} \cdot \nabla \times \mathbf{V}$, to become discontinuous. To the extent that the topology of the surfaces of vorticity flux remains intact there is no motion (or transport) of fluid relative to these surfaces. However, the flux surfaces of the vorticity can distort in shape as they move around in the fluid. Thus, vortex tubes or eddies are relatively robust objects in low viscosity fluids.

The nonlinear evolution and interactions of vortices in a fluid are governed by the vorticity evolution equation

$$\frac{\partial \boldsymbol{\omega}}{\partial t} = \nabla \times (\mathbf{V} \times \boldsymbol{\omega}) - \boldsymbol{\omega} (\nabla \cdot \mathbf{V}) + \frac{\mu^m}{\rho_m} \nabla^2 \boldsymbol{\omega} \quad (\text{A.147})$$

or,

$$\frac{d\boldsymbol{\omega}}{dt} \equiv \left(\frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla \right) \boldsymbol{\omega} = \boldsymbol{\omega} \cdot \nabla \mathbf{V} + \frac{\mu^m}{\rho_m} \nabla^2 \boldsymbol{\omega}. \quad (\text{A.148})$$

These equations are obtained by taking the curl of (A.131), which eliminates the coupling to sound waves, and assuming for simplicity that the mass density is constant. The $\nabla \times (\mathbf{V} \times \boldsymbol{\omega})$ term in (A.147) represents the advection of the vorticity vector $\boldsymbol{\omega}$ by the flow velocity \mathbf{V} — as indicated by the last line of (A.144). The $\boldsymbol{\omega} \cdot \nabla \mathbf{V}$ term on the right of (A.148) represents vortex tube stretching by gradients in the velocity flow; it vanishes for two-dimensional flows. In three-dimensional flows the vortex tube stretching term reduces the area of a vortex

but also increases its vorticity — to keep the vorticity flux C_K constant as required by Kelvin’s circulation theorem.

The ratio of the nonlinear advection of vorticity [$\nabla \times (\mathbf{V} \times \boldsymbol{\omega})$, a nonlinear “inertia” term] to the viscous dissipation of vorticity ($\mu^m \nabla^2 \boldsymbol{\omega}$) is

$$Re = \frac{\nabla \times (\mathbf{V} \times \boldsymbol{\omega})}{(\mu^m / \rho_m) \nabla^2 \boldsymbol{\omega}} \sim \frac{\rho_{m0} V_0 L_0}{\mu^m}, \quad \text{Reynolds number,} \quad (\text{A.149})$$

in which V_0 , L_0 are typical flow speeds and gradient scale lengths in the fluid. When the vorticity evolution equation is written in terms of dimensionless variables, the reciprocal of the Reynolds number is the only dimensionless parameter in the equation — as the coefficient of the viscous dissipation term. For example, for incompressible flows (i.e., ones that do not excite sound waves and are dominated by vorticities), Eq. (A.147) can be written in terms of the dimensionless variables $\bar{t} \equiv (V_0/L_0)t$, $\bar{\mathbf{V}} \equiv \mathbf{V}/V_0$, and $\bar{\nabla} \equiv L_0 \nabla$ as

$$\frac{\partial \boldsymbol{\omega}}{\partial \bar{t}} = \bar{\nabla} \times (\bar{\mathbf{V}} \times \boldsymbol{\omega}) + \frac{1}{Re} \bar{\nabla}^2 \boldsymbol{\omega}. \quad (\text{A.150})$$

Thus, all incompressible flows with the same Reynolds number and the same flow geometry will have the same flow properties. At low Reynolds numbers ($Re \lesssim 1$) the flow is laminar. For not too large Reynolds numbers vortex structures induced by the particular geometrical situation (e.g., flow past a fixed body) tend to dominate the flow pattern. For high Reynolds numbers ($Re \gtrsim 10^3$) the nonlinear vorticity advection overwhelms the viscous dissipation and the flow becomes turbulent.

In fully developed turbulence ($Re \gg 10^3$) there is a cascade of energy from macroscopically-induced large-scale vortices through nonlinear interactions of turbulent eddies of successively smaller dimensions until the scale lengths become so small that the energy in the eddies is viscously dissipated. (The effective Reynolds number is close to unity for the dissipative scale eddies.) Since the dominant eddy interaction term is the vortex stretching term $\boldsymbol{\omega} \cdot \nabla \mathbf{V}$ in (A.148), successive “generations” of the turbulent eddies become longer, thinner and have larger vorticities. Thus, the mean square vorticity, which is known as the enstrophy ($\Omega \equiv |\boldsymbol{\omega}|^2$), increases during the cascade.

For sufficiently large Reynolds numbers there is a large “inertial” range of spatial scale lengths for which the vortex interactions are predominantly nonlinear (i.e., where the large-scale “stirring” and small-scale viscous dissipation effects are negligible). In the inertial range the turbulent eddies are self-similar (i.e., of the same structure, independent of scale size, from one generation to the next one). The energy flow per unit mass $\dot{\epsilon} = (\mathbf{V} \cdot \nabla)(V^2/2)$ from one wavenumber range k to the next smaller one can be estimated by $\dot{\epsilon}_k \sim k V_k^3 \sim V_k^2 / \tau_k$ in which $\tau_k \sim (k V_k)^{-1}$ is the turbulent decorrelation or eddy turnover time at a given k . Since energy is input via “stirring” at large scales and dissipated at small scales, in steady-state the energy transfer rate from one scale to the next smaller one in the inertial range must be nearly constant. Thus, $\dot{\epsilon}_k \simeq \dot{\epsilon} \sim V_0^3 / L_0$, a constant for a given externally driven situation, and hence

$V_k \sim (\dot{\epsilon}/k)^{1/3}$. The energy $E(k)$ in the turbulent fluctuations between k and $2k$ is given approximately by $\int dk E(k) \sim k E(k) \sim V_k^2$ or $E(k) \sim \dot{\epsilon}^{2/3} k^{-5/3}$, which is the Kolomogorov spectrum for turbulence within a large inertial range. The successively smaller scale eddies have smaller velocities and energies, but larger vorticity and faster turnover rates [$\tau_k \sim (kV_k)^{-1} \sim (\dot{\epsilon}k^2)^{-1/3}$] to keep the energy flow rate in k -space constant.

In the inertial range the turbulent eddies lose their momentum on a mixing length scale $\Delta_k \sim V_k \tau_k \sim 1/k$. This leads to a Prandtl mixing length estimate for the effective diffusion coefficient [cf., (A.120)] for turbulent viscosity in the fluid of $D_{\text{eff}} \sim \mu_{\text{eff}}/\rho_m \sim \Delta_k^2/\tau_k \sim \dot{\epsilon}^{1/4}/k^{4/3}$. However, this turbulent mixing is actually dissipationless; all it does is transfer the momentum and energy to shorter scale lengths. Eventually, the eddies reach the (Kolomogorov) dissipation scale k_d^{-1} at which $1/\tau_{k_d} \sim (\mu^m/\rho_m)k_d^2$, which yields $k_d \sim \dot{\epsilon}^{1/4}/(\mu^m/\rho_m)^{3/4} \sim (Re)^{3/4}/L_0$.

Because the effects of viscosity are negligible in the inertial range and because the viscous dissipation scale length is so short [$k_d^{-1} \sim L_0/(Re)^{3/4} \ll L_0$], it is tempting to neglect it entirely. However, while its effects can be neglected for inertial range scale lengths ($1/L_0 \ll k \ll k_d$), it must be retained in general because it: 1) increases the order of the differential equation governing vorticity; 2) is important in boundary layers near material objects and other nearby vortices; and, 3) most importantly for computer simulation, provides the only energy sink (at high k) for turbulent fluctuations in a neutral fluid.

Most of the previously noted standard textbooks on mechanics, statistical mechanics and kinetic theory of gases contain introductory or intermediate level descriptions of fluid mechanics. Advanced level monographs and textbooks that specifically deal with fluid mechanics include:

Batchelor, *Introduction to Fluid Dynamics* (1967) [?]

Tennekus and Lumley, *A First Course in Turbulence* (1972) [?].

A.7 Quantum Mechanical Effects

The fundamental concept in quantum mechanics is that, owing to the wavelike nature of particles on small scale lengths, a particle's position \mathbf{q} and canonically conjugate momentum \mathbf{p} cannot simultaneously be known to arbitrarily high accuracy. Rather, the product of the uncertainties in the position and momentum, $\delta\mathbf{q}$ and $\delta\mathbf{p}$, respectively, must be Planck's constant or greater:

$$\delta\mathbf{p} \cdot \delta\mathbf{q} \geq h, \quad \text{Heisenberg uncertainty principle.} \quad (\text{A.151})$$

This relation shows the limit of applicability of mechanical causality. The uncertainty principle holds for any pair of canonically conjugate variables. Thus, it applies for energy and time, which for conservative systems are canonically conjugate variables ($p = H = \varepsilon$ and $q = t$), as well:

$$\delta\varepsilon \delta t \geq h. \quad (\text{A.152})$$

By Heisenberg's uncertainty principle, the position of a nonrelativistic particle moving with velocity \mathbf{v} in a force-free region (so that its canonical momentum \mathbf{p} is simply $m\mathbf{v}$) cannot be known to within

$$\lambda_h = h/mv, \quad \text{de Broglie wavelength.} \quad (\text{A.153})$$

In the Bohr model of the hydrogen atom an electron gyrates at constant radius a_0 around the proton nucleus of the atom. Since the rotational angle φ is a symmetry coordinate and hence totally uncertain, the Heisenberg uncertainty principle requires that the canonically conjugate action J be quantized to integer multiples (n) of Planck's constant:

$$J = \oint \mathbf{p} \cdot d\mathbf{q} = \oint p_\varphi d\varphi = 2\pi m_e a_0^2 \omega_0 = n h$$

in which the angular momentum $p_\varphi \equiv m_e a_0^2 \omega_0$ where $\omega_0 \equiv d\varphi/dt$ is the constant rotation frequency. The equilibrium radial force balance between the electric field force $e^2/(\{4\pi\epsilon_0\}a_0^2)$ and the centripital acceleration force $m_e a_0 \omega_0^2$ on the electron yields the equation

$$\frac{e^2}{\{4\pi\epsilon_0\}a_0^2} = m_e a_0 \omega_0^2.$$

Solving these two simultaneous equations for a_0 in the ground state ($n = 1$) case yields the characteristic radius of the hydrogen atom:

$$a_0 = \{4\pi\epsilon_0\} \frac{(h/2\pi)^2}{m_e e^2} \simeq 0.529 \times 10^{-10} \text{ m, Bohr radius.} \quad (\text{A.154})$$

This is the characteristic scale length for the "size" of all atoms — the range over which their electrostatic force field extends. The corresponding range over which nuclear forces extend is

$$r_e = \frac{e^2}{\{4\pi\epsilon_0\}m_e c^2} \simeq 2.82 \times 10^{-15} \text{ m, classical electron radius,} \quad (\text{A.155})$$

which is inferred from equating the electric potential energy $\sim e^2/(\{4\pi\epsilon_0\}r_e)$ from a distributed electron charge to the electron rest mass energy $m_e c^2$.

The binding energy of an electron in a Bohr atom in its ground (lowest energy) state is given by the (negative of the) potential energy of the electron when it is located at the Bohr radius from the proton plus the kinetic energy of the electron:

$$E_\infty^H = \frac{e^2}{\{4\pi\epsilon_0\}a_0} - \frac{m_e}{2} a_0^2 \omega_0^2 = \frac{1}{\{4\pi\epsilon_0\}^2} \frac{m_e e^4}{2(h/2\pi)^2} \simeq 13.6 \text{ eV,}$$

Bohr atom binding energy, (A.156)

which is also called the Rydberg energy. For electrons in the n^{th} quantum state the orbit radius increases by a factor of n^2 and the rotation frequency

ω_0 decreases by a factor of $1/n^3$; consequently, the binding energy of the state decreases by a factor of $1/n^2$. For electrons gyrating around an ion of charge Z_i , the potential and consequently the electric field force increases by a factor of Z_i . This causes the Bohr radius to decrease by a factor of $1/Z_i$ and the ionization energy to increase by a factor of Z_i^2 . Thus, neglecting fine-structure effects, the binding energy of an outer electron in a level labeled by the quantum number n (≥ 1) which is gyrating around an ion of charge Z_i is given by

$$E_\infty^Z(n) \simeq Z_i^2 E_\infty^H/n^2, \quad \text{outer electron binding energy.} \quad (\text{A.157})$$

Note that for a nucleus with a high atomic number Z the binding energy of the most tightly bound ($n = 1$, ground state) electron, which is the last one to be removed as an atom is ionized, can be very large. For example, for iron ($Z = 26$) the binding energy of the last electron is ~ 9 keV while for tungsten ($Z = 74$) it is ~ 75 keV.

The degree of ionization in a plasma can be estimated from the Saha equation which gives the population density of a particular ionization and quantum state of an atom in a gas in thermodynamic equilibrium. It can be obtained by equating the rates of ionization [$\propto n_n \exp(-U_i/T_e)$] and recombination [$\propto n_i(n_e \lambda_h^3)$] for ions in a partially ionized gas:

$$\begin{aligned} \frac{n_i}{n_n} &\simeq \frac{2}{n_e} \left(\frac{2\pi m_e T_e}{h^2} \right)^{3/2} e^{-U_i/T_e} = 2^{5/2} \frac{n_e \lambda_{De}^3}{(n_e a_0^3)^{1/2}} e^{-U_i/T_e} \\ &\simeq \frac{6 \times 10^{27}}{n_e (\text{m}^{-3})} [T_e (\text{eV})]^{3/2} e^{-U_i/T_e}, \quad \text{Saha equation,} \quad (\text{A.158}) \end{aligned}$$

in which n_e, n_i and n_n are the electron, ion and neutral density, respectively, U_i is the ionization potential and T_e is the temperature in electron volts of the assumed Maxwellian distribution of electrons. The ionization potential U_i for ionization of an atom from its ground (neutral) state to the first ionized state is given by the electron binding energy in the atom [cf., Eq. (A.157)]. It ranges from 3.9 eV for Cesium atoms to 24.6 eV for Helium.

The fractional ionization [$\equiv n_i/(n_n + n_i)$] is exponentially small for electron temperatures T_e much lower than the ionization potential U_i . The electron temperature required to attain a small degree of ionization ($\sim n_i/n_n \ll 1$) can be estimated by solving the Saha equation iteratively for T_e :

$$T_e|_{\text{ion}} \simeq \frac{U_i}{\ln \left(\frac{6 \times 10^{27} [T_e (\text{eV})]^{3/2}}{(n_i/n_n) n_e (\text{m}^{-3})} \right)} \sim (0.02-1) U_i, \quad (\text{A.159})$$

where in the last form the smallest number corresponds to interplanetary densities ($\sim 10^6 \text{ m}^{-3}$) and the largest to solid densities ($\sim 10^{29} \text{ m}^{-3}$). The T_e required to produce a fully ionized state ($n_i/n_n \gg 1$) is not much larger. Thus, for example, a nitrogen gas ($U_i = 14.5$ eV) at a density of $2.5 \times 10^{25} \text{ m}^{-3}$ (the density of room temperature air) becomes 1% ionized at $T_e \simeq 1.4$ eV, and fully ionized for $T_e \gtrsim 2.2$ eV. At lower densities the electron temperature range over which

the transition from a partially to fully ionized gas takes place is even narrower. For some examples of the variation with electron density of the T_e required for complete ionization, see Fig. ?? at the end of Chapter 1.

Note however that the ions might not be fully stripped of their electrons. In particular, for $T_e \sim 0.1\text{--}10$ keV, high Z ions might not be fully stripped because of the very large binding energy of their most tightly bound electrons. Such ions would have an ion charge $Z_i < Z$.

Some standard introductory level quantum mechanics textbooks are:

Krane, *Modern Physics* () [?]

Sproul and Phillips, *Modern Physics* () [?]

Tipler, *Modern Physics* () [?]

Gasiorowicz, *Quantum Physics* () [?]

Powell and Crasemann, *Quantum Mechanics* () [?].

A.8 Physical Constants

Fundamental Physical Constants

<u>Quantity</u>	<u>Symbol</u>	<u>Best Value</u> ⁶	<u>Relative Uncertainty ($\times 10^{-6}$)</u>
electron mass	m_e	$9.109\,389\,7 \times 10^{-31}$ kg	0.59
proton mass	m_p	$1.672\,623\,1 \times 10^{-27}$ kg	0.59
elementary charge	e	$1.602\,177\,33 \times 10^{-19}$ C	0.30
speed of light in vacuum	c	299 792 458 m/s	exact ⁷
permeability of vacuum	μ_0	$4\pi \times 10^{-7}$ H/m	exact
permittivity of vacuum	ϵ_0	$1/\mu_0 c^2$ F/m	exact
gravitational constant	G	$6.672\,59 \times 10^{-11}$ N·m ² /kg ²	128
Planck constant	h	$6.626\,075\,5 \times 10^{-34}$ J·s	0.60
Boltzmann constant	k_B	$1.380\,658 \times 10^{-23}$ J/K	8.5

SI Units And Their Abbreviations, Interrelationships

<u>Quantity</u>	<u>Name</u>	<u>Symbol</u>	<u>In Terms Of Other Units</u>
length	meter	m	10^2 cm = 10^{10} Å
mass	kilogram	kg	10^3 g
time	second	s	
electric current	ampere	A	C/s
temperature	kelvin	K	$\simeq 1/11\,604.4$ eV
amount of substance	mole	mol	
atomic unit of energy	electron volt	eV	$\simeq 1.602\,177\,33 \times 10^{-19}$ J
atomic unit of mass	amu	u	$\simeq 1.660\,540\,2 \times 10^{-27}$ kg
frequency	hertz	Hz	s^{-1} (cycles per second)
force	newton	N	$m \cdot kg \cdot s^{-2}$
pressure, stress	pascal	Pa	$N/m^2 = m^{-1} \cdot kg \cdot s^{-2}$
energy, work	joule	J	$N \cdot m = m^2 \cdot kg \cdot s^{-2}$
power	watt	W	$J/s = m^2 \cdot kg \cdot s^{-3}$
electric charge	coulomb	C	$s \cdot A$
electric potential	volt	V	$W/A = m^2 \cdot kg \cdot s^{-3} \cdot A^{-1}$
capacitance	farad	F	$C/V = m^{-2} \cdot kg^{-1} \cdot s^4 \cdot A^2$
electrical resistance	ohm	Ω	$V/A = m^2 \cdot kg \cdot s^{-3} \cdot A^{-2}$
magnetic flux	weber	Wb	$V \cdot s = m^2 \cdot kg \cdot s^{-2} \cdot A^{-1}$
magnetic flux density ⁸	tesla	T	$Wb/m^2 = kg \cdot s^{-2} \cdot A^{-1}$
inductance	henry	H	$Wb/A = m^2 \cdot kg \cdot s^{-2} \cdot A^{-2}$

⁶E.R. Cohen and B.N. Taylor, *Physics Today*, August 1998, BG7 [?].

⁷The speed of light fixes the length of the meter in terms of the second.

⁸In plasma physics magnetic field strengths are often quoted in Gauss: 1 Tesla \equiv 10 kGauss.

Other Physical Constants

<u>Quantity</u>	<u>Symbol</u>	<u>Value</u>
Avogadro constant	N_A	6.022×10^{23} #/mol
Molar gas constant	R	$8.31 \text{ J} \cdot \text{mol}^{-1} \text{K}^{-1}$
Air (20°C and 1 atmosphere)		
density	n	2.49×10^{25} molecules/m ³
sound speed	c_S	343 m/s
atmospheric pressure	p	760 Torr = 1.01×10^5 Pa
molecular weight		28.9 g/mol
viscous diffusivity	μ^m/ρ_m	1.5×10^{-5} m ² /s
Water		
density	n	3.33×10^{28} molecules/m ³
sound speed	c_S	1460 m/s
viscous diffusivity	μ^m/ρ_m	10^{-6} m ² /s
Earth		
mass	M_E	5.98×10^{24} kg
mean radius	R_E	6.37×10^6 m
gravitational acceleration	g	9.81 m/s^2
magnetic dipole moment	M_d	8.0×10^{22} A · m ²

Particle Masses

<u>Particle or Atom</u>	<u>Symbol</u>	<u>Atomic Number Z</u>	<u>Best Atomic Mass⁹Value</u>	<u>Energy Units (mc^2/e, MeV)</u>
electron	m_e		0.000 548 579 903	0.511
muon	m_μ		0.113 428 913	105.658
proton	m_p	1	1.007 276 470	938.272
neutron	m_n		1.008 664 904	939.566
deuteron	m_D	1	2.013 553 214	1 875.613
triton	m_T	1	3.016 050	2 809.853
helium	m_{He}	2	4.002 603	3 728.402
carbon	m_C	6	12.011 15	
nitrogen	m_N	7	14.006 7	
oxygen	m_O	8	15.999 4	
argon	m_{Ar}	18	39.948	
iron	m_{Fe}	26	55.845	
molybdenum	m_{Mo}	42	95.94	
tungsten	m_W	74	183.84	

⁹The unified atomic mass unit = $1.660\,540\,2 \times 10^{-27}$ kg (0.59×10^{-6} relative error) = $931.494\,32$ MeV (0.30×10^{-7} relative error). Note also that Avogadro's constant $N_A \equiv 1/u$.