Chapter 3
Kinetic theory of dilute gases

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3.1. Distribution function

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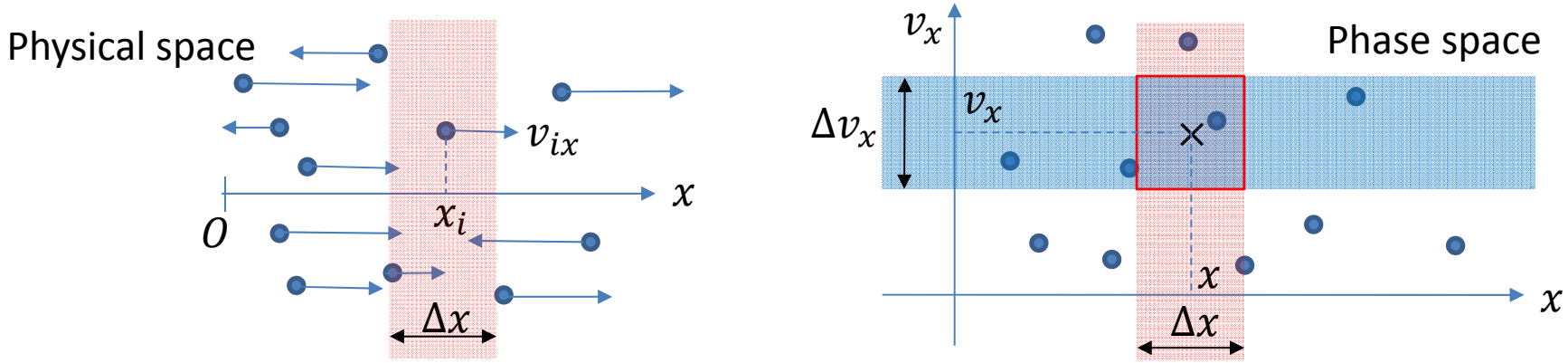
3.1. Distribution function

Illustrative example: One-dimensional motion of molecules

Let's first consider a **molecular beam** of a simple gas, where all molecules move along a given axis, e.g., axis x. Then current state of every molecule i in the beam can be characterized by its coordinate x_i and velocity v_{ix} and can be represented by a point on the plane (x, v_x). This plane is called the **phase space** (or **phase plane**). Current state (historically called *phase*) of the gas of N molecules can be represented by a set of N points on the phase plane.



Let's now assume that N is so large that there is no any practical opportunity to trace every individual molecule. Instead, let's introduce a quantity f which can describe *distribution* of molecules on the phase plane independently on their precise number, using the same approach that is usually utilized in order to characterize distribution of molecules in the physical space, i.e.

$$n(x,t) = \frac{\text{Number of molecules in the cell } \Delta x \text{ of the physical space}}{\Delta x}$$: Number density

$$f(x,v_x,t) = \frac{\text{Number of molecules in the cell } \Delta x \Delta v_x \text{ of the phase space}}{\Delta x \Delta v_x}$$: Distribution function

3.1. Distribution function

Distribution function $f(x, v_x, t)$ is equal to the average number of molecules in a unit "volume" of a phase space, i.e. $f(x, v_x, t)$ is *the number density of molecules in the phase space*. If we chose infinitely small phase volume $dxdv_x$, then

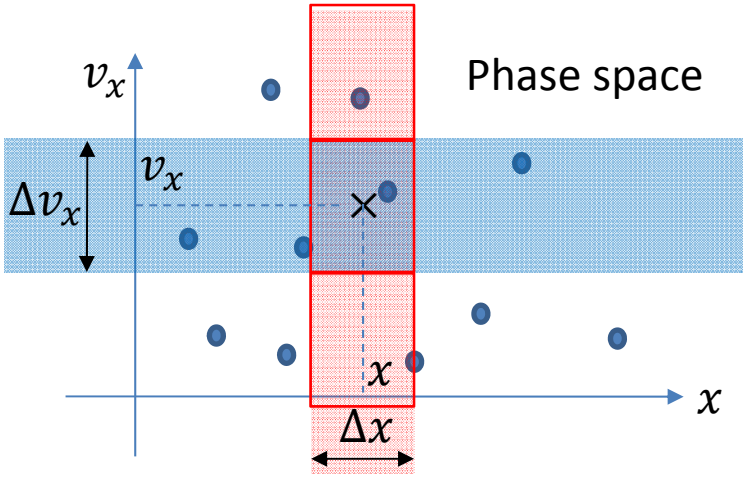
$$dN = f(x, v_x, t)dxdv_x \tag{3.1.1}$$

is equal to the average number of molecules whose phase coordinates x_i and v_{ix} at time t satisfy the conditions

$$x < x_i < x + dx, \qquad v_x < v_{ix} < v_x + dv_x,$$

i.e. the average number of molecules inside "volume" $dxdv_x$ at point (x, v_x). Eq. (3.1.1) gives the physical meaning of distribution function: It is introduces to count molecules in the phase space. The usefulness of $f(x, v_x, t)$ is based on the fact that any macroscopic gas parameter can be calculated based on $f(x, v_x, t)$ (Section 3.2).

Example: Number density. In order to find the total number of molecules ΔN in a cell Δx of the physical space, one needs to sum contributions of molecules with various velocities, i.e. contributions of cells in the red strip



$$\Delta N(x, t) \approx \sum_{all\ cells\ at\ fixed\ x} f(x, v_x, t)\Delta x \Delta v_x$$

or, if we consider infinitely small dx and dv_x,

$$dN(x, t) = n(x, t)dx = dx \int_{-\infty}^{+\infty} f(x, v_x, t)dv_x\,. \quad \Rightarrow \quad n(x, t) = \int_{-\infty}^{+\infty} f(x, v_x, t)dv_x$$

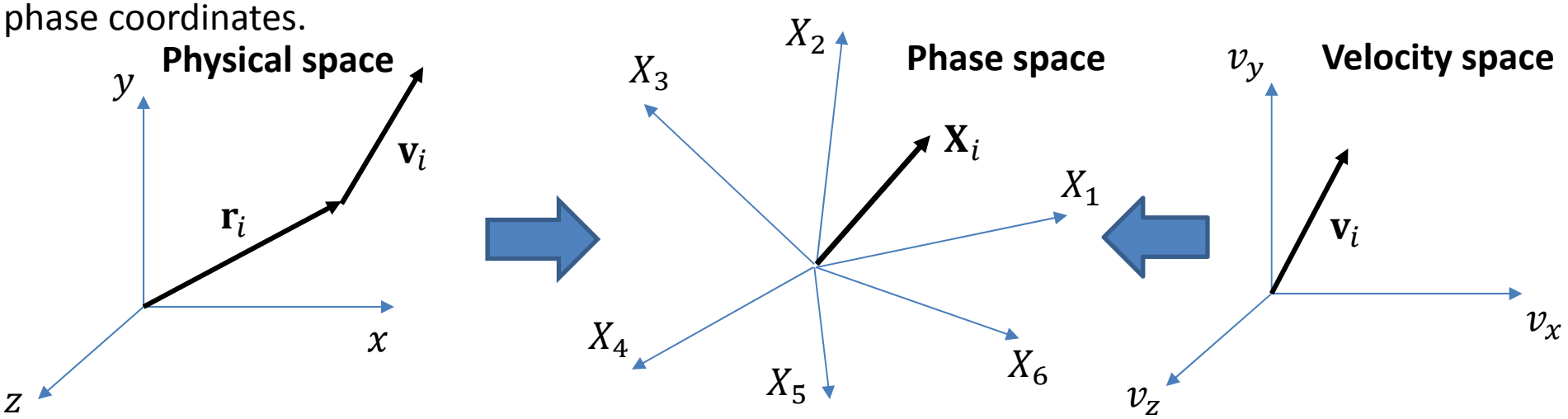
3.1. Distribution function

Phase space of molecules of a simple gas

Now our goal is to generalize the notion of the distribution function for the general case of three-dimensional (3D) motion of molecules. In the 3D case, the current state of every molecule i of a simple gas can be *completely* characterized by its Cartesian coordinates x_i, y_i, z_i and velocity components v_{ix}, v_{iy}, v_{iz}, i.e. by 6 numbers. Current position of a molecules can be represented by a point in 3D physical space and current velocity of molecules can be represented by a point in the 3D **velocity space**. However, if the goal is to describe current state of a molecule completely, then one needs to introduce 6-th dimensional **space**, where the state of every molecule can be visualized by a point with 6 **phase coordinates**

$$\mathbf{X} = (X_1, X_2, \ldots, X_6) = (x, y, z, v_x, v_y, v_z).$$

This space is called the **phase space** of molecules of a simple gas. The current state of a gas of N molecules can be *completely* represented by a set of N points in the phase space, i.e. by $6N$ phase coordinates.



3.1. Distribution function

Distribution function of gas molecules

Distribution function or **velocity distribution function (VDF) of gas molecules**

$$f = f(\mathbf{X}, t) = f(\mathbf{r}, \mathbf{v}, t) = f\left(x, y, z, v_x, v_y, v_z, t\right)$$

is equal to the average number of molecules in a unit "volume" of the phase space, i.e. *represents the number density of molecules in the phase space*. If we chose infinitely small phase volume

$$d\mathbf{X} = d\mathbf{r}d\mathbf{v} = dxdydzdv_x dv_y dv_z$$

at point $\mathbf{X}$ of the phase space, then

(3.1.2)
$$dN = f(\mathbf{r}, \mathbf{v}, t)d\mathbf{r}d\mathbf{v}$$

is equal to the average number of molecules inside that phase volume, i.e. the number of molecules whose phase coordinates x_i, y_i, z_i and velocity components v_{ix}, v_{iy}, v_{iz} at time t satisfy the conditions

(3.1.3)
$$\begin{aligned} x < x_i < x + dx, \qquad & v_x < v_{ix} < v_x + dv_x, \\ y < y_i < y + dy, \qquad & v_y < v_{iy} < v_y + dv_y, \\ z < z_i < z + dz, \qquad & v_z < v_{iz} < v_z + dv_z. \end{aligned}$$

Eq. (3.1.2) gives the physical meaning of distribution function: It is introduced to count molecules in the phase space. In the future we will use conditions given by Eq. (3.1.3) many times, so for short we will denote then as

$$\mathbf{r} < \mathbf{r}_i < \mathbf{r} + d\mathbf{r}, \qquad \mathbf{v} < \mathbf{v}_i < \mathbf{v} + d\mathbf{v},$$

or

$$\mathbf{X} < \boldsymbol{X}_i < \mathbf{X} + d\mathbf{X}.$$

3.1. Distribution function

In order to find the total number of molecules $\langle \Delta N \rangle$ in a small volume $\Delta \mathbf{r} = \Delta x \Delta y \Delta z$ at point $\mathbf{r}$ one needs to account for contribution of all molecules with coordinates satisfying the condition

$$\mathbf{r} < \mathbf{r}_i < \mathbf{r} + \Delta \mathbf{r},$$

but with arbitrary velocities. For this purpose, one can introduce a 3D mesh of cells in the velocity space with centers in nodes $(v_{x(i)}, v_{y(j)}, v_{z(k)})$ of sizes $\Delta v_x, \Delta v_y, \Delta v_z$. Then

(3.1.4) $$\langle \Delta N \rangle (x, y, z, t) \approx \sum_i \sum_j \sum_k f\left(x, y, z, v_{x(i)}, v_{x(j)}, v_{x(k)}, t\right) \Delta x \Delta y \Delta z \Delta v_x \Delta v_y \Delta v_z$$

or, if we consider infinitely small $dxdydz$ and $dv_x dv_y dv_z$,

$$\langle dN \rangle (x, y, z, t) = n(x, y, z, t) dx dy dz = dx dy dz \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f\left(x, y, z, v_x, v_y, v_z t\right) dv_x dv_y dv_z$$

and the gas **number density** is equal to

(3.1.5) $$n(x, y, z, t) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f\left(x, y, z, v_x, v_y, v_z t\right) dv_x dv_y dv_z.$$

Eq. (3.1.5) is called the **normalization condition of the distribution function**. It shows that the distribution function has unit of $[f]=[n]/[v]^3=\text{s}^3/\text{m}^6$. We will consider **triple integrals** like integral in Eq. (3.1.5) many times, so we will write them for short as follows

$$n(\mathbf{r}, t) = \int f(\mathbf{r}, \mathbf{v}, t)\, d\mathbf{v}.$$

3.2. Macroscopic gas parameters

- Density of molecular quantities
- Internal energy, thermal velocity, and temperature
- Density of fluxes of molecular quantities

3.2. Macroscopic gas parameters

Densities of molecular quantities

Let's consider some **additive** physical quantity Φ, i.e. such quantity that the value of this quantity in a volume of gas is equal to the sum of corresponding molecular quantities $\Phi = \Phi(\mathbf{r}, \mathbf{v}, t) = \Phi(\mathbf{X}, t)$ of individual molecules in this volume. Firsts, let's find the total value $d\Phi$ of Φ for all molecules, which phase coordinates at time t correspond to points inside an infinitely small "volume" of the phase space, i.e. satisfy Eq. (3.1.3). Since $d\mathbf{X}$ is small, we can assume that all molecules in this "volume" possess the same value of quantity $\Phi(\mathbf{r}, \mathbf{v}, t)$. Then $d\Phi = \Phi(\mathbf{r}, \mathbf{v}, t)dN$, where the number of molecules inside $d\mathbf{X}$ is given by Eq. (3.1.2), i.e.

(3.2.1) $$d\Phi = \Phi(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}, t) d\mathbf{r} d\mathbf{v}.$$

Now let's find the total amount $\langle d\Phi \rangle$ of Φ for all molecules in volume $d\mathbf{r}$ of physical space, i.e. molecules whose coordinates satisfy the condition $\boldsymbol{r} < \mathbf{r}_i < \mathbf{r} + d\mathbf{r}$. For this purpose one needs to sum contributions of all "volumes" in the velocity space, i.e. repeat the same operation which we already performed when formulated Eqs. (3.1.4) and (3.1.5). It results in

$$\langle d\Phi \rangle = d\mathbf{r} \int \Phi(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}.$$

Then the average value of molecular quantity $\langle \Phi \rangle (\mathbf{r}, t)$ is given by the equation

(3.2.2) $$\langle \Phi \rangle (\mathbf{r}, t) = \frac{\langle d\Phi \rangle}{\langle dN \rangle} = \frac{1}{n(\mathbf{r}, t)} \int \Phi(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}\,.$$ $[\langle \Phi \rangle]=[\Phi]$

3.2. Macroscopic gas parameters

The **density of physical quantity** Φ (physical quantity Φ per unit volume) is equal to

(3.2.3) $$\langle \Phi_V \rangle(\mathbf{r},t) = \frac{\langle d\Phi \rangle}{d\mathbf{r}} = \int \Phi(\mathbf{r},\mathbf{v},t) f(\mathbf{r},\mathbf{v},t) d\mathbf{v}\,. \qquad [\langle \Phi_V \rangle] = \frac{[\Phi]}{\mathrm{m}^3}$$

and **specific gas macroscopic parameters** (physical quantity Φ per unit mass) is equal to

(3.2.4) $$\langle \Phi_M \rangle(\mathbf{r},t) = \frac{\langle d\Phi \rangle}{m\langle dN \rangle} = \frac{1}{\rho(\mathbf{r},t)} \int \Phi(\mathbf{r},\mathbf{v},t) f(\mathbf{r},\mathbf{v},t) d\mathbf{v}\,, \qquad [\langle \Phi_V \rangle] = \frac{[\Phi]}{\mathrm{kg}}$$

where $\rho(\mathbf{r},t) = mn(\mathbf{r},t)$ is the gas mass density. According to Eqs. (3.2.2)-(3.2.4), all three types of the macroscopic parameters are connected with each other by the relationship

(3.2.5) $$\langle \Phi_V \rangle(\mathbf{r},t) = n\langle \Phi_V \rangle(\mathbf{r},t) = \rho\langle \Phi_M \rangle(\mathbf{r},t).$$

Eqs. (3.2.2)-(3.2.4) show that calculation of macroscopic parameters in the kinetic theory reduces to the integration of the distribution function $f(\mathbf{r},\mathbf{v},t)$ with various weights $\Phi(\mathbf{r},\mathbf{v},t)$ over the velocity space. The averaging operation $\langle \dots \rangle$ in Eq. (3.2.2) has two major properties:

1. It does not change a macroscopic parameter $\langle \Phi \rangle(\mathbf{r},t)$ or any quantity that does not depend on $\mathbf{v}$, i.e.

$$\big\langle \langle \Phi \rangle \big\rangle(\mathbf{r},t) = \frac{1}{n} \int \langle \Phi \rangle(\mathbf{r},t) f(\mathbf{r},\mathbf{v},t) d\mathbf{v} = \frac{\langle \Phi \rangle(\mathbf{r},t)}{n} \int f(\mathbf{r},\mathbf{v},t) d\mathbf{v} = \langle \Phi \rangle(\mathbf{r},t).$$

2. It is a linear operation in a sense that (Here a, b do not depend on $\mathbf{v}$)

$$\langle a\Phi + b\Psi \rangle = a\langle \Phi \rangle + b\langle \Psi \rangle.$$

3.2. Macroscopic gas parameters

Let's consider the most important macroscopic parameters

If $\Phi = 1$, then $\langle \Phi_V \rangle = n$ is the gas **number density**

$$n(\mathbf{r}, t) = \int f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} \ .$$

If $\Phi = m$, then $\langle \Phi_V \rangle = \rho$ is the gas **mass density**

$$\rho(\mathbf{r}, t) = \int m f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} \ .$$

If $\Phi = m\mathbf{v}$, then $\overline{\langle \Phi_M \rangle} = \mathbf{u}$ is the gas **macroscopic gas velocity**, or bulk velocity, or specific linear momentum

$$\mathbf{u}(\mathbf{r}, t) = \frac{1}{\rho(\mathbf{r}, t)} \int m\mathbf{v} f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} = \frac{1}{n(\mathbf{r}, t)} \int \mathbf{v} f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} \, .$$

If $\Phi = m\mathbf{v}^2/2$, then $\langle \Phi_M \rangle = e_{tot}$ is the gas **specific total translational energy** (total kinetic energy of molecules per unit mass)

$$e_{tot}(\mathbf{r}, t) = \frac{1}{\rho(\mathbf{r}, t)} \int \frac{m\mathbf{v}^2}{2} f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} \ .$$

and $\langle \Phi_V \rangle = E_{tot}$ is the **density of total translational energy** (total kinetic energy per unit mass)

$$E_{tot}(\mathbf{r}, t) = \int \frac{m\mathbf{v}^2}{2} f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} = \rho e_{tot}.$$

3.2. Macroscopic gas parameters

Internal energy, thermal velocity, and temperature

Velocity $\mathbf{c}$ of chaotic motion of molecule is the velocity of the molecule in a framework that moves with the gas macroscopic velocity gas velocity in the point where the molecule is located:

(3.2.6) $$\mathbf{c} = \mathbf{v} - \mathbf{u}(\mathbf{r}, t).$$

The chaotic velocity is defined by $\mathbf{v}, \mathbf{r}$, and t.

The **specific internal energy** of a simple gas e is the kinetic energy of chaotic motion of molecules per unit mass:

(3.2.7) $$e(\mathbf{r}, t) = \left\langle \frac{m\mathbf{c}^2}{2} \right\rangle_M = \frac{1}{\rho}\int \frac{m\mathbf{c}^2}{2} f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} = \frac{1}{\rho}\int \frac{m(\mathbf{v}-\mathbf{u})^2}{2} f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} =$$

$$\frac{1}{\rho}\int \frac{m\mathbf{v}^2 - 2\mathbf{v}\cdot\mathbf{u} + \mathbf{u}^2}{2} f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} = e_{tot} - \frac{\mathbf{u}^2}{2}.$$

The **density of internal energy** of a simple gas E is the kinetic energy of chaotic motion of molecules per unit mass:

$$E(\mathbf{r}, t) = \left\langle \frac{m\mathbf{c}^2}{2} \right\rangle_V = \int \frac{m\mathbf{c}^2}{2} f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} = \rho e.$$

Thus, there is a relationship between gas total and internal energies:

(3.2.8) $$e_{tot} = e + \frac{\mathbf{u}^2}{2}, \qquad E_{tot} = E + \frac{\rho\mathbf{u}^2}{2},$$

3.2. Macroscopic gas parameters

In the right-hand sides of Eq. (3.2.8), the last terms is the kinetic energy of the center-of-mass motion or macroscopic motion of the gas.

Thermal velocity C of gas is given by the equation

(3.2.9) $$C^2 = \langle \mathbf{c}^2 \rangle = \frac{1}{n}\int (\mathbf{v}-\mathbf{u})^2 f(\mathbf{r},\mathbf{v},t)d\mathbf{v} = 2e\,.$$

According to the kinetic definition, Eq. (1.3.11), **temperature** T can be defined as follows:

(3.2.10) $$\frac{k_B T}{2} = \frac{mC^2/2}{3} = \frac{m\langle \mathbf{c}^2 \rangle/2}{3} = \frac{1}{3}\frac{1}{n}\int \frac{m\mathbf{c}^2}{2} f(\mathbf{r},\mathbf{v},t)d\mathbf{v} = \frac{1}{3}\frac{E}{n}.$$

We can always calculate quantity T if we know $f(\mathbf{r},\mathbf{v},t)$. But calculations with Eq. (3.2.10) result in the true thermodynamic temperature only if $f(\mathbf{r},\mathbf{v},t)$ corresponds to the gas in an equilibrium state. We will discuss this problem later on.

There is a direct analogy between macroscopic quantities introduces in the present Section, and volume-averaged quantities defined is Section 1.2. If the continuity hypothesis is satisfied, then

$$\langle \Phi \rangle = \bar{\Phi}, \qquad \langle \Phi_V \rangle = \overline{\Phi_V}, \qquad \langle \Phi_M \rangle = \overline{\Phi_M}.$$

If the continuity hypothesis is invalid, then we cannot introduce $\bar{\Phi}$, $\overline{\Phi_V}$, and $\overline{\Phi_M}$, but quantities $\langle \Phi \rangle$, $\langle \Phi_V \rangle$, and $\langle \Phi_M \rangle$ can be introduced and used in any gas flow independently of its degree of rarefaction. Definitions of macroscopic parameters given in this Section are called **kinetic** or **statistical**. $\langle \Phi \rangle$, $\langle \Phi_V \rangle$, and $\langle \Phi_M \rangle$ are called the **ensemble-averaged** macroscopic parameters.

Density of fluxes of molecular quantities

Let's calculate a flux density of a molecular quantity $\Phi(\mathbf{r},\mathbf{v},t)$ in some point $\mathbf{r}$ of a dilute gas based on the distribution function $f(\mathbf{r},\mathbf{v},t)$. In the dilute gas, the contribution of collisional transfer of molecular quantities is small (see Section 1.5, slide 63 of Chapter 1), so that we neglect by the collisional transfer and take into account only the convective transfer.

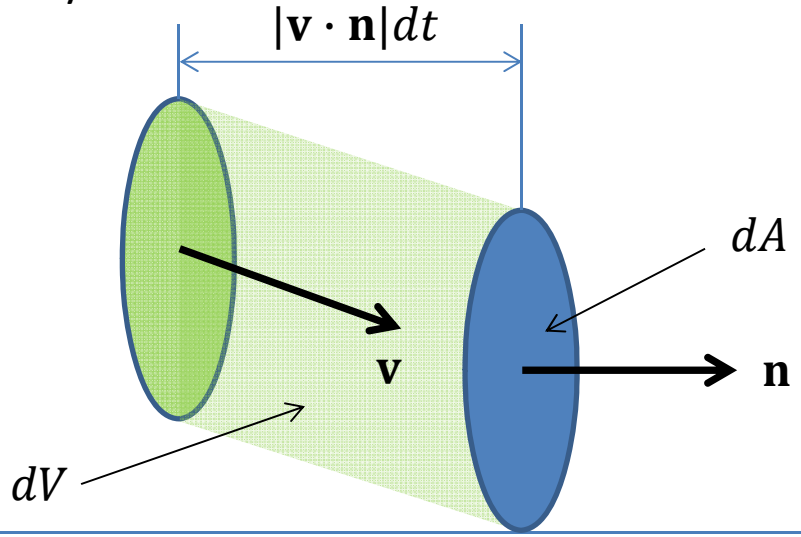
Let's introduce a surface of infinitely small area dA with the unit normal $\mathbf{n}$ in point $\mathbf{r}$ and consider the total amount $d\Phi$ of molecular quantity Φ that is transferred by molecules moving through area dA during time dt in both directions. Let's assume that $d\Phi > 0$ if quantity is transferred in the direction of normal $\mathbf{n}$ for molecules that cross dA with $\mathbf{v}\cdot\mathbf{n} > 0$. Then quantity $d\Phi$ can be represented in the form

(3.2.11) $$d\Phi = d\Phi_+ - d\Phi_-,$$

where $d\Phi_+$ and $d\Phi_-$ are amounts of Φ transferred by molecules with $\mathbf{v}\cdot\mathbf{n} > 0$ and $\mathbf{v}\cdot\mathbf{n} < 0$, correspondingly.

Let's fix velocity $\mathbf{v}$ and assume that $\mathbf{v}\cdot\mathbf{n} > 0$. Molecules with such velocity can intersect dA during dt only if at time t they are located within an inclined cylinder (marked by green in the sketch) with basement dA and height $|\mathbf{v}\cdot\mathbf{n}|dt$. The volume of this cylinder is equal to

(3.2.12) $$dV = |\mathbf{v}\cdot\mathbf{n}|dtdA.$$



3.2. Macroscopic gas parameters

Let's consider molecules from that cylinder, whose velocities satisfy equation

$$\mathbf{v} < \mathbf{v}_i < \mathbf{v} + d\mathbf{v}.$$

The total number of such molecules is given by Eq. (3.1.2):

$$dN(\mathbf{v}) = f(\mathbf{r}, \mathbf{v}, t) dV d\mathbf{v} = dt dA |\mathbf{v} \cdot \mathbf{n}| f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}.$$

Every such molecule transfers the same amount of molecular quantity $\Phi(\mathbf{r}, \mathbf{v}, t)$, so the total amount of Φ transferred by these molecules is equal to

(3.2.13) $$d\Phi(\mathbf{v}) = \Phi(\mathbf{r}, \mathbf{v}, t) dN(\mathbf{v}) = dt dA |\mathbf{v} \cdot \mathbf{n}| \Phi(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}.$$

In order to obtain $d\Phi_+$ one needs to sum contributions of molecules with various $\mathbf{v}$, i.e. integrate Eq. (3.2.13) over a part of the velocity space, which corresponds to $\mathbf{v} \cdot \mathbf{n} > 0$:

$$d\Phi_+ = \int\limits_{\mathbf{v}\cdot\mathbf{n}>0} \Phi(\mathbf{r}, \mathbf{v}, t) dN(\mathbf{v}) = dt dA \int\limits_{\mathbf{v}\cdot\mathbf{n}>0} (\mathbf{v} \cdot \mathbf{n}) \Phi(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}\,.$$

Using the same approach one can obtain

$$d\Phi_- = dt dA \int\limits_{\mathbf{v}\cdot\mathbf{n}<0} |\mathbf{v} \cdot \mathbf{n}| \Phi(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v} = -dt dA \int\limits_{\mathbf{v}\cdot\mathbf{n}<0} (\mathbf{v} \cdot \mathbf{n}) \Phi(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}\,,$$

so finally

$$d\Phi = dt dA \int (\mathbf{v} \cdot \mathbf{n}) \Phi(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}\,.$$

Then the **flux** dF_Φ of molecular quantity Φ through dA is equal to

3.2. Macroscopic gas parameters

(3.2.14) $$dF_\Phi = \frac{d\Phi}{dt} = dA\,\mathbf{n}\cdot\int \mathbf{v}\Phi(\mathbf{r},\mathbf{v},t)f(\mathbf{r},\mathbf{v},t)d\mathbf{v}.$$

Let's introduce a **vector of flux density of molecular quantity** Φ

(3.2.15) $$\mathbf{f}_\Phi(\mathbf{r},t) = \int \mathbf{v}\Phi(\mathbf{r},\mathbf{v},t)f(\mathbf{r},\mathbf{v},t)d\mathbf{v} = \langle(\mathbf{v}\Phi)_V\rangle,$$

Compare with Eq. (3.2.3)

so that finally the flux through a small surface and flux density are related to each other via the equation (see for comparison Equations in slide 61 of Chapter 1, Section 1.5)

$$dF_\Phi = dA(\,\mathbf{n}\cdot\mathbf{f}_\Phi).$$

Example: if $\Phi = m\mathbf{v}^2/2$ is the translational energy of a molecule then

$$\mathbf{f}_{tr} = \int \mathbf{v}\frac{m\mathbf{v}^2}{2}f(\mathbf{r},\mathbf{v},t)d\mathbf{v}$$

is the vector of **energy flux density** in the gas.

Concluding remarks:

- Any macroscopic gas parameter can be determined if we know the distribution function. If we know $f(\mathrm{r},\mathrm{v},t)$, we know *all* macroscopic parameters.
- Our **kinetic definition** of macroscopic parameters based on $f(\mathbf{r},\mathbf{v},t)$, Eq. (3.2.2), is in agreement with previous definition of volume-averaged molecular quantities in Section 1.2. If the continuity hypothesis is valid, then volume-averaged quantities coincide with quantities defined by Eq. (3.2.2). The major advantage of our kinetic definition, however, is that we can use it in any dilute gas flow even if the continuity hypotheses is not satisfied.

3.3. Kinetic equation

- Illustrative example: One-dimensional motion of molecules
- Kinetic equation

3.3. Kinetic equation

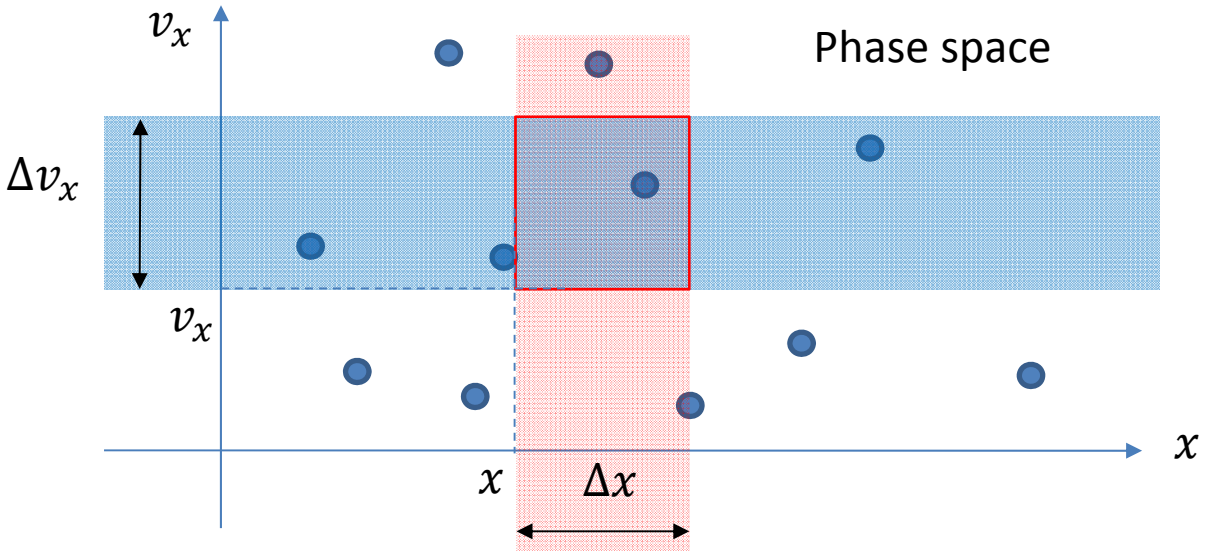
Kinetic equation is an equation, where the unknown is the velocity distribution function of gas molecules. Before derivation of the kinetic equation for $f(\mathbf{r}, \mathbf{v}, t)$, let's consider the major principles of such derivation, using the case of one-dimensional motion of molecules when $f = f(x, v_x, t)$ as an illustrative example.

Illustrative example: One-dimensional motion of molecules

Let's consider a small cell of the phase space of volume $\Delta x \Delta v_x$ around point (x, v_x). The average numbers of molecules in this cell at times t and $t + \Delta t$ are given by Eq. (3.1.1) (For the sake of simplicity, here we use slightly different notation compared to Section 3.1):

(3.3.1) $$N(t) = f(x, v_x, t)\Delta x \Delta v_x, \qquad N(t + \Delta t) = f(x, v_x, t + \Delta t)\Delta x \Delta v_x.$$

Why the number of molecules in $\Delta x \Delta v_x$ varies with time and $N(t + \Delta t) \neq N(t)$?



3.3. Kinetic equation

There are two reasons for variation of $N(t)$ in time:

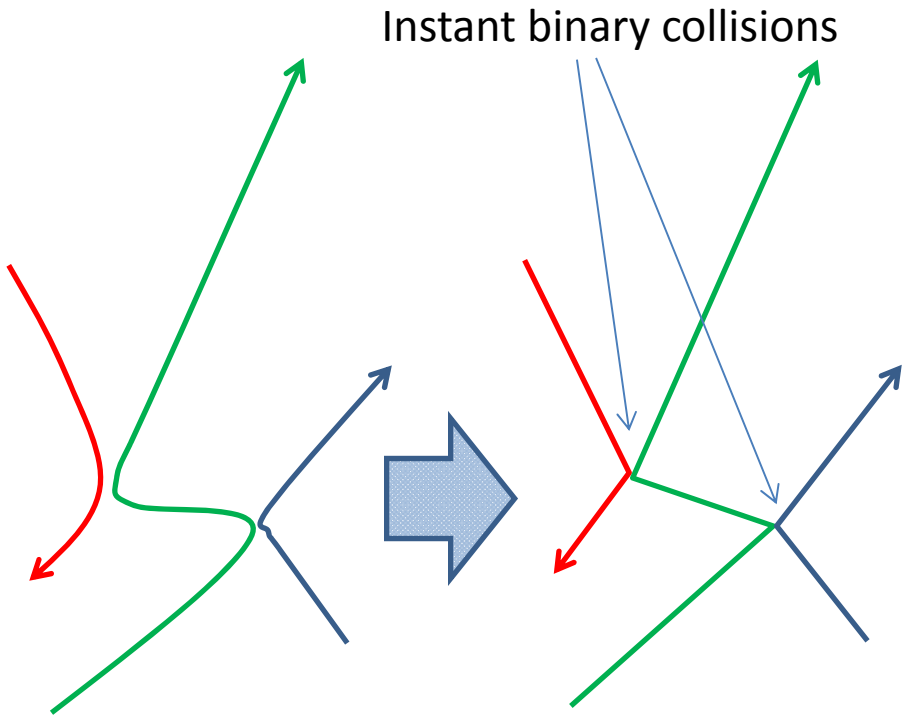
1. Continuous, collisionless motion of molecules that results in variation of coordinate and velocity of every molecule with time according to equations of motion

$$\dot{x} = v_x, \qquad \dot{v}_x = F_x(x)/m, \tag{3.3.2}$$

   where $F_x(x)$ is the **external** conservative force exerted on particle, e.g., gravity force.

2. Collisions between molecules.

The approach to derivation of kinetic equation based on the fact that the time t_c and length l_c scales of collisions (see slide 11 in Chapter 1, Section 1.1) are much smaller than any time and length scale that have to be considered based on the kinetic equation. In this case we can consider every collision as an instant jump-like change of particle velocities and approximate continuous trajectories of particles under continuous interaction forces (left part of the sketch) by non-smooth curves, where every vertex correspond to instant change of particle velocity in a collision (right part of the sketch).



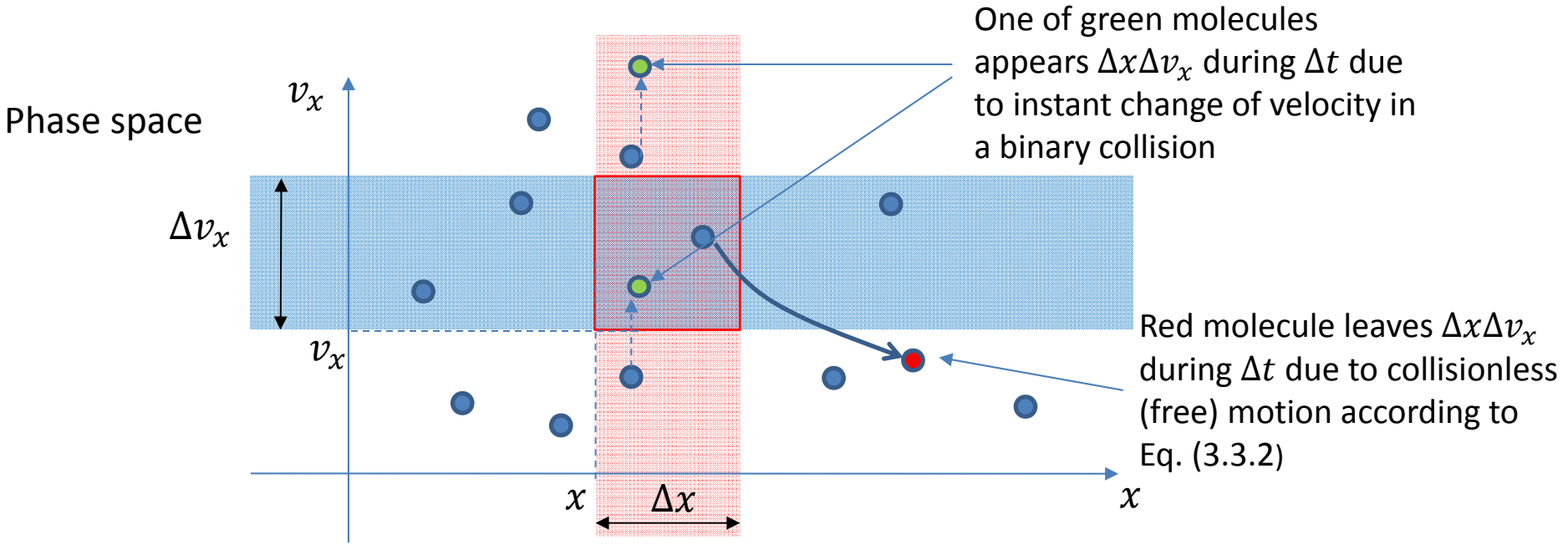
3.3. Kinetic equation

Let's assume that in the dilute gas we account for only binary collisions between molecules and, moreover every collision can be considered as an instant change of velocities of colliding molecules. Then we can split total variation $N(t+\Delta t)-N(t)$ into two parts

(3.3.3) $$N(t+\Delta t)-N(t)=\Delta N_{free}+\Delta N_{coll}.$$

This is the **equation of balance** (or **conservation**) of the number of molecules in the phase space

Under approximation of instant collisions, the mechanisms of change of number of particles in a cell of the phase space and calculate is qualitatively different (it is illustrated in the sketch) and one can calculate ΔN_{free} and ΔN_{coll} separately from each other.



3.3. Kinetic equation

Let's calculate ΔN_{free}. The volume $\Delta x \Delta v_x$ has four edges, so

$$\Delta N_{free} = \Delta N_{AB} + \Delta N_{BC} + \Delta N_{CD} + \Delta N_{DA},$$

where, e.g., ΔN_{DA} is the total average number of molecules that move through edge DA during time Δt. This number can be calculated if we notice that a molecule can move through DA during Δt only if at time t it is located not farther than $v_x \Delta t$ from DA, i.e. it is inside the green layer of phase volume $v_x \Delta t \Delta v_x$ in the sketch (here we assume that $v_x > 0$, otherwise we need to show green layer inside the cell $\Delta x \Delta v_x$). Then ΔN_{DA} is the total number of molecules in that layer. This number can be calculated again with Eq. (3.1.1):

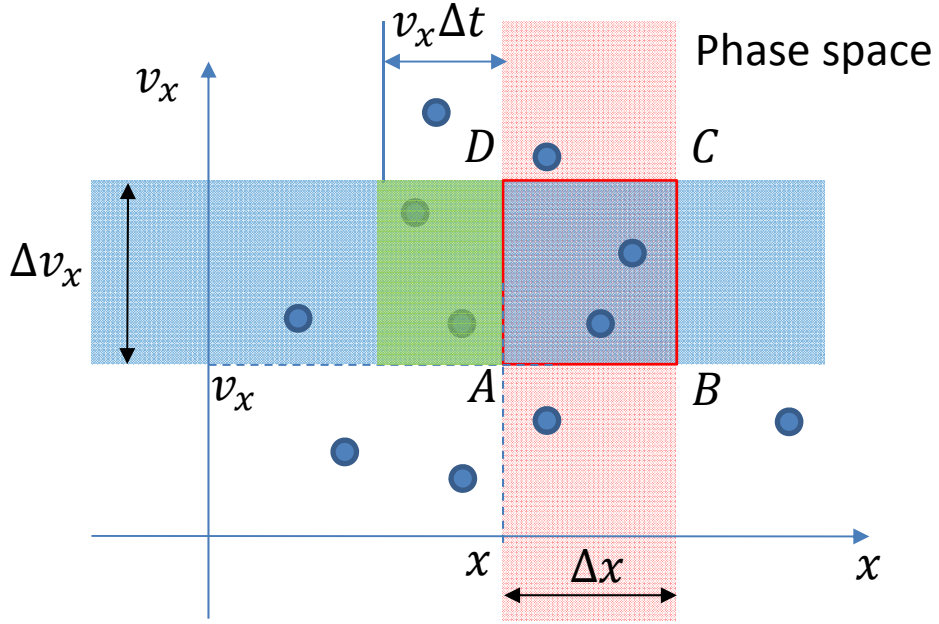
$$\Delta N_{DA} = f(x, v_x, t) v_x \Delta t \Delta v_x.$$

Using the same approach one can find that

$$\Delta N_{BC} = -f(x + \Delta x, v_x, t) v_x \Delta t \Delta v_x,$$

$$\Delta N_{AB} = f(x, v_x, t) \frac{F_x}{m} \Delta t \Delta x,$$

$$\Delta N_{CD} = -f(x, v_x + \Delta v_x, t) \frac{F_x}{m} \Delta t \Delta x.$$



3.3. Kinetic equation

In order to characterize ΔN_{coll}, let's introduce a **collision term**: such quantity $I(x, v_x, t)$ which is equal to the number of molecules that appear (if $I > 0$) or disappear (if $I < 0$) inside a unit phase volume per unit time. Then

$$\Delta N_{coll} = I(x, v_x, t)\Delta x \Delta v_x \Delta t.$$

If one inserts equations for individual terms into the equation of balance of the number of molecules in the phase space, Eq. (3.3.3), then

$$f(x, v_x, t + \Delta t)\Delta x \Delta v_x - f(x, v_x, t)\Delta x \Delta v_x = I(x, v_x, t)\Delta x \Delta v_x \Delta t +$$
$$- f(x + \Delta x, v_x, t) v_x \Delta t \Delta v_x + f(x, v_x, t) v_x \Delta t \Delta v_x - f(x, v_x + \Delta v_x, t)\frac{F_x}{m}\Delta t \Delta x$$
$$+ f(x, v_x, t)\frac{F_x}{m}\Delta t \Delta x.$$

Now let's divide the equation by $\Delta x \Delta v_x \Delta t$:

$$\frac{f(x, v_x, t + \Delta t) - f(x, v_x, t)}{\Delta t} + v_x \frac{f(x + \Delta x, v_x, t) - f(x, v_x, t)}{\Delta x}$$
$$+ \frac{F_x}{m}\frac{f(x, v_x + \Delta v_x, t) - f(x, v_x, t)}{\Delta v_x} = I(x, v_x, t)$$

and take the limits $\Delta t \to 0$, $\Delta x \to 0$, and $\Delta v_x \to 0$:

(3.3.4)
$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + \frac{F_x}{m}\frac{\partial f}{\partial v_x} = I.$$

This is the **kinetic equation** (equation where the unknown is f) for the 1D case.

3.3. Kinetic equation

Kinetic equation

Our goal now is to derive the kinetic equation in the general case of 3D molecular motion and 6-dimensional phase space. Let's consider a small volume of the phase space of size $\Delta\mathbf{X} = \Delta\mathbf{r}\Delta\mathbf{v}$ around point $\mathbf{X} = (\mathbf{r}, \mathbf{v})$. The average numbers of molecules in this volume at times t and $t + \Delta t$ are given by Eq. (3.1.2) :

$$N(t) = f(\mathbf{r}, \mathbf{v}, t)\Delta\mathbf{X}, \qquad N(t + \Delta t) = f(\mathbf{r}, \mathbf{v}, t + \Delta t)\Delta\mathbf{X}.$$

There are two reasons for variation of $N(t)$ in time:

1. Continuous, collisionless motion of molecules that results in variation of coordinate and velocity of every molecule with time according to equations of motion

$$\dot{\mathbf{X}} = \mathbf{Y}(\mathbf{X}),$$

$$\mathbf{Y}(\mathbf{X}) = (Y_1, Y_2, \dots, Y_6) = \left(v_x, v_y, v_z, \frac{F_x}{m}, \frac{F_y}{m}, \frac{F_z}{m}\right).$$

Vector $\mathbf{Y}(\mathbf{X})$ is called the **phase velocity vector**.

   where $\mathbf{F} = F_x\mathbf{i} + F_y\mathbf{j} + F_z\mathbf{k}$ is **external** conservative external force exerted on a molecule.
2. Collisions between molecules.

Let's assume that in the dilute gas we account for only binary collisions between molecules and, moreover every collision can be considered as an instant change of velocities of colliding molecules. Then we can split total variation $N(t + \Delta t) - N(t)$ into two parts

(3.3.5) $$N(t + \Delta t) - N(t) = \Delta N_{free} + \Delta N_{coll}$$

and calculate ΔN_{free} and ΔN_{coll} separately from each other.

3.3. Kinetic equation

Eq. (3.3.5) is the equation of balance of the number of molecules (conservation law for the number of molecules) in the phase space.

In order to characterize ΔN_{coll}, let's introduce a **collision term** $I(\mathbf{X}, t)$ which is equal to the number of molecules that appear (if $I > 0$) or disappear (if $I < 0$) inside a unit phase volume per unit time. Then

$$\Delta N_{coll} = I(\mathbf{X}, t)\Delta\mathbf{X}\Delta t.$$

In order to find ΔN_{free}, let's use the same approach as we used in 1D case: For n-th phase coordinate ($n = 1,2, \dots, 6$), the change of the number of molecules in $\Delta\mathbf{X}$ during Δt is equal to

$$\Delta N_{free(n)} = -f(\mathbf{X}_n, t)\Delta\mathbf{X}_n + f(\boldsymbol{X}, t)\Delta\mathbf{X}_n = -Y_n\Delta t\Delta\mathbf{X}\frac{f(\mathbf{X}_n, t) - f(\mathbf{X}, t)}{\Delta X_n}.$$

Here

$$\boldsymbol{X}_n = (X_1, \dots, X_{n-1}, X_n + \Delta X_n, \Delta X_{n+1}, \dots X_n),$$

$$\Delta\mathbf{X}_n = \Delta X_1 \dots \Delta X_{n-1} Y_n \Delta t \Delta X_{n+1} \dots \Delta X_n.$$

If one inserts equations for individual terms into the balance equation, Eq. (3.3.5), divide the equation by $\Delta\mathbf{X}\Delta t$

(3.3.6)

$$\frac{f(\mathbf{X}, t + \Delta t) - f(\mathbf{X}, t)}{\Delta t} + \sum_{n=1}^{6} Y_n \frac{f(\mathbf{X}_n, t) - f(\mathbf{X}, t)}{\Delta X_n} = I(\mathbf{X}, t),$$

and take the limits $\Delta t \to 0, \Delta X_n \to 0$, then

3.3. Kinetic equation

(3.3.7)
$$\frac{\partial f}{\partial t}+\sum_{n=1}^{6} Y_n \frac{\partial f}{\partial X_n}=I.$$

This is **kinetic equation** (equation where the unknown is the distribution function f). The term

$$\sum_{n=1}^{6} Y_n \frac{\partial f}{\partial X_n}$$

in the LHS of Eq. (3.3.7) describes a part of local variation of f due to collisionless motion of molecules and effects of external forces exerted on molecules and is called the **convective term** or **convective operator**. The **collision term** or **collision operator** I in the RHS of Eq. (3.3.7) describes local variation of f due to binary collisions between molecules. The convective term can be re-written as follows

$$\sum_{n=1}^{6} Y_n \frac{\partial f}{\partial X_n}=v_x\frac{\partial f}{\partial x}+v_y\frac{\partial f}{\partial y}+v_z\frac{\partial f}{\partial z}+\frac{F_x}{m}\frac{\partial f}{\partial v_x}+\frac{F_y}{m}\frac{\partial f}{\partial v_y}+\frac{F_z}{m}\frac{\partial f}{\partial v_z}=\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}}+\frac{\mathbf{F}}{m}\cdot\frac{\partial f}{\partial \mathbf{v}}.$$

The kinetic equation then takes the form

(3.3.8)
$$\frac{\partial f}{\partial t}+\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}}+\frac{\mathbf{F}}{m}\cdot\frac{\partial f}{\partial \mathbf{v}}=I.$$

Here we use our notation for a **gradient**. See slide 14 in Chapter 2.

The kinetic equation is the mathematical form of the conservation law of particle number in the phase space. This equation can be used for calculations of the distribution function f only if we are able to derive the collision term I in terms of f. This is the most difficult part of the work.

3.4. Boltzmann collision term. Boltzmann kinetic equation

- Collision term
- Collision term I^- for HS molecules
- Direct and reverse collisions
- Change of variables in a collision term
- Collision term I^+ for HS molecules
- Boltzmann collision integral
- Boltzmann kinetic equation
- Collisions density

3.4. Boltzmann collision term. Boltzmann kinetic equation

Collision term

The goal of this Section is to find the mathematical form of the collision term I in the kinetic equation, Eq. (3.3.8). We will find I using two assumptions:

- We consider the dilute gas and account only for binary collisions between particles. This assumption is very important and the derived collision term will be applicable only for flows of a dilute gas.
- Individual collision between molecules is described by the Hard Sphere (HS) molecular model. This assumption can be relaxed and our derivation of the collision term can be generalized for the case of any molecular model considered in Chapter 2. We use this assumption only in order to simplify calculations of the collision term.

The collision term $I(\mathbf{r},\mathbf{v},t)$ is equal to the number of molecules that appear (if $I>0$) or disappear (if $I<0$) inside a unit phase volume per unit time. Then the number of molecules that appear/disappear in the phase volume $d\mathbf{r}d\mathbf{v}$ during time dt is equal to

$$dN_{coll} = I(\mathbf{r},\mathbf{v},t)d\mathbf{r}d\mathbf{v}dt. \tag{3.4.1}$$

Let's represent the collision term and ΔN_{coll} in the form

$$I(\mathbf{r},\mathbf{v},t) = I^{+}(\mathbf{r},\mathbf{v},t) - I^{-}(\mathbf{r},\mathbf{v},t), \tag{3.4.2}$$

$$dN_{coll} = dN_{coll(+)} - dN_{coll(-)} = I^{+}(\mathbf{r},\mathbf{v},t)d\mathbf{r}d\mathbf{v}dt - I^{-}(\mathbf{r},\mathbf{v},t)d\mathbf{r}d\mathbf{v}dt.$$

3.4. Boltzmann collision term. Boltzmann kinetic equation

$dN_{coll(-)}$ is the number of molecules which phase coordinates at time t satisfy the conditions

$$\mathbf{r} < \mathbf{r}_i < \mathbf{r} + d\mathbf{r}, \qquad \mathbf{v} < \mathbf{v}_i < \mathbf{v} + d\mathbf{v},$$

and during dt they leave the phase volume $d\mathbf{r}d\mathbf{v}$ because of collisions with other molecules.

$dN_{coll(+)}$ is the number of molecules which positions in the physical space coordinates at time t satisfy the condition

$$\mathbf{r} < \mathbf{r}_i < \mathbf{r} + d\mathbf{r}$$

and velocities are arbitrary, but during dt these molecules participate in such collisions that post-collisional velocity of these molecules $\mathbf{v'}_i$ satisfy the condition

$$\mathbf{v} < \mathbf{v'}_i < \mathbf{v} + d\mathbf{v},$$

i.e. *after the collision* these molecules appear in the phase volume $d\mathbf{r}d\mathbf{v}$ around point $(\mathbf{r}, \mathbf{v})$.

Let's note that by choosing sufficiently short time interval dt we can guarantee that every molecule can participate during dt in no more than one collision. Thus, $dN_{coll(-)}$ and $dN_{coll(+)}$ can be calculated as *numbers of collisions* between molecules with desired pre- or post-collisional phase coordinates.

We will calculate $dN_{coll(-)}$ and $dN_{coll(+)}$ separately from each other using the following approach:

- Initially, we divide all molecules into such groups that the number of molecules in every group and the number of binary collisions between them are easy to calculate.
- Then we account for contributions of various pairs of molecular groups into the total $dN_{coll(-)}$ and $dN_{coll(+)}$.

3.4. Boltzmann collision term. Boltzmann kinetic equation

Collsion term I^- for HS molecules

Let's consider **group 1** of molecules whose phase coordinates at time t satisfy the conditions

$$\mathbf{r} < \mathbf{r}_i < \mathbf{r} + d\mathbf{r}, \qquad \mathbf{v} < \mathbf{v}_i < \mathbf{v} + d\mathbf{v}.$$

The number of such molecules is equal to

$$dN_1 = f(\mathbf{r}, \mathbf{v}, t) d\mathbf{r} d\mathbf{v}.$$

Let's introduce **group 2** of molecules whose velocity at time t satisfy the condition

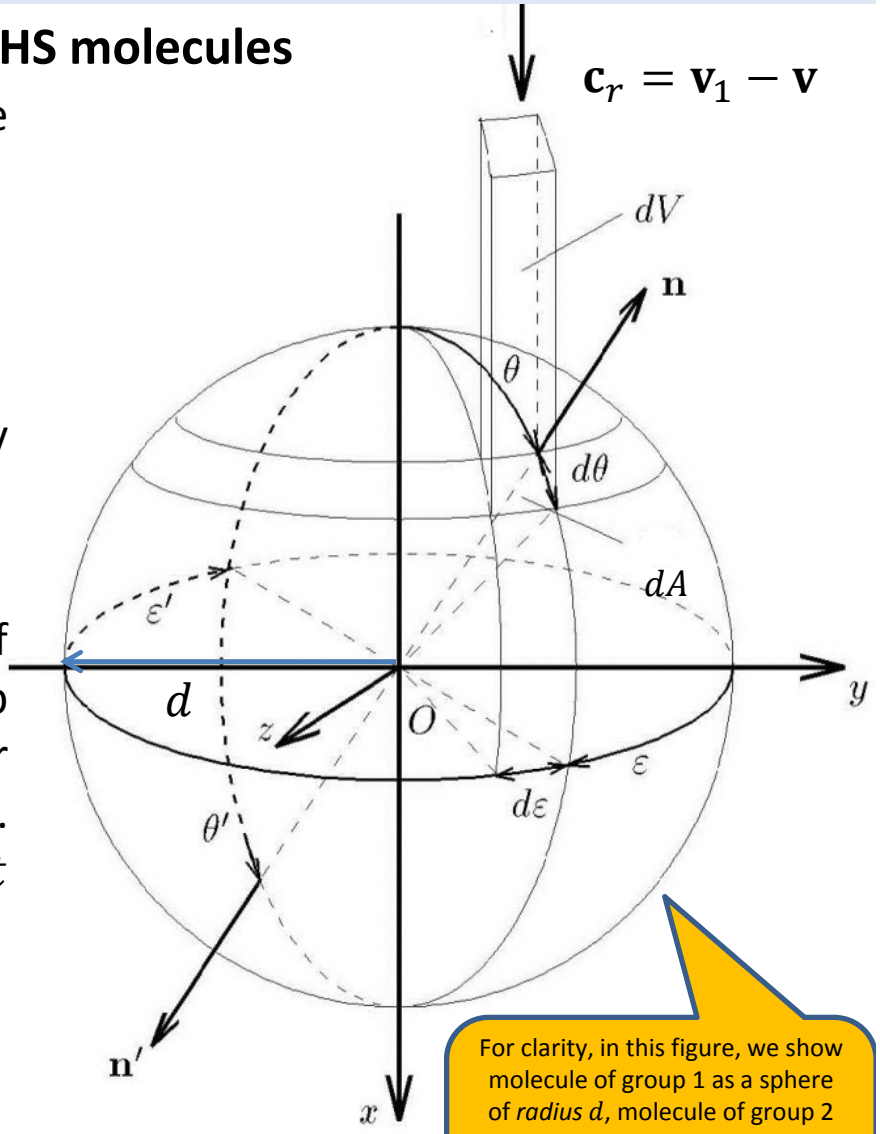
$$\mathbf{v}_1 < \mathbf{v}_i < \mathbf{v}_1 + d\mathbf{v}_1$$

and coordinates are such that every molecule of group 2 during dt collides with a molecule of group 1 and during the collision the center-to center vector $\mathbf{n}$ is within the solid angle $d\Omega = \sin\theta \, d\theta d\varepsilon$. Molecules of group 2 must be located at time t within the "parallelepiped" of volume

$$dV = c_r dt dA |\cos\theta| = |\mathbf{c}_r \cdot \mathbf{n}| dt dA,$$
$$dA = d^2 d\Omega = d^2 \sin\theta \, d\theta d\varepsilon.$$

The number of molecules in group 2 is equal to

$$dN_2 = dt f(\mathbf{r}, \mathbf{v}_1, t) |\mathbf{c}_r \cdot \mathbf{n}| d^2 \sin\theta \, d\theta d\varepsilon d\mathbf{v}_1.$$



For clarity, in this figure, we show molecule of group 1 as a sphere of *radius d*, molecule of group 2 is shown as a point. All notation is in agreement with notation used in figures on slides 24, 25, and 31 of Chapter 2.

3.4. Boltzmann collision term. Boltzmann kinetic equation

Then the number of collisions between molecules of groups 1 and 2 during dt is equal to

(3.4.3) $$dI_{12} = dN_1 dN_2 = dt d\mathbf{r} d\mathbf{v} f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_1, t) |\mathbf{c}_r \cdot \mathbf{n}| d^2 \sin\theta \, d\theta d\varepsilon d\mathbf{v}_1.$$

In order to obtain the full number of collisions $dN_{coll(-)}$ between molecules of group 1 and all other molecules, we need to integrated Eq. (3.4.3) for all possible directions of $\mathbf{n}$, i.e. at

$$0 \le \theta \le \frac{\pi}{2}, \qquad 0 \le \varepsilon \le 2\pi.$$

(Here $\theta \le \pi/2$ because only in this case $\mathbf{c}_r \cdot \mathbf{n} < 0$. This condition must be fulfilled for any real collision) and for all velocities $\mathbf{v}_1$ of molecules in group 2:

$$dN_{coll(-)} = I^- dt d\mathbf{r} d\mathbf{v} = dt d\mathbf{r} d\mathbf{v} \int_0^{2\pi} \int_0^{\pi/2} f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_1, t) |\mathbf{c}_r \cdot \mathbf{n}| d^2 \sin\theta \, d\theta d\varepsilon d\mathbf{v}_1 \, .$$

which immediately gives

(3.4.4) $$I^-(\mathbf{r}, \mathbf{v}, t) = \int_0^{2\pi} \int_0^{\pi/2} f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_1, t) |\mathbf{c}_r \cdot \mathbf{n}| d^2 \sin\theta \, d\theta d\varepsilon d\mathbf{v}_1.$$

Calculation of I^+ is a more complicated task. In order to do it, we will solve first two auxiliary problems.

3.4. Boltzmann collision term. Boltzmann kinetic equation

Direct and reverse collisions

Let's recall the relationships between velocities of molecules before and after a collision, Eq. (2.2.11) and (2.2.12):

$$\mathbf{c}'_r = \mathbf{c}_r - 2(\mathbf{c}_r \cdot \mathbf{n})\mathbf{n},$$

(3.4.5)

$$\mathbf{v}' = \mathbf{v} + [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n},$$

$$\mathbf{v}'_1 = \mathbf{v}_1 - [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n}.$$

Note that all these equations were first established for the HS molecules, but then we found that they are applicable to any molecular model of a simple gas. Corresponding, the results we are going to obtain now are applicable to any molecular model of the simple gas.

First, let's find velocities of molecules before the collisions, $\mathbf{v}$ and $\mathbf{v}_1$, as functions of their velocities after the collisions, $\mathbf{v}'$ and $\mathbf{v}'_1$. We know (see Eq. (2.2.10)) that during a collision the normal component of relative velocity ($\mathbf{c}_r = \mathbf{v}_1 - \mathbf{v}$) changes its sign, i.e., $(\mathbf{c}'_r \cdot \mathbf{n}) = -(\mathbf{c}_r \cdot \mathbf{n})$. Then

$$\mathbf{c}_r = \mathbf{c}'_r + 2(\mathbf{c}_r \cdot \mathbf{n})\mathbf{n} = \mathbf{c}'_r - 2(\mathbf{c}'_r \cdot \mathbf{n})\mathbf{n},$$

(3.4.6)

$$\mathbf{v} = \mathbf{v}' - [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n} = \mathbf{v}' + [(\mathbf{v}'_1 - \mathbf{v}') \cdot \mathbf{n}]\mathbf{n},$$

$$\mathbf{v}_1 = \mathbf{v}'_1 + [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n} = \mathbf{v}'_1 - [(\mathbf{v}'_1 - \mathbf{v}') \cdot \mathbf{n}]\mathbf{n}.$$

Thus we see, that equations for pre-collisional velocities as functions of post-collisional ones are identical to Eq. (3.4.5).

3.4. Boltzmann collision term. Boltzmann kinetic equation

Let's note that formally the results of calculations with Eq. (2.4.5) and (2.4.6) do not change if we replace $\mathbf{n}$ with $-\mathbf{n}$. Physically, a collision at given $\mathbf{v}$ and $\mathbf{v}_1$ can happen only if $\mathbf{c}_r \cdot \mathbf{n} < 0$ (it corresponds to $\theta < \pi/2$). Such a collision is called the **direct collision**. Let's introduce a new unit vector $\mathbf{n}' = -\mathbf{n}$ and calculate $\mathbf{c}'_r \cdot \mathbf{n}'$:

$$\mathbf{c}'_r \cdot \mathbf{n}' = -(\mathbf{c}'_r \cdot \mathbf{n}) = \mathbf{c}_r \cdot \mathbf{n} < 0.$$

Thus, potentially a collision can occur with velocities of molecules velocities $\mathbf{v}'$ and $\mathbf{v}'_1$ and center-to-center vector $\mathbf{n}'$. Such a collision is called the **reverse collision with respect to the given direct**. One can use Eq. (3.4.5) and (3.4.6) in order to calculate velocities of molecules $\mathbf{v}''$ and $\mathbf{v}''_1$ after the reverse collision:

$$\mathbf{v}'' = \mathbf{v}' + [(\mathbf{v}'_1 - \mathbf{v}') \cdot \mathbf{n}']\mathbf{n}' = \mathbf{v} + [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n} - [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n} = \mathbf{v},$$

(3.4.7)

$$\mathbf{v}''_1 = \mathbf{v}'_1 - [(\mathbf{v}'_1 - \mathbf{v}') \cdot \mathbf{n}']\mathbf{n}' = \mathbf{v}_1 - [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n} + [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n} = \mathbf{v}_1.$$

Thus, after the reverse collision, molecules take velocities that they had before the direct collision. The direct and reverse collisions are mutually reverse.

This consideration also shows that if we want to find velocities of molecules before a direct collision, they can be found as velocities after the corresponding reverse collision.

3.4. Boltzmann collision term. Boltzmann kinetic equation

Change of variables in the collision term

Let's consider an equation

(3.4.8) $$dI = a(\mathbf{v}', \mathbf{v}'_1)d\mathbf{v}'d\mathbf{v}'_1,$$

where $\mathbf{v}'$ and $\mathbf{v}'_1$ have physical meaning of particle velocities before a collision with given $\mathbf{n}'$. Let's find the form of this equation after the change of variables from $\mathbf{v}'$ and $\mathbf{v}'_1$ to $\mathbf{v}''$ and $\mathbf{v}''_1$ where the latter have meaning of velocities after the collision with given $\mathbf{n}'$, i.e. are related to $\mathbf{v}'$ and $\mathbf{v}'_1$ by means of Eq. (3.4.5):

$$\mathbf{v}'' = \mathbf{v}' + [(\mathbf{v}'_1 - \mathbf{v}') \cdot \mathbf{n}']\mathbf{n}', \qquad \mathbf{v}''_1 = \mathbf{v}'_1 - [(\mathbf{v}'_1 - \mathbf{v}') \cdot \mathbf{n}']\mathbf{n}'.$$

Prerequisite: Variable change in definite integrals (see calculus).

One-dimensional case: Variable change $x'' = g(x')$, $x' = h(x'')$; $h(x'')$ is inverse to $g(x')$.

$$I = \int_a^b a(x')dx' = \int_{g(a)}^{g(b)} a(h(x''))\frac{dh}{dx''}dx'', \qquad \text{or} \qquad dI = a(x')dx' = a(h(x''))\frac{dh}{dx''}dx''.$$

Two-dimensional case: Variable change $x_1'' = g_1(x'_1, x'_2)$, $x_2'' = g_2(x'_1, x'_2)$; inverse transformation $x_1' = h_1(x''_1, x''_2)$, $x_2' = h_2(x''_1, x''_2)$.

$$I = \iint_{D'} a(x'_1, x'_2)dx'_1dx'_2 = \iint_{D''} a(h_1(x''_1, x''_2), h_2(x''_1, x''_2))|J|dx''_1dx''_2$$

or $$dI = a(x'_1, x'_2)dx'_1dx'_2 = a(h_1(x''_1, x''_2), h_2(x''_1, x''_2))|J|dx''_1dx''_2,$$

where

$$J = \det\begin{bmatrix} \frac{\partial x'_1}{\partial x''_1} & \frac{\partial x'_1}{\partial x''_2} \\ \frac{\partial x'_2}{\partial x''_1} & \frac{\partial x'_2}{\partial x''_2} \end{bmatrix}$$

is the **Jacobinan**, i.e. the determinant of the **Jacobian matrix**.

The same rule works independently on the number of variables and we can use it in order to transform Eq. (3.4.8). It means that we need to find analogs of functions h_i, i.e. pre-collisional velocities as functions of post-collisional ones. But we already solved this problem and found (see Eq. (3.4.6)) that

(3.4.9) $$\mathbf{v}' = \mathbf{v}'' + [(\mathbf{v}''_1 - \mathbf{v}'') \cdot \mathbf{n}']\mathbf{n}', \qquad \mathbf{v}'_1 = \mathbf{v}''_1 - [(\mathbf{v}''_1 - \mathbf{v}'') \cdot \mathbf{n}']\mathbf{n}'.$$

Then

$$dI = a(\mathbf{v}'' + [(\mathbf{v}''_1 - \mathbf{v}'') \cdot \mathbf{n}']\mathbf{n}', \mathbf{v}''_1 - [(\mathbf{v}''_1 - \mathbf{v}'') \cdot \mathbf{n}']\mathbf{n}')|J|d\mathbf{v}''d\mathbf{v}''_1,$$

where

$$J = \det\left[\frac{\partial(\mathbf{v}', \mathbf{v}'_1)}{\partial(\mathbf{v}'', \mathbf{v}''_1)}\right]$$

is the Jacobian of the variable transformation given by Eq. (3.4.9). It can be shown that $J = -1$, so that finally

(3.4.10) $$dI = a(\mathbf{v}'' + [(\mathbf{v}''_1 - \mathbf{v}'') \cdot \mathbf{n}']\mathbf{n}', \mathbf{v}''_1 - [(\mathbf{v}''_1 - \mathbf{v}'') \cdot \mathbf{n}']\mathbf{n}')d\mathbf{v}''d\mathbf{v}''_1.$$

3.4. Boltzmann collision term. Boltzmann kinetic equation

Collsion term I^+ for the HS molecules

Let's consider **group 3** of molecules whose phase coordinates at time t satisfy the conditions

$$\mathbf{r} < \mathbf{r}_i < \mathbf{r} + d\mathbf{r}, \qquad \mathbf{v}' < \mathbf{v}_i < \mathbf{v}' + d\mathbf{v}'.$$

The number of such molecules is equal to

$$dN_3 = f(\mathbf{r}, \mathbf{v}', t) d\mathbf{r} d\mathbf{v}'.$$

Let's introduce **group 4** of molecules whose velocity at time t satisfy the condition

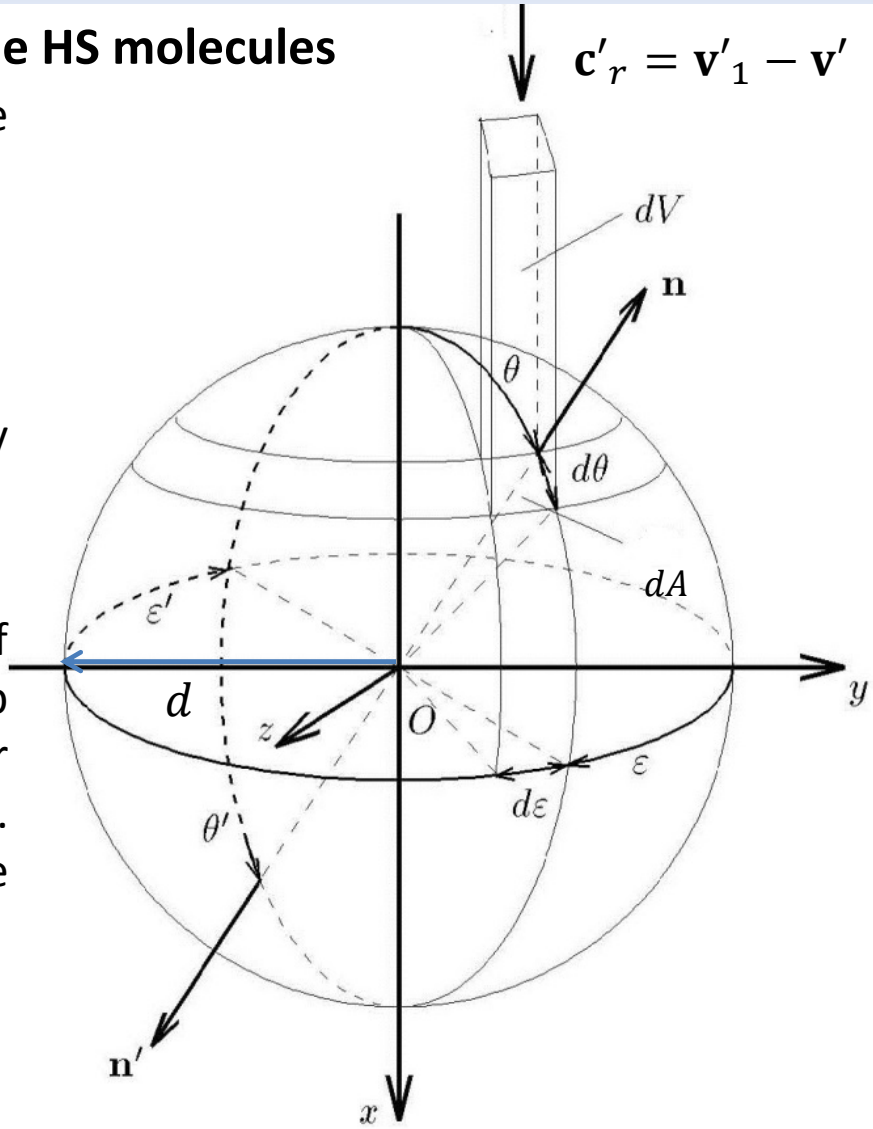
$$\mathbf{v}'_1 < \mathbf{v}'_i < \mathbf{v}'_1 + d\mathbf{v}'_1$$

and coordinates are such that every molecule of group 2 during dt collides with a molecule of group 1 and during the collision the center-to center vector $\mathbf{n}$ is within the solid angle $d\Omega' = \sin\theta'\, d\theta' d\varepsilon$. Molecules of group 4 must be located at time t within the "parallelepiped" of volume

$$dV' = c_r dt dA' |\cos\theta'| = |\mathbf{c}_r \cdot \mathbf{n}'| dt dA',$$
$$dA' = d^2 d\Omega' = d^2 \sin\theta'\, d\theta' d\varepsilon'.$$

The number of molecules in group 4 is equal to

$$dN_4 = dt f(\mathbf{r}, \mathbf{v}'_1, t) |\mathbf{c}'_r \cdot \mathbf{n}'| d^2 \sin\theta'\, d\theta' d\varepsilon' d\mathbf{v}'_1.$$



3.4. Boltzmann collision term. Boltzmann kinetic equation

Then the number of collisions between molecules of groups 3 and 4 during dt is equal to

(3.4.11) $$dI_{34} = dN_3 dN_4 = dt d\mathbf{r} d\mathbf{v}' f(\mathbf{r}, \mathbf{v}', t) f(\mathbf{r}, \mathbf{v}'_1, t) |\mathbf{c}'_r \cdot \mathbf{n}| d^2 \sin\theta' \, d\theta' d\varepsilon' d\mathbf{v}'_1.$$

Unfortunately, dI_{34} does not allow one to directly calculate $dN_{coll(+)}$, because dI_{34} depends only on velocities *before* the collision, but in order to calculate $dN_{coll(+)}$ one needs to impose restrictions on velocities of molecules *after* collisions. In order to solve this issue, let's make a change of variables in Eq. (3.4.11): Let's replace velocities before the collision, by velocities after the collision that are calculated based on Eq. (3.4.5), i.e.

$$\mathbf{v}'' = \mathbf{v}' + [(\mathbf{v}'_1 - \mathbf{v}') \cdot \mathbf{n}']\mathbf{n}', \qquad \mathbf{v}''_1 = \mathbf{v}'_1 - [(\mathbf{v}'_1 - \mathbf{v}') \cdot \mathbf{n}']\mathbf{n}'.$$

Then, according to Eq. (3.4.10), one can obtain

$$I_{34} = \Delta t d\mathbf{r} d\mathbf{v}'' f(\mathbf{r}, \mathbf{v}'' + [(\mathbf{v}''_1 - \mathbf{v}'') \cdot \mathbf{n}']\mathbf{n}', t) \times$$
$$f(\mathbf{r}, \mathbf{v}''_1 - [(\mathbf{v}''_1 - \mathbf{v}'') \cdot \mathbf{n}']\mathbf{n}', t) |\mathbf{c}''_r \cdot \mathbf{n}'| d^2 \sin\theta' \, d\theta' d\varepsilon' d\mathbf{v}''_1.$$

Now I_{34} depends on post-collisional velocities. In order to calculate $dN_{coll(+)}$, let's impose the restrictions on the post-collisional values of $\mathbf{v}''$: Let's consider such $\mathbf{v}''$ and $d\mathbf{v}''$ that after a collision a molecule of group 3 falls into group 1, i.e.

$$\mathbf{v}'' = \mathbf{v}, \qquad d\mathbf{v}'' = d\mathbf{v}.$$

Then

(3.4.12) $$I_{34} = \Delta t d\mathbf{r} d\mathbf{v} f(\mathbf{r}, \mathbf{v} + [(\mathbf{v}''_1 - \mathbf{v}) \cdot \mathbf{n}']\mathbf{n}', t) \times$$
$$f(\mathbf{r}, \mathbf{v}''_1 - [(\mathbf{v}''_1 - \mathbf{v}) \cdot \mathbf{n}']\mathbf{n}', t) |(\mathbf{v}''_1 - \mathbf{v}) \cdot \mathbf{n}'| d^2 \sin\theta' \, d\theta' d\varepsilon' d\mathbf{v}''_1.$$

3.4. Boltzmann collision term. Boltzmann kinetic equation

In order to obtain the full number of such collisions $dN_{coll(+)}$ that the first colliding molecule falls into group 1 after the collision, one needs to integrated Eq. (3.4.12) for all possible directions of $\mathbf{n}'$, i.e. at

$$\frac{\pi}{2} \le \theta' \le \pi, \qquad 0 \le \varepsilon' \le 2\pi.$$

Here $\theta' \ge \pi/2$ because only in this case $(\mathbf{v''}_1 - \mathbf{v}) \cdot \mathbf{n}' > 0$, which is required for post-collisional velocities at any real collision) and for all velocities $\mathbf{v''}_1$ of molecules in group 4:

$$dN_{coll(+)} = I^+ dt d\mathbf{r} d\mathbf{v} = dt d\mathbf{r} d\mathbf{v} \times$$

$$\int_0^{2\pi} \int_{\pi/2}^{\pi} f(\mathbf{r}, \mathbf{v} + [(\mathbf{v''}_1 - \mathbf{v}) \cdot \mathbf{n}']\mathbf{n}', t) f(\mathbf{r}, \mathbf{v''}_1 - [(\mathbf{v''}_1 - \mathbf{v}) \cdot \mathbf{n}']\mathbf{n}', t) |(\mathbf{v''}_1 - \mathbf{v}) \cdot \mathbf{n}'| d^2 \sin\theta' \, d\theta' d\varepsilon' d\mathbf{v''}_1$$

Let's change the notation of the integration variables $\mathbf{v}_1 = \mathbf{v''}_1$ and make the variable change

$$\theta = \pi - \theta', \qquad \varepsilon = \varepsilon' + \pi.$$

Then $\mathbf{n}'$ transforms into $\mathbf{n}$ and

$$I^+(\mathbf{r}, \mathbf{v}, t) = \int_0^{2\pi} \int_0^{\pi/2} f(\mathbf{r}, \mathbf{v} + [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n}, t) f(\mathbf{r}, \mathbf{v}_1 - [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n}, t) |(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}| d^2 \sin\theta \, d\theta d\varepsilon d\mathbf{v}_1 \quad (3.4.13)$$

3.4. Boltzmann collision term. Boltzmann kinetic equation

Boltzmann collision term

In order to simplify the form of I^- and I^- let's introduce a special notation for distribution functions in these integrals:

$$f = f(\mathbf{r}, \mathbf{v}, t), \qquad f_1 = f(\mathbf{r}, \mathbf{v}_1, t),$$
$$f' = f(\mathbf{r}, \mathbf{v} + [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n}, t), \qquad f'_1 = f(\mathbf{r}, \mathbf{v}_1 - [(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}]\mathbf{n}, t).$$

Then Eqs. (3.4.4) and (3.4.13) can be written as ($\sigma = d^2/4$ is the differential cross-section for the HS molecules)

$$I^-(\mathbf{r}, \mathbf{v}, t) = 4 \int_0^{2\pi} \int_0^{\pi/2} \int f f_1 |\mathbf{c}_r \cdot \mathbf{n}| \sigma \sin\theta \, d\theta d\varepsilon d\mathbf{v}_1 \,,$$

$$I^+(\mathbf{r}, \mathbf{v}, t) = 4 \int_0^{2\pi} \int_0^{\pi/2} \int f' f'_1 |\mathbf{c}_r \cdot \mathbf{n}| \sigma \sin\theta \, d\theta d\varepsilon d\mathbf{v}_1 \,.$$

Everywhere in Chapter 3, $\mathbf{c}_r$ and c_r denote relative velocity *before* a collision. These quantities were denoted also as $\mathbf{C}_r$ and C_r in Chapter 2.

The collision term in the form

(3.4.14a) $$I_B = I^+(\mathbf{r}, \mathbf{v}, t) - I^-(\mathbf{r}, \mathbf{v}, t) = 4 \int_0^{2\pi} \int_0^{\pi/2} \int \left(f' f'_1 - f f_1\right) |\mathbf{c}_r \cdot \mathbf{n}| \sigma \sin\theta \, d\theta d\varepsilon d\mathbf{v}_1.$$

is called the **Boltzmann collision term**. It was obtained for the HS molecules. It can be proved, however, that Eq. (3.4.13) can be used for any molecular model if $\sigma = \sigma(\pi - 2\theta, |\mathbf{v}_1 - \mathbf{v}|)$ is the differential cross section for that molecular model.

3.4. Boltzmann collision term. Boltzmann kinetic equation

The Boltzmann collision term can be viewed as a difference of two collision terms, $I^-(\mathbf{r},\mathbf{v},t)$ and $I^+(\mathbf{r},\mathbf{v},t)$, which are called the **collision integrals of direct and reverse collisions**.

One can re-write the Boltzmann collision terms in various forms depending on variables that are used in order to characterize the relative position of molecules before a collision. Instead of θ, one can use the deflection angle $\chi = \pi - 2\theta$ or collision parameter b. Then one can make the change of variables in the collision integral (note that $|\boldsymbol{c}_r \cdot \mathbf{n}| = c_r \cos\theta$)

$$bdbd\varepsilon = \sigma(\chi, c_r)\sin\chi\, d\chi d\varepsilon = 4\sigma(\chi, c_r)\cos\theta\sin\theta\, d\theta d\varepsilon$$

and write I_B also in the forms

(3.4.14b) $$I_B(\mathbf{r},\mathbf{v},t) = \int \int_0^{2\pi} \int_0^{\pi} (f'f'_1 - ff_1) c_r \sigma(c_r,\chi)\sin\chi\, d\chi d\varepsilon d\mathbf{v}_1 ,$$

(3.4.14c) $$I_B(\mathbf{r},\mathbf{v},t) = \int \int_0^{2\pi} \int_0^{r_{max}} (f'f'_1 - ff_1) c_r b db d\varepsilon d\mathbf{v}_1 .$$

Boltzmann Equation

The kinetic equation where the collision term is equal to the Boltzmann collision term is called the **Boltzmann kinetic equation**:

(3.4.15) $$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m}\cdot\frac{\partial f}{\partial \mathbf{v}} = \int \int_0^{2\pi} \int_0^{r_{max}} (f'f'_1 - ff_1) c_r b db d\varepsilon d\mathbf{v}_1 .$$

3.4. Boltzmann collision term. Boltzmann kinetic equation

The Boltzmann equation is the major equation of the kinetic theory of dilute gases: If we are able to solve the Boltzmann equation and find the velocity distribution function, then we can find any macroscopic gas parameters.

The Boltzmann equation is a non-linear **integro-differential equation** with respect to a function with 7 independent variables. The exact solutions of the Boltzmann equation are known only for a few very special cases. The numerical solution of the full Boltzmann equations is difficult even for modern computers. The major difficulties in the numerical solution come from the necessity to calculate the fifth-dimensional integral in the Boltzmann collision term.

We derive the Boltzmann collision integral using roughly the same approach which was used by L. Boltzmann. This method of derivation of the Boltzmann equation is called **phenomenological**. It was later on found that the Boltzmann equation can be derived directly from the equations of motion of individual gas molecules. It was done for the first time by the Russian scientist N. Bogolubov in 1946. Currently, a few quite different approaches for derivation of the Boltzmann equation from the equations of motion of individual molecules are known.

Collision density

The approach we used to calculate I_B can be also used to calculate the **collision density** Z: number of binary collisions in a unit volume of gas per unit time (see Section 1.4). Equation

$$dN_{coll(-)} = dtd\mathbf{r}d\mathbf{v}\int_0^{2\pi}\int_0^{\pi} f(\mathbf{r},\mathbf{v},t)f(\mathbf{r},\mathbf{v}_1,t)c_r\sigma(c_r,\chi)\sin\chi\, d\chi d\varepsilon d\mathbf{v}_1$$

defines the number of collisions between molecules of group 1 and other molecules during dt.

3.4. Boltzmann collision term. Boltzmann kinetic equation

In order to find the total number of binary collisions in volume $d\mathbf{r}$ during dt one needs to account for contributions of all possible velocities of molecules in group 1, i.e. perform integration over $\mathbf{v}$. In the resultant equation, one also needs to account for coefficient ½, because two molecules participate in every binary collision:

$$Z(\mathbf{r},t)dtd\mathbf{r} = dtd\mathbf{r}\frac{1}{2}\int\int f(\mathbf{r},\mathbf{v},t)f(\mathbf{r},\mathbf{v}_1,t)c_r\int_0^{2\pi}\int_0^{\pi}\sigma(c_r,\chi)\sin\chi\, d\chi d\varepsilon d\mathbf{v}_1 d\mathbf{v}.$$

Since (see also Eq. (2.5.13))

$$\int_0^{2\pi}\int_0^{\pi}\sigma(\chi,c_r)\sin\chi\, d\chi d\varepsilon = \sigma_T(c_r),$$

one can finally obtain

(3.4.16) $$Z(\mathbf{r},t) = \frac{1}{2}\int\int f(\mathbf{r},\mathbf{v},t)f(\mathbf{r},\mathbf{v}_1,t)c_r\sigma_T(c_r)d\mathbf{v}_1 d\mathbf{v}.$$

Other collisional properties, including the **collision frequency** z, **mean free time** τ and **mean free path** λ can be derived in terms of Z (see Section 1.4):

(3.4.17) $$Z = \frac{1}{2}nz, \qquad \tau = \frac{1}{z}, \qquad \lambda = \tau C,$$

where λ depends on the adopted value of the characteristic velocity C.

More accurately, $\lambda = \tau v_*$, where the characteristic velocity v_* is not necessarily equal to C, but can be chosen based on different considerations.

3.5. Boltzmann H-theorem

- Integral lemma
- Collisional invariants
- Boltzmann equation in a spatially homogeneous gas without external fields
- Boltzmann H-theorem in a homogeneous gas

3.5. Boltzmann H-theorem

Boltzmann H-theorem is a very important assertion, which states that *solutions of the Boltzmann equation are in agreement with the second law of thermodynamics*. In order to prove this theorem one needs first to consider and prove an additional statement about properties of the Boltzmann collision term. This statement, integral lemma, will be also used later on in order to establish a relationship between the Boltzmann kinetic equation and macroscopic equations of gas dynamics.

Integral lemma

Let consider the Boltzmann collision term

$$I_B(\mathbf{r},\mathbf{v},t)=\int_0^{2\pi}\int_0^{r_{max}}\left(f'f'_1-ff_1\right)c_r b db d\varepsilon d\mathbf{v}_1,$$

multiply it by a molecular quantity $\Phi(\mathbf{r},\mathbf{v},t)$, and then integrate over velocity $\mathbf{v}$:

(3.5.1)
$$\Delta\Phi(\mathbf{r},t)=\int\Phi(\mathbf{r},\mathbf{v},t)I_B(\mathbf{r},\mathbf{v},t)d\mathbf{v}=\int\int_0^{2\pi}\int_0^{r_{max}}\Phi(\mathbf{r},\mathbf{v},t)\left(f'f'_1-ff_1\right)c_r b db d\varepsilon d\mathbf{v}_1 d\mathbf{v}.$$

Integral lemma:
The quantity $\Delta\Phi(\mathrm{r},t)$ given by Eq. (3.5.1) can be represented in the following *symmetrical* form:

(3.5.2)
$$\Delta\Phi(\mathbf{r},t)=\frac{1}{4}\int\int_0^{2\pi}\int_0^{r_{max}}\left(\Phi+\Phi_1-\Phi'-\Phi'_1\right)\left(f'f'_1-ff_1\right)c_r b db d\varepsilon d\mathbf{v}_1 d\mathbf{v}.$$

where $\Phi=\Phi(\mathbf{r},\mathbf{v},t)$, $\Phi_1=\Phi(\mathbf{r},\mathbf{v}_1,t)$, $\Phi'=\Phi(\mathbf{r},\mathbf{v}',t)$, and $\Phi'_1=\Phi(\mathbf{r},\mathbf{v}'_1,t)$.

3.5. Boltzmann H-theorem

Proof:

As the first step, let's change in Eq. (3.5.1) the notation for integration variables, i.e. rename integration variables: $\mathbf{v}_1 = \mathbf{v}$, $\mathbf{v} = \mathbf{v}_1$. Then

$$\Delta\Phi(\mathbf{r},t) = \int\int\int_0^{2\pi}\int_0^{r_{max}} \Phi(\mathbf{r},\mathbf{v}_1,t)\left(f'f'_1 - ff_1\right)c_r b db d\varepsilon d\mathbf{v}_1 d\mathbf{v}. \tag{3.5.3}$$

Now let's make in Eq. (3.5.1) and (3.5.3) the variable change: Let's change variables $\mathbf{v}$ and $\mathbf{v}_1$ into $\mathbf{v}'$ and $\mathbf{v}'_1$ according to Eq. (3.4.5). The we can use the rule given by Eq. (3.4.6) and obtain

$$\Delta\Phi(\mathbf{r},t) = \int\int\int_0^{2\pi}\int_0^{r_{max}} \Phi(\mathbf{r},\mathbf{v}' + [(\mathbf{v}'_1 - \mathbf{v}')\cdot\mathbf{n}]\mathbf{n}\,,t)\left(f'f'_1 - ff_1\right)c_r b db d\varepsilon d\mathbf{v}'_1 d\mathbf{v}'.$$

$$\Delta\Phi(\mathbf{r},t) = \int\int\int_0^{2\pi}\int_0^{r_{max}} \Phi(\mathbf{r},\mathbf{v}'_1 - [(\mathbf{v}'_1 - \mathbf{v}')\cdot\mathbf{n}]\mathbf{n}\,,t)\left(f'f'_1 - ff_1\right)c_r b db d\varepsilon d\mathbf{v}'_1 d\mathbf{v}'.$$

In the last two equations we can again rename variables $\mathbf{v}_1 = \mathbf{v}'_1$, $\mathbf{v} = \mathbf{v}'$:

$$\Delta\Phi(\mathbf{r},t) = -\int\int\int_0^{2\pi}\int_0^{r_{max}} \Phi'\left(f'f'_1 - ff_1\right)c_r b db d\varepsilon d\mathbf{v}'_1 d\mathbf{v}'. \tag{3.5.4}$$

$$\Delta\Phi(\mathbf{r},t) = -\int\int\int_0^{2\pi}\int_0^{r_{max}} \Phi'_1\left(f'f'_1 - ff_1\right)c_r b db d\varepsilon d\mathbf{v}'_1 d\mathbf{v}'. \tag{3.5.5}$$

By calculating the sum of Eqs. (3.5.1), (3.5.3)-(3.5.5), we find $\Delta\Phi(\mathbf{r},t)$ in the form of Eq. (3.5.2).

3.5. Boltzmann H-theorem

Collisional invariants

Let's consider some molecular quantity $\Phi(\mathbf{r},\mathbf{v},t)$, which is conserved during a binary collision between molecules, i.e.

(3.5.6) $$\Phi(\mathbf{r},\mathbf{v},t)+\Phi_1(\mathbf{r},\mathbf{v}_1,t)=\Phi(\mathbf{r},\mathbf{v}+[(\mathbf{v}_1-\mathbf{v})\cdot\mathbf{n}]\mathbf{n},t)+\Phi_1(\mathbf{r},\mathbf{v}_1-[(\mathbf{v}_1-\mathbf{v})\cdot\mathbf{n}]\mathbf{n},t)$$

at arbitrary $\mathbf{n}$. Then such a molecular quantity is called the **collisional invariant**.

Note that according to the integral lemma, $\Delta\Phi(\mathbf{r},t)=0$ for any collisional invariant.

It can be proved that among all possible collisional invariants, one can choose a group of such **independent collisional invariants** $\Phi_{(m)}$ $(m=1,\dots,M)$, that any other invariant can be represented as a linear combination of independent ones, i.e. in the form

$$\Phi(\mathbf{r},\mathbf{v},t)=\sum_{m=1}^{M} a_{(m)}(\mathbf{r},t)\Phi_{(m)}(\mathbf{r},\mathbf{v},t).$$

The number of independent invariants is equal to the number of independent conservation laws in a molecular collision. In a simple gas (identical atoms, no internal degrees of freedom, no chemical reactions), the number M of independent conservation laws is equal to 3, and the following invariants can be considered as independent ones:

(3.5.7) $$\Phi=1,\qquad \Phi=m\mathbf{v},\qquad \Phi=\frac{m\mathbf{v}^2}{2}.$$

Then any other collisional invariant can be represented in the form

(3.5.8) $$\Phi(\mathbf{r},\mathbf{v},t)=a(\mathbf{r},t)+\mathbf{b}(\mathbf{r},t)\cdot(m\mathbf{v})+c(\mathbf{r},t)\frac{m\mathbf{v}^2}{2}.$$

3.5. Boltzmann H-theorem

Boltzmann equation in a spatially homogeneous gas without external fields

Gas or gas flow is called (**spatially**) **homogeneous**, if the distribution function does not depend on coordinates $\mathbf{r}$, i.e. if $f = f(\mathbf{v}, t)$.

Note that according to the kinetic definition of macroscopic gas parameters (Section 3.2), in a spatially homogeneous gas all macroscopic parameters also do not depend on coordinate and can be functions of only time.

Let's consider a homogeneous gas ($\partial f/\partial \mathbf{r} = 0$) without external fields ($\mathbf{F} = 0$). Then $f(\mathbf{v}, t)$ must be a solution of the **spatially homogeneous Boltzmann equation without external fields**:

(3.5.9)
$$\frac{\partial f}{\partial t} = I_B.$$

Boltzmann H-theorem

Let's consider a homogeneous gas without external fields. In order to find a solution of the Boltzmann equation (3.5.9) one needs to impose only an **initial condition** at time $t = 0$:

(3.5.10)
$$f(\mathbf{v}, 0) = f_0(\mathbf{v}).$$

Then Eq. (3.5.9) predicts how $f(\mathbf{v}, t)$ evolves in time due to collisions between molecules.

Boltzmann H-theorem:

For any molecular model describing collisions between molecules and for arbitrary $f_0(\mathbf{v})$, a solution of Eq. (3.5.9) satisfies the following condition: The **Boltzmann H-function** $H(t)$

(3.5.11)
$$H(t) = \int [\log f(\mathbf{v}, t)] f(\mathbf{v}, t) d\mathbf{v}$$

is a non-increasing function of time, i.e. $dH/dt \leq 0$.

3.5. Boltzmann H-theorem

Proof:

Note that any $f = f(\mathbf{v}, t)$ must satisfy the normalization condition, Eq. (3.5.1):

(3.5.12) $$n(t) = \int f(\mathbf{v}, t)\, d\mathbf{v}.$$

This improper integral converges only if $f(\mathbf{v}, t) \to 0$ at $|\mathbf{v}| \to \infty$. Thus, there is an uncertainty $\infty \cdot 0$ at $|\mathbf{v}| \to \infty$ under the integral in Eq. (3.5.11) and first of all one needs to prove that the integral in Eq. (3.5.11) converges. Let's skip this part of the proof, but note that convergence of $H(t)$ given by Eq. (3.5.11) can be proved as a consequence of the limited value of the total gas energy. In other word, one can prove that if (see slide 11)

(3.5.13) $$\rho(t) e_{tot}(t) = \int \frac{m\mathbf{v}^2}{2} f(\mathbf{v}, t) d\mathbf{v} < \infty,$$

then the integral in Eq. (3.5.11) converges. Now let's calculate the derivative dH/dt:

(3.5.14) $$\frac{dH}{dt} = \frac{d}{dt}\int f \log f \, d\mathbf{v} = \int [\log f + 1] \frac{\partial f}{\partial t} d\mathbf{v} = \int [\log f + 1] I_B d\mathbf{v}$$

Here we use Eq. (3.5.6)

and note that the RHS in Eq. (3.5.14) has the form of quantity $\Delta\Phi$ in Eq. (3.5.1) if $\Phi(\mathbf{r}, \mathbf{v}, t) = \log f(\mathbf{v}, t) + 1$. Then one can use the integral lemma, Eq. (3.5.2) in order to transform the RHS in Eq. (3.5.14). Since

$$(\log f + 1) + (\log f' + 1) - (\log f_1 + 1) - \left(\log f'_1 + 1\right) = \log \frac{f f'}{f_1 f'_1},$$

3.5. Boltzmann H-theorem

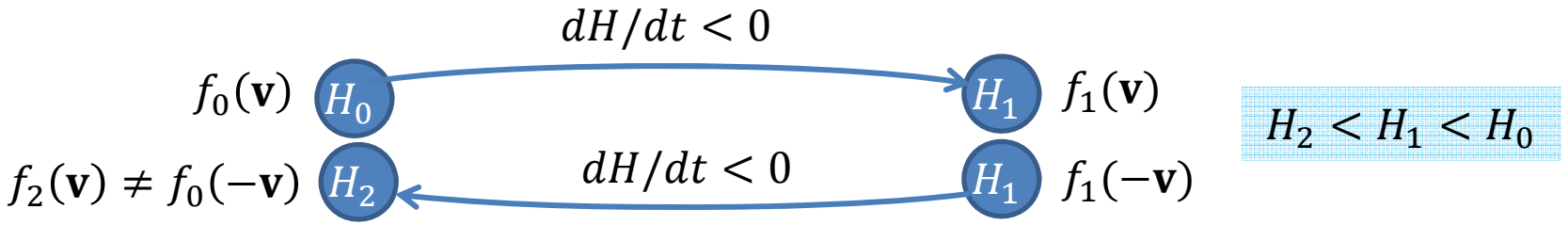
then

$$\frac{dH}{dt} = \frac{1}{4}\int\int\int_0^{2\pi}\int_0^{r_{max}} \log\frac{ff'}{f_1 f'_1}\left(f'f'_1 - ff_1\right)c_r b\,db\,d\varepsilon\,d\mathbf{v}_1\,d\mathbf{v}.$$

One can see that the integrand in the last equation is a non-positive function: if $ff_1 \geq f'f'_1$ then $f'f'_1 - ff_1 \leq 0$, but $\log(ff'/f_1f'_1) \geq 0$; if $ff_1 \leq f'f'_1$ then $f'f'_1 - ff_1 \geq 0$, but $\log(ff'/f_1f'_1) \leq 0$. Thus, $dH/dt \leq 0$ and the H-theorem is proved.

The Boltzmann H-theorem shows that the Boltzmann equation describes **non-reversible processes** in gases in agreement with the second law of thermodynamics.

Let's consider a process described by Eq. (3.5.9) where the distribution function varies during time interval $[0, t_1]$ from $f_0(\mathbf{v})$ with H-function equal to H_0 to some $f_1(\mathbf{v}) = f(\mathbf{v}, t_1)$ with H_1. In this process, the H-function decreases, $dH/dt < 0$, according to the H-theorem. If this process is **reversible**, then Eq. (3.5.9) must have a solution with initial condition $f_1(-\mathbf{v})$ (sign "-" means reversing the direction of motion of every molecule) which leads to the initial state with the distribution function $f_0(-\mathbf{v})$. But during the reverse motion the H-function again can only decrease to value H_2. As a result, the gas cannot return to the state with the initial value of H_0.



3.6. Statistical equilibrium. Maxwell-Boltzmann distribution function. Entropy

- Statistical equilibrium in a spatially homogeneous gas without external fields
- Maxwell-Boltzmann equilibrium distribution function
- Characteristic velocities of chaotic motion
- Equilibrium collisional properties of a VHS gas
- Boltzmann entropy

Statistical equilibrium in a spatially homogeneous gas without external fields

Accurate proof of the Boltzmann H-theorem shows that if the condition given by Eq. (3.5.12) is satisfied, then the H-function for a process with given $f_0(\mathbf{v})$ is limited from below, i.e. such constant C exists that $H(t) < C$ for any t. It is shown in calculus that any function, which is limited from below and not increasing, must have a limit at $t \to \infty$. Thus,

$$H(t) \to H_M = const \quad \text{at} \quad t \to \infty.$$

According to Eq. (3.5.13), $dH/dt \to 0$ only if

$$\frac{\partial f}{\partial t} = I_B \to 0 \qquad \text{at} \qquad t \to \infty$$

and, thus,

$$f(\mathbf{v}, t) \to f_M(\mathbf{v}) \qquad \text{at} \qquad t \to \infty,$$

i.e. any solution of Eq. (3.5.6), with increasing time, approaches a special time-independent state with the distribution function $f_M(\mathbf{v})$, which turns I_B into zero, i.e. satisfies the equation

(3.6.1)
$$\int_0^{2\pi} \int_0^{r_{max}} \left(f'_M f'_{M1} - f_M f_{M1}\right) c_r b db d\varepsilon d\mathbf{v}_1 = 0.$$

If gas is in the state with the velocity distribution function $f_M(\mathbf{v})$, then it will stay in this state forever unless external conditions change. This limit time-independent state of the gas is called the **state of (full) statistical equilibrium** and $f_M(\mathbf{v})$ is called the **equilibrium distribution function**. The process of transition from arbitrary initial state $f_0(\mathbf{v})$ to the equilibrium state $f_M(\mathbf{v})$, described by Eq. (3.5.9), is called **relaxation**.

3.6. Statistical equilibrium. Maxwell-Boltzmann distribution function. Entropy

One can say that, according to the Boltzmann H-theorem, the Boltzmann kinetic equation in the spatially homogeneous gas without external fields describes the process of non-reversible relaxation from arbitrary initial state to the state of full statistical equilibrium.

Maxwell-Boltzmann distribution function

The equilibrium distribution function $f_M(\mathbf{v})$ in the case of spatially homogeneous gas without external fields is called the **Maxwell-Boltzmann** (or **Maxwell**) **distribution function**.

This function must satisfy Eq. (3.6.1). It can be proved that this equation can be satisfied only if the integrand is equal to zero at arbitrary b, ε, and $\mathbf{v}_1$, i.e.

$$f'_M f'_{M1} = f_M f_{M1}.$$

Let's take logarithm of the last equation:

$$\log f'_M + \log f'_{M1} = \log f_M + \log f_{M1}\,.$$

Now one can see (compare with Eq. (3.5.6)) that $\log f_M$ is the collisional invariant, and can be represented in the form of a linear combination of independent invariants given by Eq. (3.5.8)

$$\log f_M(\mathbf{v}) = \tilde{a} + \tilde{\mathbf{b}}\cdot(m\mathbf{v}) + \tilde{c}\,\frac{m\mathbf{v}^2}{2}$$

or

$$f_M(\mathbf{v}) = a\exp\left[-c\,\frac{m(\mathbf{v}-\mathbf{b})^2}{2}\right]. \qquad (3.6.2)$$

One can write that
$(\mathbf{v}-\mathbf{b})^2 = \mathbf{v}^2 - 2\mathbf{b}\cdot\mathbf{v} + \mathbf{b}^2$
and, thus,
$\tilde{a} = \log a - \frac{cm\mathbf{b}^2}{2}$,
$\tilde{\mathbf{b}} = c\mathbf{b}$, $\quad \tilde{c} = -c$

Note that the normalization condition requires $f(\mathbf{v},t) \to 0$ at $|\mathbf{v}| \to \infty$ and, thus, $c > 0$ ($\tilde{c} < 0$).

3.6. Statistical equilibrium. Maxwell-Boltzmann distribution function. Entropy

The functional form of $f_M(\mathbf{v})$ is completely defined by Eq. (3.6.2). Constants a, $\mathbf{b}$, and c can be derived in terms of macroscopic gas parameters in the equilibrium state. Let' use for this purpose the densities of independent collisional invariants, i.e. apply Eq. (3.2.3) to molecular quantities in Eq. (3.5.7) [Here the equation for energy is taken in the form of Eq. (3.2.10)]:

(3.6.3) $$n = \int f_M(\mathbf{v})\, d\mathbf{v}\,, \qquad mn\mathbf{u} = \int m\mathbf{v}\, f_M(\mathbf{v})\, d\mathbf{v}\,, \qquad \frac{3nk_BT}{2} = \int \frac{m(\mathbf{v}-\mathbf{u})^2}{2} f_M(\mathbf{v})\, d\mathbf{v}\,.$$

Let's insert Eq. (3.6.2) into all integrals in Eqs. (3.6.3). In order to calculate integrals of the exponential function, we will use the so-called **Poisson integral** J established in calculus:

$$J = \int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{\pi}.$$

For the number density:

$$n = a \int_{-\infty}^{+\infty} \exp\left[-\frac{cm(v_x-b_x)^2}{2}\right] dv_x \times \int_{-\infty}^{+\infty} \exp\left[-\frac{cm(v_y-b_y)^2}{2}\right] dv_y \times \int_{-\infty}^{+\infty} \exp\left[-\frac{cm(v_z-b_z)^2}{2}\right] dv_z.$$

$$\int_{-\infty}^{+\infty} \exp\left[-\frac{cm(v_x-b_x)^2}{2}\right] dv_x = \sqrt{\frac{2}{cm}} \int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{\frac{2}{cm}} J = \sqrt{\frac{2\pi}{cm}}.$$

Variable change $x = \sqrt{\frac{cm}{2}}(v_x - b_x)$

$$n = a\left(\frac{2\pi}{cm}\right)^{3/2}. \qquad (3.6.4)$$

3.6. Statistical equilibrium. Maxwell-Boltzmann distribution function. Entropy

For the gas macroscopic velocity:

$$nu_x = a\int_{-\infty}^{+\infty} v_x \exp\left[-\frac{cm(v_x-b_x)^2}{2}\right]dv_x \times \int_{-\infty}^{+\infty} \exp\left[-\frac{cm(v_y-b_y)^2}{2}\right]dv_y \times \int_{-\infty}^{+\infty} \exp\left[-\frac{cm(v_z-b_z)^2}{2}\right]dv_z.$$

$$\int_{-\infty}^{+\infty} v_x \exp\left[-\frac{cm(v_x-b_x)^2}{2}\right]dv_x = \sqrt{\frac{2}{cm}}\left(\int_{-\infty}^{+\infty} xe^{-x^2}dx + b_x\int_{-\infty}^{+\infty} e^{-x^2}dx\right) = b_x\sqrt{\frac{2\pi}{cm}}.$$

(3.6.5)
$$nu_x = a\left(\frac{2\pi}{cm}\right)^{3/2} b_x.$$

From the comparison of Eqs. (3.6.4) and (3.6.5) one can conclude that $b_x = u_x$ and

(3.6.6)
$$\mathbf{b} = \mathbf{u}.$$

For the internal energy:

$$\frac{3nk_BT}{m} = a\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\left[c_x^2+c_y^2+c_z^2\right]\exp\left[-c\frac{m(c_x^2+c_y^2+c_z^2)}{2}\right]dc_xdc_ydc_z = a(J_2J_0J_0 + J_0J_2J_0 + J_0J_0J_2)$$

$$= 3aJ_2J_0J_0,$$

where

$$J_0 = \int_{-\infty}^{+\infty}\exp\left[-c\frac{mc_x^2}{2}\right]dc_x = \sqrt{\frac{2\pi}{cm}}, \qquad J_2 = \int_{-\infty}^{+\infty} c_x^2\exp\left[-c\frac{mc_x^2}{2}\right]dc_x = \left(\frac{2}{cm}\right)^{3/2}\int_{-\infty}^{+\infty} x^2e^{-x^2}dx\,.$$

The last integral can be reduced to the Poisson integral by the integration by parts:

$$\int_{-\infty}^{+\infty} x^2 e^{-x^2} dx = -\frac{1}{2}\int_{-\infty}^{+\infty} x e^{-x^2} d(-x^2) = -\frac{1}{2}\int_{-\infty}^{+\infty} x d\left(e^{-x^2}\right) = -\frac{1}{2}\left[x e^{-x^2}\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} e^{-x^2} dx\right] = \frac{\sqrt{\pi}}{2}.$$

Then

$$\frac{3nk_BT}{m} = 3a\left(\frac{2}{cm}\right)^{3/2}\frac{\sqrt{\pi}}{2}\sqrt{\frac{2\pi}{cm}}\sqrt{\frac{2\pi}{cm}} \qquad \Rightarrow \qquad nk_BT = a\left(\frac{2\pi}{cm}\right)^{\frac{3}{2}}\frac{1}{c}.$$

Let's compare the last equation with Eq. (3.6.4):

$$n = a\left(\frac{2\pi}{cm}\right)^{3/2}$$

We see that

(3.6.7) $$c = \frac{1}{k_BT}, \qquad a = \frac{n}{(2\pi k_BT/m)^{3/2}},$$

and the Maxwell-Boltzmann function takes the form

(3.6.8) $$f_M(\mathbf{v}) = \frac{n}{(2\pi k_BT/m)^{3/2}}\exp\left[-\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_BT}\right].$$

We obtained Eq. (3.6.8) as the *exact* solution of the Boltzmann equation for the state of full statistical equilibrium. If we introduce the gas constant $R = k_B/m$, then

(3.6.9) $$f_M(\mathbf{v}) = \frac{n}{(2\pi RT)^{3/2}}\exp\left[-\frac{(\mathbf{v}-\mathbf{u})^2}{2RT}\right].$$

Characteristic velocities of chaotic motion

In terms of velocities of chaotic motion $\mathbf{c} = \mathbf{v} - \mathbf{u}$, the Maxwell-Boltzmann distribution function in Eq. (3.6.9) can be written as follows

$$f_M(\mathbf{c}) = \frac{n}{(2\pi RT)^{3/2}} \exp\left[-\frac{\mathbf{c}^2}{2RT}\right].$$

We can use it in order to characterize the distribution of absolute chaotic velocity $c = |\mathbf{c}|$. If we use spherical coordinates (c, χ, ε) in order to represent the Cartesian components of vector $\mathbf{c}$ (see also slide 33 in Chapter 2, Section 2.5), then

$$c_x = c\cos\chi\,, \qquad c_y = c\sin\chi\cos\varepsilon\,, \qquad c_z = c\sin\chi\sin\varepsilon\,, \qquad dc_x dc_y dc_z = c^2\sin\chi\, d\chi d\varepsilon,$$

and distribution function of absolute values c can be found in the form:

(3.6.10) $$f_M(c) = \frac{n}{(2\pi RT)^{3/2}} c^2 \exp\left[-\frac{c^2}{2RT}\right] \int_0^{2\pi}\int_0^{\pi} \sin\chi\, d\chi d\varepsilon = \frac{4\pi n}{(2\pi RT)^{3/2}} c^2 \exp\left[-\frac{c^2}{2RT}\right].$$

Value $dN = f_M(c)\, dc$ is equal to the average number of molecules in the equilibrium state with magnitudes of chaotic velocities in the range $c < |\mathbf{c}_i| \le c + dc$.

Then one can introduce three different measures of chaotic velocity.

1. The **mean square velocity of chaotic motion** C

(3.6.11) $$C = \left(\frac{1}{n}\int \mathbf{c}^2 f_M(\mathbf{c}) d\mathbf{c}\right)^{1/2} = \sqrt{3RT}.$$

3.6. Statistical equilibrium. Maxwell-Boltzmann distribution function. Entropy

2. The **mean velocity of chaotic motion** C_a

(3.6.12)
$$C_a = \frac{1}{n}\int_0^\infty c\, f_M(c)dc = \sqrt{\frac{8}{\pi}RT}.$$

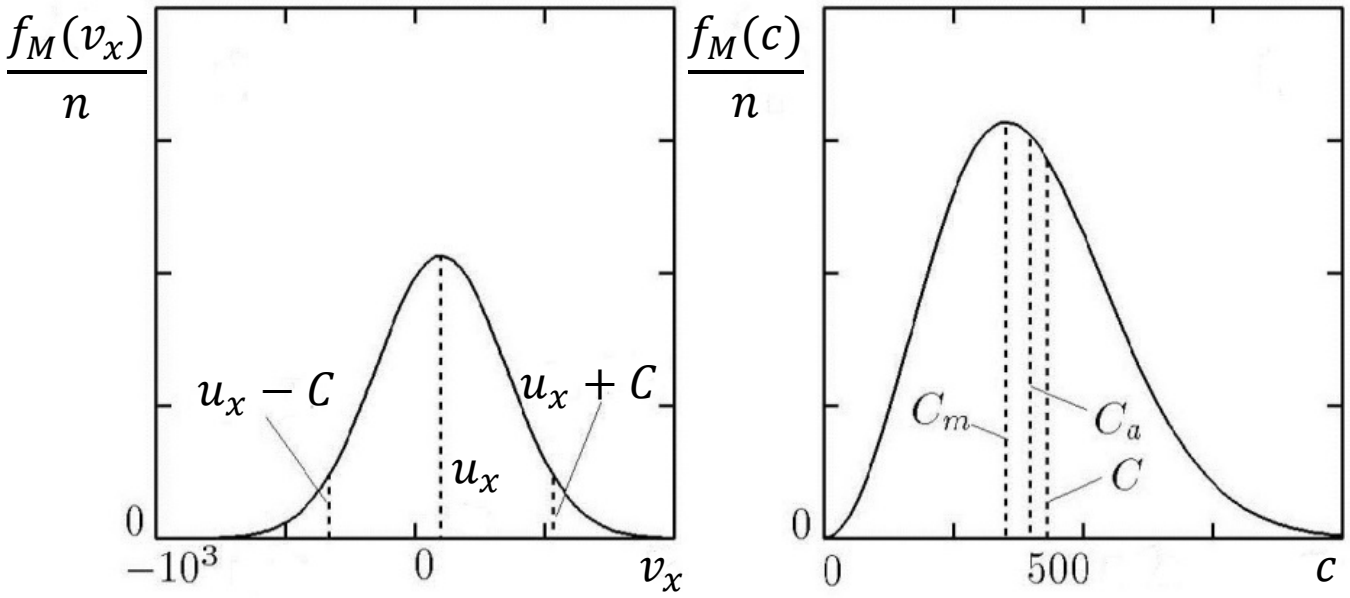
3. The **most probable chaotic velocity** C_m, i.e. value of c which corresponds to maximum $f_M(c)$:
$$C_m = \sqrt{2RT}.$$

In order to find C_m, one needs to find derivative

(3.6.13)
$$\frac{d}{dc}\left(c^2 \exp\left[-\frac{c^2}{2RT}\right]\right) = \left[2c - \frac{c^3}{RT}\right]\exp\left[-\frac{c^2}{2RT}\right].$$

The derivative is equal to zero at $c = C_m = \sqrt{2RT}$.

Maxwell-Boltzmann distribution in Ar at $u_x = 100$ m/s and $T = 300$ K:



Equilibrium collisional properties of a VHS gas

Let's calculate collision density Z of a VHS gas in the equilibrium state. Z is given by Eq. (3.4.16):

$$Z = \frac{1}{2}\int\int f(\mathbf{r},\mathbf{v},t) f(\mathbf{r},\mathbf{v}_1,t) c_r \sigma_T(c_r) d\mathbf{v}_1 d\mathbf{v}$$

where we used the equilibrium distribution function and $\sigma_T(C_r)$ for VHS gas given by Eq. (2.6.6)

$$\sigma_T(c_r) = \pi d^2\,(c_r) = \sigma_{T,Ref}\left(\frac{c_{r,Ref}}{c_r}\right)^{\varpi}.$$

where $\varpi = 2\omega - 1$, and ω is the viscosity index in Eq. (2.6.7). Then

$$Z_M = \frac{\sigma_{T,Ref}\left(c_{r,Ref}\right)^{\varpi}}{2}\int\int f_M(\mathbf{v})\, f_M(\mathbf{v}_1)|\mathbf{v}_1 - \mathbf{v}|^{1-\varpi}\, d\mathbf{v}_1 d\mathbf{v}.$$

The integral can be calculated and reduced to

(3.6.14)
$$Z_M = \frac{\sigma_{T,Ref} n^2}{\sqrt{2}}\Gamma\left(\frac{4-\varpi}{2}\right)\left(\frac{c_{r,Ref}}{\sqrt{4RT}}\right)^{\varpi} C_a,$$

where $\Gamma(x)$ is the **gamma function**:

(3.6.15)
$$\Gamma(x) = \int_0^{\infty} \xi^{x-1} e^{-\xi} d\xi\,.$$

Then (see Eqs. (3.4.17)):

(3.6.16) $$z_M = \frac{2Z_M}{n} = \sqrt{2}\sigma_{T,Ref} n \Gamma\left(\frac{4-\varpi}{2}\right)\left(\frac{c_{r,Ref}}{\sqrt{4RT}}\right)^{\varpi} C_a, \qquad \tau_M = \frac{1}{z_M}.$$

Traditionally, λ_M is defined based on C_a:

(3.6.17) $$\lambda_M = \tau_M C_a = \frac{1}{\sqrt{2}\sigma_{T,Ref} n \Gamma\left(\frac{4-\varpi}{2}\right)}\left(\frac{\sqrt{4RT}}{c_{r,Ref}}\right)^{\varpi}$$

Traditionally $v_* = C_a$. Note we defined λ earlier based on the means square veloicity C: See comment in slide 41 of this Chapter.

Mean free path depends on temperature if $\varpi \neq 0$.

If we use Eq. (2.6.11) which defines $c_{r,Ref}$ in the VHS model, then equation for Z_M, z_M, and λ_M can be re-written in terms of the reference temperature T_{Ref} and viscosity index ω:

(3.6.18) $$Z_M = \frac{\sigma_{T,Ref} n^2}{\sqrt{2}} C_a \left(\frac{T_{Ref}}{T}\right)^{\omega-\frac{1}{2}}, \quad z_M = \sqrt{2}\sigma_{T,Ref} n C_a \left(\frac{T_{Ref}}{T}\right)^{\omega-\frac{1}{2}}, \quad \lambda_M = \frac{1}{\sqrt{2}\sigma_{T,Ref} n}\left(\frac{T}{T_{Ref}}\right)^{\omega-\frac{1}{2}}.$$

For the HS molecules $\omega = 1/2$, $\sigma_{T,Ref} = \sigma_T = const$, and equations above reduce to

(3.6.19) $$Z_M = \frac{\sigma_T n^2}{\sqrt{2}} C_a, \qquad z_M = \sqrt{2}\sigma_T n C_a, \qquad \tau_M = \frac{1}{\sqrt{2}\sigma_T n C_a}, \qquad \lambda_M = \frac{1}{\sqrt{2}\sigma_T n}.$$

Compare these equations with estimates obtained in Section 1.4.

Boltzmann entropy

Let's calculate the Boltzmann H-function given by Eq. (3.5.11) under equilibrium conditions:

$$H_M = \int f_M(\mathbf{v}) \log f_M(\mathbf{v})\, d\mathbf{v}.$$

If we insert into this equation the Maxwell-Boltzmann distribution, Eq. (3.6.9), we obtain

(3.6.20) $$H_M = n \log \frac{mn}{T^{3/2}} + const.$$

In thermodynamics, the **specific entropy** of ideal and calorically perfect monatomic ($c_V = (3/2)R, \gamma = c_p/c_V = 5/3$) gas is equal to

(3.6.21) $$s = c_V \log \frac{T}{\rho^{2/3}} + const\,,$$

where the choice of the constant is arbitrary (only the change of entropy makes since in the classical thermodynamics). Let's show that s can be written in terms of H_M:

$$s = \frac{3}{2}\frac{k_B}{m} \log \frac{T}{\rho^{2/3}} + const = -\frac{k_B}{mn} n \log \frac{\rho}{T^{\frac{3}{2}}} + const = -\, k_B \frac{H_M}{\rho} + const.$$

Thus, the specific Boltzmann H-function H_M/ρ in the equilibrium state is proportional to entropy s.

3.6. Statistical equilibrium. Maxwell-Boltzmann distribution function. Entropy

According to the second law of thermodynamics, entropy of any closed system cannot decrease with time. But according to the Boltzmann H-theorem, $-k_B H_M$ possess the same property: In any process described by the homogeneous Boltzmann equation, it cannot decrease. Thus, the solutions of the Boltzmann equation are in agreement with the second law of thermodynamics. This is the reason to define the entropy density (density per unit volume) in the kinetic theory for arbitrary, non-equilibrium state as

(3.6.22) $$S(\mathbf{r},t) = s\rho = -k_B \int f(\mathbf{r},\mathbf{v},t)\log f(\mathbf{r},\mathbf{v},t)\, d\mathbf{v} + C(\rho).$$

This quantity $S(\mathbf{r},t)$ is called the **Boltzmann entropy**.

The Boltzmann entropy, however, coincides with entropy in classical thermodynamics only in the equilibrium state.

3.7. Gas-surface interaction. Kinetic boundary condition

- Scattering of gas molecules on interphase boundaries
- Conditional scattering probability density function
- Kinetic boundary condition on an impenetrable surface at rest
- Condition of impenetrability
- Stress and heat flux on a surface at rest

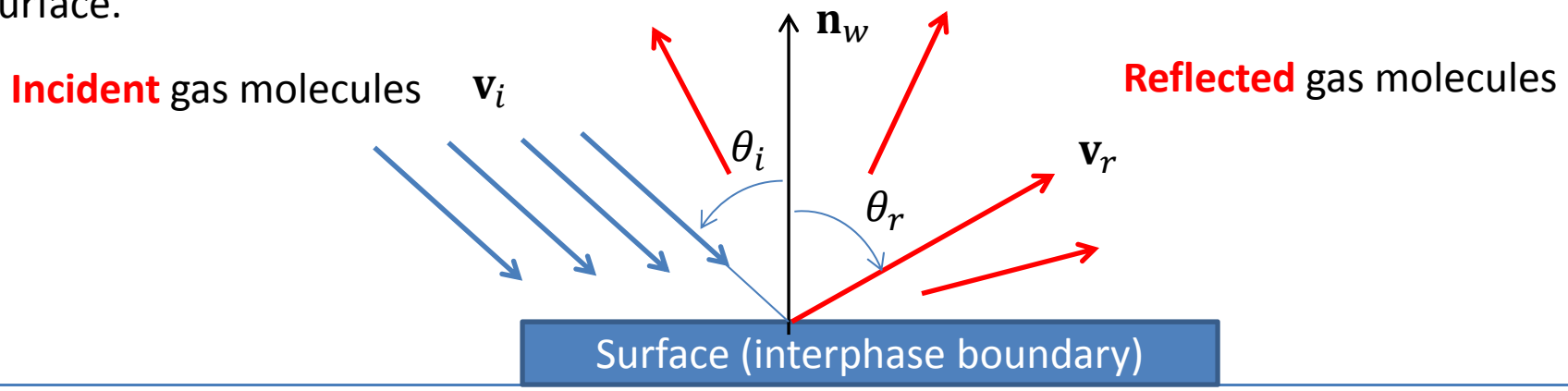
3.7. Gas-surface interaction. Kinetic boundary condition

In the majority of applications, we consider gas flows around some wall, obstacles, or bodies. In order to solve the Boltzmann equation in such flows we need to supply this equation with **kinetic boundary conditions**, which describe the process of interaction of gas molecules with the surfaces of bodies or **interphase boundaries** in terms of the distribution function. The goal of this Section is to derive such boundary conditions for an **impenetrable surface at rest**.

Scattering of gas molecules on interphase boundaries

Interaction of gas with a body surface reduces to interaction of individual gas molecules with individual atoms of the surface material. The result of interaction (velocity of a gas molecule when its interaction with all atoms of surface materials is terminated) depends on numerous factors including incident velocity, surface temperature and roughness, presence of impurities, position of a molecule with respect to individual atoms of the crystalline lattice, etc.

Physical experiment show that if we direct a monoenergetic molecular beam (flux of gas molecules with identical velocity vectors) to a surface, different molecules after interaction with the surface will attain different velocities. This phenomenon is called **scattering** of molecules on a surface.



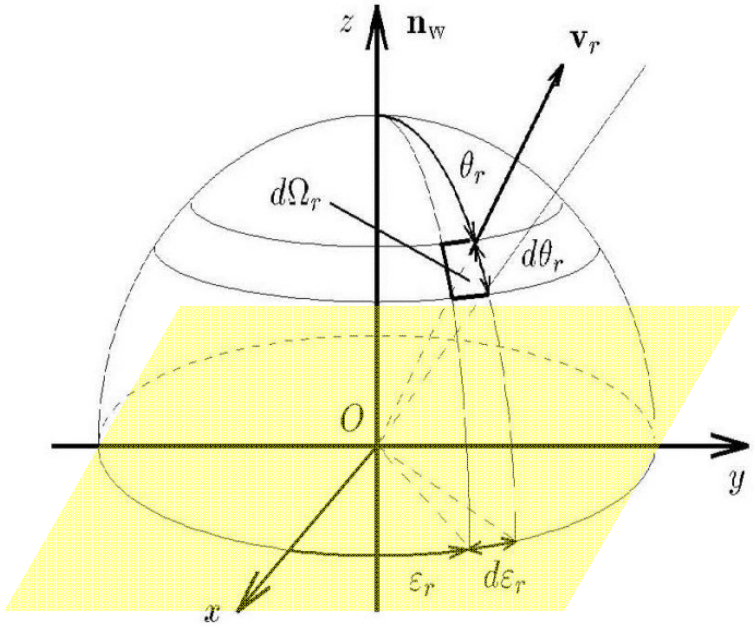
3.7. Gas-surface interaction. Kinetic boundary condition

Experimentally, the angular distribution of reflected molecules can be characterized by a **scattering indicatrix** $I(\theta_r, \varepsilon_r)$, where angles θ_r and ε_r characterize the direction of the velocity vector $\mathbf{v}_r$ of a gas molecule after reflection from the surface.

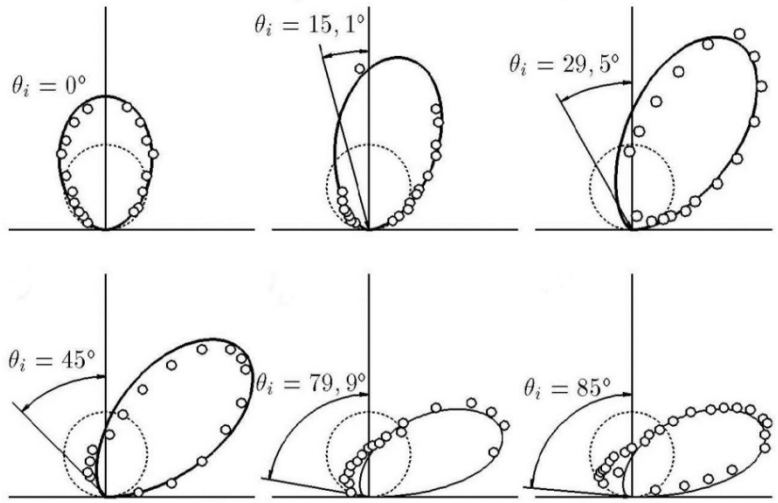
If we know that the total number of molecules reflected from a unit area per unit time is equal to N and dN molecules were reflected into the solid angle $d\Omega_r = \sin\theta_r \, d\theta_r d\varepsilon_r$, then

$$\frac{dN}{N} = I(\theta_r, \varepsilon_r) d\Omega_r. \tag{3.7.1}$$

The indicatrix $I(\theta_r, \varepsilon_r)$ defines the probability of scattering into different solid angles. Quite often the indicatrix does not depend on ε_r and can be shown only as a function of θ_r. Currently, experimental indicatrix are known for various surfaces and gases.



Indicatrix for a monocrystal of LiF



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3.7. Gas-surface interaction. Kinetic boundary condition

Conditional scattering probability density function

In the kinetic theory, the scattering of gas molecules at the interphase boundaries is considered as a random process and modelled based on known distribution function for velocity vectors of reflected molecules. Scattering indicatrix is insufficient to completely characterize the velocity distribution of reflected molecules, because it contains information about only directions of $\mathbf{v}_r$, and does contain information about distribution of absolute values of velocity.

Let's assume that we consider interaction of gas molecules with a smooth surface, which has a known vector of the external unit normal $\mathbf{n}_w$, fix the velocity vector of incident molecules $\mathbf{v}_i$, and know that among all $N(\mathbf{v}_i)$ molecules reflected from a surface with unit area per unit time $dN(\mathbf{v}_r, d\mathbf{v}_r|\mathbf{v}_i)$ molecules has velocity vectors $\mathbf{v}_{n(r)}$ from the range

$$\mathbf{v}_r < \mathbf{v}_{n(r)} < \mathbf{v}_r + d\mathbf{v}_r.$$

Then

(3.7.2)
$$dP\left(\mathbf{v}_r < \mathbf{v}_{n(r)} < \mathbf{v}_r + d\mathbf{v}_r \middle| \mathbf{v}_i\right) = \frac{dN(\mathbf{v}_r, d\mathbf{v}_r|\mathbf{v}_i)}{N(\mathbf{v}_i)}$$

is the probability to find a reflected molecule with velocity $\mathbf{v}_{n(r)}$ in the given range. Let's represent this probability in the form

(3.7.3)
$$dP\left(\mathbf{v}_r < \mathbf{v}_{n(r)} < \mathbf{v}_r + d\mathbf{v}_r \middle| \mathbf{v}_i\right) = S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w)d\mathbf{v}_r,$$

where $S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w)$ is the **scattering probability density function** (SPDF) found under condition that incident molecule has velocity $\mathbf{v}_i$ and interaction happens in a surface point with normal $\mathbf{n}_w$. We will show that, if we know $S(\mathbf{v}_i \to \mathbf{v}_r)$, then we can formulate a unique kinetic boundary condition for the Boltzmann equation on an impenetrable surface.

3.7. Gas-surface interaction. Kinetic boundary condition

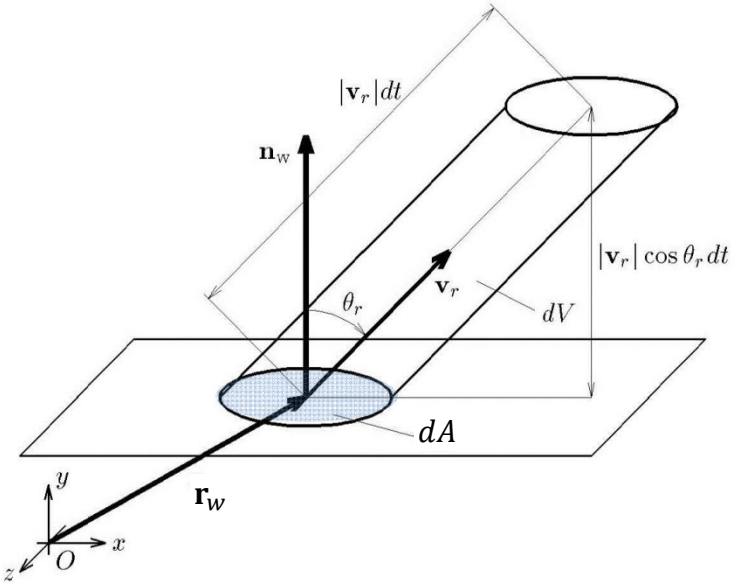
The SPDF $S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w)$, as any PDF in statistics, must satisfy the **normalization condition:**

(3.7.4)
$$\int\limits_{\mathbf{v}_r\cdot\mathbf{n}_w\geq 0} S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w)d\,\mathbf{v}_r = 1,$$

which is the mathematical form of condition that the surface is impenetrable: Any incident gas molecule must leave the surface and total probability of reflection is equal to 1. If we introduce a local system of coordinates where axis Oy is directed along $\mathbf{n}_w$, then Eq. (3.7.4) takes the form

$$\int\limits_{-\infty}^{+\infty}\int\limits_{0}^{+\infty}\int\limits_{-\infty}^{+\infty} S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w)dv_{rx}dv_{ry}dv_{rz} = 1.$$

Kinetic boundary condition on an impenetrable surface at rest



Let's consider molecules that are reflected from dA during dt with velocities from the range

$$\mathbf{v}_r < \mathbf{v}_{n(r)} < \mathbf{v}_r + d\mathbf{v}_r. \qquad (3.7.5)$$

The number of such molecules is equal to

$$dN_r = dAdt|\mathbf{v}_r\cdot\mathbf{n}_w|f(\mathbf{r}_w,\mathbf{v}_r,t)d\mathbf{v}_r. \qquad (3.7.6)$$

Let's consider molecules that fall at dA during dt with velocities from the range

$$\mathbf{v}_i < \mathbf{v}_{n(i)} < \mathbf{v}_i + d\mathbf{v}_i. \qquad (3.7.7)$$

The number of such molecules is equal to

$$dN_i = dAdt|\mathbf{v}_i\cdot\mathbf{n}_w|f(\mathbf{r}_w,\mathbf{v}_i,t)d\mathbf{v}_i. \qquad (3.7.8)$$

3.7. Gas-surface interaction. Kinetic boundary condition

Now, using Eqs. (3.7.2) and (3.7.3), we can find the number of incident molecules whose velocities after the reflection satisfy Eq. (3.7.5):

(3.7.9) $$dN_{ri} = dN_{ri} S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w) d\mathbf{v}_i = dA dt d\mathbf{v}_r |\mathbf{v}_i \cdot \mathbf{n}_w| S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w) f(\mathbf{r}_w, \mathbf{v}_i, t) d\mathbf{v}_i.$$

In order to obtain the total number of reflected molecules with velocities from the range given by Eq. (3.7.5), one needs to account for contributions of all incident molecules, i.e. perform integration of Eq. (3.7.9) over velocities $\mathbf{v}_i$ of incident molecules:

(3.7.10) $$dN_r = dA dt d\mathbf{v}_r \int\limits_{\mathbf{v}_i \cdot \mathbf{n}_w \le 0} |\mathbf{v}_i \cdot \mathbf{n}_w| S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w) f(\mathbf{r}_w, \mathbf{v}_i, t) d\mathbf{v}_i \ .$$

Eqs. (3.7.6) and (3.7.10) define the same quantity. If we equate the right-hand sides, we obtain

(3.7.11) $$|\mathbf{v}_r \cdot \mathbf{n}_w| f(\mathbf{r}_w, \mathbf{v}_r, t) = \int\limits_{\mathbf{v}_i \cdot \mathbf{n}_w \le 0} |\mathbf{v}_i \cdot \mathbf{n}_w| S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w) f(\mathbf{r}_w, \mathbf{v}_i, t) d\mathbf{v}_i \ .$$

or

(3.7.12) At $\mathbf{v}_r \cdot \mathbf{n}_w > 0$: $$f(\mathbf{r}_w, \mathbf{v}_r, t) = \int\limits_{\mathbf{v}_i \cdot \mathbf{n}_w \le 0} \frac{|\mathbf{v}_i \cdot \mathbf{n}_w|}{|\mathbf{v}_r \cdot \mathbf{n}_w|} S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w) f(\mathbf{r}_w, \mathbf{v}_i, t) d\mathbf{v}_i.$$

Distribution function of reflected molecules

Distribution function of incident molecules

This is the **kinetic boundary condition** on an impenetrable surface. It allows one to calculate the distribution function of reflected molecules through the distribution function of incident ones.

if we introduce the **scattering kernel**

(3.7.13) $$V(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w) = \frac{|\mathbf{v}_i \cdot \mathbf{n}_w|}{|\mathbf{v}_r \cdot \mathbf{n}_w|} S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w),$$

then the boundary conditions takes the form

(3.7.14) $$\text{At} \quad \mathbf{v}_r \cdot \mathbf{n}_w > 0: \quad f(\mathbf{r}_w, \mathbf{v}_r, t) = \int\limits_{\mathbf{v}_i \cdot \mathbf{n}_w \le 0} V(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w) f(\mathbf{r}_w, \mathbf{v}_i, t) d\mathbf{v}_i.$$

The scattering kernel completely defines the physical model of interaction of gas molecules with an impenetrable interphase boundary.

Condition of impenetrability

Let's take the boundary condition in the form of Eq. (3.7.11), integrated it over velocities of reflected molecules:

(3.7.15) $$\mathbf{n}_w \cdot \int\limits_{\mathbf{v}_r \cdot \mathbf{n}_w > 0} \mathbf{v}_r f(\mathbf{r}_w, \mathbf{v}_r, t) d\mathbf{v}_r$$
$$= -\mathbf{n}_w \cdot \int\limits_{\mathbf{v}_i \cdot \mathbf{n}_w \le 0} \mathbf{v}_i \left(\int\limits_{\mathbf{v}_r \cdot \mathbf{n}_w > 0} S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w) d\mathbf{v}_r \right) f(\mathbf{r}_w, \mathbf{v}_i, t) d\mathbf{v}_i \ ,$$

and use the normalization condition, Eq. (3.7.4). By combining two integrals into one, we obtain

i.e. normal to the surface component of gas velocity is equal to zero. This is the "standard" **condition of impenetrability** in the continuum gas dynamics. We showed that this condition is a consequence of the kinetic boundary condition and normalization condition given by Eq. (3.7.4).

Stress and heat flux on a surface at rest

In Section 3.4, we introduced a vector of flux density of molecular quantity $\Phi(\mathbf{r},\mathbf{v},t)$ in the form

$$\mathbf{f}_\Phi(\mathbf{r},t) = \langle(\mathbf{v}\Phi)_V\rangle = \int \mathbf{v}\Phi(\mathbf{r},\mathbf{v},t)f(\mathbf{r},\mathbf{v},t)d\mathbf{v}\,.$$

This equation can be used in order to calculate the stress vector and heat flux on a surface. The amount of molecular quantity $\Phi(\mathbf{r},\mathbf{v},t)$ transferred to the surface due to reflection of gas molecules from a unit area with external normal $\mathbf{n}_w$ per unit time is equal to

(3.7.16) $$Q_w = -\mathbf{n}_w \cdot \int \mathbf{v}\Phi(\mathbf{r}_w,\mathbf{v},t)f(\mathbf{r}_w\mathbf{v},t)d\mathbf{v} = -\int (\mathbf{n}_w\cdot\mathbf{v})\Phi(\mathbf{r}_w,\mathbf{v},t)f(\mathbf{r}_w,\mathbf{v},t)d\mathbf{v}\,.$$

Here we multiply the vector quantities in integrals by $-\mathbf{n}_w$, because $\Phi(\mathbf{r},\mathbf{v},t)$ transferred *from gas to the surface* if $(\mathbf{n}_w\cdot\mathbf{v}) < 0$. Now let's represent the integral as a sum of two integrals: One for incident molecules and another one for reflected molecules:

$$Q_w$$

$$= -\int\limits_{\mathbf{v}_i\cdot\mathbf{n}_w\le 0} (\mathbf{n}_w\cdot\mathbf{v}_i)\Phi(\mathbf{r}_w,\mathbf{v}_i,t)f(\mathbf{r}_w,\mathbf{v}_i,t)d\mathbf{v}_i - \int\limits_{\mathbf{v}_r\cdot\mathbf{n}_w>0} (\mathbf{n}_w\cdot\mathbf{v}_r)\Phi(\mathbf{r}_w,\mathbf{v}_r,t)f(\mathbf{r}_w,\mathbf{v}_r,t)d\mathbf{v}_r\,.$$

This equation then can be represented in the form

3.7. Gas-surface interaction. Kinetic boundary condition

$$Q_w = Q_i - Q_r,$$

$$Q_i = \int\limits_{\mathbf{v}_i \cdot \mathbf{n}_w \le 0} |\mathbf{n}_w \cdot \mathbf{v}_i| \Phi(\mathbf{r}_w, \mathbf{v}_i, t) f(\mathbf{r}_w, \mathbf{v}_i, t) d\mathbf{v}_i \,, \tag{3.7.17}$$

$$Q_r = \int\limits_{\mathbf{v}_r \cdot \mathbf{n}_w > 0} |\mathbf{n}_w \cdot \mathbf{v}_r| \Phi(\mathbf{r}_w, \mathbf{v}_r, t) f(\mathbf{r}_w, \mathbf{v}_r, t) d\mathbf{v}_r \,.$$

where Q_i is the amount of quantity Φ which is brought to unit area per unit time by incident molecules, and Q_r is the amount of quantity Φ which is removed from unit area per unit time by reflected molecules. Note that according to the boundary condition given by Eq. (3.7.14), both Q_i and Q_r can be found if we know the distribution function of incident molecules.

Examples:

1. Transfer (or exchange) between surface and gas by the number of molecules is described by the **number density flux** ($\Phi(\mathbf{r}, \mathbf{v}, t) = 1$):

$$J_w = -\int (\mathbf{n}_w \cdot \mathbf{v}) f(\mathbf{r}_w, \mathbf{v}, t) d\mathbf{v} = J_i - J_r,$$

(3.7.18)

$$J_i = \int\limits_{\mathbf{v}_i \cdot \mathbf{n}_w \le 0} |\mathbf{n}_w \cdot \mathbf{v}_i| f(\mathbf{r}_w, \mathbf{v}_i, t) d\mathbf{v}_i \,, \qquad J_r = \int\limits_{\mathbf{v}_r \cdot \mathbf{n}_w > 0} |\mathbf{n}_w \cdot \mathbf{v}_r| f(\mathbf{r}_w, \mathbf{v}_r, t) d\mathbf{v}_r \,.$$

Note that according to the impenetrability condition, Eq. (3.7.15) $J_i = J_r$ and $J_w = 0$.

3.7. Gas-surface interaction. Kinetic boundary condition

2. Transfer (or exchange) between surface and gas by the linear momentum is described by the **stress vector** $\mathbf{p}_w$ ($\Phi(\mathbf{r},\mathbf{v},t) = m\mathbf{v}$):

$$\mathbf{p}_w = -m\int (\mathbf{n}_w\cdot\mathbf{v})\mathbf{v} f(\mathbf{r}_w,\mathbf{v},t)d\mathbf{v} = \mathbf{p}_i - \mathbf{p}_r,$$

(3.7.19)

$$\mathbf{p}_i = m\int\limits_{\mathbf{v}_i\cdot\mathbf{n}_w\le 0} |\mathbf{n}_w\cdot\mathbf{v}_i|\mathbf{v}_i f(\mathbf{r}_w,\mathbf{v}_i,t)d\mathbf{v}_i\,, \qquad \mathbf{p}_r = m\int\limits_{\mathbf{v}_r\cdot\mathbf{n}_w>0} |\mathbf{n}_w\cdot\mathbf{v}_r|\mathbf{v}_r f(\mathbf{r}_w,\mathbf{v}_r,t)d\mathbf{v}_r\,.$$

Stress vector can be represented as a sum of the **normal**, $\mathbf{p}_{wn}$, and **tangential**, $\mathbf{p}_{wt}$, stresses:

(3.7.20) $$\mathbf{p}_w = \mathbf{p}_{wn} + \mathbf{p}_{wt}, \qquad \mathbf{p}_{wn} = (\mathbf{p}_{wn}\cdot\mathbf{n}_w)\mathbf{n}_w.$$

Pressure p_w at the surface is equal to the absolute value of the normal stress ($\mathbf{p}_{wn}\cdot\mathbf{n}_w < 0$):

(3.7.21) $$\mathbf{p}_{wn} = -p_w\mathbf{n}_w.$$

3. Transfer (or exchange) of energy from gas to the surface is described by the **heat flux** q_w ($\Phi(\mathbf{r},\mathbf{v},t) = m\mathbf{v}^2/2$):

$$q_w = -\int (\mathbf{n}_w\cdot\mathbf{v})\frac{m\mathbf{v}^2}{2} f(\mathbf{r}_w,\mathbf{v},t)d\mathbf{v} = q_i - q_r,$$

(3.7.22)

$$q_i = \int\limits_{\mathbf{v}_i\cdot\mathbf{n}_w\le 0} |\mathbf{n}_w\cdot\mathbf{v}_i|\frac{m\mathbf{v}_i^2}{2} f(\mathbf{r}_w,\mathbf{v}_i,t)d\mathbf{v}_i\,, \qquad q_r = \int\limits_{\mathbf{v}_r\cdot\mathbf{n}_w>0} |\mathbf{n}_w\cdot\mathbf{v}_r|\frac{m\mathbf{v}_r^2}{2} f(\mathbf{r}_w,\mathbf{v}_r,t)d\mathbf{v}_r\,.$$

3.8. Models of specular, diffuse, and specular-diffuse scattering

- Model of specular scattering
- Maxwell model of diffuse scattering
- Model of specular-diffuse scattering

3.8. Models of specular, diffuse, and specular-diffuse scattering

The goal of this section is to introduce the most popular (and simplest) models that describe interaction of gas molecules with an impenetrable surface. Such models must be formulated in terms of the scattering PDF $S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w)$ in the boundary condition

(3.8.1) At $\mathbf{v}_r \cdot \mathbf{n}_w > 0$: $f(\mathbf{r}_w, \mathbf{v}_r, t) = \int\limits_{\mathbf{v}_i \cdot \mathbf{n}_w \le 0} \frac{|\mathbf{v}_i \cdot \mathbf{n}_w|}{|\mathbf{v}_r \cdot \mathbf{n}_w|} S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w) f(\mathbf{r}_w, \mathbf{v}_i, t) d\mathbf{v}_i.$

There are two approaches how it can be done.

1. Direct, when a model $S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w)$ is introduced based on consideration of mechanics of individual interactions of gas molecules with a surface.

2. Indirect, when some assumption are made about the form of the distribution function of reflected molecules $f(\mathbf{r}_w, \mathbf{v}_r, t)$. Then $S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w)$ can be obtained as a solution of the integral Eq. (3.8.1). In this case, $S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w)$ can be easily found if one assumes that the SPDF does not depend on the velocity of incident molecules, i.e. $S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w) = S(\mathbf{v}_r|\mathbf{n}_w)$. Then

$$f(\mathbf{r}_w, \mathbf{v}_r, t) = \frac{S(\mathbf{v}_r|\mathbf{n}_w)}{|\mathbf{v}_r \cdot \mathbf{n}_w|} \int\limits_{\mathbf{v}_i \cdot \mathbf{n}_w \le 0} |\mathbf{v}_i \cdot \mathbf{n}_w| f(\mathbf{r}_w, \mathbf{v}_i, t) d\mathbf{v}_i = \frac{S(\mathbf{v}_r|\mathbf{n}_w)}{|\mathbf{v}_r \cdot \mathbf{n}_w|} J_i$$

or

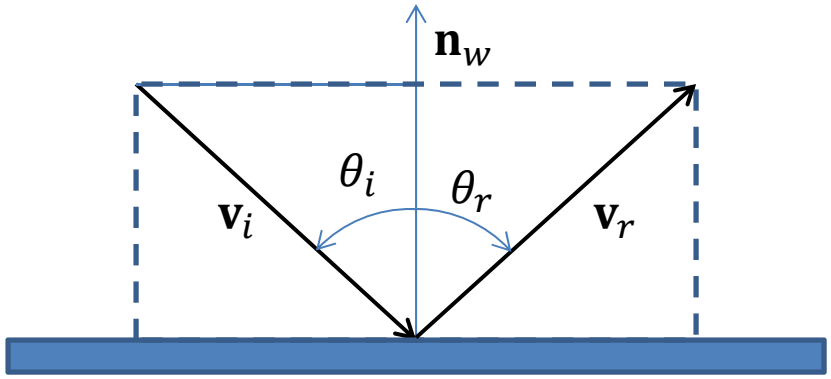
(3.8.2) $$S(\mathbf{v}_r|\mathbf{n}_w) = \frac{|\mathbf{v}_r \cdot \mathbf{n}_w| f(\mathbf{r}_w, \mathbf{v}_r, t)}{J_i}.$$

We will use both direct and indirect approaches in order to establish $S(\mathbf{v}_r|\mathbf{n}_w)$ for simplest models of gas-surface interaction.

3.8. Models of specular, diffuse, and specular-diffuse scattering

Model of specular scattering

In the **model of specular scattering**, the velocity of a molecules transforms during interaction with a surface like a velocity of hard sphere molecules during a binary collision: Normal to the surface velocity changes its direction to the opposite one, and tangential velocity does not change.



$$\mathbf{v}_r \cdot \mathbf{n}_w = -\mathbf{v}_i \cdot \mathbf{n}_w, \qquad \mathbf{v}_r - (\mathbf{v}_r \cdot \mathbf{n}_w)\mathbf{n}_w = \mathbf{v}_i - (\mathbf{v}_i \cdot \mathbf{n}_w)\mathbf{n}_w,$$

(3.8.3)
$$\mathbf{v}_r = \mathbf{v}_i - 2(\mathbf{v}_i \cdot \mathbf{n}_w)\mathbf{n}_w.$$

Thus, velocity of a molecule after reflection is not random, it is completely defined by velocity of the incident molecule and by the direction of the normal. Correspondingly, the scattering PDF can be represented by the **generalized Dirac delta-function** δ_3:

(3.8.4)
$$S(\mathbf{v}_i \to \mathbf{v}_r|\mathbf{n}_w) = \delta_3(\mathbf{v}_r - (\mathbf{v}_i - 2(\mathbf{v}_i \cdot \mathbf{n}_w)\mathbf{n}_w)).$$

Generalized Dirac delta-function appears in statistics every time when we introduce a PDF for a non-random variable. The major properties of the Dirac functions are as follows:

3.8. Models of specular, diffuse, and specular-diffuse scattering

$$\delta_3(\mathbf{v}_r - \mathbf{a}) = 0 \quad \text{for all} \quad \mathbf{v}_r \neq \mathbf{a},$$

$$\int f(\mathbf{v}_r)\delta_3(\mathbf{v}_r - \mathbf{a})d\mathbf{v}_r = f(\mathbf{a}).$$

Then, after inserting the scattering PDF for the model of specular scattering into the boundary condition given by Eq. (3.8.1), one can find the relationship between the distribution functions of reflected and incident molecules:

(3.8.5) $$\text{At} \quad \mathbf{v}_r \cdot \mathbf{n}_w > 0: \quad f(\mathbf{r}_w, \mathbf{v}_r, t) = f(\mathbf{r}_w, \mathbf{v}_r - 2(\mathbf{v}_r \cdot \mathbf{n}_w)\mathbf{n}_w, t).$$

After inserting this $f(\mathbf{r}_w, \mathbf{v}_r, t)$ into the definition of the pressure vector and heat flux an the surface, one can obtain

(3.8.6)
$$\mathbf{p}_{rn} = -\mathbf{p}_{in}, \qquad \mathbf{p}_{rt} = \mathbf{p}_{it}, \qquad q_r = q_i,$$

$$\mathbf{p}_{wn} = 2\mathbf{p}_{in}, \qquad \mathbf{p}_{wt} = 0, \qquad q_w = 0.$$

Thus, for the model of specular scattering, the tangential stress and heat flux at the surface are equal to zero, and the effect of the gas on the surface reduces only to the normal stress.

This conclusion is in agreement with the definition of the model of specular scattering:

$$\mathbf{v}_r - (\mathbf{v}_r \cdot \mathbf{n}_w)\mathbf{n}_w = \mathbf{v}_i - (\mathbf{v}_i \cdot \mathbf{n}_w)\mathbf{n}_w, \qquad m\mathbf{v}_r^2/2 = m\mathbf{v}_i^2/2,$$

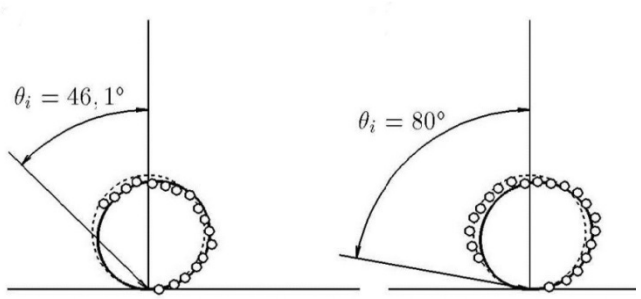
with no transfer of tangential momentum and energy from individual molecule to the surface.

3.8. Models of specular, diffuse, and specular-diffuse scattering

Maxwell model of diffuse scattering

Experiments show that scattering indicatrix for engineering surfaces is almost independent of the velocities of incident molecules. This results can be explained by multiple interactions between gas molecules and atoms composing the body. As a result, gas molecules come to thermal equilibrium with atoms of the surface and reflected molecules have an equilibrium distribution of velocities.

Indicatrix for scattering from polished LiF



Hurlbut, RAND Rept 339, 1959, V. 21, N. 1

In the **Maxwell model of diffuse scattering** is its assumed that the distribution function of reflected molecules is the Maxwell-Boltzmann equilibrium distribution at some relaxation temperature T_r and zero macroscopic velocity:

(3.8.7) $$\text{At} \quad \mathbf{v}_r \cdot \mathbf{n}_w > 0: \quad f(\mathbf{v}_r) = \frac{n_r}{(2\pi R T_r)^{3/2}} \exp\left[-\frac{\mathbf{v}_r^2}{2RT_r}\right],$$

where n_r is the number density of reflected molecules. This density is not a free parameter of the model, but is given by the condition of surface impenetrability that reduces to

(3.8.8) $$J_i = J_r = \int\limits_{\mathbf{v}_r \cdot \mathbf{n}_w > 0} |\mathbf{n}_w \cdot \mathbf{v}_r| f(\mathbf{v}_r) d\mathbf{v}_r = \frac{n_r}{2}\sqrt{\frac{2RT_r}{\pi}}.$$

Thus, the Maxwell model has the only one free parameter T_r that is usually chosen to be equal to the surface temperature T_w: $T_r = T_w$.

3.8. Models of specular, diffuse, and specular-diffuse scattering

Let's assume that the scattering PDF does not depend on $\mathbf{v}_i$. Then we can use Eq. (3.8.2) in order to find $S(\mathbf{v}_r|\mathbf{n}_w)$:

$$S(\mathbf{v}_r|\mathbf{n}_w) = \frac{|\mathbf{v}_r \cdot \mathbf{n}_w| f(\mathbf{r}_w, \mathbf{v}_r, t)}{J_i} = \frac{|\mathbf{v}_r \cdot \mathbf{n}_w|}{\frac{n_r}{2}\sqrt{\frac{2RT_r}{\pi}}} \frac{n_r}{(2\pi RT_r)^{3/2}} \exp\left[-\frac{\mathbf{v}_r^2}{2RT_r}\right].$$

where we used Eq. (3.8.8) for J_i. Finally

(3.8.9)
$$S(\mathbf{v}_r|\mathbf{n}_w) = \frac{|\mathbf{v}_r \cdot \mathbf{n}_w|}{2\pi(RT_r)^2} \exp\left[-\frac{\mathbf{v}_r^2}{2RT_r}\right].$$

By using Eq. (3.8.7) for calculation of the contribution of the reflected molecules to the stress vector and heat flux given by Eqs. (3.7.19) and (3.7.22), one can find that

(3.8.10)
$$\mathbf{p}_{rn} = \frac{mJ_i}{2}\sqrt{2\pi RT_r}\mathbf{n}_w, \qquad \mathbf{p}_{rt} = 0, \qquad q_r = 2J_i k_B T_r,$$

$$\mathbf{p}_{wn} = \mathbf{p}_{in} - \frac{mJ_i}{2}\sqrt{2\pi RT_r}\mathbf{n}_w, \qquad \mathbf{p}_{wt} = \mathbf{p}_{it}, \qquad q_w = q_i - 2J_i k_B T_r.$$

Thus, the model of diffuse scattering produces non-zero tangential stress and heat flux. The actual values of stress and heat flux depend on the distribution function of incident molecules (distribution function of incident molecules defines J_i, $\mathbf{p}_{in}$, $\mathbf{p}_{it}$, and q_i in Eq. (3.8.10)) and relaxation temperature T_r.

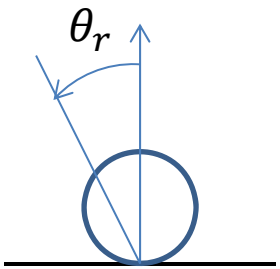
3.8. Models of specular, diffuse, and specular-diffuse scattering

It can be shown that the scattering indicatrix for the model of diffuse scattering is given by the equation

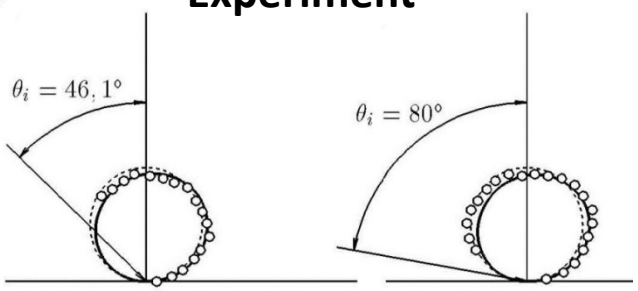
$$I(\theta_r, \varepsilon_r) = \frac{\cos\theta_r}{\pi}.$$

This scattering indicatrix or **cosine law of scattering** is close to experimentally established indicatrix for engineering surfaces.

Cosine law



Experiment



Model of specular-diffuse scattering

Comparison of simulation results obtained based on the model of diffuse scattering with results of measurements of the tangential stress and heat fluxes at surfaces in rarefied gas flows show that the model of diffuse scattering is usually slightly overestimates $\mathbf{p}_{wt}$ and q_w. Physically, it happens because of a correlation between directions of motion of incident and reflected molecules, which is completely neglected in the model of diffuse scattering. One can get better agreement with experiments, assuming assumes that some small fraction of molecules exhibits a specular scattering, and the rest of molecules is scattered diffusively.

In the **model of specular-diffuse scattering**, it is assumed that fraction α_t of all molecules ($0 \leq \alpha_t \leq 1$) exhibit diffuse scattering and $1 - \alpha_t$ molecules exhibits specular scattering. Then the scattering PDF and distribution function of reflected molecules can be represented in the form of linear combinations of corresponding functions/SPDFs for models of diffuse and specular scattering:

3.8. Models of specular, diffuse, and specular-diffuse scattering

$$S(\mathbf{v}_r|\mathbf{n}_w) = \alpha_t \frac{|\mathbf{v}_r \cdot \mathbf{n}_w|}{2\pi(RT_r)^2} \exp\left[-\frac{\mathbf{v}_r^2}{2RT_r}\right] + (1-\alpha_t)\delta_3\big(\mathbf{v}_r - (\mathbf{v}_i - 2(\mathbf{v}_i \cdot \mathbf{n}_w)\mathbf{n}_w)\big),$$

$$f(\mathbf{v}_r) = \alpha_t \frac{n_r}{(2\pi RT_r)^{3/2}} \exp\left[-\frac{\mathbf{v}_r^2}{2RT_r}\right] + (1-\alpha_t) f(\mathbf{r}_w, \mathbf{v}_r - 2(\mathbf{v}_r \cdot \mathbf{n}_w)\mathbf{n}_w, t). \quad (3.8.11)$$

Then the equations for stresses and heat flux take the form:

$$\mathbf{p}_{rn} = \alpha_t \frac{mJ_i}{2}\sqrt{2\pi RT_r}\mathbf{n}_w - (1-\alpha_t)\mathbf{p}_{in},$$

$$\mathbf{p}_{rt} = (1-\alpha_t)\mathbf{p}_{it},$$

$$q_r = \alpha_t 2J_i k_B T_r + (1-\alpha_t)q_i, \quad (3.8.12)$$

$$\mathbf{p}_{wn} = (2-\alpha_t)\mathbf{p}_{in} - \alpha_t \frac{mJ_i}{2}\sqrt{2\pi RT_r}\mathbf{n}_w,$$

$$\mathbf{p}_{wt} = \alpha_t \mathbf{p}_{it},$$

$$q_w = \alpha_t(q_i - 2J_i k_B T_r).$$

Since $\mathbf{p}_{wt} = \alpha_t \mathbf{p}_{it}$, coefficient α_t is called **the tangential momentum accommodation coefficient**. It can be considered as a probability of diffuse scattering of any individual molecules during the interaction with the body surface. Physical experiments show that usually α_t is a conservative parameter and varies in the range

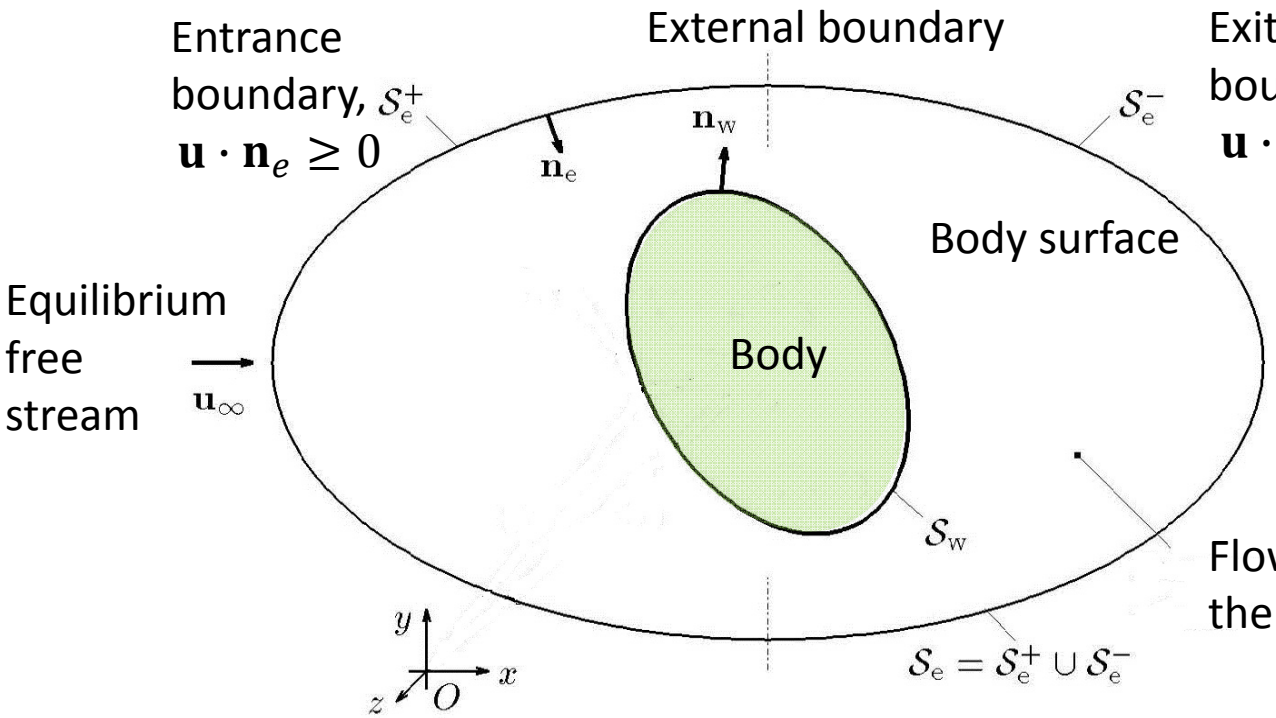
$$0.8 - 0.9 \le \alpha_t \le 1.$$

3.9. Formulation of problems in RGD. Boltzmann equation in reduced units

- Formulation of problem in the rarefied gas aerodynamics
- The Boltzmann equation in reduced units
- Flow regimes of the dilute gas. Local equilibrium

3.9. Formulation of problems in RGD. Boltzmann equation in reduced units

Formulation of problem in the rarefied gas aerodynamics



Aerodynamics is the branch of gas dynamics, which focuses on flows around bodies.

Flow domain, where we solve the Boltzmann equation

The form of boundary conditions that is required in order to obtain a unique solution of a mathematical problem is dictated by corresponding theorem of existence and uniqueness. Mathematically, the theorem of existence and uniqueness for solutions for the non-homogeneous Boltzmann equation is not proven yet.

Experience of practical calculations show that a solution of the Boltzmann equation exists and unique if, in any point of the boundary (including the external boundary and the body surface), the velocity distribution function is defined for molecules moving from outside to inside the flow domain, i.e. at $\mathbf{v} \cdot \mathbf{n}_e \geq 0$. The distribution function for molecules moving from inside to outside of the computational domain, i.e. at $\mathbf{v} \cdot \mathbf{n}_e < 0$, must not be constrained by boundary conditions and is defined as a result of the solution.

3.9. Formulation of problems in RGD. Boltzmann equation in reduced units

The kinetic problem of finding a rarefied gas flow around a given body includes

- **The Boltzmann equation:**

(3.9.1) $$\frac{\partial f}{\partial t}+\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}}+\frac{\mathbf{F}}{m}\cdot\frac{\partial f}{\partial \mathbf{v}}=\int_0^{2\pi}\int_0^{\pi}(f'f'_1-ff_1)c_r\sigma(c_r,\chi)\sin\chi\, d\chi d\varepsilon d\mathbf{v}_1\,.$$

- **The molecular model** describing the differential cross section of gas molecules. For instance, for the VHS model:

(3.9.2) $$\sigma(c_r,\chi)=\frac{1}{4}d_{Ref}^2\left(\frac{c_{r,Ref}}{c_r}\right)^{\varpi}\,.$$

- **The model of the external force.** For instance for the constant gravity force with gravitational acceleration $\mathbf{g}$:

(3.9.3) $$\mathbf{F}(\mathbf{r})=m\mathbf{g}.$$

- **The boundary condition at the external boundary.** Usually gas in the free stream is assumed to be in the state of the global equilibrium. Then, if the external boundary is placed far enough from the body surface and one can neglect the perturbations that the body introduces into the free stream, the following condition can be used:

(3.9.4) $$\text{At}\quad \mathbf{v}\cdot\mathbf{n}_e>0,\qquad f(\mathbf{r},\mathbf{v},t)=f_\infty(\mathbf{v})\,,$$
$$f_\infty(\mathbf{v})=\frac{n_\infty}{(2\pi k_B T_\infty/m)^{3/2}}\exp\left[-\frac{m(\mathbf{v}-\mathbf{u}_\infty)^2}{2k_B T_\infty}\right].$$

3.9. Formulation of problems in RGD. Boltzmann equation in reduced units

- **Boundary condition at the impenetrable body surface:**

(3.9.5) $$\text{At} \quad \mathbf{v}_r \cdot \mathbf{n}_w > 0: \quad f(\mathbf{r}_w, \mathbf{v}_r, t) = \int\limits_{\mathbf{v}_i \cdot \mathbf{n}_w \le 0} \frac{|\mathbf{v}_i \cdot \mathbf{n}_w|}{|\mathbf{v}_r \cdot \mathbf{n}_w|} S(\mathbf{v}_i \to \mathbf{v}_r | \mathbf{n}_w) f(\mathbf{r}_w, \mathbf{v}_i, t) d\mathbf{v}_i.$$

- **The physical model of interaction between gas molecules.** In the case of the model of specular-diffuse scattering:

(3.9.6) $$S(\mathbf{v}_r | \mathbf{n}_w) = \alpha_t \frac{|\mathbf{v}_r \cdot \mathbf{n}_w|}{2\pi (RT_r)^2} \exp\left[-\frac{\mathbf{v}_r^2}{2RT_r}\right] + (1-\alpha_t)\delta_3(\mathbf{v}_r - (\mathbf{v}_i - 2(\mathbf{v}_i \cdot \mathbf{n}_w)\mathbf{n}_w)).$$

- **Initial condition** that describe distribution function in the computational domain at $t = 0$:

(3.9.7) $$\text{At } t = 0: \quad f(\mathbf{r}, \mathbf{v}, 0) = f_0(\mathbf{r}, \mathbf{v}).$$

Quite often $f_0(\mathbf{r}, \mathbf{v})$ is unknown or steady-state solution of the problem is sought by converging to the steady state from arbitrary initial state. Then the initial distribution function can be chosen, e.g., in the form of the equilibrium distribution function in the free stream

(3.9.8) $$f_0(\mathbf{r}, \mathbf{v}) = f_\infty(\mathbf{v}).$$

The solution of the problem given by Eqs. (3.9.1)-(3.9.8) depends on

$$m, d_{Ref}^2 \left(c_{r,Ref}\right)^{\varpi}, \varpi, \qquad \mathbf{g}, \qquad n_\infty, \mathbf{u}_\infty, T_\infty, \qquad \text{body shape}, T_r, \alpha_t.$$

The Boltzmann equation in reduced units

Let's introduce the **scales** (characteristic values) of various physical quantities:

$$L_*, t_*, v_*, \pi d_{Ref}^2, F_*, n_*.$$

The scale for the distribution function then can be established based on the normalization condition given by Eq. (3.1.5):

$$n_* \frac{n}{n_*} = f_* v_*^3 \int \frac{f}{f_*} d\frac{v_x}{v_*} d\frac{v_y}{v_*} d\frac{v_z}{v_*} \quad \Rightarrow \quad f_* = \frac{n_*}{v_*^3}.$$

Then let's introduce the physical quantities in reduced units as follows

$$\bar{\mathbf{r}} = \frac{\mathbf{r}}{L_*}, \qquad \bar{t} = \frac{t}{t_*}, \qquad \bar{\mathbf{v}} = \frac{\mathbf{v}}{v_*}, \qquad \bar{c}_r = \frac{c_r}{v_*}, \qquad \bar{\sigma} = \frac{\sigma}{\pi d_{Ref}^2}, \qquad \bar{\mathbf{F}} = \frac{\mathbf{F}}{F_*}, \qquad \bar{f} = \frac{f}{f_*},$$

re-write the Boltzmann equation in terms of reduced units

$$\frac{f_*}{t_*}\frac{\partial \bar{f}}{\partial \bar{t}} + \frac{f_* v_*}{L_*} \bar{\mathbf{v}} \cdot \frac{\partial \bar{f}}{\partial \bar{\mathbf{r}}} + \frac{f_* F_*}{v_* m} \bar{\mathbf{F}} \cdot \frac{\partial \bar{f}}{\partial \bar{\mathbf{v}}} = f_*^2 \pi d_{Ref}^2 v_*^4 \int_0^{2\pi} \int_0^{\pi} \left(\bar{f}' \bar{f}'_1 - \bar{f} \bar{f}_1 \right) \bar{c}_r \bar{\sigma} \left(\bar{c}_r, \chi \right) \sin\chi \, d\chi d\varepsilon d\bar{\mathbf{v}}_1 ,$$

and then divide all terms in the equation by $f_*/v_* L_*$:

(3.9.9) $$Sh \frac{\partial \bar{f}}{\partial \bar{t}} + \bar{\mathbf{v}} \cdot \frac{\partial \bar{f}}{\partial \bar{\mathbf{r}}} + \frac{1}{Fr} \bar{\mathbf{F}} \cdot \frac{\partial \bar{f}}{\partial \bar{\mathbf{v}}} = \frac{1}{Kn} \int_0^{2\pi} \int_0^{\pi} \left(\bar{f}' \bar{f}'_1 - \bar{f} \bar{f}_1 \right) \bar{c}_r \bar{\sigma} \left(\bar{c}_r, \chi \right) \sin\chi \, d\chi d\varepsilon d\bar{\mathbf{v}}_1 ,$$

where Sh, Fr, and Kn are dimensionless numbers:

(3.9.10) $$Sh = \frac{L_*}{t_* v_*}, \qquad Fr = \frac{m v_*^2}{F_* L_*}, \qquad Kn = \frac{\lambda_*}{L_*}, \qquad \lambda_* = \frac{1}{\pi d_{Ref}^2 n_*}.$$

The **Strouhal number** Sh is equal to the ratio of the length scale to the characteristic path of a molecule during the characteristic time. Sh characterizes the effects of unsteadiness in the flow. If $Sh \ll 1$, then the effects of unsteadiness are small and we can consider the **steady-state flow** by solving the **steady-state Boltzmann equation** when

$$\frac{\partial f}{\partial t} = 0.$$

The **Froude number** Fr is equal to the ratio of the characteristic kinetic energy of a molecule to the characteristic work of the external force on the path L_*. It characterizes the effect of the external field on the motion of molecules. If $Fr \gg 1$, then the effect of the external force on the motion of molecules is negligible (work of the force is negligible compared to the kinetic energy, so $\mathbf{F}$ cannot change substantially the velocities of molecules). When one can solve the **Boltzmann equation without external fields**, i.e. with

$$\mathbf{F} = 0.$$

The **Knudsen number** Kn is the ratio of the characteristic mean free path of gas molecules to the characteristic flow length scale. It characterizes the effect of binary collisions on the flow. If $Kn \gg 1$, then one can neglect collisions and solve a **collisionless Boltzmann equation**

(3.9.11) $$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0.$$

Flow regimes of the dilute gas. Local equilibrium

- The case of $Kn \gg 1$ corresponds to the **free molecular flow regime**.
- The case of $Kn \sim 1$ corresponds to the **transitional flow regime**. In this case, one needs to solve the full non-linear integro differential Boltzmann equation.
- The case of $Kn \ll 1$ corresponds to the **continuum flow regime**. In the limit $Kn \to 0$, the Boltzmann equation reduces to

$$\int_0^{2\pi}\int_0^{r_{max}}\int \left(f'f'_1 - ff_1\right)c_r b db d\varepsilon d\mathbf{v}_1 = 0. \tag{3.9.12}$$

Rarefied gas flows, where the distribution function satisfies equation (3.9.12), are called the **locally equilibrium flows**. We already know (see slide 48) that the solution of Eq. (3.9.12) has the form of Maxwell-Boltzmann equilibrium distribution function. In the considered case, however, macroscopic parameters in this function are not necessarily constant, but can vary with $\mathbf{r}$ and t. So the **locally equilibrium solution** of the Boltzmann equation takes the form

$$f_L(\mathbf{r},\mathbf{v},t) = \frac{n(\mathbf{r},t)}{(2\pi k_B T(\mathbf{r},t)/m)^{3/2}} \exp\left[-\frac{m(\mathbf{v}-\mathbf{u}(\mathbf{r},t))^2}{2k_B T(\mathbf{r},t)}\right]. \tag{3.9.13}$$

Equations with respect to $n(\mathbf{r},t)$, $\mathbf{u}(\mathbf{r},t)$, and $T(\mathbf{r},t)$ can be obtained by inserting Eq. (3.9.13) into the Boltzmann equation in the form of Eq. (3.9.11). This problem will be briefly considered in the end of Section 3.10.

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

- Transfer equation for molecular quantities
- Transfer equation for molecular quantities depending on the chaotic velocity
- Macroscopic conservation laws
- Stress tensor and heat flux vector
- Euler equations

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

The goal of this section is to show that macroscopic conservation laws in the continuum gas dynamics can be obtained as *exact* consequences of the Boltzmann kinetic equation.

Transfer equation for molecular quantities

Let consider the Boltzmann kinetic equation, Eq. (3.4.15),

$$\frac{\partial f}{\partial t}+\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}}+\frac{\mathbf{F}}{m}\cdot\frac{\partial f}{\partial \mathbf{v}}=\int_0^{2\pi}\int_0^{r_{max}}\left(f'f'_1-ff_1\right)c_r b db d\varepsilon d\mathbf{v}_1\,, \tag{3.10.1}$$

multiply this equation by some molecular quantity $\Phi(\mathbf{r},\mathbf{v},t)$, and integrate the equation over velocity $\mathbf{v}$. Then we obtain the equation

$$I_t+I_r+I_v=\Delta\Phi, \tag{3.10.2}$$

where

$$I_t(\mathbf{r},t)=\int\Phi\frac{\partial f}{\partial t}d\mathbf{v}\,,\qquad I_r(\mathbf{r},t)=\int\Phi\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}}d\mathbf{v}\,,\qquad I_v(\mathbf{r},t)=\frac{\mathbf{F}}{m}\cdot\int\Phi\frac{\partial f}{\partial \mathbf{v}}d\mathbf{v}\,,$$

(3.10.3)

$$\Delta\Phi(\mathbf{r},t)=\int\Phi(\mathbf{r},\mathbf{v},t)I_B(\mathbf{r},\mathbf{v},t)d\mathbf{v}=\int\int_0^{2\pi}\int_0^{r_{max}}\Phi(\mathbf{r},\mathbf{v},t)\left(f'f'_1-ff_1\right)c_r b db d\varepsilon d\mathbf{v}_1 d\mathbf{v}.$$

Quantities I_t, I_r, and I_v are not macroscopic parameters, since integrals contain derivatives of f, but any macroscopic parameter must be represented in the form given by Eq. (3.2.2), i.e.

$$n(\mathbf{r},t)\langle\Phi\rangle(\mathbf{r},t)=\int\Phi(\mathbf{r},\mathbf{v},t)f(\mathbf{r},\mathbf{v},t)d\mathbf{v}\ . \tag{3.10.4}$$

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

Let's derive I_t, I_r, and I_v in terms of macroscopic parameters using the rule for calculation of the derivative of a product,

$$\frac{\partial(\Phi f)}{\partial a} = \frac{\partial \Phi}{\partial a} f + \Phi \frac{\partial f}{\partial a},$$

where variable a stands for $t, x, y, z, v_x, v_y, v_z$. Let's also use the following notation for the **divergence** of a vector field $\mathbf{a}(\mathbf{r})$:

$$\mathrm{div}_{\mathbf{r}}\, \mathbf{a} = \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{a} = \frac{\partial a_x}{\partial x} + \frac{\partial a_y}{\partial y} + \frac{\partial a_z}{\partial z}.$$

Then

$$I_t = \int \Phi \frac{\partial f}{\partial t} d\mathbf{v} = \int \left(\frac{\partial(\Phi f)}{\partial t} - \frac{\partial \Phi}{\partial t} f \right) d\mathbf{v} = \frac{\partial}{\partial t} \int \Phi f d\mathbf{v} - \int \frac{\partial \Phi}{\partial t} f d\mathbf{v} = \frac{\partial (n\langle \Phi \rangle)}{\partial t} - n \left\langle \frac{\partial \Phi}{\partial t} \right\rangle,$$

$$I_r = \int \Phi \frac{\partial}{\partial \mathbf{r}} \cdot (\mathbf{v} f) d\mathbf{v} = \int \left(\frac{\partial}{\partial \mathbf{r}} \cdot (\mathbf{v} \Phi f) - \frac{\partial}{\partial \mathbf{r}} \cdot (\mathbf{v}\Phi) f \right) d\mathbf{v} = \frac{\partial}{\partial \mathbf{r}} \cdot (n\langle \mathbf{v}\Phi \rangle) - n \left\langle \frac{\partial}{\partial \mathbf{r}} \cdot (\mathbf{v}\Phi) \right\rangle.$$

Transformation of I_v has a peculiarity related to the fact that differentiation under the integral and integration are performed for the same variables $\mathbf{v}$. Let's first represent I_v in the form

$$I_v = \frac{F_x}{m} \int \Phi \frac{\partial f}{\partial v_x} d\mathbf{v} + \frac{F_y}{m} \int \Phi \frac{\partial f}{\partial v_y} d\mathbf{v} + \frac{F_z}{m} \int \Phi \frac{\partial f}{\partial v_z} d\mathbf{v} = \frac{F_x}{m} I_x + \frac{F_y}{m} I_y + \frac{F_z}{m} I_z,$$

and calculate, e.g., I_x:

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

$$I_x = \int \Phi \frac{\partial f}{\partial v_x} d\mathbf{v} = \int \left(\frac{\partial (\Phi f)}{\partial v_x} - \frac{\partial \Phi}{\partial v_x} f \right) d\mathbf{v} = \int \frac{\partial (\Phi f)}{\partial v_x} d\mathbf{v} - n \left\langle \frac{\partial \Phi}{\partial v_x} \right\rangle,$$

$$\int \frac{\partial (\Phi f)}{\partial v_x} d\mathbf{v} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left(\int_{-\infty}^{+\infty} \frac{\partial (\Phi f)}{\partial v_x} dv_x \right) dv_y dv_z = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left(\int_{-\infty}^{+\infty} \frac{\partial (\Phi f)}{\partial v_x} dv_x \right) dv_y dv_z .$$

Now let's use the **fundamental theorem of calculus**:

$$\int_a^b \frac{dF}{dx} dx = F(b) - F(a).$$

Then

$$\int \frac{\partial (\Phi f)}{\partial v_x} d\mathbf{v} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left(\Phi f \Big|_{v_x \to -\infty}^{v_x \to +\infty} \right) dv_y dv_z = 0,$$

because the condition

$$\Phi(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}, t) \xrightarrow[|\mathbf{v}| \to \infty]{} 0$$

is necessary for convergence of the integral in Eq. (3.10.4) and existence of the macroscopic parameter $\langle \Phi \rangle$. Then finally

$$I_v(\mathbf{r}, t) = -n \frac{\mathbf{F}}{m} \cdot \left\langle \frac{\partial \Phi}{\partial \mathbf{v}} \right\rangle.$$

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

Now let's insert the obtained equations for I_t, I_r, and I_v into equation (3.10.2):

(3.10.5) $$\frac{\partial(n\langle\Phi\rangle)}{\partial t}+\frac{\partial}{\partial\mathbf{r}}\cdot(n\langle\mathbf{v}\Phi\rangle)=n\left(\left\langle\frac{\partial\Phi}{\partial t}\right\rangle+\left\langle\mathbf{v}\cdot\frac{\partial\Phi}{\partial\mathbf{r}}\right\rangle+\frac{\mathbf{F}}{m}\cdot\left\langle\frac{\partial\Phi}{\partial\mathbf{v}}\right\rangle\right)+\Delta\Phi.$$

This is the **macroscopic transfer equation** for the molecular quantity Φ. All terms in this equation with exception of $\Delta\Phi$ are represented in terms of macroscopic parameters of various molecular quantities.

Transfer equation for molecular quantities depending on the chaotic velocity

Let's consider a molecular quantity Ψ that depends on the velocity of the chaotic motion of molecule $\mathbf{c}$ (see Eq. (3.2.6)):

(3.10.6) $$\Psi=\Psi(\mathbf{r},\mathbf{c},t),\qquad \mathbf{c}=\mathbf{v}-\mathbf{u}(\mathbf{r},t).$$

Example of such quantity Ψ is the kinetic energy of chaotic motion, $m\mathbf{c}^2/2$, see slide 13. We can apply Eq. (3.10.5) for Ψ if we introduce

(3.10.7) $$\Phi(\mathbf{r},\mathbf{v},t)=\Psi(\mathbf{r},\mathbf{v}-\mathbf{u}(\mathbf{r},t),t).$$

Then in the left-hand side of Eq. (3.10.5) individual macroscopic parameters can be re-written as follows:

$$n\langle\Phi\rangle=n\langle\Psi\rangle,\qquad n\langle\mathbf{v}\Phi\rangle=n\langle(\mathbf{c}+\mathbf{u})\Psi\rangle=n\langle\mathbf{c}\Psi\rangle+n\mathbf{u}\langle\Psi\rangle.$$

In the right-hand side of Eq. (3.10.5) individual macroscopic parameters can be re-written using the chain rule for calculation of derivatives, for instance:

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

$$\frac{\partial \Phi}{\partial t} = \frac{\partial}{\partial t}\Psi(\mathbf{r}, \mathbf{v} - \mathbf{u}(\mathbf{r}, t), t) = \frac{\partial \Psi}{\partial t} - \frac{\partial \Psi}{\partial c_x}\frac{\partial u_x}{\partial t} - \frac{\partial \Psi}{\partial c_y}\frac{\partial u_y}{\partial t} - \frac{\partial \Psi}{\partial c_z}\frac{\partial u_z}{\partial t} = \frac{\partial \Psi}{\partial t} - \frac{\partial \mathbf{u}}{\partial t}\cdot\frac{\partial \Psi}{\partial \mathbf{c}}.$$

Then

$$\left\langle \frac{\partial \Phi}{\partial t} \right\rangle = \left\langle \frac{\partial \Psi}{\partial t} \right\rangle - \frac{\partial \mathbf{u}}{\partial t}\cdot\left\langle \frac{\partial \Psi}{\partial \mathbf{c}} \right\rangle,$$

$$\left\langle \mathbf{v}\cdot\frac{\partial \Phi}{\partial \mathbf{r}} \right\rangle = \left\langle (\mathbf{c}+\mathbf{u})\cdot\left(\frac{\partial \Psi}{\partial \mathbf{r}} - \frac{\partial \mathbf{u}}{\partial \mathbf{r}}\cdot\frac{\partial \Psi}{\partial \mathbf{c}}\right) \right\rangle = \left\langle \mathbf{c}\cdot\frac{\partial \Psi}{\partial \mathbf{r}} \right\rangle + \mathbf{u}\cdot\left\langle \frac{\partial \Psi}{\partial \mathbf{r}} \right\rangle - \left\langle \mathbf{c}\cdot\frac{\partial \mathbf{u}}{\partial \mathbf{r}}\cdot\frac{\partial \Psi}{\partial \mathbf{c}} \right\rangle - \mathbf{u}\cdot\frac{\partial \mathbf{u}}{\partial \mathbf{r}}\cdot\left\langle \frac{\partial \Psi}{\partial \mathbf{c}} \right\rangle,$$

$$\frac{\mathbf{F}}{m}\cdot\left\langle \frac{\partial \Phi}{\partial \mathbf{v}} \right\rangle = \frac{\mathbf{F}}{m}\cdot\left\langle \frac{\partial \Psi}{\partial \mathbf{c}} \right\rangle,$$

where

(3.10.8)

$$\frac{\partial \mathbf{u}}{\partial \mathbf{r}} = \begin{bmatrix} \frac{\partial u_x}{\partial x} & \frac{\partial u_y}{\partial x} & \frac{\partial u_z}{\partial x} \\ \frac{\partial u_x}{\partial y} & \frac{\partial u_y}{\partial y} & \frac{\partial u_z}{\partial y} \\ \frac{\partial u_x}{\partial z} & \frac{\partial u_y}{\partial z} & \frac{\partial u_z}{\partial z} \end{bmatrix}$$

is the **second-rank tensor (matrix) of the velocity gradient**.

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

Now by inserting all obtained equations for individual terms into Eq. (3.10.5), one can find the **transfer equation molecular quantity Ψ depending on the chaotic velocity:**

(3.10.9)
$$\frac{\partial(n\langle\Psi\rangle)}{\partial t}+\frac{\partial}{\partial\mathbf{r}}\cdot(n\langle\mathbf{c}\Psi\rangle)+\frac{\partial}{\partial\mathbf{r}}\cdot(n\mathbf{u}\langle\Psi\rangle)=$$
$$n\left(\left\langle\frac{\partial\Psi}{\partial t}\right\rangle-\frac{\partial\mathbf{u}}{\partial t}\cdot\left\langle\frac{\partial\Psi}{\partial\mathbf{c}}\right\rangle+\left\langle\mathbf{c}\cdot\frac{\partial\Psi}{\partial\mathbf{r}}\right\rangle+\mathbf{u}\cdot\left\langle\frac{\partial\Psi}{\partial\mathbf{r}}\right\rangle-\left\langle\mathbf{c}\cdot\frac{\partial\mathbf{u}}{\partial\mathbf{r}}\cdot\frac{\partial\Psi}{\partial\mathbf{c}}\right\rangle-\mathbf{u}\cdot\frac{\partial\mathbf{u}}{\partial\mathbf{r}}\cdot\left\langle\frac{\partial\Psi}{\partial\mathbf{c}}\right\rangle+\frac{\mathbf{F}}{m}\cdot\left\langle\frac{\partial\Psi}{\partial\mathbf{c}}\right\rangle\right)+\Delta\Psi.$$

We can slightly simplify this equation if, similar to the continuum mechanics, introduce a **material derivative**

(3.10.10)
$$\frac{Da}{Dt}=\frac{\partial a}{\partial t}+u_x\frac{\partial a}{\partial x}+u_y\frac{\partial a}{\partial y}+u_z\frac{\partial a}{\partial z}=\frac{\partial a}{\partial t}+\mathbf{u}\cdot\frac{\partial a}{\partial\mathbf{r}}$$

that describes the time rate of change of physical quantity $a(\mathbf{r},t)$ in a **material element**, i.e. in a portion of fluid moving with the macroscopic velocity $\mathbf{u}$. Then we can re-write the sum of the first and last terms in the left-hand side of Eq. (3.10.9) as

$$\frac{\partial(n\langle\Psi\rangle)}{\partial t}+\frac{\partial}{\partial\mathbf{r}}\cdot(n\mathbf{u}\langle\Psi\rangle)=\frac{\partial(n\langle\Psi\rangle)}{\partial t}+\mathbf{u}\cdot\frac{\partial(n\langle\Psi\rangle)}{\partial\mathbf{r}}+n\langle\Psi\rangle\frac{\partial}{\partial\mathbf{r}}\cdot\mathbf{u}=\frac{D(n\langle\Psi\rangle)}{Dt}+n\langle\Psi\rangle\frac{\partial}{\partial\mathbf{r}}\cdot\mathbf{u}$$

and also combine the first and fourth terms as well second and sixth terms in the right-hand side of Eq. (3.10.9). Finally we obtain the transfer equation in the form:

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

(3.10.11)
$$\frac{D(n\langle\Psi\rangle)}{Dt}+n\langle\Psi\rangle\frac{\partial}{\partial\mathbf{r}}\cdot\mathbf{u}+\frac{\partial}{\partial\mathbf{r}}\cdot(n\langle\mathbf{c}\Psi\rangle)=$$
$$n\left(\left\langle\frac{D\Psi}{Dt}\right\rangle-\frac{D\mathbf{u}}{Dt}\cdot\left\langle\frac{\partial\Psi}{\partial\mathbf{c}}\right\rangle+\left\langle\mathbf{c}\cdot\frac{\partial\Psi}{\partial\mathbf{r}}\right\rangle-\left\langle\mathbf{c}\cdot\frac{\partial\mathbf{u}}{\partial\mathbf{r}}\cdot\frac{\partial\Psi}{\partial\mathbf{c}}\right\rangle+\frac{\mathbf{F}}{m}\cdot\left\langle\frac{\partial\Psi}{\partial\mathbf{c}}\right\rangle\right)+\Delta\Psi.$$

Macroscopic conservation laws

Now let's apply Eq. (3.10.11) for three particular molecular quantities:

(3.10.12)
$$\Psi=1,\qquad\Psi=m\mathbf{c},\qquad\Psi=\frac{m\mathbf{c}^2}{2}.$$

Every such molecular quantity is conserved during the binary collision and thus, is the collisional invariant (see slide 45 in this Chapter). Then according to the integral lemma (slide 43 in this Chapter), $\Delta\Psi=0$ for any molecular quantity in Eq. (3.10.12). In addition, these quantities do not depend on t and $\mathbf{r}$, so that

$$\frac{D\Psi}{Dt}=0,\qquad\frac{\partial\Psi}{\partial\mathbf{r}}=0.$$

Then Eq. (3.10.11) reduces to

$$\frac{D(n\langle\Psi\rangle)}{Dt}+n\langle\Psi\rangle\frac{\partial}{\partial\mathbf{r}}\cdot\mathbf{u}+\frac{\partial}{\partial\mathbf{r}}\cdot(n\langle\mathbf{c}\Psi\rangle)=n\left(\frac{\mathbf{F}}{m}\cdot\left\langle\frac{\partial\Psi}{\partial\mathbf{c}}\right\rangle-\frac{D\mathbf{u}}{Dt}\cdot\left\langle\frac{\partial\Psi}{\partial\mathbf{c}}\right\rangle-\left\langle\mathbf{c}\cdot\frac{\partial\mathbf{u}}{\partial\mathbf{r}}\cdot\frac{\partial\Psi}{\partial\mathbf{c}}\right\rangle\right).$$

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

Transfer equation for $\Psi = 1$:

$$\langle \Psi \rangle = 1, \qquad \langle \mathbf{c}\Psi \rangle = \langle \mathbf{c} \rangle = 0, \qquad \frac{\partial \Psi}{\partial \mathbf{c}} = 0.$$

Then

(3.10.13)
$$\frac{Dn}{Dt} + n\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{u} = 0.$$

This is the **continuity equation** of continuum mechanics, which is the mathematical form of the number (mass) of molecules conservation law. Thus, the transfer equation for $\Psi = 1$ coincides with the continuity equation.

Transfer equation for $\Psi = m\mathbf{c}$:

$$\langle \Psi \rangle = \langle m\mathbf{c} \rangle = 0, \qquad \frac{\partial \Psi}{\partial \mathbf{c}} = m\mathbf{I} = m\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

where $\mathbf{I}$ is the **metric tensor** (In Cartesian coordinates, components of $\mathbf{I}$ form the **identity matrix**). Then

$$\left\langle \mathbf{c} \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{r}} \cdot \frac{\partial \Psi}{\partial \mathbf{c}} \right\rangle = \left\langle \mathbf{c} \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{r}} \right\rangle = m\langle \mathbf{c} \rangle \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{r}} = 0$$

and we obtain the equation

$$\frac{\partial}{\partial \mathbf{r}} \cdot (n\langle m\mathbf{cc} \rangle) = mn\left(\frac{\mathbf{F}}{m} - \frac{D\mathbf{u}}{Dt}\right), \qquad \text{or}$$

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

(3.10.14)
$$mn\frac{D\mathbf{u}}{Dt}=\frac{\partial}{\partial\mathbf{r}}\cdot\mathbf{S}+n\mathbf{F},$$

where

Components of the symmetric tensor satisfy the condition $s_{ij}=s_{ji}$, so any symmetric tensor has only 6 different components.

(3.10.15a)
$$\mathbf{S}=\begin{bmatrix}s_{xx} & s_{xy} & s_{xz}\\ s_{yx} & s_{yy} & s_{yz}\\ s_{zx} & s_{zy} & s_{zz}\end{bmatrix}$$

is the second-rank **symmetric** tensor with components

(3.10.15b)
$$s_{ij}=s_{ji}=-n\langle mc_ic_j\rangle=-m\int c_ic_j\,f\,d\mathbf{v}=-m\int(v_i-u_i)(v_j-u_j)\,f\,d\mathbf{v}.$$

Equation (3.10.14) coincides with the **momentum equation** of continuum mechanics, which is the mathematical form of the linear momentum conservation law, if we assume that Eqs. (3.10.15) define **the stress tensor** $\mathbf{S}$ in the gas. Thus, the transfer equation for $\Psi=m\mathbf{c}$ coincides with the momentum equation.

Transfer equation for $\Psi=m\mathbf{c}^2/2$:

(3.10.16)
$$n\langle\Psi\rangle=n\left\langle\frac{m\mathbf{c}^2}{2}\right\rangle=E,\qquad\frac{\partial\Psi}{\partial\mathbf{c}}=m\mathbf{c},\qquad\left\langle\frac{\partial\Psi}{\partial\mathbf{c}}\right\rangle=\langle m\mathbf{c}\rangle=0,$$

where nE is the internal energy density (internal energy per unit volume). Then one can obtain the transfer equation in the form

$$\frac{DE}{Dt}+E\frac{\partial}{\partial\mathbf{r}}\cdot\mathbf{u}+\frac{\partial}{\partial\mathbf{r}}\cdot\left(n\left\langle\mathbf{c}\frac{m\mathbf{c}^2}{2}\right\rangle\right)=-n\left\langle\mathbf{c}\cdot\frac{\partial\mathbf{u}}{\partial\mathbf{r}}\cdot m\mathbf{c}\right\rangle$$

These terms cancel each other due to Eq. (3.10.13)

or

$$n\frac{D(E/n)}{Dt}+\frac{E}{n}\left(\frac{Dn}{Dt}+n\frac{\partial}{\partial\mathbf{r}}\cdot\mathbf{u}\right)=-\frac{\partial}{\partial\mathbf{r}}\cdot\mathbf{q}-n\left\langle\mathbf{c}\cdot\frac{\partial\mathbf{u}}{\partial\mathbf{r}}\cdot m\mathbf{c}\right\rangle, \tag{3.10.17}$$

where

$$\mathbf{q}=n\left\langle\mathbf{c}\frac{m\mathbf{c}^2}{2}\right\rangle=\int\mathbf{c}\frac{m\mathbf{c}^2}{2}f\,d\mathbf{v}. \tag{3.10.18}$$

Let's show that the last term in Eq. (3.10.17) can be written in terms of the stress tensor. For this purpose, let's introduced a new operation for second-rand tensors which is called the **double scalar (double dot) product**:

$$\mathbf{S}:\mathbf{E}=\begin{bmatrix}s_{xx}&s_{xy}&s_{xz}\\s_{yx}&s_{yy}&s_{yz}\\s_{zx}&s_{zy}&s_{zz}\end{bmatrix}:\begin{bmatrix}e_{xx}&e_{xy}&e_{xz}\\e_{yx}&e_{yy}&e_{yz}\\e_{zx}&e_{zy}&e_{zz}\end{bmatrix}=\sum_{i=x,y,z}\sum_{j=x,y,z}s_{ij}e_{ji}\,.$$

Then the last term in Eq. (3.10.17) can be written as follows:

$$-n\left\langle\mathbf{c}\cdot\frac{\partial\mathbf{u}}{\partial\mathbf{r}}\cdot m\mathbf{c}\right\rangle=-n\left\langle(m\mathbf{cc}):\frac{\partial\mathbf{u}}{\partial\mathbf{r}}\right\rangle=-n\langle m\mathbf{cc}\rangle:\frac{\partial\mathbf{u}}{\partial\mathbf{r}}=\mathbf{S}:\frac{\partial\mathbf{u}}{\partial\mathbf{r}}.$$

The last term can be written in a form generally accepted in continuum mechanics if the components of the velocity gradient tensor are represented as follows

This equation can be proved by writing the left- and right-hand sides in the component form

$$\frac{\partial u_j}{\partial r_i}=\frac{1}{2}\left(\frac{\partial u_j}{\partial r_i}+\frac{\partial u_i}{\partial r_j}\right)+\frac{1}{2}\left(\frac{\partial u_j}{\partial r_i}-\frac{\partial u_i}{\partial r_j}\right).$$

Then the tensor of the velocity gradient can be represented in the form

$$\frac{\partial \mathbf{u}}{\partial \mathbf{r}} = \mathbf{E} + \boldsymbol{\Omega}\,, \tag{3.10.19}$$

where $\mathbf{E}$ is the symmetric **strain rate tensor** with components

$$E_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial r_i} + \frac{\partial u_i}{\partial r_j}\right) \tag{3.10.20}$$

and $\boldsymbol{\Omega}$ is the **skew-symmetric** tensor with components

$$\Omega_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial r_i} - \frac{\partial u_i}{\partial r_j}\right).$$

Components of the skew-symmetric tensor satisfy the condition $s_{ij} = -s_{ji}$, so $s_{ii} = 0$ and any skew-symmetric tensor has only 3 different components.

Three different components of tensor $\boldsymbol{\Omega}$ forms the **vector of vorticity** $\boldsymbol{\omega}$

$$\boldsymbol{\omega} = \frac{1}{2}\,\mathrm{rot}\,\mathbf{u} = \Omega_{23}\mathbf{i} + \Omega_{13}\mathbf{j} + \Omega_{12}\mathbf{k}.$$

One can prove that double scalar product of any symmetric tensor $\mathbf{S}$ and skew-symmetric tensor $\boldsymbol{\Omega}$ is equal to zero, $\mathbf{S}:\boldsymbol{\Omega} = 0$, and, thus, $\mathbf{S}:\partial\mathbf{u}/\partial\mathbf{r} = \mathbf{S}:\mathbf{E}$. Then the equation of energy transfer finally takes the form

$$n\frac{D(E/n)}{Dt} = -\frac{\partial}{\partial \mathbf{r}}\cdot\mathbf{q} + \mathbf{S}:\mathbf{E}. \tag{3.10.21}$$

Equation (3.10.21) coincides with the **energy equation** of continuum mechanics, which is the mathematical form of the energy conservation law, if we assume that Eqs. (3.10.15) and (3.10.18) define the stress tensor $\mathbf{S}$ and **heat flux vector** $\mathbf{q}$ in the gas, correspondingly. Thus, the transfer equation for $\Psi = m\mathbf{c}^2/2$ coincides with the energy equation.

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

Stress tensor and heat flux vector

We showed that the transfer equations reduce to the continuum conservation laws if equations

$$\mathbf{S} = -n\langle m\mathbf{cc}\rangle, \qquad s_{ij} = -n\langle mc_i c_j\rangle = -\int mc_i c_j\, f d\mathbf{v},$$

$$\mathbf{q} = n\left\langle \mathbf{c}\frac{m\mathbf{c}^2}{2}\right\rangle = \int \mathbf{c}\frac{m\mathbf{c}^2}{2} f d\mathbf{v}$$

define the stress vector and hear flux vector in the gas. These are the **kinetic definitions** of the stress tensor and heat flux vector.

The system of conservation laws then takes the form

$$\frac{Dn}{Dt} + n\frac{\partial}{\partial \mathbf{r}}\cdot\mathbf{u} = 0, \qquad mn\frac{D\mathbf{u}}{Dt} = \frac{\partial}{\partial \mathbf{r}}\cdot\mathbf{S} + n\mathbf{F}, \qquad n\frac{D(E/n)}{Dt} = -\frac{\partial}{\partial \mathbf{r}}\cdot\mathbf{q} + \mathbf{S}:\mathbf{E}. \tag{3.10.22}$$

In this system of equation, the mass of molecule m is known, the external force $\mathbf{F}$ is assumed be a known function of coordinates, and the deformation rate tensor $\mathbf{E}$ is defined by the velocity vector, Eq. (3.10.20). Then five scalar equations (3.20.22) includes 14 unknowns:

n, E, 3 components of $\mathbf{u}$, 6 components of $\mathbf{S}$, and 3 components of $\mathbf{q}$.

The system is not closed. It is possible to obtain from Eq. (3.10.11) additional transfer equations with respect to $\mathbf{S}$ and $\mathbf{q}$, but these equations will include new unknown macroscopic parameters. In any system of transfer equations the number of unknowns is larger than the number of equations and such system cannot be solved without additional assumptions.

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

In general, it is possible to obtain approximate additional equation for components of $\mathbf{S}$ and $\mathbf{q}$ only in the continuum flow regime at $Kn << 1$, i.e. if the local state of the flow is close to local equilibrium state. For this purpose, special mathematical methods of analysis of solution of the Boltzmann equation are developed. Two the most general methods are

- Method of moments.
- Chapman-Enskog method.

In particular the Chapman-Enskog method shows that, if deviations from the local equilibrium are small, then the equations for $\mathbf{S}$ and $\mathbf{q}$ reduce to the **Fourier law of heat conduction** and **Newton law of viscous drag** and the closed system of transfer equations coincides with the system of **Navier-Stokes equations** for compressible gas.

Euler equations

Let's assume that in the limit $Kn \to 0$, gas flow is in the local equilibrium state and the distribution function is given by Eq. (3.9.13)

$$f_L(\mathbf{r},\mathbf{v},t) = \frac{n(\mathbf{r},t)}{(2\pi k_B T(\mathbf{r},t)/m)^{3/2}} \exp\left[-\frac{m(\mathbf{v}-\mathbf{u}(\mathbf{r},t))^2}{2k_B T(\mathbf{r},t)}\right]. \tag{3.10.23}$$

We can use this equation in order to find E, $\mathbf{S}$, and $\mathbf{q}$ in terms of macroscopic parameters n, $\mathbf{u}$, and T, and thus, to obtain a close systems of gas dynamic equations. If we insert Eq. (3.10.23) into Eq. (3.10.16), (3.10.15), and (3.10.18), then we obtain:

$$E = n\left\langle \frac{m\mathbf{c}^2}{2} \right\rangle = \int \frac{m\mathbf{c}^2}{2} f_L(\mathbf{r},\mathbf{v},t)d\mathbf{v} = \frac{3}{2} n k_B T; \tag{3.10.24}$$

3.10. Macroscopic gas dynamics equations. Stress tensor and heat flux vector

This equation coincides with the **equation of state of calorically perfect gas**, Eq. (1.3.13);

(3.10.25) $$\mathbf{S} = -n\langle m\mathbf{cc}\rangle = -m\int \mathbf{cc}\, f_L(\mathbf{r},\mathbf{v},t)\, d\mathbf{v} = -p\mathbf{I} = \begin{bmatrix} -p & 0 & 0 \\ 0 & -p & 0 \\ 0 & 0 & -p \end{bmatrix},$$

(3.10.26) $$p = nk_BT;$$

The last equation coincides with the **equation of state of ideal gas**, Eq. (1.3.11);

(3.10.27) $$\mathbf{q} = n\left\langle \mathbf{c}\frac{m\mathbf{c}^2}{2}\right\rangle = \int \mathbf{c}\frac{m\mathbf{c}^2}{2} f_L(\mathbf{r},\mathbf{v},t)\, d\mathbf{v} = 0.$$

Eqs. (3.10.25) and (3.10.26) show that in the limit of $Kn \to 0$ viscous stress and heat fluxes disappear, and only normal stresses, where p is the **pressure**, exist in the gas. Thus, the assumption of the local equilibrium results in the model of inviscid and thermally non-conducting ideal and calorically perfect gas. The conservation laws reduce for this model to

(3.10.28) $$\frac{Dn}{Dt} + n\frac{\partial}{\partial \mathbf{r}}\cdot\mathbf{u} = 0, \qquad mn\frac{D\mathbf{u}}{Dt} = -\frac{\partial p}{\partial \mathbf{r}} + n\mathbf{F}, \qquad n\frac{D(E/n)}{Dt} = -p\frac{\partial}{\partial \mathbf{r}}\cdot\mathbf{u},$$
$$\frac{E}{n} = \frac{3}{2}k_BT, \qquad p = nk_BT.$$

These equations form a closed system (7 equations, 7 unknows). In continuum gas dynamics, these equations are known as the **Euler equations**. We showed that the Euler equations are the exact consequences of the Boltzmann equation under conditions of local equilibrium.