

6. BOUNDARY CONDITIONS

When the Boltzmann equation is posed over a spatial domain with a boundary, it must be supplemented with boundary conditions. Boundary effects can dominate the solution when mean-free-paths are comparable to length scales in the spatial domain. Because this is often the regime one is in when one wants to solve the Boltzmann equation, the treatment of boundary conditions is central to the subject.

There are many kinds of boundaries. There are physical boundaries such as the wall of a container or piston that confines the gas. There are open boundaries such as the mouth of a valve or nozzle through which gas is either injected into or expelled from the domain. Boundaries can be either stationary or moving. They can move in a prescribed way independent of the gas, or in an unprescribed way that is influenced by the gas. For example, a piston can have a prescribed position as a function of time, or it can exert a prescribed containing force on the gas and move accordingly. The most complicated kind of boundaries are those that are free to take on a wide variety of shapes in response to the gas — so-called free boundaries. Examples of free boundaries include a confining membrane or liquid surface. Finally, there are artificial boundaries that are introduced to make a problem computationally manageable. For example, artificial boundaries are needed when computing the aerodynamics of a reentering spacecraft. We will not model all the types of boundaries mentioned above. Rather, we will select some for detailed treatment, others for sketchy treatment, and others for neglect.

6.1. Stationary, Perfectly Reflecting Boundaries. Perfectly reflecting boundaries are ones at which every molecule striking it is reflected back in some altered state. Molecules are neither created nor destroyed at such a boundary. Each molecule that strikes such a boundary will certainly have its momentum changed, and possibly its energy too. The walls of a container that physically confine a gas are often modeled as perfectly reflecting boundaries.

Let $\partial\Omega|_R$ denote that part of $\partial\Omega$ which is a perfectly reflecting boundary. We will begin by considering the case where $\partial\Omega|_R$ is stationary. We will assume that at each point $x \in \partial\Omega|_R$ there is a unique tangent plane with outward unit normal $n(x) \in \mathbb{S}^{D-1}$. Molecules with velocities v such that $n \cdot v > 0$ are moving towards the boundary, while those with velocities v such that $n \cdot v < 0$ are moving away from the boundary into the domain. For every $t > 0$ we must specify boundary values for $F(v, x, t)$ on the set of incoming velocities along $\partial\Omega|_R$ in terms of the boundary values for $F(v, x, t)$ on the set of outgoing velocities along $\partial\Omega|_R$. In other words, for each $t > 0$ we must specify $F(v, x, t)$ on the set

$$(6.1a) \quad \Gamma_R^- = \left\{ (v, x) \in \mathbb{R}^D \times \partial\Omega|_R : n(x) \cdot v < 0 \right\},$$

in terms of $F(v', x', t')$ for $t' \in [0, t]$ on the set

$$(6.1b) \quad \Gamma_R^+ = \left\{ (v', x') \in \mathbb{R}^D \times \partial\Omega|_R : n(x') \cdot v' > 0 \right\}.$$

In ideal gas regimes most of the gas molecules that interact with the reflecting boundary will not be influenced by other gas molecules. The relationship giving $F(v, x, t)$ on Γ_R^- in terms of $F(v', x', t')$ on $\Gamma_R^+ \times [0, t]$ will therefore be taken to be linear.

We will also assume that the spatial and temporal scales over which most molecules interact with the boundary are comparable with the spatial and temporal scales of an intermolecular interaction, which are neglected in our kinetic model. The linear relationship giving $F(v, x, t)$ on Γ_- in terms of $F(v', x', t')$ on $\Gamma_R^+ \times [0, t]$ will therefore be taken to be local in space and time. In other words, $F(v, x, t)$ on Γ_R^- will be related linearly to $F(v', x, t)$ on Γ_R^+ .

Finally, we will assume the boundary material is in local thermal equilibrium characterized by a so-called wall temperature $\theta_W = \theta_W(x, t)$. This temperature can either be prescribed or be influenced by the gas. The assumption that a boundary is in local thermal equilibrium is usually good because the molecules of the boundary material are usually far denser than those of the gas. Indeed, the molecules of a solid boundary material are in constant contact and behave collectively. Therefore they typically interact with each other many times between their interactions with gas molecules. The molecules of the boundary material also generally are heavier than those of the gas. Therefore their momentum and energy are changed less by interactions with gas molecules than by interactions with each other.

The rate at which molecules of mass m with velocity v' strike a differential area $dA(x)$ of the boundary surface with outward normal $n(x)$ is given by

$$(6.2a) \quad \frac{1}{m} n \cdot v' F(v', x, t) dv' dA(x).$$

The rate at which molecules of mass m with velocity v move away from the differential area $dA(x)$ with outward normal $n(x)$ is given by

$$(6.2b) \quad \frac{1}{m} |n \cdot v| F(v, x, t) dv dA(x).$$

If we let $R(v, v')$ be the probability density that a molecule which strikes the boundary surface with velocity v' will move away from it with velocity v then we can express the general reflection boundary condition as

$$(6.3a) \quad |n \cdot v| F(v, x, t) = \int_{n \cdot v' > 0} R(v, v') n \cdot v' F(v', x, t) dv' \quad \text{for every } (v, x) \in \Gamma_R^-.$$

where the so-called redistribution kernel $R(v, v')$ satisfies

$$(6.3b) \quad \begin{aligned} (1) \quad & R(v, v') \geq 0 \quad \text{for every } n \cdot v < 0 \text{ and } n \cdot v' > 0, \\ (2) \quad & \int_{n \cdot v < 0} R(v, v') dv = 1 \quad \text{for every } n \cdot v' > 0, \\ (3) \quad & |n \cdot v| M(v; \theta_W) = \int_{n \cdot v' > 0} R(v, v') n \cdot v' M(v'; \theta_W) dv' \quad \text{for every } n \cdot v < 0, \end{aligned}$$

where $\theta_W(x, t)$ is the wall temperature and the so-called wall Maxwellian $M(v; \theta_W)$ is given by

$$(6.4) \quad M(v; \theta_W) = \mathcal{M}(v; 1, 0, \theta_W).$$

Here we have suppressed the fact that R can depend on (x, t) , typically through the normal $n(x)$ and/or the wall temperature $\theta_W(x, t)$.

Conditions **(1)** and **(2)** in (6.3b) state that for each v' the kernel $R(v, v')$ is a probability density in v over $n \cdot v < 0$, which is another way of saying the boundary is perfectly reflecting. Condition **(3)** states that the boundary condition (6.3a) is satisfied when F is a local Maxwellian in the form $F(v, x, t) = \rho(x, t) M(v; \theta_W(x, t))$ for some mass density ρ .

Sometimes condition **(3)** is replaced by the so-called *detail-balance* condition

$$(6.5) \quad R(v, v') n \cdot v' M(v'; \theta_W) = R(v', v) |n \cdot v| M(v; \theta_W) \quad \text{for every } n \cdot v < 0 \text{ and } n \cdot v' > 0.$$

This statement of symmetry holds for many redistribution kernel models. It is easily checked that this condition plus **(2)** implies **(3)**.

To better understand the general class of perfectly reflecting boundary conditions (6.3), it is helpful to consider some specific models.

6.1.1. *Specular Reflection Model.* If the boundary is modeled as a smooth hard surface then a molecule striking it with velocity v' will be elastically reflected with a velocity v given by

$$(6.6) \quad v = v' - 2nn \cdot v' = (I - 2nn^T)v'.$$

This is called *specular reflection*. Each such reflection conserves the energy of the molecule because $|v|^2 = |v'|^2$. It also conserves the tangential momentum of the molecule because $v - v'$ is always in the normal direction.

Now consider $F(v, x, t)$ at a point $(v, x) \in \Gamma_-$. By (6.6) a molecule with reflected velocity v can only have been produced by striking the surface with velocity v' given by

$$v' = v - 2nn \cdot v = (I - 2nn^T)v.$$

The so-called specular reflection boundary condition is therefore

$$(6.7) \quad F(v, x, t) = F(v - 2nn \cdot v, x, t) \quad \text{for every } (v, x) \in \Gamma_-.$$

The corresponding redistribution kernel is given by

$$(6.8) \quad R_S(v, v') = \delta(v' - v + 2nn \cdot v).$$

This kernel satisfies all the conditions in (6.3b) and the detailed-balance symmetry (6.5). Of course, on molecular length scales no surface is smooth. Consequently, few reflections will be truly specular. Therefore this boundary condition represents an ideal.

6.1.2. *Isotropic Reflection Model.* If the boundary is modeled as a rough hard surface then a molecule striking it with velocity v' will be elastically reflected to have velocity $v = |v'|o$ where o is an arbitrary unit vector such that $n \cdot o < 0$. Each such reflection conserves the energy of the molecule because $|v|^2 = |v'|^2$.

The vector o should be drawn from a probability distribution that depends on the normal n and the direction $o' = v'/|v'|$. When the microscopic dynamics is rotationally invariant the underlying probability density will be a function of the cosines $o \cdot o'$, $o \cdot n$, and $o' \cdot n$. Rather than deriving such a probability density from a model for the molecular structure of the surface, we will simply draw o from the uniform distribution. This is called *isotropic reflection*.

Now consider $F(v, x, t)$ at a point $(v, x) \in \Gamma_-$. A molecule reflected with velocity v can only have been produced by striking the surface with velocity $v' = |v|o'$ where o' is a unit vector such that $n \cdot o' > 0$. By (6.2a) molecules strike the surface at a rate proportional to $n \cdot o'$. Therefore the so-called isotropic reflection boundary condition is

$$(6.9a) \quad F(v, x, t) = \frac{1}{c_1} \int_{n \cdot o' > 0} n \cdot o' F(|v|o', x, t) do' \quad \text{for every } (v, x) \in \Gamma_-^-,$$

where the constant c_1 is given by

$$(6.9b) \quad c_1 = \int_{n \cdot o' > 0} n \cdot o' do'.$$

The corresponding redistribution kernel is given by

$$(6.10) \quad R_I(v, v') = \frac{|n \cdot v|}{c_1 |v|^D} \delta(|v'| - |v|).$$

This kernel satisfies all the conditions in (6.3b) and the detailed-balance symmetry (6.5).

Remark. The microscopic roughness being modeled here is not in contradiction with our assumption that $\partial\Omega$ varies on the scales of a mean-free-path or longer.

6.1.3. *Thermal Reflection Model.* If the boundary is modeled as a rough surface at a so-called wall temperature $\theta_W = \theta_W(x, t)$ such that a molecule striking it with velocity v' will be thermalized and re-emitted with a velocity v drawn from the Maxwellian density $M(v; \theta_W)$.

The so-called thermal reflection boundary condition is therefore

$$(6.11) \quad F(v, x, t) = \left(\frac{2\pi}{\theta_W}\right)^{\frac{1}{2}} M(v; \theta_W) \int_{n \cdot v' > 0} n \cdot v' F(v', x, t) dv' \quad \text{for every } (v, x) \in \Gamma_R^-.$$

The corresponding redistribution kernel is given by

$$(6.12) \quad R_T(v, v') = |n \cdot v| \left(\frac{2\pi}{\theta_W}\right)^{\frac{1}{2}} M(v; \theta_W).$$

This kernel satisfies all the conditions in (6.3b) and the detailed-balance symmetry (6.5).

6.1.4. *Simple Composite Models.* We can build more realistic models of perfectly reflecting boundaries by simply taking convex combinations of the idealized kernels given by (6.8), (6.10), and (6.12):

$$(6.13) \quad R(v, v') = \alpha_S R_S(v, v') + \alpha_I R_I(v, v') + \alpha_T R_T(v, v'),$$

where $\alpha_S, \alpha_I, \alpha_T \geq 0$ with $\alpha_S + \alpha_I + \alpha_T = 1$. Here α_S, α_I , and α_T commonly are called accommodation coefficients. They are the probabilities that a molecule striking the surface will undergo specular, isotropic, or thermal reflection. Such composite kernels satisfy all the conditions in (6.3b) and the detailed-balance symmetry (6.5).

Remark. In 1879 Maxwell [5] proposed such a model with $\alpha_I = 0$, in which case α_T is the so-called the Maxwell accommodation coefficient. This Maxwell model was the only one used to model reflecting boundaries until the late 1960s. Its major shortcoming is that it has only the one free parameter α_T , which is not enough to capture all important boundary phenomena.

Remark. Better models of reflecting boundaries were developed so that simulations could better match experimental observations. The Cercignani-Lampis model [1, 3] is among the best examples of such developments. It has two free parameters, which is the number needed to capture most important boundary phenomena.

6.2. **Stationary, Absorbing-Emitting Boundaries.** Perfectly emitting-absorbing boundaries are ones at which every molecule striking it is absorbed, while molecules are emitted from it in a prescribed way that only depends on properties like the velocity, orientation, and temperature of the boundary.

Let $\partial\Omega|_A$ denote that part of $\partial\Omega$ which is a perfectly absorbing-emitting boundary. We will begin by considering the case where $\partial\Omega|_A$ is stationary. We will assume that at each point $x \in \partial\Omega|_A$ there is a unique tangent plane with outward unit normal $n(x) \in \mathbb{S}^{D-1}$. For every $t > 0$ we must specify boundary values for $F(v, x, t)$ on the set

$$(6.14) \quad \Gamma_A^- = \left\{ (v, x) \in \mathbb{R}^D \times \partial\Omega|_S : n(x) \cdot v < 0 \right\}.$$

The boundary condition will have the form

$$(6.15) \quad F(v, x, t) = F^{\text{bd}}(v, x, t) \quad \text{for every } (v, x) \in \Gamma_A^-.$$

where $F^{\text{bd}}(v, x, t)$ is a specified density of emitted molecules. At a perfectly absorbing boundary we set $F^{\text{bd}}(v, x, t) = 0$. At the boundary of a reservoir of gas molecules in the local thermal equilibrium characterized by a mass density $\rho^{\text{bd}}(x, t)$ and a temperature $\theta^{\text{bd}}(x, t)$ we set

$$(6.16) \quad F^{\text{bd}}(v, x, t) = \mathcal{M}(\rho^{\text{bd}}(x, t), 0, \theta^{\text{bd}}(x, t)) \quad \text{for every } (v, x) \in \Gamma_A^-.$$

6.3. Reflecting Boundaries and Conservation Laws. For every collision invariant $\zeta = \zeta(v)$ we have the local conservation law

$$\partial_t \langle \zeta F \rangle + \nabla_x \cdot \langle v \zeta F \rangle = 0.$$

Upon integrating this over Ω and applying the divergence theorem we obtain

$$(6.17) \quad \frac{d}{dt} \int_{\Omega} \langle \zeta F \rangle dx = - \int_{\partial\Omega} n \cdot \langle v \zeta F \rangle dA(x).$$

This will yield a global conservation law whenever the above integrals make sense and the right-hand side vanishes.

If $\partial\Omega$ is perfectly reflecting and F satisfies a boundary condition of the form (6.3) then the normal component of the flux on the right-hand side of (6.17) is

$$(6.18) \quad \begin{aligned} n \cdot \langle v \zeta F \rangle &= \int_{n \cdot v' > 0} \zeta' n \cdot v' F' dv' - \int_{n \cdot v < 0} \zeta |n \cdot v| F dv \\ &= \int_{n \cdot v' > 0} \left(\zeta' - \int_{n \cdot v < 0} \zeta R(v, v') dv \right) n \cdot v' F' dv'. \end{aligned}$$

If we set $\zeta = 1$ then condition **(2)** in (6.3b) implies that

$$(6.19) \quad n \cdot \langle v F \rangle = 0 \quad \text{for every } x \in \partial\Omega.$$

Therefore mass is globally conserved for every reflecting boundary condition of the form (6.3). The same cannot be said for momentum or energy. Here we show that some models of reflecting boundaries can have additional conservation laws that are consistent with the geometry of Ω .

6.3.1. Specular Reflection Model. For the specular reflection kernel (6.8) we have

$$\zeta(v') - \int_{n \cdot v < 0} \zeta(v) R_S(v, v') dv = \zeta(v') - \zeta(v' - 2nn \cdot v').$$

Upon setting $\zeta = v$ and $\zeta = \frac{1}{2}|v|^2$, we obtain

$$\begin{aligned} v' - \int_{n \cdot v < 0} v R_S(v, v') dv &= 2nn \cdot v', \\ |v'|^2 - \int_{n \cdot v < 0} |v|^2 R_S(v, v') dv &= 0. \end{aligned}$$

By (6.18) we see that

$$\left. \begin{aligned} n \cdot \langle v \otimes v F \rangle &= 2n \int_{n \cdot v' > 0} (n \cdot v')^2 F' dv', \\ n \cdot \langle v \frac{1}{2}|v|^2 F \rangle &= 0, \end{aligned} \right\} \text{for every } x \in \partial\Omega.$$

The specular reflection boundary condition (6.7) thereby globally conserves mass and energy. Moreover, it globally conserves momentum in every direction $\hat{t} \in \mathbb{S}^{D-1}$ such that $\hat{t} \cdot n(x) = 0$ at every $x \in \partial\Omega$. Such \hat{t} will exist only for those domains Ω with a translational symmetry.

6.3.2. *Isotropic Reflection Model.* For the isotropic reflection kernel (6.10) we have

$$\zeta(v') - \int_{n \cdot v < 0} \zeta(v) R_I(v, v') dv = \zeta(v') - \frac{1}{c_1} \int_{n \cdot o < 0} \zeta(|v'|o) |n \cdot o|,$$

where c_1 is given by (6.9b). Upon letting $\zeta = v$ and $\zeta = \frac{1}{2}|v|^2$, we obtain

$$\begin{aligned} v' - \int_{n \cdot v < 0} v R_I(v, v') dv &= v' - \frac{|v'|}{c_1} \int_{n \cdot o < 0} o |n \cdot o| do = v' + \frac{c_2}{c_1} |v'| n, \\ |v'|^2 - \int_{n \cdot v < 0} |v|^2 R_I(v, v') dv &= |v'|^2 - \frac{|v'|^2}{c_1} \int_{n \cdot o < 0} |n \cdot o| do = 0, \end{aligned}$$

where the constant c_2 is given by

$$c_2 = \int_{n \cdot o' > 0} (n \cdot o')^2 do'.$$

By (6.18) we see that

$$\left. \begin{aligned} n \cdot \langle v \otimes v F \rangle &= \int_{n \cdot v' > 0} \left(v' + \frac{c_2}{c_1} |v'| n \right) n \cdot v' F' dv', \\ n \cdot \langle v \frac{1}{2} |v|^2 F \rangle &= 0, \end{aligned} \right\} \text{ for every } x \in \partial\Omega.$$

The isotropic reflection boundary condition (6.9a) thereby globally conserves mass and energy.

6.3.3. *Thermal Reflection Model.* For the thermal reflection kernel (6.12) we have

$$\zeta(v') - \int_{n \cdot v < 0} \zeta(v) R_T(v, v') dv = \zeta(v') - \left(\frac{2\pi}{\theta_W} \right)^{\frac{1}{2}} \int_{n \cdot v < 0} \zeta(v) |n \cdot v| M(v; \theta_W) dv.$$

Upon letting $\zeta = v$ and $\zeta = \frac{1}{2}|v|^2$ we obtain

$$\begin{aligned} v' - \int_{n \cdot v < 0} v R_T(v, v') dv &= v' - \left(\frac{2\pi}{\theta_W} \right)^{\frac{1}{2}} \int_{n \cdot v < 0} v |n \cdot v| M(v; \theta_W) dv \\ &= v' + n \left(\frac{2\pi}{\theta_W} \right)^{\frac{1}{2}} \int_{n \cdot v < 0} (n \cdot v)^2 M(v; \theta_W) dv \\ &= v' + n \left(\frac{\pi\theta_W}{2} \right)^{\frac{1}{2}}, \\ |v'|^2 - \int_{n \cdot v < 0} |v|^2 R_T(v, v') dv &= |v'|^2 - \left(\frac{2\pi}{\theta_W} \right)^{\frac{1}{2}} \int_{n \cdot v < 0} |v|^2 |n \cdot v| M(v; \theta_W) dv \\ &= |v'|^2 - \left(\frac{2\pi}{\theta_W} \right)^{\frac{1}{2}} \int_{n \cdot v < 0} |n \cdot v|^3 M(v; \theta_W) dv - (D-1)\theta_W \\ &= |v'|^2 - (D+1)\theta_W. \end{aligned}$$

By (6.18) we see that

$$\left. \begin{aligned} n \cdot \langle v \otimes v F \rangle &= \int_{n \cdot v' > 0} \left(v' + n \left(\frac{\pi\theta_W}{2} \right)^{\frac{1}{2}} \right) n \cdot v' F' dv', \\ n \cdot \langle v \frac{1}{2} |v|^2 F \rangle &= \int_{n \cdot v' > 0} \left(\frac{1}{2} |v'|^2 - \frac{D+1}{2} \theta_W \right) n \cdot v' F' dv', \end{aligned} \right\} \text{ for every } x \in \partial\Omega.$$

The thermal reflection boundary condition (6.11) thereby globally conserves only mass.

6.4. Reflecting Boundaries and Dissipation Laws. The local entropy dissipation law is

$$\partial_t \langle F \log(F) \rangle + \nabla_x \cdot \langle v F \log(F) \rangle \leq 0.$$

Upon integrating this over Ω and applying the divergence theorem, we obtain

$$(6.20) \quad \frac{d}{dt} \int_{\Omega} \langle F \log(F) \rangle dx \leq - \int_{\partial\Omega} n \cdot \langle v F \log(F) \rangle dA(x).$$

This would yield a global dissipation law for entropy whenever the above integrals make sense and the right-hand side is nonpositive. However, here we will show that generally a quantity different from the entropy obeys a global dissipation law when boundaries are reflecting.

Let $\partial\Omega$ be perfectly reflecting such that F satisfies a boundary condition of the form (6.3) with a wall temperature $\theta_W(x, t)$. By (6.4) and (6.19) we know that on $\partial\Omega$ we have

$$n \cdot \langle v M_W \rangle = 0, \quad n \cdot \langle v F \rangle = 0.$$

Then the normal component of the flux on the right-hand side of (6.20) can be expressed as

$$(6.21) \quad \begin{aligned} n \cdot \langle v F \log(F) \rangle &= n \cdot \left\langle v F \log\left(\frac{F}{\rho M_W}\right) \right\rangle - \frac{n \cdot \langle v \frac{1}{2} |v|^2 F \rangle}{\theta_W} \\ &= n \cdot \left\langle v \left(F \log\left(\frac{F}{\rho M_W}\right) - F + \rho M_W \right) \right\rangle - \frac{n \cdot \langle v \frac{1}{2} |v|^2 F \rangle}{\theta_W} \\ &= n \cdot \left\langle v \eta\left(\frac{F}{\rho M_W}\right) \rho M_W \right\rangle - \frac{n \cdot \langle v \frac{1}{2} |v|^2 F \rangle}{\theta_W}, \end{aligned}$$

where $\rho = \langle F \rangle$ and the function η is defined by

$$\eta(Z) = Z \log(Z) - Z + 1 \quad \text{for every } Z \in \mathbb{R}_+.$$

It is easy to check that η is a strictly convex function over \mathbb{R}_+ with minimum value $\eta(1) = 0$. Then

$$(6.22) \quad \begin{aligned} \left\langle \eta\left(\frac{F}{\rho M_W}\right) n \cdot v \rho M_W \right\rangle &= \int_{n \cdot v' > 0} \eta\left(\frac{F'}{\rho M'_W}\right) n \cdot v' \rho M'_W dv' \\ &\quad - \int_{n \cdot v < 0} \eta\left(\frac{F}{\rho M_W}\right) |n \cdot v| \rho M_W dv. \end{aligned}$$

The Jensen inequality states that for every nontrivial, finite, nonnegative Borel measure $d\nu$ and for every nonnegative $G \in L^1(d\nu)$ we have

$$\eta\left(\frac{1}{|\nu|} \int G d\nu\right) \leq \frac{1}{|\nu|} \int \eta(G) d\nu.$$

Below we apply this with $G = F'/(\rho M'_W)$ and $d\nu(v') = R(v, v') n \cdot v' \rho M'_W dv'$ over $n \cdot v' > 0$, so that by conditions **(1)** and **(3)** of (6.3b) the Borel measure $d\nu(v')$ is nonnegative with

$$|\nu| = \int_{n \cdot v' > 0} R(v, v') n \cdot v' \rho M'_W dv' = |n \cdot v| \rho M_W.$$

Then the boundary condition (6.3a) followed by the Jensen inequality yields

$$\begin{aligned} \eta\left(\frac{F}{\rho M_W}\right) &= \eta\left(\frac{1}{|n \cdot v| \rho M_W} \int_{n \cdot v' > 0} R(v, v') n \cdot v' F' dv'\right) \\ &\leq \frac{1}{|n \cdot v| M_W} \int_{n \cdot v' > 0} R(v, v') n \cdot v' M'_W \eta\left(\frac{F'}{\rho M'_W}\right) dv'. \end{aligned}$$

When we multiply this inequality by $|n \cdot v| M_W$, integrate the result over $n \cdot v < 0$, and then apply condition (2) of (6.3b), we obtain

$$\begin{aligned} \int_{n \cdot v < 0} \eta\left(\frac{F}{\rho M_W}\right) |n \cdot v| M_W \, dv &\leq \int_{n \cdot v < 0} \int_{n \cdot v' > 0} R(v, v') n \cdot v' M'_W \eta\left(\frac{F'}{\rho M'_W}\right) \, dv' \, dv \\ &= \int_{n \cdot v' > 0} n \cdot v' M'_W \eta\left(\frac{F'}{\rho M'_W}\right) \, dv', \end{aligned}$$

whereby it follows from (6.22) that

$$\left\langle \eta\left(\frac{F}{\rho M_W}\right) n \cdot v \rho M_W \right\rangle \geq 0 \quad \text{for every } x \in \partial\Omega.$$

We conclude from (6.21) that

$$(6.23) \quad n \cdot \langle v F \log(F) \rangle \geq -\frac{n \cdot \langle v \frac{1}{2} |v|^2 F \rangle}{\theta_W} \quad \text{for every } x \in \partial\Omega.$$

This inequality was discovered by Darrozès and Guiraud [4] in 1966.

The Darrozès-Guiraud inequality (6.23) leads to global dissipation laws of quantities that depend on the nature of the boundary conditions. We say a reflecting boundary condition of the form (6.3) is *insulating* when there is no energy exchange between the gas and the boundary material — i.e. when

$$n \cdot \langle v \frac{1}{2} |v|^2 F \rangle = 0 \quad \text{for every } x \in \partial\Omega.$$

We saw that the specular reflection (6.7) and isotropic reflection (6.9) models are insulating. Indeed, any reflecting boundary condition which does not change the speed of the molecules is insulating. The Darrozès-Guiraud inequality (6.23) implies that the entropy obeys a global dissipation law for domains Ω with insulating boundaries.

When the domain Ω has a reflecting boundary condition of the form (6.3) that at every $x \in \partial\Omega$ is either insulating or corresponds to a constant wall temperature θ_W then the Darrozès-Guiraud inequality (6.23) implies there is a global dissipation law for the quantity

$$\int_{\Omega} \langle F \log(F) \rangle \, dx + \frac{1}{\theta_W} \int_{\Omega} \langle \frac{1}{2} |v|^2 F \rangle \, dx.$$

This quantity is related to the Helmholtz free energy of thermodynamics, which is minimized at equilibrium when a system is in contact with a heat reservoir at temperature θ_W . It is equivalent to the relative entropy with respect to the wall Maxwellian M_W (which depends only on v)

$$\int_{\Omega} \left\langle F \log\left(\frac{F}{M_W}\right) - F + M_W \right\rangle \, dx.$$

More generally, if M_W is consistent with the restriction of a global Maxwellian $M(v, x, t)$ to $\partial\Omega$ then there can be a global dissipation law for the relative entropy with respect to M .

6.5. Moving Boundaries. There are two kinds of moving boundaries: ones whose motion is prescribed, and ones whose motion depends on the state of the gas — so called free boundaries. An example of a prescribed moving boundary is a piston with a predetermined position in a cylinder or the surface of an airfoil being controlled by a pilot. An example of a free boundary is a piston applying a position-dependant force in a cylinder or a liquid-gas interface. A moving piston often is modeled as a rigid body; an airfoil often is modeled as flexible structure; while a liquid-gas interface typically is deformable.

We will consider the Boltzmann equation over a prescribed spatial domain $\Omega(t)$. Let $\partial\Omega|_R(t)$ denote that part of $\partial\Omega(t)$ which is a perfectly reflecting boundary. We will assume that at each point $x \in \partial\Omega|_R(t)$ there is a unique tangent plane with outward unit normal $n(x, t)$ and a velocity $u_W(x, t)$ at which the boundary is moving. Molecules with velocities v such that $n \cdot (v - u_W) > 0$ are moving towards the boundary, while those velocities v such that $n \cdot (v - u_W) < 0$ are moving away from the boundary into the domain. For every $t > 0$ we must specify boundary values for $F(v, x, t)$ on the set of incoming velocities along $\partial\Omega|_R(t)$ in terms of the boundary values for $F(v, x, t)$ on the set of outgoing velocities along $\partial\Omega|_R(t)$. In other words, for each $t > 0$ we must specify $F(v, x, t)$ on the set

$$(6.24a) \quad \Gamma_R^-(t) = \left\{ (v, x) \in \mathbb{R}^D \times \partial\Omega|_R(t) : n(x, t) \cdot (v - u_W(x, t)) < 0 \right\},$$

in terms of $F(v', x', t')$ for $t' \in [0, t]$ on the set

$$(6.24b) \quad \Gamma_R^+(t) = \left\{ (v', x') \in \mathbb{R}^D \times \partial\Omega|_R(t) : n(x', t) \cdot (v' - u_W(x, t)) > 0 \right\}.$$

The rate at which molecules of mass m with velocity v' are impinging a differential area $dA(x)$ with outward normal $n(x, t)$ moving with velocity $u_W(x, t)$ is given by

$$(6.25a) \quad \frac{1}{m} n \cdot (v' - u_W) F' dv' dA(x).$$

The rate at which molecules of mass m with velocity v are moving away from a differential area $dA(x)$ with outward normal $n(x, t)$ moving with velocity $u_W(x, t)$ is given by

$$(6.25b) \quad \frac{1}{m} |n \cdot (v - u_W)| F dv dA(x).$$

Now we assume that the motion of the boundary is sufficiently slow that its motion can be considered uniform during on a time scale over which most molecules interact with the it. We can then model the

$$(6.26) \quad |n \cdot (v - u_W)| F(v, x, t) = \int_{n \cdot (v' - u_W) > 0} R(v - u_W, v' - u_W) n \cdot (v' - u_W) F(v', x, t) dv'$$

for every $(v, x) \in \Gamma_R^-(t)$.

where the redistribution kernel R is as before.

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