Problems

4.16. Collisional heat flux in dense gases. Obtain the collisional contribution to the heat flux $\vec{q}_C$, performing an analysis similar to that applied to obtain the collisional stress tensor (4.91). Compute the collision integral for $\varphi = mc^2/2$ in the Enskog equation and render it as a divergence, $-\vec{\nabla}\cdot\vec{q}$. Show that it has the structure discussed in Section 2.6.3, where the third contribution (potential transport) is not present for hard spheres.

The heat flux $\vec{J}_e$ is defined by the conservation equation

$$\frac{\partial \rho_e}{\partial t} = -\vec{\nabla}\cdot\vec{J}_e \ , \tag{2.42}$$

where the energy density ρ_e is

$$\rho_e = \rho_\varphi = \frac{3}{2}k_{\mathrm{B}}T[f] = \frac{1}{n(\vec{r},t)}\int \frac{m}{2}(\vec{c}-\vec{v})^2\, f(\vec{r},\vec{c})\, d^3\vec{c} \ . \tag{4.44}$$

The Enskog equation is given by the Enskog collision operator

$$\begin{aligned} \frac{d\,f}{d\,t} &= J_{\text{Enskog}}[f](\vec{c}) \qquad (4.87)\\ :=& D^2\int[\chi(\vec{r}-\vec{n}/2)f(\vec{r},\vec{c}\,')f(\vec{r}-\vec{n},\vec{c}_1') - \chi(\vec{r}+\vec{n}/2)f(\vec{r},\vec{c})f(\vec{r}+\vec{n},\vec{c}_1)](\vec{g}\cdot\hat{n})\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{c}_1 \ , \end{aligned}$$

where $\vec{n} = D\hat{n}$.

The collision integral for $\varphi(\vec{c}) = m\vec{c}^{\,2}/2$ is defined as integrating $\varphi(\vec{c})J_{\text{Enskog}}[f](\vec{c})$ over $d^3\vec{c}$:

$$\begin{aligned} I_\varphi &= \frac{m}{2}\int \vec{c}^{\,2}J_{\text{Enskog}}[f](\vec{c})d^3\vec{c} = \frac{m}{2}\int \vec{c}^{\,2}[J_+ - J_-]d^3\vec{c} \qquad (1)\\ &= \frac{D^2 m}{2}\int \vec{c}^{\,2}[\chi(\vec{r}-\vec{n}/2)f(\vec{r},\vec{c}\,')f(\vec{r}-\vec{n},\vec{c}_1') - \chi(\vec{r}+\vec{n}/2)f(\vec{r},\vec{c})f(\vec{r}+\vec{n},\vec{c}_1)](\vec{g}\cdot\hat{n})\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{c}_1\, d^3\vec{c} \ , \end{aligned}$$

which we can split into the direct collision, coming from J_-,

$$I_{\varphi-} = \frac{m}{2}\int \vec{c}^{\,2}J_- d^3\vec{c} = \frac{D^2 m}{2}\int \vec{c}^{\,2}\chi(\vec{r}+\vec{n}/2)f(\vec{r},\vec{c})f(\vec{r}+\vec{n},\vec{c}_1)(\vec{g}\cdot\hat{n})\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{c}_1\, d^3\vec{c} \ , \tag{2}$$

and the inverse collision, coming from J_+

$$I_{\varphi+} = \frac{m}{2}\int \vec{c}^{\,2}J_+ d^3\vec{c} = \frac{D^2 m}{2}\int \vec{c}^{\,2}\chi(\vec{r}-\vec{n}/2)f(\vec{r},\vec{c}\,')f(\vec{r}-\vec{n},\vec{c}_1')(\vec{g}\cdot\hat{n})\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{c}_1\, d^3\vec{c} \ . \tag{3}$$

- As a first step we exchange the names of the physical momenta in the inverse collision:

  $$(\vec{c},\vec{c}_1) \leftrightarrow (\vec{c}\,',\vec{c}_1') \qquad \Rightarrow \quad (\vec{g},\hat{n}) \leftrightarrow (\vec{g}\,',-\hat{n}) \ , \tag{4}$$

  which induces the reversal of $\hat{n}$:

  $$I_{\varphi+} = \frac{D^2 m}{2}\int \vec{c}\,'^2\chi(\vec{r}+\vec{n}/2)f(\vec{r},\vec{c})f(\vec{r}+\vec{n},\vec{c}_1)(-\vec{g}\,'\cdot\hat{n})\Theta(-\vec{g}\,'\cdot\hat{n})\, d^2(-\hat{n})\, d^3\vec{c}_1'\, d^3\vec{c}\,' \ . \tag{5}$$

- using the collision rule for hard spheres (exercise 4.5) we have

  $$\vec{g}' = \vec{g} - 2(\vec{g}\cdot\hat{n})\hat{n} \ , \tag{6}$$

  giving

  $$(-\vec{g}\,'\cdot\hat{n}) = -[(\vec{g}\cdot\hat{n}) - 2(\vec{g}\cdot\hat{n})(\hat{n}\cdot\hat{n})] = -(\vec{g}\cdot\hat{n}) + 2(\vec{g}\cdot\hat{n})\cdot 1 = (\vec{g}\cdot\hat{n}) \ , \tag{7}$$

  leading to

  $$I_{\varphi+} = \frac{D^2 m}{2}\int \vec{c}\,'^2\chi(\vec{r}+\vec{n}/2)f(\vec{r},\vec{c})f(\vec{r}+\vec{n},\vec{c}_1)(\vec{g}\cdot\hat{n})\Theta(\vec{g}\cdot\hat{n})\,(-1)^2 d^2\hat{n}\, d^3\vec{c}_1'\, d^3\vec{c}\,' \ . \tag{8}$$

- remembering that the phase-space for $d^3\vec{c}_1'\, d^3\vec{c}'$ is the same as for $d^3\vec{c}_1\, d^3\vec{c}$, we can change the integral to the original integration variables:

$$I_{\varphi+} = \frac{D^2 m}{2}\int \vec{c}'^2 \chi(\vec{r}+\vec{n}/2) f(\vec{r},\vec{c}) f(\vec{r}+\vec{n},\vec{c}_1)(\vec{g}\cdot\hat{n})\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{c}_1\, d^3\vec{c}\ , \tag{9}$$

which allows us to write the collision integral $I_\varphi = I_{\varphi+} - I_{\varphi-}$ as

$$I_{\varphi} = \frac{D^2 m}{2}\int (\vec{c}'^2 - \vec{c}^2) \chi(\vec{r}+\vec{n}/2) f(\vec{r},\vec{c}) f(\vec{r}+\vec{n},\vec{c}_1)(\vec{g}\cdot\hat{n})\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{c}_1\, d^3\vec{c}\ . \tag{10}$$

- using again the collision rule we can evaluate

$$\begin{aligned}\vec{c}'^2 - \vec{c}^2 &= (\vec{c} - [\vec{g}\cdot\hat{n}]\hat{n})^2 - \vec{c}^2 = \vec{c}^2 - 2(\vec{g}\cdot\hat{n})(\vec{c}\cdot\hat{n}) + (\vec{g}\cdot\hat{n})^2\hat{n}^2 - \vec{c}^2 = (\vec{g}\cdot\hat{n})(\vec{g} - 2\vec{c}\cdot\hat{n}) \quad (11)\\ &= (\vec{g}\cdot\hat{n})([-\vec{c}_1 - \vec{c}]\cdot\hat{n}) = -(\vec{g}\cdot\hat{n})([2\vec{C} - \frac{m_0 - m_1}{M}\vec{g}]\cdot\hat{n}) \doteq -2(\vec{g}\cdot\hat{n})(\vec{C}\cdot\hat{n})\ .\end{aligned}$$

- interchanging the integration variables $\vec{c} \leftrightarrow \vec{c}_1$ results in the change $\vec{g} \to -\vec{g}$ by the definition of $\vec{g}$ and also $\hat{n} \to -\hat{n}$ due to the orientation of $\hat{n}$ from $\vec{c}$ to $\vec{c}_1$, but not $\vec{C}$. Then we get

$$I_{\varphi}' = \frac{D^2 m}{2}\int 2(\vec{g}\cdot\hat{n})(\vec{C}\cdot\hat{n}) \chi(\vec{r}-\vec{n}/2) f(\vec{r},\vec{c}_1) f(\vec{r}-\vec{n},\vec{c})(\vec{g}\cdot\hat{n})\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{c}_1\, d^3\vec{c}\ , \tag{12}$$

which is the same as I_φ, eq. (10).

- Averaging over I_φ and I_φ' we get

$$\begin{aligned}I_\varphi^{\text{ave}} &= \tfrac{1}{2}(I_\varphi + I_\varphi')\\ &= \frac{D^2 m}{2}\int -(\vec{g}\cdot\hat{n})(\vec{C}\cdot\hat{n}) \chi(\vec{r}+\vec{n}/2) f(\vec{r},\vec{c}) f(\vec{r}+\vec{n},\vec{c}_1)(\vec{g}\cdot\hat{n})\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{c}_1\, d^3\vec{c}\\ &+ \frac{D^2 m}{2}\int (\vec{g}\cdot\hat{n})(\vec{C}\cdot\hat{n}) \chi(\vec{r}-\vec{n}/2) f(\vec{r}-\vec{n},\vec{c}) f(\vec{r},\vec{c}_1)(\vec{g}\cdot\hat{n})\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{c}_1\, d^3\vec{c}\\ &= \frac{D^2 m}{2}\int [\chi(\vec{r}-\vec{n}/2) f(\vec{r}-\vec{n},\vec{c}) f(\vec{r},\vec{c}_1) - \chi(\vec{r}+\vec{n}/2) f(\vec{r},\vec{c}) f(\vec{r}+\vec{n},\vec{c}_1)]\\ &\qquad (\vec{C}\cdot\hat{n})(\vec{g}\cdot\hat{n})^2\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{c}_1\, d^3\vec{c}\ .\end{aligned} \tag{13}$$

- following the book

$$\begin{aligned}&[\chi(\vec{r}-\vec{n}/2) f(\vec{r}-\vec{n},\vec{c}) f(\vec{r},\vec{c}_1) - \chi(\vec{r}+\vec{n}/2) f(\vec{r},\vec{c}) f(\vec{r}+\vec{n},\vec{c}_1)]\\ &= -\vec{\nabla}\cdot\hat{n}\int_0^1 \chi(\vec{r}-s\vec{n}/2) f(\vec{r}-s\vec{n},\vec{c}) f(\vec{r}+(1-s)\vec{n},\vec{c}_1) ds\ ,\end{aligned} \tag{4.90}$$

we can write (2.42) with

$$\vec{J}_e := \frac{D^2 m}{2}\int \hat{n}\int_0^1 \chi(\vec{r}-s\vec{n}/2) f(\vec{r}-s\vec{n},\vec{c}) f(\vec{r}+(1-s)\vec{n},\vec{c}_1) ds (\vec{C}\cdot\hat{n})(\vec{g}\cdot\hat{n})^2\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{c}_1\, d^3\vec{c}\ . \tag{14}$$

Taylor expanding the function around $\vec{r}$ with the abbreviations $\chi = \chi(\vec{r})$, $f = f(\vec{r}, \vec{c})$, and $f_1 = f(\vec{r}, \vec{c}_1)$ we get with changing to Jacobi coordinates

$$\begin{aligned}
I_\varphi^{\text{ave}} &= \frac{D^2 m}{2} \int \Big[[\chi - \tfrac{1}{2}\vec{n}\cdot(\vec{\nabla}\chi)][f - \vec{n}\cdot(\vec{\nabla}f)]f_1 - [\chi + \tfrac{1}{2}\vec{n}\cdot(\vec{\nabla}\chi)]f[f_1 + \vec{n}\cdot(\vec{\nabla}f_1)]\Big] \\
&\qquad (\vec{C}\cdot\hat{n})(\vec{g}\cdot\hat{n})^2\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{C}\, d^3\vec{g} \\
&= \frac{D^2 m}{2} \int \Big[\chi f f_1 - \tfrac{1}{2}\vec{n}\cdot(\vec{\nabla}\chi) f f_1 - \chi\vec{n}\cdot(\vec{\nabla}f) f_1 + \tfrac{1}{2}[\vec{n}\cdot(\vec{\nabla}\chi)][\vec{n}\cdot(\vec{\nabla}f)]f_1 \\
&\qquad - \chi f f_1 - \tfrac{1}{2}\vec{n}\cdot(\vec{\nabla}\chi) f f_1 - \chi f \vec{n}\cdot(\vec{\nabla}f_1) - \tfrac{1}{2}[\vec{n}\cdot(\vec{\nabla}\chi)]f[\vec{n}\cdot(\vec{\nabla}f_1)]\Big] \\
&\qquad (\vec{C}\cdot\hat{n})(\vec{g}\cdot\hat{n})^2\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{C}\, d^3\vec{g} \\
&= -\frac{D^2 m}{2} \int \vec{n}\cdot\Big[(\vec{\nabla}\chi) f f_1 + \chi(\vec{\nabla}f) f_1 + \chi f(\vec{\nabla}f_1)\Big]\,(\vec{C}\cdot\hat{n})(\vec{g}\cdot\hat{n})^2\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{C}\, d^3\vec{g} \\
&+ \frac{D^2 m}{4}[\vec{n}\cdot(\vec{\nabla}\chi)]\,\vec{n}\cdot\int\Big[-(\vec{\nabla}f)f_1 + f(\vec{\nabla}f_1)\Big]\,(\vec{C}\cdot\hat{n})(\vec{g}\cdot\hat{n})^2\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{C}\, d^3\vec{g} \\
&= -\frac{D^3 m}{2}\vec{\nabla}\cdot\int \hat{n}\,\chi f f_1 (\vec{C}\cdot\hat{n})(\vec{g}\cdot\hat{n})^2\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{C}\, d^3\vec{g} \\
&+ \frac{D^4 m}{4}\int [\hat{n}\cdot(\vec{\nabla}\chi)]\,\hat{n}\cdot\Big[-[\vec{\nabla}f(\vec{C}+\tfrac{1}{2}\vec{g})]f(\vec{C}-\tfrac{1}{2}\vec{g}) + f(\vec{C}+\tfrac{1}{2}\vec{g})[\vec{\nabla}f(\vec{C}-\tfrac{1}{2}\vec{g})]\Big] \\
&\qquad (\vec{C}\cdot\hat{n})(\vec{g}\cdot\hat{n})^2\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{C}\, d^3\vec{g} \\
&= -\vec{\nabla}\cdot\vec{J}_e + \mathbf{rest}\ .
\end{aligned} \tag{15}$$

Taylor expanding also in the velocities around $f(\vec{C}) = f$ we get **to first order in** $\frac{\partial f}{\partial \vec{c}}$

$$\begin{aligned}
\mathbf{rest} &= \frac{D^4 m}{4}\int (\nabla_{\hat{n}}\chi)\,\Big[-[\nabla_{\hat{n}}(f(\vec{C}) + \tfrac{1}{2}\vec{g}\cdot\frac{\partial}{\partial\vec{c}}f(\vec{C}))](f(\vec{C}) - \tfrac{1}{2}\vec{g}\cdot\frac{\partial}{\partial\vec{c}}f(\vec{C})) \\
&\qquad + (f(\vec{C}) + \tfrac{1}{2}\vec{g}\cdot\frac{\partial}{\partial\vec{c}}f(\vec{C}))[\nabla_{\hat{n}}(f(\vec{C}) - \tfrac{1}{2}\vec{g}\cdot\frac{\partial}{\partial\vec{c}}f(\vec{C}))]\Big] \\
&\qquad (\vec{C}\cdot\hat{n})(\vec{g}\cdot\hat{n})^2\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{C}\, d^3\vec{g} \\
&= \frac{D^4 m}{4}\int (\nabla_{\hat{n}}\chi)\,\Big[-(\nabla_{\hat{n}}f)f - \frac{1}{2}(\vec{g}\cdot\frac{\partial\nabla_{\hat{n}}f}{\partial\vec{c}})f + \frac{1}{2}(\nabla_{\hat{n}}f)(\vec{g}\cdot\frac{\partial f}{\partial\vec{c}}) + \frac{1}{4}(\vec{g}\cdot\frac{\partial\nabla_{\hat{n}}f}{\partial\vec{c}})(\vec{g}\cdot\frac{\partial f}{\partial\vec{c}}) \\
&\qquad + f(\nabla_{\hat{n}}f) + \frac{1}{2}(\vec{g}\cdot\frac{\partial f}{\partial\vec{c}})(\nabla_{\hat{n}}f) - \frac{1}{2}f(\vec{g}\cdot\frac{\partial\nabla_{\hat{n}}f}{\partial\vec{c}}) - \frac{1}{4}(\vec{g}\cdot\frac{\partial f}{\partial\vec{c}})(\vec{g}\cdot\frac{\partial\nabla_{\hat{n}}f}{\partial\vec{c}})\Big] \\
&\qquad (\vec{C}\cdot\hat{n})(\vec{g}\cdot\hat{n})^2\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{C}\, d^3\vec{g} \\
&= \frac{D^4 m}{4}\int (\nabla_{\hat{n}}\chi)\,\vec{g}\cdot\left[\frac{\partial f}{\partial\vec{c}}(\nabla_{\hat{n}}f) - f\frac{\partial\nabla_{\hat{n}}f}{\partial\vec{c}}\right](\vec{C}\cdot\hat{n})(\vec{g}\cdot\hat{n})^2\Theta(\vec{g}\cdot\hat{n})\, d^2\hat{n}\, d^3\vec{C}\, d^3\vec{g}\ .
\end{aligned} \tag{16}$$

This integral integrates over an odd power of $\vec{g}$ and hence vanishes.