Solving homogeneous Boltzmann equation in spherical coordinates

Let us denote the velocity vector as $\mathbf{v}$ and its magnitude as v. In the spatially homogeneous case of collisions between electrons and immobile (infinitely heavy) neutrals the Boltzmann equation takes the form

$$\partial_t f(\mathbf{v},t) = \int\limits_{S^2} B(v,\omega)\left(f(\mathbf{v}',t) - f(\mathbf{v},t)\right)\, d\omega$$

Projecting the equation onto a test function $\phi(\mathbf{v})$ gives the following variational formulation

$$\partial_t \int\limits_{\mathbb{R}^3} f(\mathbf{v},t)\phi(\mathbf{v})\, d\mathbf{v} = \int\limits_{\mathbb{R}^3}\int\limits_{S^2} B(v,\omega)\left(f(\mathbf{v}',t) - f(\mathbf{v},t)\right)\phi(\mathbf{v})\, d\omega\, d\mathbf{v}$$

Assume $f(\mathbf{v})$ deviates from the Maxwell-Boltzmann velocity distribution[1] only slightly

$$f(\mathbf{v}) = M(v)\left(1 + h(\mathbf{v},t)\right)$$

where $M(v)$ denotes

$$M(v) = \frac{n}{\left(v_{\text{th}}\sqrt{\pi}\right)^3} e^{-\left(\frac{v}{v_{\text{th}}}\right)^2}$$

This leads to

$$\begin{aligned}\int\limits_{\mathbb{R}^3} M(v)\partial_t h(\mathbf{v},t)\phi(\mathbf{v})\, d\mathbf{v} &= \int\limits_{\mathbb{R}^3}\int\limits_{S^2} B(v,\omega)\left(M(v') - M(v)\right)\phi(\mathbf{v})\, d\omega\, d\mathbf{v} \\ &+ \int\limits_{\mathbb{R}^3}\int\limits_{S^2} B(v,\omega)\left(M(v')h(\mathbf{v}',t) - M(v)h(\mathbf{v},t)\right)\phi(\mathbf{v})\, d\omega\, d\mathbf{v}\end{aligned}$$

One option is to approximate $h(\mathbf{v},t)$ in Cartesian coordinates using Hermite polynomials

$$h(\mathbf{v},t) \approx \sum_{i,j,k} h_{i,j,k}(t) P_i\left(\frac{v_x}{v_{\text{th}}}\right) P_j\left(\frac{v_y}{v_{\text{th}}}\right) P_k\left(\frac{v_z}{v_{\text{th}}}\right)$$

which satisfy the property

$$\int\limits_{-\infty}^{+\infty} e^{-x^2} P_i(x) P_{i'}(x)\, dx \sim \delta_{ii'}$$

[1] Not sure what's the right thing to call it, but this is essentially a three-dimensional Gaussian distribution and should not be confused with the Maxwell-Boltzmann distribution which describes distribution for speed and $\sim v^2 e^{-\frac{v}{v_{\text{th}}}}$

Here another option is summarized: approximate $h(\mathbf{v},t)$ in spherical coordinates using a combination of real-valued spherical harmonics with either the so-called "Maxwell" polynomials or the more traditional associated Laguerre polynomials

$$h(\mathbf{v},t) \approx \sum_{k,l,m} h_{k,l,m}(t) P_k\left(\frac{v}{v_{\text{th}}}\right) Y_{lm}(v_\theta, v_\phi)$$
$$h(\mathbf{v},t) \approx \sum_{k,l,m} h_{k,l,m}(t) L_k\left(\frac{v^2}{v_{\text{th}}^2}\right) Y_{lm}(v_\theta, v_\phi)$$

Let us define the "Maxwell" polynomials as

$$\int\limits_0^{+\infty} \frac{4}{\sqrt{\pi}} x^2 e^{-x^2} P_k(x) P_{k'}(x)\, dx = \delta_{kk'}$$

and the associated Laguerre polynomials as

$$\int\limits_0^{+\infty} \frac{4}{\sqrt{\pi}} x^2 e^{-x^2} L_k\left(x^2\right) L_{k'}\left(x^2\right) dx = \delta_{kk'}$$

or, equivalently,

$$\int\limits_0^{+\infty} \frac{2}{\sqrt{\pi}} \sqrt{y} e^{-y} L_k(y) L_{k'}(y)\, dy = \delta_{kk'}$$

Such polynomials can be generated (up to the normalization constant) by the following recursive relation

$$\begin{aligned} P_{-1}(x) &= 0, \\ P_0(x) &= 1, \\ P_{n+1}(x) &= (x - a_n) P_n(x) - b_n P_{n-1}(x), \end{aligned}$$

where

$$a_n = \frac{\langle x P_n, P_n \rangle}{\langle P_n, P_n \rangle}, \quad b_n = \frac{\langle P_n, P_n \rangle}{\langle P_{n-1}, P_{n-1} \rangle}, \quad \langle f, g \rangle = \int\limits_0^{\infty} f(x) g(x) \frac{4}{\sqrt{\pi}} x^2 e^{-x^2}\, dx$$

(If only first several polynomials are needed we could probably just generated them analytically in Mathematica. I wrote a short script for that if needed.)

A few first of such polynomials are given by

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= \sqrt{\frac{2\pi}{3\pi - 8}} x - 2\sqrt{\frac{2}{3\pi - 8}}, \\ P_2(x) &= \frac{6\pi\sqrt{2}x^2 - 16\sqrt{2}x^2 - 4\sqrt{2\pi}x + 32\sqrt{2} - 9\sqrt{2}\pi}{2\sqrt{224 - 156\pi + 27\pi^2}}, \\ P_3(x) &= \frac{18\pi^{3/2}x^3 - 56\sqrt{\pi}x^3 - 42\pi x^2 + 128x^2 - 45\pi^{3/2}x + 144\sqrt{\pi}x + 81\pi - 256}{\sqrt{-28672 + 30216\pi - 10530\pi^2 + 1215\pi^3}}, \end{aligned}$$

Note that with the chosen normalization constant

$$\int_0^{+\infty} M(v) P_i\left(\frac{v}{v_{\text{th}}}\right) P_{i'}\left(\frac{v}{v_{\text{th}}}\right) v^2\, dv = \frac{n}{4\pi}\delta_{ii'}$$

The real-valued spherical Y_{lm} harmonics can be defined through the complex-valued spherical harmonics

$$Y_l^m(\theta,\phi) = \sqrt{(2l+1)\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\phi}$$

where P_l^m are associated Legendre polynomials, as

$$Y_{lm}(\theta,\phi) = \begin{cases} \sqrt{2}(-1)^m \Im\left[Y_l^m\right], & m<0 \\ Y_l^0, & m=0 \\ \sqrt{2}(-1)^m \Re\left[Y_l^m\right], & m>0 \end{cases}$$

They satisfy

$$\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} Y_{lm} Y_{l'm'}\, d\omega = 4\pi\delta_{ll'}\delta_{mm'}$$

Using the same expansion for test functions

$$\phi(\mathbf{v}) = P_p\left(\frac{v}{v_{\text{th}}}\right) Y_{sq}(v_\theta, v_\phi)$$

one gets

$$\partial_t h_{k,l,m}(t) = M_{k,l,m} + \sum_{p,q,s} L_{k,l,m}^{p,q,s} h_{p,q,s}(t)$$

where

$$M_{k,l,m} = \frac{1}{n}\int_0^{+\infty} M(v) v^2 P_k\left(\frac{v}{v_{\text{th}}}\right) \int_{S^2}\int_{S^2} \left(\frac{M(v')}{M(v)} - 1\right) B(v,\omega) Y_{ml}(v_\theta, v_\phi)\, d\omega\, dv_\omega\, dv$$

$$\begin{aligned} L_{k,l,m}^{p,q,s} = {} & \frac{1}{n}\int_0^{+\infty} M(v) v^2 P_p\left(\frac{v}{v_{\text{th}}}\right) \int_{S^2}\int_{S^2} B(v,\omega) Y_{qs}(v_\theta, v_\phi) \times \\ & \times \left(\frac{M(v')}{M(v)} P_k\left(\frac{v'}{v_{\text{th}}}\right) Y_{lm}\left(v'_\theta, v'_\phi\right) - P_k\left(\frac{v}{v_{\text{th}}}\right) Y_{lm}(v_\theta, v_\phi)\right) d\omega\, dv_\omega\, dv \end{aligned}$$

Note that for elastic collisions $v = v'$

$$\begin{aligned} M_{k,l,m} &= 0 \\ L_{k,l,m}^{p,q,s} &= \frac{1}{n}\int_0^{+\infty} M(v) v^2 P_p\left(\frac{v}{v_{\text{th}}}\right) P_k\left(\frac{v}{v_{\text{th}}}\right) \int_{S^2}\int_{S^2} B(v,\omega) Y_{qs}(v_\theta, v_\phi) \times \\ &\quad \times \left(Y_{lm}\left(v'_\theta, v'_\phi\right) - Y_{lm}(v_\theta, v_\phi)\right) d\omega\, dv_\omega\, dv \end{aligned}$$

As an option, for calculating integrals of the form

$$\int\limits_0^{+\infty} \frac{4}{\sqrt{\pi}} x^2 e^{-x^2} f(x)\,dx$$

we can use the Gauss or Gauss-Radau quadratures associated with the "Maxwell" polynomials, that is

$$\int\limits_0^{+\infty} \frac{4}{\sqrt{\pi}} x^2 e^{-x^2} f(x)\,dx \approx \sum_{i=0}^{N} w_i f(x_i).$$

The calculation of nodes and weights is done based on the coefficients a_n and b_n from the recurrence relation. Specifically, the Gauss nodes $\{x_i\}_{i=0}^N$ are the eigenvalues of matrix

$$J = \begin{pmatrix} a_0 & \sqrt{b_1} & & & \\ \sqrt{b_1} & a_0 & \sqrt{b_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{b_{N-2}} & a_{N-1} & \sqrt{b_{N-1}} \\ & & & \sqrt{b_{N-1}} & a_N \end{pmatrix}$$

and the weights $\{w_i\}_{i=0}^N$ are given by

$$w_i = \frac{1}{\mathbf{p_i}^T \mathbf{p_i}}, \quad \text{where} \quad \mathbf{p}_i = \begin{pmatrix} P_0(x_i) \\ \vdots \\ P_N(x_i) \end{pmatrix}, \quad i = 0, \ldots, N.$$

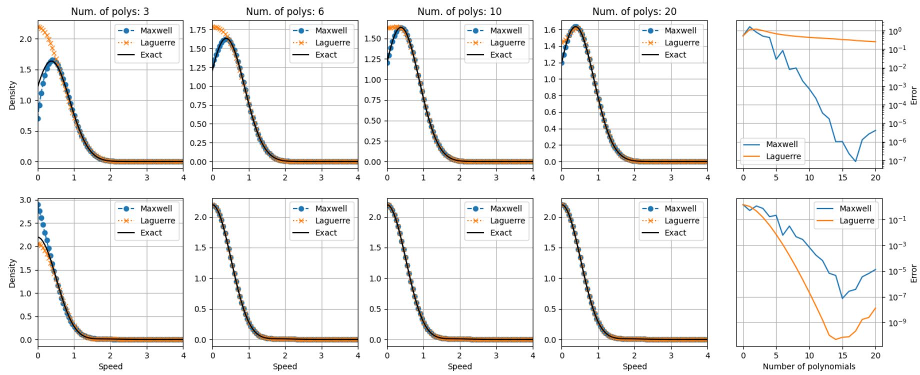

Figure 1: Compare $f(v)$. Top: $f(v) = (1.2 + \sin(v))e^{-v^2}$, bottom: $f(v) = (1.2 + \cos(v))e^{-v^2}$

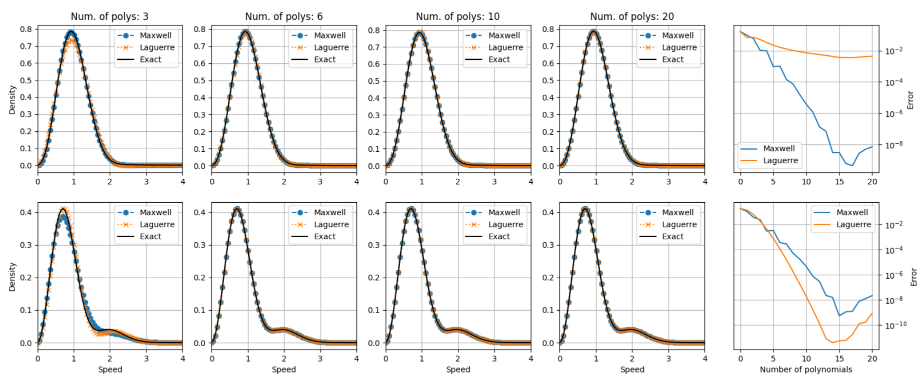

Figure 2: Compare $f(v)v^2$. Top: $f(v) = (1.2 + \sin(v))e^{-v^2}$, bottom: $f(v) = (1.2 + \cos(v))e^{-v^2}$

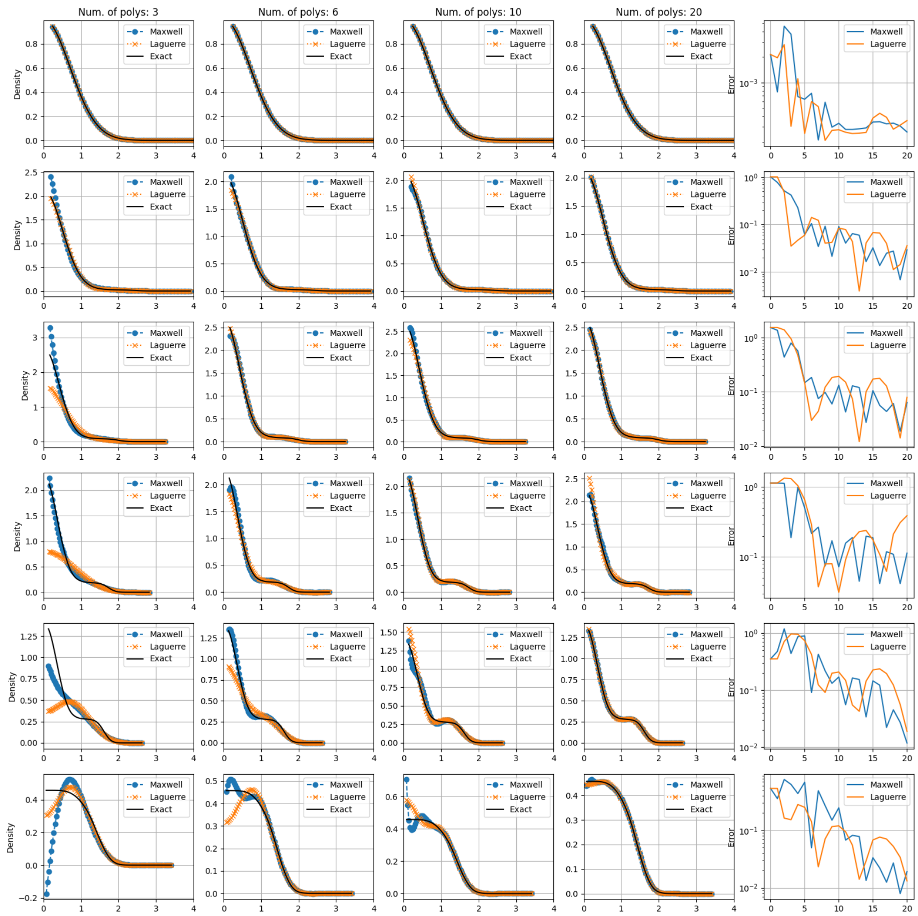

Figure 3: Compare $f(v)$.

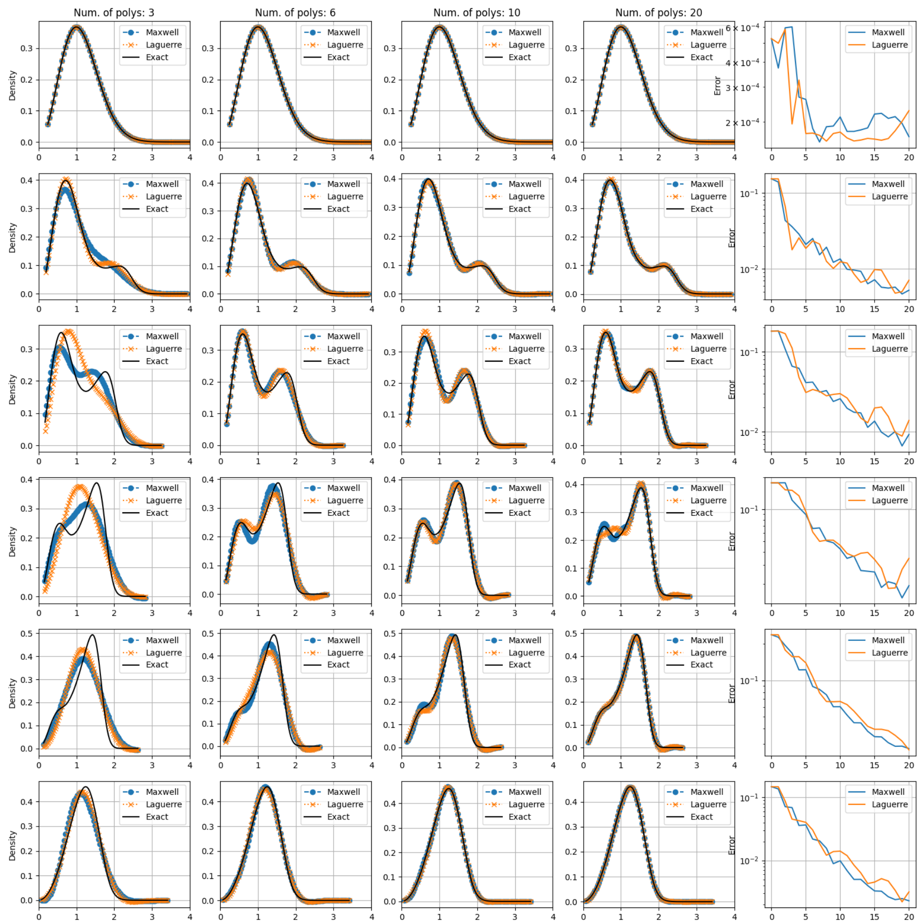

Figure 4: Compare $f(v)v^2$.