Shock wave structure for Generalized Burnett Equations

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To the memory of Carlo Cercignani

Abstract

Stationary shock wave solutions for Generalized Burnett Equations (GBE) [A. V. Bobylev, J. Stat. Phys. **132**, 569 (2008)] are studied. Based on results of [M. Bisi, M. P. Cassinari, M. Groppi, Kinet. Relat. Models **1**, 295 (2008)], we choose a unique (optimal) form of GBE, and solve numerically the shock wave problem for various Mach numbers. The results are compared with numerical solutions of Navier–Stokes equations and with the Mott–Smith approximation for the Boltzmann equation (all calculations are done for Maxwell molecules), since it is believed that the Mott–Smith approximation yields better results for strong shocks. The comparison shows that GBE yield certain improvement of the Navier–Stokes results for moderate Mach numbers.

1 Introduction

We continue in this paper to study equations of hydrodynamics (derived from the Boltzmann equation) at the Burnett level. The well–known instability [1] of classical Burnett equations became a starting point for several different methods to regularize these equations (see [2, 3, 4] and the references therein for a review). We use in this paper the approach of one of the authors [2] based on the idea of "small" changes of variables. In other words, we consider the equations not for true hydrodynamic variables (density ρ^{tr}, bulk velocity $\mathbf{u}^{tr}$, and temperature T^{tr}), but for slightly modified quantities

$$\rho = \rho^{tr} + O(\varepsilon^2)\,, \qquad \mathbf{u} = \mathbf{u}^{tr} + O(\varepsilon^2)\,, \qquad T = T^{tr} + O(\varepsilon^2)\,, \tag{1}$$

for which the standard notations $(\rho, \mathbf{u}, T)$ are used. A small parameter ε denotes the Knudsen number, i.e. a mean free path divided by a typical macroscopic length.

It was shown in [5] how this approach leads to the so–called generalized Burnett equations (GBE). These equations are not defined uniquely, they depend on two free parameters $\theta_{1,2} \geq 0$. A possible choice of the parameters was discussed in [5, 6] on the basis of solutions to some linear problems. The authors of these papers presented several arguments in favour of the choice $\theta_1 = 1$, $\theta_2 = 0$. Therefore we consider the corresponding version of GBE (GBE (1,0,0) in the notation of [5]) in the present paper. Our aim is to study the shock–wave profile for different Mach numbers in order to see if GBE lead to certain improvement of the Navier–Stokes approximation. We shall consider below the case of Maxwell molecules, since this is the only model for which the classical Burnett equations are known in fully explicit form.

We would like to mention that Carlo Cercignani was always interested in the problem of the shock wave structure (in particular, the case of infinite Mach number). The papers [7, 8, 9, 10] can be considered as a part of his contribution to this problem. We regret that it is too late now to discuss our results with him.

The paper is organized as follows. The unique form of GBE, used in the paper, is discussed in detail in Section 2. The statement of the problem for shock–wave solutions and transition to dimensionless variables is given in Section 3. The Mott–Smith approximation for the Boltzmann equation is explained in Section 4. We use this approximation for comparison with our numerical results in Section 5 because of numerical evidence [11] that it works relatively good for strong shocks. Another reference model is for us the classical Navier–Stokes equations. The shock profiles for all three models are compared for different Mach numbers in Section 5.

2 Generalized Burnett Equations

First we define a unique version of GBE which corresponds to values of parameters ($\theta_1 = 1$, $\theta_2 = 0$), in [5]. Equalities (1) for this version read

$$\rho = \rho^{tr}, \qquad \mathbf{u} = \mathbf{u}^{tr}, \qquad T = T^{tr} + \frac{\varepsilon^2}{\rho} \operatorname{div} \left(\frac{\mathbf{R}}{\rho} \right), \tag{2}$$

where

$$\mathbf{R} = a(T)\, \nabla(\log \rho) + b(T)\, \nabla(\log T)\,, \tag{3}$$

with coefficients $a(T)$ and $b(T)$ having for Maxwell molecules the following form

$$a(T) = \frac{13}{18}\, \eta^2 T^2\,, \qquad b(T) = \frac{2}{3}\, \eta^2 T^2\,, \qquad \eta = \text{const.} \tag{4}$$

The constant parameter η is given by equality

$$\eta^{-1} = \frac{3}{2}\, \pi \int_{-1}^{1} g(\mu)\, (1-\mu^2)\, d\mu\,, \qquad g(\cos\theta) = |\mathbf{V}|\ \sigma(|\mathbf{V}|, \theta)\,, \tag{5}$$

where $\sigma(|\mathbf{V}|, \theta)$ is the differential scattering cross–section for Maxwell molecules, $|\mathbf{V}|$ is the absolute value of relative velocity of colliding particles, $\theta \in [0, \pi]$ is the scattering angle.

Generalized Burnett Equations for variables $(\rho, \mathbf{u}, T)$ read [5]

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho\, \mathbf{u}) = 0\,, \\
&\rho\, \hat{\mathcal{D}} u_\alpha + \frac{\partial p}{\partial x_\alpha} + \frac{\partial \Pi_{\alpha\beta}}{\partial x_\beta} = 0\,, \\
&\frac{3}{2}\, \rho\, \hat{\mathcal{D}} T + p\, \operatorname{div}(\mathbf{u}) + \Pi_{\alpha\beta} \frac{\partial u_\alpha}{\partial x_\beta} + \operatorname{div}(\mathbf{Q}) = 0, \qquad \alpha, \beta = 1, 2, 3,
\end{aligned} \tag{6}$$

where the Einstein convention on repeated indices is used and

$$\begin{aligned}
&\hat{\mathcal{D}} = \partial_t + \mathbf{u} \cdot \partial_{\mathbf{x}}\,, \qquad\qquad p = \rho\, T\,, \\
&\Pi_{\alpha\beta} = \varepsilon\, \pi^{NS}_{\alpha\beta} + \varepsilon^2 \left(\pi^B_{\alpha\beta} - \delta_{\alpha\beta} \operatorname{div} \left(\frac{\mathbf{R}}{\rho} \right) \right), \\
&Q_\alpha = \varepsilon\, q^{NS}_\alpha + \varepsilon^2 q^B_\alpha + \frac{\varepsilon^2}{\rho} \left\{ 3\, R_\beta \overline{\frac{\partial u_\alpha}{\partial x_\beta}} + \left(\frac{3}{2}\, a + b \right) \frac{\partial}{\partial x_\alpha} (\operatorname{div}(\mathbf{u})) \right\},
\end{aligned} \tag{7}$$

in the case of Maxwell molecules. Here

$$\overline{\Psi_{\alpha\beta}} = \frac{1}{2} \left(\Psi_{\alpha\beta} + \Psi_{\beta\alpha} - \frac{2}{3}\, \delta_{\alpha\beta}\, \Psi_{\gamma\gamma} \right),$$

and the upper indices NS and B denote Navier–Stokes and Burnett terms respectively. In particular, the Navier–Stokes terms are

$$\pi^{NS}_{\alpha\beta} = -\, 2\, \eta\, T\, \overline{\frac{\partial u_\alpha}{\partial x_\beta}}\,, \qquad\qquad q^{NS}_\alpha = -\, \frac{15}{4}\, \eta\, T\, \frac{\partial T}{\partial x_\alpha}\,. \tag{8}$$

The Burnett terms $\pi^B_{\alpha\beta}$ and q^B_α for Maxwell molecules can be found in books [12, 13, 14], and in the paper [2]. For brevity we present below these and other terms for the simplest case of one–dimensional flow:

$$\rho = \rho(x, t)\,, \qquad \mathbf{u} = (u(x, t), 0, 0)\,, \qquad T = T(x, t), \quad x \in \mathbb{R}\,. \tag{9}$$

Then, Eqs. (6) read

$$\begin{aligned}
&\rho_t + (\rho\, u)_x = 0\,, \\
&\rho\, (u_t + u\, u_x) + p_x + \Pi_x = 0\,, \\
&\frac{3}{2}\, \rho\, (T_t + u\, T_x) + p\, u_x + \Pi\, u_x + Q_x = 0\,,
\end{aligned} \tag{10}$$

where lower indices denote partial derivatives, Π and Q denote respectively xx–component of $\Pi_{\alpha\beta}$ and x–component of Q_α. These functions are given by

$$\begin{aligned}
&\Pi = -\, \frac{4}{3}\, \eta\, T u_x + \pi^B - \left(\frac{R}{\rho} \right)_x\,, \\
&Q = -\frac{15}{4}\, \eta\, T T_x + q^B + \frac{1}{\rho} \left[2\, R\, u_x + \left(\frac{3}{2}\, a + b \right) u_{xx} \right], \\
&R = a \frac{\rho_x}{\rho} + b\, \frac{T_x}{T}\,, \qquad a = a(T) = \frac{13}{18}\, \eta^2 T^2\,, \qquad b = b(T) = \frac{2}{3}\, \eta^2 T^2\,,
\end{aligned} \tag{11}$$

where

$$
\begin{aligned}
\pi^B &= \frac{2\,\eta^2}{9\,\rho}\left[4\,T u_x^2 + 9(T\,T_x)_x - 6\,T\left(\frac{p_x}{\rho}\right)_x\right], \\
q^B &= \frac{\eta^2 T}{8\,\rho}\left[95\,T_x u_x - 16\,T\,u_x\frac{\rho_x}{\rho} - 14\,T\,u_{xx}\right].
\end{aligned}
\tag{12}
$$

Note that the Knudsen number ε in Eqs. (7) is used as a formal parameter and we set $\varepsilon = 1$ in the final results. Thus, we obtain

$$
\Pi = -\frac{4}{3}\,\eta T u_x + \frac{2\,\eta^2}{3\,\rho}\left[-\frac{37}{12}\,\frac{T^2}{\rho}\,\rho_{xx} + \frac{25}{6}\,\frac{T^2}{\rho^2}\,\rho_x^2 + \frac{4}{3}\,T\,u_x^2 + 2\,T_x^2 - \frac{19}{6}\,\frac{T}{\rho}\,\rho_x\,T_x\right], \tag{13}
$$

$$
Q = -\frac{15}{4}\,\eta\,T T_x + \frac{\eta^2 T}{3\,\rho^2}\left(\frac{317}{8}\,\rho\,T_x - \frac{5}{3}\,T\,\rho_x\right)u_x\,. \tag{14}
$$

Eqs. (10), with the constitutive equations (13), (14), are the final one–dimensional version of Generalized Burnett Equations (GBE), which we study in this paper. Equations (1) for this version read

$$
\rho = \rho^{tr}, \qquad u = u^{tr}, \qquad T^{tr} = T - \frac{\eta^2}{\rho}\left(\frac{13}{18}\,\frac{T^2\rho_x}{\rho^2} + \frac{2}{3}\,\frac{T T_x}{\rho}\right)_x \tag{15}
$$

where the parameter η is given in Eqs. (5). This parameter is important for comparison with solutions of the Boltzmann equation. Note that Eqs. (10), (13), (14) are simpler than the classical Burnett equations since they contain only one third derivative ρ_{xxx}.

The conservative form of Eqs. (10) reads

$$
\begin{aligned}
&\rho_t + (\rho\,u)_x = 0\,, \\
&(\rho\,u)_t + \Big(\rho\,u^2 + \rho\,T + \Pi\Big)_x = 0\,, \\
&\Big[\rho(u^2 + 3T)\Big]_t + \Big[\rho\,u(u^2 + 5T) + 2(u\,\Pi + Q)\Big]_x = 0\,.
\end{aligned}
\tag{16}
$$

These equations will be used below for study of shock waves.

3 Shock wave solutions

Equations (10), (13), (14) are Galilei–invariant. In other words, the transformation

$$
\rho(x,t) = \tilde\rho(x+ct,t)\,, \qquad u(x,t) = -c+\tilde u(x+ct,t)\,, \qquad T(x,t) = \tilde T(x+ct,t)\,, \tag{17}
$$

with any constant $c \in \mathbb{R}$, leads to the same Eqs. (10), (13), (14) for $\tilde\rho(x,t)$, $\tilde u(x,t)$, $\tilde T(x,t)$. If these functions do not depend on time t, then $(\tilde\rho, \tilde u, \tilde T)$ are stationary solutions of Eqs. (10), (13), (14). The transformation (17) defines in this case travelling waves, moving with constant velocity $(-c)$. It is convenient for our goals to assume that $c > 0$ and to introduce boundary conditions

$$
\tilde\rho(-\infty) = \rho_-\,, \qquad \tilde u(-\infty) = \tilde u_- = c\,, \qquad \tilde T(-\infty) = T_-\,, \tag{18}
$$

which correspond to unperturbed gas in front of the shock.

Thus, we consider stationary Eqs. (10), (13), (14) for $(\tilde\rho, \tilde u, \tilde T)$ on the whole real line $-\infty < x < \infty$ with boundary conditions (18). Equations (10) can be presented in the conservative form (16). Then, we integrate Eqs. (16) and obtain, omitting all tildas,

$$\rho\, u = J_1\,, \qquad \rho(u^2+T)+\Pi = J_2\,, \qquad \rho\, u(u^2+5T)+2(u\,\Pi+Q) = J_3\,, \tag{19}$$

where constant fluxes $J_{1,2,3}$ are given by

$$J_1 = \rho_-\, c\,, \qquad J_2 = \rho_-(c^2+T_-)\,, \qquad J_3 = \rho_-\, c(c^2+5\,T_-) \tag{20}$$

and Π and Q are defined in Eqs. (13) and (14). Note that the speed of sound at $x \to -\infty$ (unperturbed gas) is equal to $c_0 = (5\,T_-/3)^{1/2}$, therefore

$$c = M\,\sqrt{\frac{5\,T_-}{3}}\,, \tag{21}$$

where M denotes the Mach number. It is well known (at the formal level) that the shock wave solution exists for $M > 1$ with limiting values

$$\rho(\infty) = \rho_+\,, \qquad u(\infty) = u_+\,, \qquad T(\infty) = T_+\,, \tag{22}$$

satisfying Rankine–Hugoniot conditions

$$\rho_+\, u_+ = J_1\,, \qquad \rho_+(u_+^2+T_+) = J_2\,, \qquad J_1(u_+^2+5\,T_+) = J_3\,. \tag{23}$$

Then we obtain (see Eqs. (20))

$$\rho_+ = \frac{4\,\rho_-\, c^2}{c^2+5\,T_-}\,, \qquad u_+ = \frac{c^2+5\,T_-}{4\,c}\,, \qquad T_+ = \frac{(c^2+5\,T_-)(3\,c^2-T_-)}{16\,c^2}\,, \tag{24}$$

assuming that $c > (5\,T_-/3)^{1/2}$.

The density $\rho(x)$ can be eliminated from Eqs. (19) since

$$\rho(x) = \frac{J_1}{u(x)} = \frac{\rho_-\, c}{u(x)}\,. \tag{25}$$

Then Eqs. (19) can be written in the form

$$\begin{gathered} J_1(u^2+T)+u(\Pi-J_2) = 0\,,\\ J_1(u^2+5\,T)+2(u\,\Pi+Q)-J_3 = 0\,, \end{gathered} \tag{26}$$

where now

$$\begin{aligned} \Pi &= -\frac{4}{3}\,\eta\, T u_x + \frac{2\,\eta^2}{3\,J_1}\, u\left(\frac{37}{12}\, T^2\frac{u_{xx}}{u} - 2\,T^2\,\frac{u_x^2}{u^2} + \frac{4}{3}\, T\, u_x^2 + 2\,T_x^2 + \frac{19}{6}\,\frac{T}{u}\, u_x T_x\right),\\ Q &= -\frac{15}{4}\,\eta\, T\, T_x + \frac{\eta^2 T}{3\,J_1}\, u\, u_x\left(\frac{317}{8}\, T_x + \frac{5}{3}\, T\,\frac{u_x}{u}\right). \end{aligned} \tag{27}$$

Eqs. (26) can be transformed to

$$\begin{aligned} &J_1(u^2+T)+u(\Pi-J_2)=0\,,\\ &J_1(3\,T-u^2)+2\,Q+2\,J_2\,u-J_3=0\,, \end{aligned} \tag{28}$$

where Π and Q are given in Eqs. (27). It is convenient to pass to dimensionless variables. We denote

$$\hat{x}=\frac{\rho_+\,x}{\eta\,u_+}\,,\qquad u(x)=u_+\,\hat{u}(\hat{x})\,,\qquad T(x)=T_+\,\hat{T}(\hat{x})\,,\qquad S=\frac{u_+^2}{T_+}\,, \tag{29}$$

and omit hats below. Then

$$\begin{aligned} \Pi&=\rho_+\,T_+\left[-\frac{4}{3}\,Tu_x+\frac{2\,u}{3\,S}\left(\frac{37}{12}\,T^2\frac{u_{xx}}{u}-2\,T^2\,\frac{u_x^2}{u^2}+\frac{4\,S}{3}\,T\,u_x^2+2\,T_x^2+\frac{19}{6}\,\frac{T}{u}\,u_xT_x\right)\right],\\ Q&=\frac{\rho_+\,T_+^2}{u_+}\left[-\frac{15}{4}\,T\,T_x+\frac{T}{3}\,u\,u_x\left(\frac{317}{8}\,T_x+\frac{5}{3}\,T\,\frac{u_x}{u}\right)\right]. \end{aligned} \tag{30}$$

Similarly, we obtain from Eqs. (28)

$$\begin{aligned} &T+S\,u^2+u\left(\frac{\Pi}{\rho_+\,T_+}-1-S\right)=0\,,\\ &3\,T-S\,u^2+2\,\frac{Q}{\rho_+\,u_+\,T_+}+2(1+S)u-(S+5)=0\,. \end{aligned} \tag{31}$$

Finally we denote $u_x=w$ and obtain from Eqs. (30), (31) the following set of three first order ODE:

$$\begin{aligned} u_x&=w\,,\\ T_x&=\frac{12}{T(317\,u\,w-90)}\left[-\frac{10}{9}\,T^2w^2+S^2u^2-2\,S(1+S)u-3\,S\,T+S(S+5)\right]\\ &=A(u,T,w)\,,\\ w_x&=\frac{2}{37\,T^2}\left[-12\,A^2u-19\,ATw+12\,T^2\,\frac{w^2}{u}-8\,S\,Tw^2u+12\,S\,Tw\right.\\ &\left.-9\,S\,\frac{T}{u}-9\,S^2u+9\,S(1+S)\right]=B(u,T,w)\,. \end{aligned} \tag{32}$$

These equations coincide with Eqs. (33) from [6], where the stability of their stationary solutions were studied. Asymptotic values of $u(x)$, $T(x)$, $w(x)$ at infinity can be found from Eqs. (24), (29). We obtain

$$\begin{aligned} &u(\infty)=T(\infty)=1\,,\qquad w(\infty)=0\,,\\ &u(-\infty)=\frac{S+5}{4\,S}\,,\qquad T(-\infty)=\frac{(S+5)(3\,S-1)}{16\,S}\,,\qquad w(-\infty)=0\,. \end{aligned} \tag{33}$$

Hence,

$$\rho_-=\rho_+\,\frac{4\,S}{S+5}\,,\qquad c=u_+\,\frac{S+5}{4\,S}\,,\qquad T_-=T_+\,\frac{(S+5)(3\,S-1)}{16\,S}\,,\qquad S=\frac{u_+^2}{T_+}\,, \tag{34}$$

in the notations of Eqs. (18). The parameter S can be expressed therefore through the Mach number M of the shock wave. We obtain

$$M^2 = \frac{3\,c^2}{5\,T_-} = \frac{3(S+5)}{5(3\,S-1)} \qquad \Rightarrow \qquad S = \frac{5(M^2+3)}{3(5\,M^2-1)}\,. \tag{35}$$

The parameter S decreases from $S = 5/3$ to $S = 1/3$, when M increases from $M = 1$ to $M = \infty$. A convenience of such units is that all terms of Eqs. (32), (33) remain finite in the formal limit $M = \infty$ (infinitely strong wave).

Note that $w = A(u,T,w) = B(u,T,w) = 0$, if $u = u(\pm\infty)$, $T = T(\pm\infty)$, $w = w(\pm\infty)$ from Eqs. (33). Hence, these values of (u,T,w) correspond to singular points of the dynamical system

$$u_x = w\,, \qquad T_x = A(u,T,w)\,, \qquad w_x = B(u,T,w)\,. \tag{36}$$

The shock wave solution is a heteroclinic orbit of this dynamical system, which begins at $x = -\infty$ at the supersonic singular point (provided $M > 1$ or, equivalently, $S < 5/3$) and ends at $x = \infty$ at the subsonic singular point. It follows from results of [6] that the supersonic point is an unstable node, whereas the subsonic end is a saddle point, which has only one (out of three) eigenvalue with negative real part that corresponds to incoming phase trajectory. To be more precise, the linearization of Eqs. (32) near $(u = 1,\ T = 1,\ w = 0)$ in its standard exponential form

$$u = 1 + \tilde{u}\,\mathrm{e}^{\lambda x} + \ldots, \qquad T = 1 + \tilde{T}\,\mathrm{e}^{\lambda x} + \ldots, \qquad w = \tilde{w}\,\mathrm{e}^{\lambda x} + \ldots, \tag{37}$$

where dots denote nonlinear in $(\tilde{u},\tilde{T},\tilde{w})$ terms, leads for $0 < S < 5/3$ to three different eigenvalues λ: one real negative and the other two complex conjugate with positive real part (they can also be real positive for small $S > 0$). Actually, this is a saddle point for $S < 5/3$ and an unstable node for $S > 5/3$ ($S = 5/3$ or, equivalently, $M = 1$ is a bifurcation point for Eqs. (32)). Similar linearization near $(u(-\infty),\ T(-\infty),\ 0)$ leads for $S < 5/3$ to three eigenvalues λ with positive real part. This means that the dimension $\mathtt{d}_A^{st}$ of stable manifold near the subsonic end $x = \infty$ is equal to one, whereas the similar dimension $\mathtt{d}_B^{st}$ near the supersonic end $x = -\infty$ (note that $x < 0$!) is equal to three. Hence, we have an equality $\mathtt{d}_B^{st} = \mathtt{d}_A^{st} + 2$, which is also fulfilled for general Discrete Velocity Models of the Boltzmann equation with arbitrary number of velocities [15]. This equality is not valid for Navier–Stokes equations, $\mathtt{d}_B^{st} = \mathtt{d}_A^{st} + 1$ in that case. Hence, GBE (32) yield certain improvement of NSE in a qualitative picture of solutions (see also [6] for discussion of half–space problems).

Our goal is to show that Eqs. (10) improve Navier–Stokes approximation for the shock wave problem. In order to do this we need to compare our results with exact solutions of similar problem for the Boltzmann equation. Such solutions, however, are not known. On the other hand, numerical data [11] show that lower moments $\rho(x)$, $u(x)$, $T(x)$ of the distribution function, obtained by Monte Carlo method, are very close for strong shocks to similar hydrodynamic moments of approximate Mott–Smith solutions of the Boltzmann equation. Therefore we explain briefly in Section 4 how to construct such solutions and compare the solutions of all three models in Section 5.

4 Mott–Smith solutions of the Boltzmann equations

The plane stationary Boltzmann equation for Maxwell molecules for a distribution function $f(x, \mathbf{v})$, $x \in \mathbb{R}$, $\mathbf{v} = (v_1, v_2, v_3) \in \mathbb{R}^3$, can be written in the following weak form

$$\frac{d}{dx} \int_{\mathbb{R}^3} v_x \, \psi(\mathbf{v}) \, f(x, \mathbf{v}) \, d\mathbf{v} = \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \langle \Delta \psi \rangle f(x, \mathbf{v}) f(x, \mathbf{w}) \, d\mathbf{v} \, d\mathbf{w} \,, \tag{38}$$

where $\psi(\mathbf{v})$ is any "good" test function,

$$\langle \Delta \psi \rangle = \int_{S^2} g\left(\frac{\mathbf{V} \cdot \boldsymbol{\omega}}{|\mathbf{V}|}\right) \left[\psi\left(\mathbf{U} + \frac{|\mathbf{V}|}{2} \boldsymbol{\omega}\right) + \psi\left(\mathbf{U} - \frac{|\mathbf{V}|}{2} \boldsymbol{\omega}\right) - \psi(\mathbf{v}) - \psi(\mathbf{w})\right] d\boldsymbol{\omega} \,, \tag{39}$$

where

$$\mathbf{V} = \mathbf{v} - \mathbf{w} \,, \qquad \mathbf{U} = \frac{1}{2}(\mathbf{v} + \mathbf{w}) \,, \qquad |\boldsymbol{\omega}| = 1 \,, \qquad g(\cos\theta) = |\mathbf{V}| \, \sigma(|\mathbf{V}|, \theta) \,,$$

where $\sigma(|\mathbf{V}|, \theta)$ is a differential cross–section, $0 \le \theta \le \pi$ is a scattering angle. The connection of $f(x, \mathbf{v})$ with hydrodynamic quantities $(\rho, \mathbf{u}, T)$ is given by

$$\begin{gathered} \rho(x) = \int_{\mathbb{R}^3} f(x, \mathbf{v}) \, d\mathbf{v} \,, \qquad \mathbf{u}(x) = \frac{1}{\rho} \int_{\mathbb{R}^3} \mathbf{v} \, f(x, \mathbf{v}) \, d\mathbf{v} \\ T(x) = \frac{1}{3\,\rho} \int_{\mathbb{R}^3} |\mathbf{v} - \mathbf{u}|^2 f(x, \mathbf{v}) \, d\mathbf{v} \,. \end{gathered} \tag{40}$$

We are interested in this paper in a specific solution of Eq. (38), which corresponds to the shock wave moving in the negative direction in x with the speed $c > 0$. This means that we have to consider a solution $f(x, \mathbf{v})$, which tends for $x \to -\infty$ and $x \to \infty$ to Maxwellians $M_-(\mathbf{v})$ and $M_+(\mathbf{v})$ respectively, where

$$M_\pm(\mathbf{v}) = \rho_\pm \, (2\pi \, T_\pm)^{-3/2} \exp\left[-\frac{(v_x - u_\pm)^2 + v_y^2 + v_z^2}{2\,T_\pm}\right]. \tag{41}$$

The values of parameters $(\rho_\pm, u_\pm, T_\pm)$ are exactly the same as in Eqs. (18), (24).

The Mott–Smith solution (see, for example, the book [11]) is an approximate solution of Eq. (38), having the following form:

$$f_{MS}(x, \mathbf{v}) = \Theta(x) \, M_-(\mathbf{v}) + \Big[1 - \Theta(x)\Big] M_+(\mathbf{v}) \,, \tag{42}$$

where $\Theta(-\infty) = 1$, $\Theta(+\infty) = 0$. It is clear that this function with any such $0 \le \Theta(x) \le 1$ is non–negative and satisfies Eqs. (38) for $\psi(\mathbf{v}) = 1, \mathbf{v}, |\mathbf{v}|^2$. For any other $\psi(\mathbf{v}) = \psi(v_x, |\mathbf{v}|)$ we obtain from Eq. (38) the following equation for $\Theta(x)$

$$\frac{d\Theta}{dx} = \lambda[\psi] \, \Theta(1 - \Theta) \,, \qquad \lambda[\psi] = \frac{A[\psi]}{B[\psi]} \,, \tag{43}$$

where

$$\begin{aligned} A[\psi] &= \int_{\mathbb{R}^3 \times \mathbb{R}^3} \langle \Delta \psi \rangle M_+(\mathbf{v}) M_-(\mathbf{w}) \, d\mathbf{v} \, d\mathbf{w} \,, \\ B[\psi] &= \int_{\mathbb{R}^3} \Big[M_-(\mathbf{v}) - M_+(\mathbf{v})\Big] \, v_x \, \psi(\mathbf{v}) \, d\mathbf{v} \,. \end{aligned} \tag{44}$$

In the typical case $\psi = v_x^2$ we obtain after some calculations

$$\lambda[v_x^2] = -\frac{1}{3\,\eta}\,\frac{\rho_+(u_+ - u_-)^2}{u_-(T_+ - T_-)}\,, \tag{45}$$

in the notations of Eqs. (5). A weakness of the Mott–Smith approximation is that the parameter $\lambda[\psi]$ in Eq. (43) is very sensitive to the choice of the test function $\psi(\mathbf{v})$. On the other hand, it is known [11] that the approximation with $\psi = v_x^2$ is in very good agreement with DSMC simulation for hard spheres for a wide range of Mach numbers. This is the main reason why we chose the Mott–Smith approximation with $\psi = v_x^2$ and the Navier–Stokes solutions as two reference solutions for comparison with solutions of Eqs. (32).

The general solution of Eq. (43) reads

$$\Theta(x) = \Big[1 + C\,\exp(-\,\lambda x)\Big]^{-1}\,, \tag{46}$$

where the arbitrary constant C is due to translational invariance in x. We choose $C = 1$ and $\lambda = \lambda[v_x^2]$ given in Eq. (45). Note that $T_+ > T_-$ and therefore $\lambda[v_x^2] < 0$. Hence, $\Theta(x)$ satisfies boundary conditions at $x = \pm\infty$. Then Eq. (42) is equivalent to

$$\begin{aligned} f_{MS}(x, \mathbf{v}) &= M_-(\mathbf{v}) + \frac{1}{2}\Big[M_+(\mathbf{v}) - M_-(\mathbf{v})\Big](1 + \tanh\, y)\,, \\ y &= -\,\frac{1}{2}\,\lambda[v_x^2]\,x = \frac{1}{6\,\eta}\,\frac{\rho_+(u_+ - u_-)^2}{u_-(T_+ - T_-)}\,x = a(S)\,\hat{x}\,, \end{aligned} \tag{47}$$

where (see Eqs. (29), (34))

$$\begin{aligned} \hat{x} &= \frac{\rho_+}{\eta\,u_+}\,x\,, \qquad\qquad S = \frac{u_+^2}{T_+} < \frac{5}{3}\,, \\ a(S) &= \frac{u_+(u_+ - u_-)^2}{6\,u_-(T_+ - T_-)} = S\,\frac{u_+\left(1 - \frac{u_-}{u_+}\right)^2}{6\,u_-\left(1 - \frac{T_-}{T_+}\right)} = \frac{2S(5 - 3S)}{3(S+1)(S+5)}\,. \end{aligned} \tag{48}$$

Hence, for any "good" test function $\psi(\mathbf{v})$

$$C_{MS}[\psi] = D[\psi]\,\frac{1}{2}(1 + \tanh y)\,, \qquad\qquad y = a(S)\hat{x}\,, \tag{49}$$

where

$$\begin{aligned} C_{MS}[\psi] &= \int_{\mathbb{R}^3}\Big[f_{MS}(\mathbf{v}) - M_-(\mathbf{v})\Big]\,\psi(\mathbf{v})\,d\mathbf{v}\,, \\ D[\psi] &= \int_{\mathbb{R}^3}\Big[M_+(\mathbf{v}) - M_-(\mathbf{v})\Big]\,\psi(\mathbf{v})\,d\mathbf{v}\,. \end{aligned} \tag{50}$$

For comparison with solutions of Eqs. (32) we need just functions $(\rho_{MS}, u_{MS}, T_{MS})$. Taking $\psi = 1$ in Eq. (49) we obtain

$$\rho_{MS}(x) - \rho_- = (\rho_+ - \rho_-)\frac{1}{2}(1 + \tanh y)\,. \tag{51}$$

Then $u_{MS}(x)$ can be obtained from conservation law

$$u_{MS}(x) = \frac{\rho_\pm\, u_\pm}{\rho_{MS}(x)}\,, \tag{52}$$

whereas $T_{MS}(x)$ can be obtained from Eq. (49) with $\psi = |\mathbf{v}|^2$

$$\rho_{MS}\left(u_{MS}^2 + 3\,T_{MS}\right) - \rho_-(u_-^2 + 3\,T_-) = \Big[\rho_+(u_+^2 + 3\,T_+) - \rho_-(u_-^2 + 3\,T_-)\Big]\frac{1}{2}(1 + \tanh y)\,. \tag{53}$$

Eqs. (51)–(53) define $(\rho_{MS}, u_{MS}, T_{MS})$ as functions of $y = a(S)\,\hat{x}$, in the notation of Eqs. (48). The next step is to use these functions for comparison with solutions of equations of hydrodynamics.

5 Comparison of results for different models

Our goal in this section is to solve equations (32), (33) and to compare the solutions with similar results from (a) Navier–Stokes equations and (b) Mott–Smith approximation described in Section 4. The Navier–Stokes equations can be obtained directly from Eqs. (30)–(31) by omitting Burnett terms. The resulting system of two ODE for $u(x) = u_{NS}(x)$ and $T(x) = T_{NS}(x)$ (lack of third derivative reduces dimension of dynamical system) reads

$$\begin{aligned} &\frac{4}{3}\,T\,u_x + 1 + S = S\,u + \frac{T}{u}\,,\\ &\frac{15}{2\,S}\,T\,T_x + S + 5 = -\,S\,u^2 + 2(1+S)u + 3\,T\,, \end{aligned} \tag{54}$$

$$\begin{aligned} S &= \frac{5(M^2+3)}{3(5\,M^2-1)}\,, \qquad & u(\infty) = T(\infty) = 1\,,\\ u(-\infty) &= \frac{S+5}{4\,S}\,, \qquad & T(-\infty) = \frac{(S+5)(3\,S-1)}{16\,S}\,. \end{aligned} \tag{55}$$

It is clear that these equations and Eqs. (32), (33) are invariant under translations $x \to x + \text{const}$. However, we can choose a unique solution by demanding that

$$\rho(0) = \frac{1}{2}\Big[\rho(\infty) + \rho(-\infty)\Big]\,, \tag{56}$$

or, equivalently,

$$u^{-1}(0) = \frac{1}{2}\Big[u^{-1}(\infty) + u^{-1}(-\infty)\Big]\,, \tag{57}$$

since $\rho(x)\,u(x) = \text{const}$. Note that the Mott–Smith solutions (51)–(53) are already chosen in such a way that the above conditions for $\rho(0)$ and $u(0)$ are satisfied. To keep the same notation in all three cases we need to denote

$$\begin{aligned} y &= \frac{2\,S(5-3\,S)}{3(S+1)(S+5)}\,\hat{x}\,, \qquad & \rho_{MS}(x) = \rho_+\,\hat{\rho}_{MS}(\hat{x})\,,\\ u_{MS}(x) &= u_+\,\hat{u}_{MS}(\hat{x})\,, \qquad & T_{MS}(x) = T_+\,\hat{T}_{MS}(\hat{x})\,, \end{aligned} \tag{58}$$

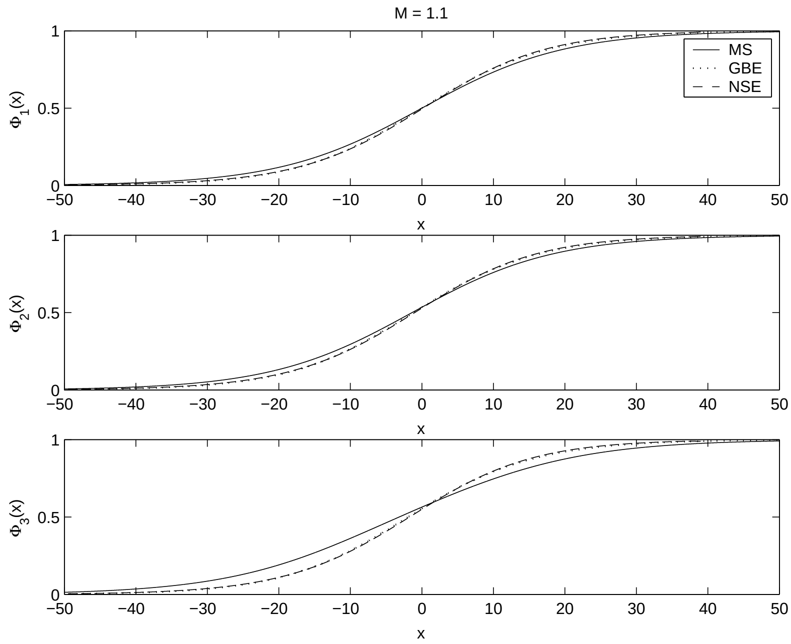

Figure 1: Profiles of the shock-wave and of the Mott-Smith solution for $M = 1.1$: GBE (dotted line), NSE equations (dashed line), MS solution (solid line).

in Eqs. (51)–(53) and then omit hats in final results. Note that

$$\rho(0) = \rho_{NS}(0) = \rho_{MS}(0) = \frac{1}{2}\Big[\rho(\infty) + \rho(-\infty)\Big]. \tag{59}$$

It is convenient to choose for comparison three normalized functions

$$\Phi_1(x) = \frac{\rho(x) - \rho(-\infty)}{\rho(\infty) - \rho(-\infty)}\,, \qquad \Phi_2(x) = \frac{u(x) - u(-\infty)}{u(\infty) - u(-\infty)}\,,$$
$$\Phi_3(x) = \frac{T(x) - T(-\infty)}{T(\infty) - T(-\infty)}\,. \tag{60}$$

Then obviously $\Phi_i(-\infty) = 0$, $\Phi_i(\infty) = 1$, $i = 1, 2, 3$. Moreover, $0 < \Phi_i(x) < 1$ for all $i = 1, 2, 3$ are monotone functions provided $\rho(x)$, $u(x)$ and $T(x)$ are monotone functions.

Thus, we fix a Mach number $M > 1$, solve numerically Eqs. (32), (33) and Navier–Stokes equations (54), (55), and then present functions $\Phi_{1,2,3}(x)$ for the three models on Figs. 1–8. Shock profiles for GBE are not clearly visible on Figs. 1 and 3, because they are very close to the corresponding curves for NSE when $M = 1.1$ (Fig. 1) and for MS approximation when $M = 2$ (Fig. 3).

It is expected that Navier–Stokes solutions are good for relatively small M, whereas the Mott–Smith approximation is better for large M. If this assumption is true, then it is clear from our results that GBE (32) improve results of Navier–Stokes approximation for large Mach numbers (strong shocks).

As expected, all three models yield similar results for weak shocks ($M = 1.1$, Figs. 1 and 2; $M = 2$, Figs. 3 and 4). We also present on Figs. 2 and 4 the corresponding phase

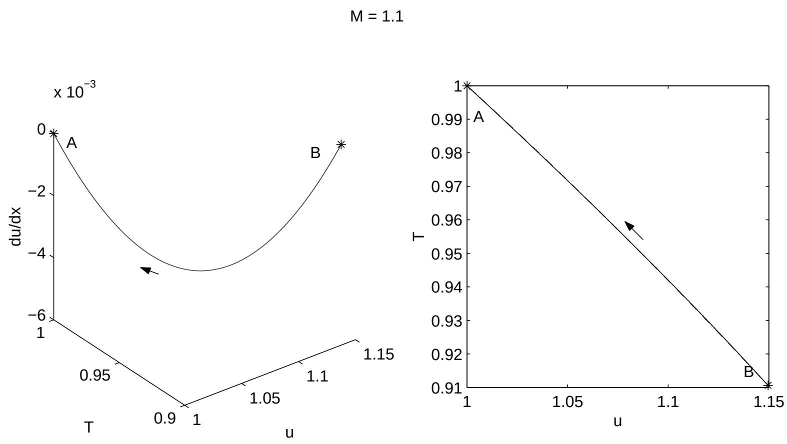

Figure 2: (Left) Shock-wave curve in the phase space for GBE for $M = 1.1$. (Right) Comparison between the projection of the shock-wave curve in the (u, T) plane for GBE (solid line) and the shock-wave for NSE equations (dashed line).

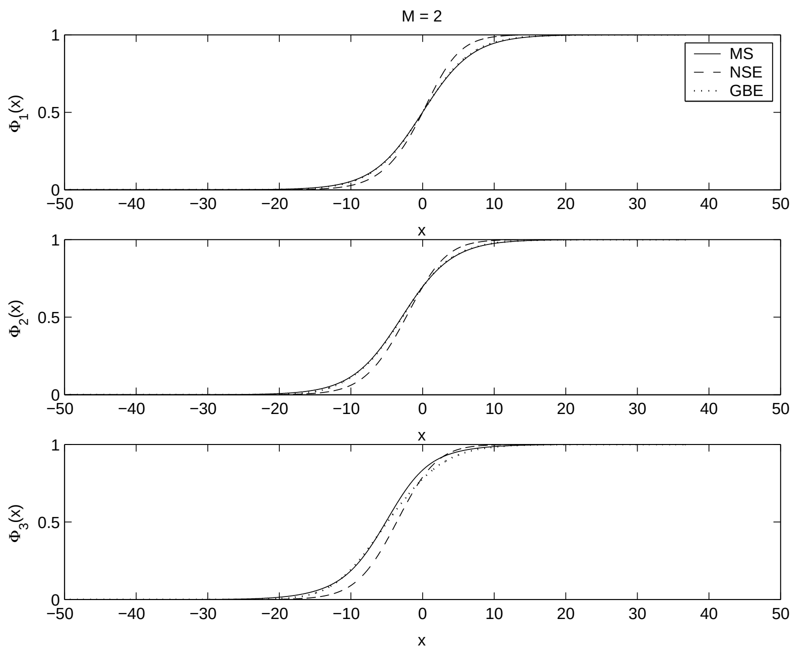

Figure 3: Profiles of the shock-wave and of the Mott-Smith solution for $M = 2$: GBE (dotted line), NSE equations (dashed line), MS solution (solid line).

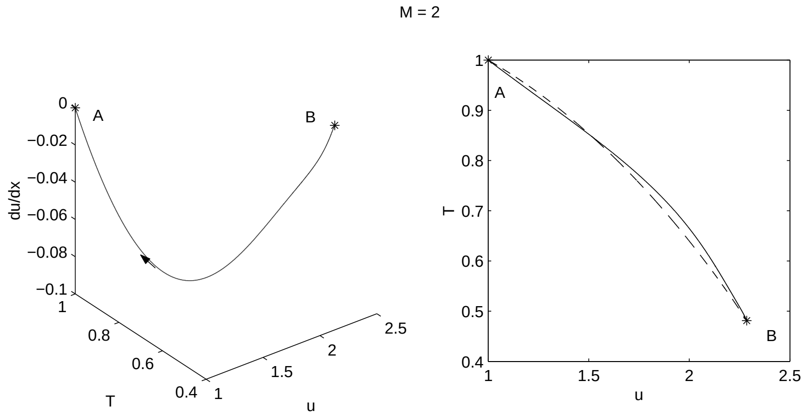

Figure 4: (Left) Shock-wave curve in the phase space for GBE for $M = 2$. (Right) Comparison between the projection of the shock-wave curve in the (u, T) plane for GBE (solid line) and the shock-wave for NSE equations (dashed line).

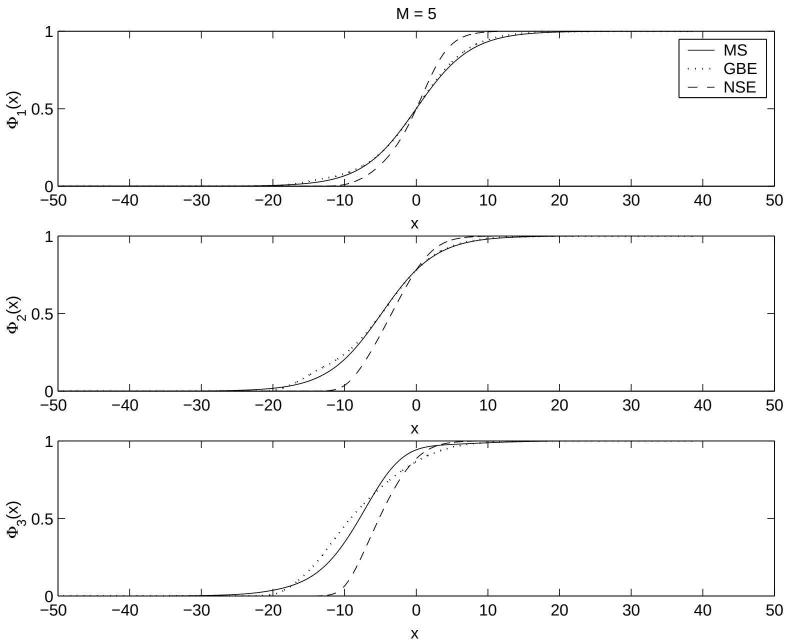

Figure 5: Profiles of the shock-wave and of the Mott-Smith solution for $M = 5$: GBE (dotted line), NSE equations (dashed line), MS solution (solid line).

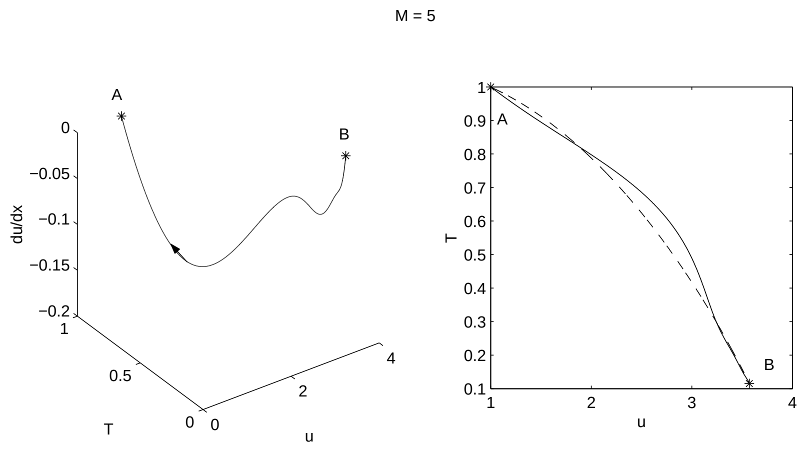

Figure 6: (Left) Shock-wave curve in the phase space for GBE for $M = 5$. (Right) Comparison between the projection of the shock-wave curve in the (u, T) plane for GBE (solid line) and the shock-wave for NSE equations (dashed line).

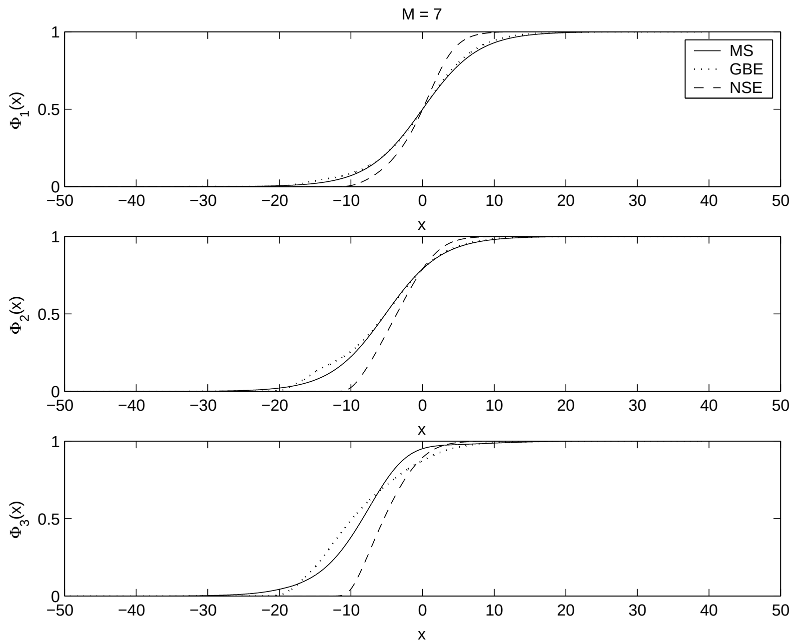

Figure 7: Profiles of the shock-wave and of the Mott-Smith solution for $M = 7$: GBE (dotted line), NSE equations (dashed line), MS solution (solid line).

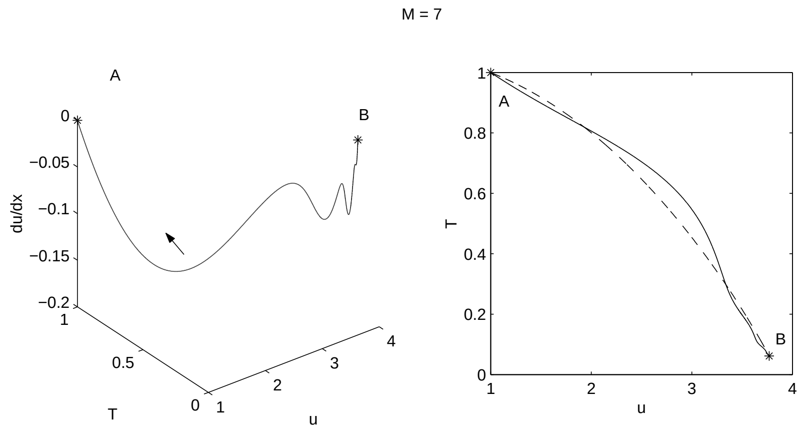

Figure 8: (Left) Shock-wave curve in the phase space for GBE for $M = 7$. (Right) Comparison between the projection of the shock-wave curve in the (u, T) plane for GBE (solid line) and the shock-wave for NSE equations (dashed line).

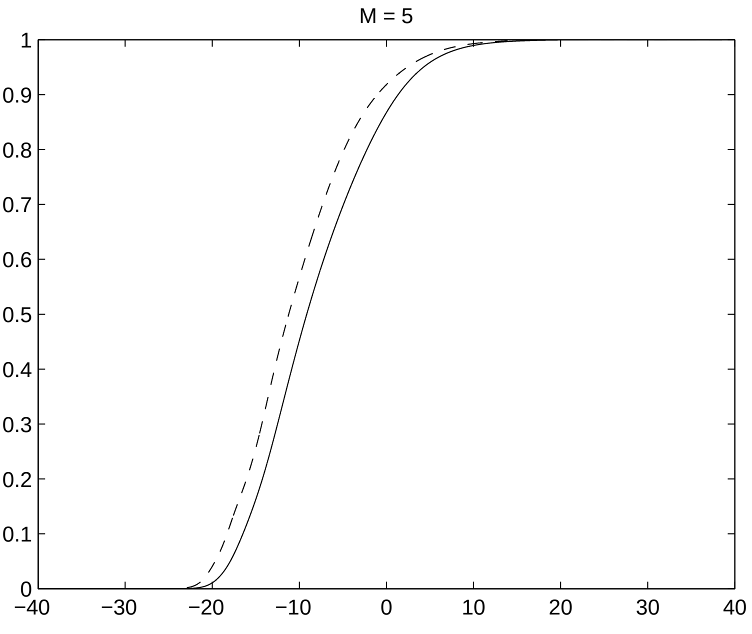

Figure 9: Comparison between the shock–wave profile of “true” temperature (dashed line) and auxiliary temperature (solid line) for $M = 5$.

trajectory in the phase space (u, T, w) of dynamical system (32). The direction of the phase trajectories are always from the supersonic state B $(x = -\infty)$ to the subsonic state A $(x = \infty)$. Similar curves for Navier–Stokes equations were studied in detail in [16]. The difference becomes more visible for strong shocks with $M = 5$ (Figs. 5, 6) and $M = 7$ (Figs. 7, 8). In all these cases the results obtained form GBE (32) are closer to Mott–Smith solutions than to solutions of the Navier–Stokes system. At the same time the projection of the phase trajectory to the plane (u, T) remains relatively close to similar curve for Navier–Stokes equations even for $M = 5$ (Fig. 6) and $M = 7$ (Fig. 8).

Strictly speaking, we should use for comparison not the function $T(x)$ from Eqs. (32), but

$$T^{tr}(x) = T - \frac{1}{\rho\, S}\left(\frac{13}{18}\,\frac{T^2\,\rho_x}{\rho^2} + \frac{2}{3}\,\frac{T\,T_x}{\rho}\right)_x \tag{61}$$

obtained from transformation (15). We do not do it for two reasons: (a) the difference is negligible for small Mach numbers and (b) it becomes visible (see Fig. 9) for larger M near the front of the shock, where, generally speaking, no hydrodynamics can be applied because of large gradients. The shock wave problem is therefore not very good test for equations of hydrodynamics. The most important result, however, is that our equations (32) are apparently uniquely solvable for all Mach numbers $M > 1$ (this assumption is supported by linear stability analysis of subsonic and supersonic states from [6]). They yield qualitatively correct results, improving the Navier–Stokes approximation for moderate Mach numbers.

We also present some data on thickness of the shock and asymmetry of the density profile. According to the book of Carlo Cercignani [17], in our dimensionless units the thickness of the shock is defined as

$$\delta = \frac{1}{\Phi_1'(0)} \tag{62}$$

where $x = 0$ is the central point of the shock $(\Phi_1(0) = 0.5)$. Values corresponding to the examples of our paper are reported in Table I.

	M=1.1	M=2	M=5	M=7
GBE	$\delta = 35.0$	$\delta = 13.7$	$\delta = 14.6$	$\delta = 14.8$
NSE	$\delta = 34.6$	$\delta = 10.8$	$\delta = 9.89$	$\delta = 9.86$
MS	$\delta = 39.7$	$\delta = 14.0$	$\delta = 15.2$	$\delta = 15.6$

Table I.

The asymmetries of the shock profiles can be captured by measuring the areas

$$A^- = \int_{-\infty}^{0} \Phi_1(x)\, dx\,, \qquad\qquad A^+ = \int_{0}^{+\infty} (1 - \Phi_1(x))\, dx\,. \tag{63}$$

Results corresponding to our cases are reported in Table II.

	M=1.1	M=2	M=5	M=7
GBE	$A^- = 5.94$ $A^+ = 6.15$	$A^- = 2.36$ $A^+ = 2.36$	$A^- = 2.74$ $A^+ = 2.45$	$A^- = 2.80$ $A^+ = 2.48$
NSE	$A^- = 6.06$ $A^+ = 5.91$	$A^- = 1.96$ $A^+ = 1.70$	$A^- = 1.79$ $A^+ = 1.47$	$A^- = 1.78$ $A^+ = 1.46$
MS	$A^- = 6.87$ $A^+ = 6.87$	$A^- = 2.43$ $A^+ = 2.43$	$A^- = 2.64$ $A^+ = 2.64$	$A^- = 2.70$ $A^+ = 2.70$

Table II.

6 Conclusions

We studied the shock wave structure for Generalized Burnett Equations [5]. The previous results obtained in [6] suggest a unique choice of parameters of GBE and therefore we considered precisely this unique version of GBE in this paper. The advantage of this version is that third derivatives of $\mathbf{u}(\mathbf{x}, t)$ and $T(\mathbf{x}, t)$ are absent in the equations. Therefore GBE are even simpler than classical (unstable) Burnett equations. We confined ourselves to the case of Maxwell molecules since it is the only case, for which all Burnett terms are known in explicit form.

The shock wave problem reduces for GBE to a set of three nonlinear ODE. The shock wave solution is, in terminology of the theory of dynamical systems [18], a heteroclinic orbit that connects two singular points of the corresponding vector field. This solution was studied for different Mach numbers and compared with solutions of Navier–Stokes equations and with the Mott–Smith approximation for the Boltzmann equations. The results show that GBE yield certain improvement of the Navier–Stokes approximation for moderate Mach numbers. It is also important that GBE have, roughly speaking, the correct difference $\Delta = 2$ of dimensions of stable manifolds near subsonic and supersonic singular points (see [15] for details). This means that a qualitative picture of solutions of GBE is, in some sense, more similar to the Boltzmann equations than in the case of Navier–Stokes equations.

At least two problems in this area remain open: (a) similar one–dimensional flows for non–Maxwell gases (hard spheres, for example) and (b) boundary conditions and multi–dimensional flows. We hope to return to these problems in the future.

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