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Bobylev's instability

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In 1982 Bobylev [A.V. Bobylev, *Sov. Phys. Dokl.* **27**, 29 (1982)] made a linear stability analysis of the Burnett equations and showed that beyond a certain critical reduced wave number there exist normal modes that grow exponentially, concluding that the Burnett equations are linearly unstable. We have partially extended his analysis, originally made for Maxwellian molecules, for any interaction potential and argue that his results can be reinterpreted as to give a bound for the Knudsen number above which the Burnett equations are not valid.

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The question regarding the stability of the solutions to the equations of hydrodynamics for given initial and boundary conditions has been of utmost importance [1]. In particular, since hydrodynamic equations for dilute gases are obtained from the Boltzmann equation by seeking, either solutions in power series in terms of Knudsen's parameter through the Chapman–Enskog method, or as truncated approximations using Grad's moment method, and in both cases the transport coefficients are in principle obtainable for given intermolecular potentials, the validity of their solution becomes an important question. In 1982 Bobylev [2] claimed that for the case of Maxwellian molecules, whereas the Navier–Stokes approximation yields equations which are stable against small perturbations, for the equilibrium state characterized by constant temperature (T_0), constant mass density (ρ_0), and zero hydrodynamic velocity ($\mathbf{u}=\mathbf{0}$), this is not the case for the next approximation in Knudsen's parameter, namely, for the Burnett equations. In fact he showed that small perturbations to the equilibrium solution which are periodic in the space variable with a wavelength smaller than some critical length are exponentially unstable. This fact is now referred to in the literature as Bobylev's instability.

On the other hand, the Burnett approximation of hydrodynamics has been recently shown to provide substantial improvement on many features of the flow occurring in several problems in hydrodynamics. This is the case for a plane Poiseuille flow [3], and others [4]. But perhaps the most spectacular of them arises in the calculation of the profiles of a shock wave at large Mach numbers. There, it has been shown by many workers in the field that the Burnett approximation substantially improves the accuracy of the different profiles in the shock wave when compared with the direct Monte Carlo simulations [5] or molecular dynamics [6]. Nevertheless, in the study of this problem, it was found that the solutions of the Burnett equations do exhibit certain "instabilities" that have been associated to Bobylev's instability [7,8],

in the case of the time dependent code, or to a bifurcation for a Mach number of value ≈ 2.69 in the stationary situation [9]. Without entering here into a detailed analysis of these features, which will be soon published, the question is if the results obtained by Bobylev can be sustained for more general models and if affirmative can they be casted in terms of Knudsen's parameter. This means, can we find a critical value for Knudsen's parameter beyond which the solutions to the Burnett equations are unstable?

The purpose of this communication is to show that this is indeed the case and further we will see that the analysis partially holds true independently of the interatomic potential. This answer provides then a rather clear cut significance to the gradient expansion in the Chapman–Enskog method [10] of solving Boltzmann's equation.

To pursue our objective we start from the conservation equations which, for the longitudinal flow, $\mathbf{u}(\mathbf{r},t)=u(x,t)\hat{i}$, are written as

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial}{\partial x}(u(x,t)\rho(x,t))=0, \quad (1)$$

$$\frac{\partial u(x,t)}{\partial t} + u(x,t)\frac{\partial u(x,t)}{\partial x} = -\frac{1}{\rho(x,t)}\frac{\partial P_{xx}}{\partial x}, \quad (2)$$

$$\begin{aligned} \frac{\partial T(x,t)}{\partial t} + u(x,t)\frac{\partial T(x,t)}{\partial x} = & -\frac{2m}{3k_B\rho(x,t)}\left(P_{xx}(x,t)\frac{\partial u(x,t)}{\partial x} \right. \\ & \left. + \frac{\partial q_x(x,t)}{\partial x}\right), \end{aligned} \quad (3)$$

where m is the mass, k_B Boltzmann's constant, $P_{xx}(x,t)$ the xx component of the pressure tensor and $q_x(x,t)$ the x component of the heat flux. $\rho(x,t)$, $u(x,t)$, and $T(x,t)$ are the local values of the mass density, the velocity and the tem-

perature, respectively. The components y and z of momentum conservation give no additional information.

The constitutive equations for P_{xx} and q_x contain the hydrostatic pressure, the usual Navier–Newton–Fourier contributions and the Burnett terms, which correspond to the second order in the gradients expansion. The pressure tensor is given by [10]

$$\begin{aligned}
P_{xx} = & \frac{\rho k_B T}{m} - \frac{4}{3} \eta \frac{\partial u}{\partial x} + \frac{2}{3} \omega_1 \eta^2 \frac{m}{\rho k_B T} \left(\frac{\partial u}{\partial x} \right)^2 \\
& + \frac{2}{3} \omega_2 \frac{\eta^2}{\rho T} \left[\frac{1}{\rho^2} \left(\frac{\partial \rho}{\partial x} \right)^2 - \frac{1}{\rho} \frac{\partial \rho}{\partial x} \frac{\partial T}{\partial x} \right. \\
& \left. - \frac{1}{\rho^2} \frac{\partial^2 \rho}{\partial x^2} - \frac{\partial^2 T}{\partial x^2} - \frac{14}{9} \left(\frac{\partial u}{\partial x} \right)^2 \right] \\
& + \frac{2}{3} \omega_3 \frac{\eta^2}{\rho T} \frac{\partial^2 T}{\partial x^2} + \frac{2}{3} \omega_4 \frac{\eta^2 m}{\rho^2 k_B T^2} \left[\frac{k_B T}{m} \frac{\partial \rho}{\partial x} \frac{\partial T}{\partial x} \right. \\
& \left. + \frac{\rho k_B}{m} \left(\frac{\partial T}{\partial x} \right)^2 \right] + \frac{2}{3} \omega_5 \frac{\eta^2}{\rho T^2} \left(\frac{\partial T}{\partial x} \right)^2 + \frac{2}{9} \omega_6 \frac{\eta^2 m}{\rho k_B T} \left(\frac{\partial u}{\partial x} \right)^2,
\end{aligned} \quad (4)$$

and the heat flux, to the same approximation, is

$$\begin{aligned}
q_x = & -\lambda \frac{\partial T}{\partial x} + \frac{\theta_1 \eta^2}{\rho T} \frac{\partial u}{\partial x} \frac{\partial T}{\partial x} - \frac{8}{3} \theta_2 \frac{\eta^2}{\rho T} \frac{\partial u}{\partial x} \frac{\partial T}{\partial x} \\
& - \frac{2}{3} \theta_2 \frac{\eta^2}{\rho} \frac{\partial^2 u}{\partial x^2} + \frac{2}{3} \theta_3 \frac{\eta^2 m}{\rho^2 k_B T} \left(\frac{k_B T}{m} \frac{\partial \rho}{\partial x} + \frac{\rho k_B}{m} \frac{\partial T}{\partial x} \right) \frac{\partial u}{\partial x} \\
& + \frac{2}{3} \theta_4 \frac{\eta^2}{\rho} \frac{\partial^2 u}{\partial x^2} + 2 \theta_5 \frac{\eta^2}{\rho T} \frac{\partial T}{\partial x} \frac{\partial u}{\partial x},
\end{aligned} \quad (5)$$

where η is the shear viscosity, λ the thermal conductivity and the ω 's and θ 's are the Burnett coefficients. They have been explicitly calculated for hard spheres as well as for Maxwell molecules [10].

Equations (1)–(5) are the complete set in the Burnett approximation that we want to study. They have as a solution the equilibrium state characterized by $\mathbf{u} = \mathbf{0}$, $\rho = \rho_0 = \text{constant}$ and $T = T_0 = \text{constant}$. We now wonder if this solution is stable under small perturbations. In order to study the stability conditions the system is perturbed, in the following manner:

$$\begin{aligned}
T(x, t) &= T_0 [1 + \epsilon T'(x, t)], \\
\rho(x, t) &= \rho_0 [1 + \epsilon \rho'(x, t)], \\
u(x, t) &= \sqrt{\frac{k_B T_0}{m}} \epsilon u'(x, t),
\end{aligned} \quad (6)$$

where all primed quantities are dimensionless and different orders in ϵ indicate the order of approximation. We also define a dimensionless length (s) and time (t') in terms of the mean free path (l), namely

$$l = \frac{\eta_0}{\rho_0} \sqrt{\frac{m}{k_B T_0}}, \quad s = \frac{x}{l}, \quad t' = \frac{\rho_0 k_B T_0}{\eta_0 m} t, \quad (7)$$

where η_0 is the shear viscosity evaluated at the temperature of the equilibrium state. By means of this transformation and substitution of the constitutive equations (4) and (5) into Eqs. (1)–(3) we obtain that to first order in ϵ ,

$$\frac{\partial \rho'}{\partial t'} + \frac{\partial u'}{\partial s} = 0, \quad (8)$$

$$\begin{aligned}
\frac{\partial u'}{\partial t'} = & -\frac{\partial}{\partial s} (\rho' + T') + \frac{4}{3} \frac{\partial^2 u'}{\partial s^2} + \frac{2\omega_2}{3} \frac{\partial^3 \rho'}{\partial s^3} \\
& - \frac{2}{3} (\omega_3 - \omega_2) \frac{\partial^3 T'}{\partial s^3},
\end{aligned} \quad (9)$$

$$\frac{\partial T'}{\partial t'} = -\frac{2}{3} \frac{\partial u'}{\partial s} + f \frac{\partial^2 T'}{\partial s^2} - \frac{4}{9} (\theta_4 - \theta_2) \frac{\partial^3 u'}{\partial s^3}, \quad (10)$$

where $f = 2m\lambda_0/3k_B\eta_0$ is the Eucken factor and λ_0 the thermal conductivity at the temperature T_0 . The first Sonine expansion gives $f = 5/2$ [10], a result which is independent of the interatomic potential and is in very good agreement with the experimental data [10]. We shall use this value from now on. Also, Eqs. (8)–(10) are valid for any interatomic potential.

Let us now introduce normal modes, namely,

$$\begin{aligned}
\rho'(s, t') &= \tilde{\rho} \exp(\Omega t' + iks), \quad T'(s, t') = \tilde{T} \exp(\Omega t' + iks), \\
u'(s, t') &= \tilde{u} \exp(\Omega t' + iks), \quad \text{Im}(k) = 0,
\end{aligned} \quad (11)$$

and substitute in Eqs. (8)–(10). This leads to a system of three equations for variables $\tilde{\rho}$, \tilde{T} , and \tilde{u} whose determinant must be set equal to zero, a condition that guarantees the existence of a nontrivial solution. This leads finally to the equation,

$$\begin{aligned}
18\Omega^3 + 69\Omega^2 k^2 + 30\Omega k^2 + 18\Omega k^4 \left[\frac{10}{3} - \frac{4}{9} (\theta_4 - \theta_2 + \omega_3 \right. \\
\left. - \omega_2) + \frac{2\omega_2}{3} \right] + \frac{16}{3} (\omega_3 - \omega_2) (\theta_4 - \theta_2) \Omega k^6 + 45k^4 \\
\left. + 30\omega_2 k^6 = 0. \right.
\end{aligned} \quad (12)$$

Since the previous dispersion relation depends only on the magnitude of k we will restrict the forthcoming discussion for positive values of k .

For the remaining part of the analysis we do require the values of the transport coefficients so we shall use those computed for Maxwellian molecules and for rigid spheres. In the former case [10],

$$\theta_2 = \frac{45}{8}, \quad \theta_4 = 3, \quad \omega_2 = 2, \quad \omega_3 = 3, \quad (13)$$

and Eq. (12) reduces to

$$\begin{aligned}
18\Omega^3 + 69\Omega^2 k^2 + 97\Omega k^4 - 14\Omega k^6 + 30\Omega k^2 + 45k^4 + 60k^6 \\
= 0.
\end{aligned} \quad (14)$$

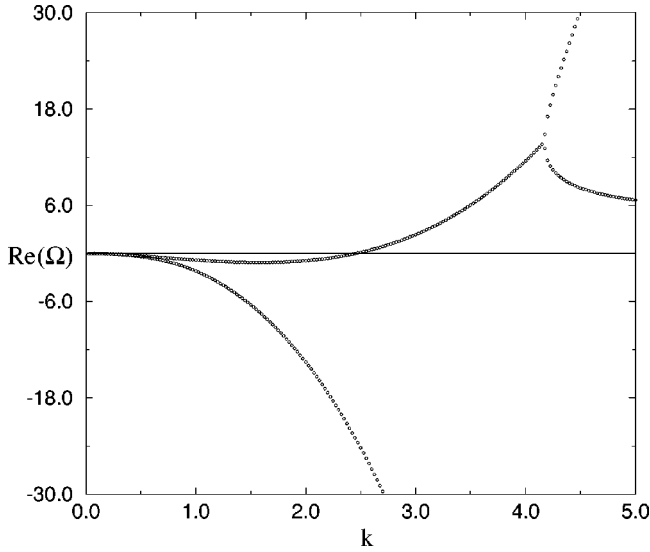


FIG. 1. Real parts of the eigenvalues (circles) as function of k for the Maxwell model.

Equation (14) differs from the result obtained by Bobylev [see Eq. (6) in Ref. [2]] in that the last term is four times larger. However substitution of Eq. (13) into Eqs. (8)–(10) reproduces the results given by Bobylev [see Eqs. (3) and (4) in Ref. [2]]. It is also pertinent to mention that the corresponding equation for the Navier–Stokes approximation is easily obtained from Eq. (15) setting $\omega_2 = \omega_3 = \theta_2 = \theta_4 = 0$ to yield

$$18\Omega^3 + 69\Omega^2k^2 + 30\Omega k^2 + 60\Omega k^4 + 45k^4 = 0, \quad (15)$$

which is also given by Bobylev. Also, for rigid spheres we have

$$\theta_2 = 5.821\,875, \theta_4 = 2.418, \omega_2 = 2.028, \omega_3 = 2.418, \quad (16)$$

and the polynomial (12) reduces to

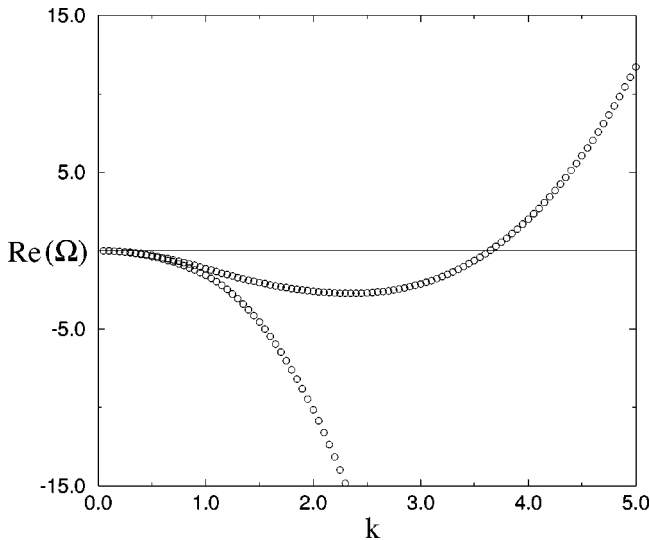


FIG. 2. Real parts of the eigenvalues (circles) as function of k for the rigid sphere model.

$$18\Omega^3 + 69\Omega^2k^2 + 108.447\Omega k^4 - 7.080\,06\Omega k^6 + 30\Omega k^2 + 45k^4 + 60.84k^6 = 0. \quad (17)$$

If we now analyze the real part of the roots of Eqs. (14) and (17) we obtain the behavior shown in Figs. 1 and 2. This clearly indicates that there exists a critical reduced wave number (k_c), such that for $k > k_c$ there is a root whose real part is positive thus implying the existence of an instability at $k_c \approx 2.5$ and $k_c \approx 3.65$ for the Maxwell model and rigid sphere model, respectively.

To interpret this result we recall that Knudsen's number is defined as

$$\mathcal{K}_n = \frac{l}{L}, \quad (18)$$

where L is a characteristic length of the phenomena under consideration. The main point here is the selection of the characteristic length appropriate to the behavior of normal modes. Thus for perturbations in the density, velocity or temperature, this implies that

$$L^{-1} = \left| \frac{\partial \rho'}{\partial x} \right| / |\rho'|, \quad L^{-1} = \left| \frac{\partial T'}{\partial x} \right| / |T'|,$$

$$\text{or } L^{-1} = \left| \frac{\partial u'}{\partial x} \right| / |u'|.$$

However all definitions of L are equivalent and equal to k/l , so that $\mathcal{K}_n = k$ and the local values of the Knudsen's number become global quantities. This implies that Bobylev's results may be interpreted alternatively by stating that Burnett equations are stable against small perturbations provided that Knudsen number is smaller than k_c . This result may surprise some readers since presumably the Chapman–Enskog solution of Boltzmann's equation is valid only if $\mathcal{K}_n \ll 1$, how small is never stated. Here however, as in Bobylev's analysis, we have not been concerned with the convergence of the series. On the other hand, as pointed out by Bobylev [2], since the Burnett equations are nonlinear it is to be expected that their nonlinearity leads to the appearance of a finite number of harmonics for finite times. Thus even if modes with $k > k_c$ are not present one may expect that the nonlinearities will generate them and so one may be tempted to conclude that our interpretation is incorrect. We have done calculations to second order in the perturbation ($u(x,t) = \sqrt{k_B T_0/m} [\epsilon u'(x,t) + \epsilon^2 u''(x,t)]$) and will consider only the case of the hydrodynamic velocity since the results for the density and the temperature are analogous. Assuming that the first order perturbation (u') corresponds to a single mode we find that the perturbation $u''(x,t)$ is of the form,

$$u''(x,t) = u_0'' \exp(2\Omega t' + 2iks), \quad (19)$$

where u_0'' is a constant and k and Ω are determined from the linear hydrodynamic stability analysis. So, Bobylev's remark that higher harmonics are generated by nonlinearities is true but if the real part of Ω is negative, which is valid provided that $k < k_c$ as shown in Figs. 1 and 2, then the second harmonic does not give rise to an instability. The same argument can be used to show that the higher harmonics of the

form $\exp(n\Omega t' + niks)$, where n is a positive integer, are stable if $k < k_c$. A more detailed analysis is beyond the scope of this paper.

Bobylev's instability and other problems associated with the Burnett equations, or with the Chapman–Enskog expansion, has lead some workers in the field to search for other ways of dealing with the gradient expansion such as regularization techniques proposed by Rosenau [11] and the partial summation techniques as have been used by Gorban and Karlin and others [12–14]. Other authors have considered a subset or a superset of the Burnett equations [7,8] so that the corresponding equations are stable under small perturbations, or have used macroscopic arguments to derive Burnett like equations that are free from some problems associated with their origin as power series expansions [15].

On the other hand, the Navier–Stokes equations are linearly stable for all Knudsen numbers as follows from Eq. (15) [2], while this is a nice property of them it would be naive to claim that their description is correct for all Knudsen numbers as is clear from the following simple order of

magnitude estimation; under standard conditions, the mean free path is about 10^{-5} cm [10], for $k = 10^3$ it follows that L is of order 10^{-8} cm which is about the atomic diameter, a distance for which the description in terms of macroscopic quantities (continuum description) is completely unreliable.

The main result of this work is to point out that the hydrodynamic instability found by Bobylev [2] does not come as a surprise if we realize that the Burnett equations are expected to be valid for small Knudsen numbers. When this condition is not satisfied then there is no *a priori* reason to expect that the Burnett equations remain valid and their instability may be interpreted as a manifestation of the fact that we are outside of their range of validity. In fact, the value of k_c gives a quantitative criterion about the validity limits.

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