

Bobylev-Krook-Wu Modes for Multicomponent Gas Mixtures

Yu. N. Grigoryev*

*Institute of Computational Technologies, Siberian Branch of Russian Academy of Sciences,
Novosibirsk, 630090, Russia*

S. V. Meleshko

*Institute of Theoretical and Applied Mechanics, Siberian Branch of Russian Academy of Sciences,
Novosibirsk, 630090, Russia
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Exact invariant solutions of the spatially uniform Boltzmann equations, the so-called Bobylev-Krook-Wu modes, are presented in the explicit form for an arbitrary N -species gas mixture. The corresponding necessary and sufficient conditions imposed on the molecular parameters are formulated. The completeness of the results obtained is supported by the rigorous group analysis of the Boltzmann equations. [S0031-9007(98)06421-7]

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About two decades ago Bobylev [1] and, independently, Krook and Wu [2] obtained the exact solution of the Boltzmann kinetic equation (BE) for spatially uniform temporal relaxation of one-component gas. Now this solution is commonly known as the Bobylev-Krook-Wu (BKW) mode. The BKW mode is of physical interest for explicit modeling of some nonequilibrium threshold processes such as chemical reactions, thermonuclear fusion, etc. [2]. From this point of view, the analogous solutions for N -component gas mixture could be of even greater interest. The generalization of the solution to an arbitrary N -species gas mixture was announced by the authors [2] in [3]. However, their results have been actually presented for $N = 2$ only and even in this case appeared incomplete. It seemed [4] that the conditions of the BKW mode existence formulated in [3] could be weakened. As a matter of fact, the BKW modes were not considered in [4]. Recently, in [5] the BKW modes were obtained for a binary gas mixture but only in the asymptotic limit when the ratio of species masses tends to zero. In this case the authors of [5] have practically dealt with a single BE as in [1,2].

In this Letter we present the comprehensive results on the BKW modes for an arbitrary N -component mixture of monatomic gases. They are based on the rigorous calculation of the widest Lie group transformations admissible by the system of the BE. The Lie group allows us to describe uniquely the complete class of the invariant BKW solutions, in particular, the BKW modes that are the only members of the class expressed in elementary functions.

As in [3,4], we study gas of N species of molecules with Maxwellian interaction. The homogeneous relaxation is defined by the set of N velocity distribution functions (DF), $f_\alpha(\mathbf{v}_\alpha, t)$, which are the solutions of the Cauchy problem for the BE system [6]. For such a problem there are conservation laws of species concentrations and total kinetic energy of molecules. Under the chosen system of the dimensionless variables they are expressed as

$$n_\alpha(t) = \int d\mathbf{v}_\alpha f_\alpha(\mathbf{v}_\alpha, t) = n_\alpha(0), \quad \sum_{\alpha=1}^N n_\alpha = 1, \quad (1)$$

$$E(t) = \sum_{\alpha=1}^N \int d\mathbf{v}_\alpha v_\alpha^2 f_\alpha(\mathbf{v}_\alpha, t) = E(0) = 3. \quad (2)$$

We use the Bobylev approach [1,4] to the BE in terms of the Fourier transformation of the DF $\varphi_\alpha(\mathbf{k}_\alpha, t) = \int d\mathbf{v}_\alpha e^{i\mathbf{k}_\alpha \mathbf{v}_\alpha} f_\alpha(\mathbf{v}_\alpha, t)$. Then the BE system for DF isotropic in the velocity space is transformed to the system

$$\begin{aligned} \frac{\partial \varphi_\alpha(x_\alpha, t)}{\partial t} &= \sum_{\beta=1}^N \sigma_{\alpha\beta} \int_0^1 ds \\ &\times [\varphi_\alpha(x_\alpha(1 - \varepsilon_{\alpha\beta}s))\varphi_\beta(x_\alpha \varepsilon_{\alpha\beta}s) \\ &\quad - \varphi_\alpha(x_\alpha)\varphi_\beta(0)], \quad \alpha = 1, \dots, N, \end{aligned} \quad (3)$$

where $x_\alpha = k_\alpha^2/2$, $\varepsilon_{\alpha\beta} = 4m_\alpha m_\beta / (m_\alpha + m_\beta)^2$, and m_α is a molecular mass of α species. For simplicity we restrict our consideration to the Maxwellian isotropic scattering model as in [3]. Here $\sigma_{\alpha\beta}$ is a constant in the cross section for collision of α series with β series.

The conservation laws (1),(2) turn into the relations

$$\begin{aligned} \varphi_\alpha(0, t) &= n_\alpha, \quad \alpha = 1, \dots, N; \\ \sum_{\alpha=1}^N \frac{\partial \varphi_\alpha(0, t)}{\partial x_\alpha} &= -1. \end{aligned} \quad (4)$$

Using our approach [7] to the group analysis of the equations with nonlocal (integral) operators (see also Ref. [8]) the widest Lie group G^4 admissible by the system (3) was calculated. The basis of the group G^4 consists of the infinitesimal generators

$$\begin{aligned} X_1 &= \partial_t, & X_2 &= \sum_{\alpha=1}^N x_\alpha \varphi_\alpha \partial_{\varphi_\alpha}, \\ X_3 &= \sum_{\alpha=1}^N x_\alpha \partial_{x_\alpha}, & X_4 &= \sum_{\alpha=1}^N \varphi_\alpha \partial_{\varphi_\alpha} - t \partial_t. \end{aligned}$$

Here the action of the operator $\partial_{\varphi_\alpha}$ on the integrals in (3) is the Freshet differentiation. The class of the invariant BKW solutions is determined by the generator $X = X_2 - X_3 + c^{-1}X_1$, where c is some constant. Therefore, as in [1], one can search for the BKW solutions in the following form:

$$\varphi_\alpha(x_\alpha, t) = n_\alpha \exp(y_\alpha - x_\alpha) \left(1 + \sum_{k=1}^{\infty} a_k^{(\alpha)} \frac{y_\alpha^k}{k!} \right), \quad (5)$$

$$y_\alpha = \theta_0 e^{ct} x_\alpha.$$

The energy conservation law (4) gives the restriction

$$\sum_{\alpha=1}^N n_\alpha a_1^{(\alpha)} = -1. \quad (6)$$

By the substitution of Eqs. (5) in Eqs. (3) the recurrent systems of linear equations are derived for the coefficients $\mathbf{a}_k = (a_k^{(1)}, \dots, a_k^{(N)})$, $k = 1, \dots$;

$$(cE - B_k)\mathbf{a}_k = -cE\mathbf{a}_{k-1} + \mathbf{f}_k, \quad (7)$$

where the elements of the matrices B_k are expressed as

$$b_{\alpha\alpha}^{(k)} = \frac{1}{k(k+1)} \left[n_\alpha \sigma_{\alpha\alpha} (1-k) + \sum_{\beta=1}^N {}'n_\beta \sigma_{\alpha\beta} \sum_{m=2}^{k+1} (-1)^{m-1} \binom{k+1}{m} \varepsilon_{\alpha\beta}^{m-1} \right], \quad b_{\alpha\beta}^{(k)} = \frac{1}{k(k+1)} n_\alpha \sigma_{\alpha\beta} \varepsilon_{\alpha\beta}^k,$$

$$f_k^{(\alpha)} = \frac{1}{k(k+1)} \sum_{m=1}^{k-1} \left[n_\alpha \sigma_{\alpha\alpha} a_m^{(\alpha)} a_{k-m}^{(\alpha)} + \sum_{\beta=1}^N {}'n_\beta \sigma_{\alpha\beta} I(\varepsilon_{\alpha\beta}, k-m+1, m+1) a_m^{(\alpha)} a_{k-m}^{(\beta)} \right], \quad k > 1.$$

Here, the $I(\varepsilon, k, p)$ is a quotient of incomplete Euler beta function; the prime in the sum means the absence of the term with the index $\beta = \alpha$.

By virtue of the recurrent character of the system (5) one can cut the series in Eqs. (7) off if and only if $\mathbf{a}_2 = \mathbf{a}_3 = 0$. Then the inverse Fourier transformation of such a segment gives the BKW modes

$$f_\alpha(v_\alpha, t) = \frac{n_\alpha}{[2\pi T(t)]^{3/2}} \left[1 - a_1^{(\alpha)} \frac{1-T(t)}{T(t)} \left(\frac{v_\alpha^2}{2T(t)} - \frac{3}{2} \right) \right] \exp\left(-\frac{v_\alpha^2}{2T(t)} \right), \quad \alpha = 1, \dots, N, \quad T(t) = 1 - \theta_0 e^{ct}, \quad (8)$$

where the constant θ_0 is determined by the arbitrary choice of time origin. It is essential to emphasize that here in contrast to [3] the identical temperature functions for all the species are not postulated, but are the consequence of the strict calculation of the BKW class generator.

To nullify \mathbf{a}_2 in any case the uniformity of the corresponding system (7) is necessary. This is equivalent to the requirement $c\mathbf{a}_1 = \mathbf{f}_2$. If the parameter c coincides with none of the nonzero eigenvalues of the matrix B_1 , then the solution of the system (7) for $k=1$, satisfying Eq. (6), is $\mathbf{a}_1 = (-1, \dots, -1)$. From the uniformity condition, the following restrictions are obtained:

$$c = -\frac{1}{6} \left[n_\alpha \sigma_{\alpha\alpha} + \sum_{(\beta)} {}'n_\beta \sigma_{\alpha\beta} (3 - 2\varepsilon_{\alpha\beta}) \varepsilon_{\alpha\beta} \right], \quad (9)$$

$$\alpha = 1, \dots, N.$$

Under these conditions the matrices $(cE - B_k)$, $k = 2, 3$, have simultaneously the rank $p = N - 1$. In other words, both of the matrices B_2, B_3 have a simple "resonant" eigenvalue c in the form (9). If we nullify any single component of vectors \mathbf{a}_2 and \mathbf{a}_3 , then the series in (5) will be broken. As a result we obtain the BKW modes (8). In this case the BKW modes are non-negative for $v_\alpha \in [0, \infty)$, $t > 0$, when $\theta_0 \in [0, 2/5]$.

The necessary expression for parameter c ,

$$c = -\frac{1}{6N} \sum_{\alpha=1}^N \left[n_\alpha \sigma_{\alpha\alpha} + \sum_{(\beta)} {}'n_\beta \sigma_{\alpha\beta} (3 - 2\varepsilon_{\alpha\beta}) \varepsilon_{\alpha\beta} \right],$$

can be derived by the symmetrization of the conditions (9). As can be readily seen this is a direct generalization of obtaining the BKW mode in one-component gas [1].

However, in the multicomponent gas mixture there is another way to obtain the BKW modes. Let the molecular parameters satisfy the following set of constraints:

$$c = -\frac{1}{2} \sigma_{\alpha\beta} \varepsilon_{\alpha\beta}, \quad \alpha < \beta, \quad \alpha = 1, \dots, r, \quad (10)$$

$$\beta = 2, \dots, N.$$

Then c is an r -multiple eigenvalue of the matrix B_1 . Thus, the solution of the system (7) for $k=1$ satisfying (6) is $a_1^{(\alpha)} = -a^{(\alpha)}$, $\alpha = 1, \dots, r$; $a_1^{(\alpha)} = -(1 - \sum_{\alpha=1}^r n_\alpha a^{(\alpha)}) / \sum_{\alpha=r+1}^N n_\alpha$, $\alpha \geq r$. Here, the coefficients $a^{(\alpha)}$ are arbitrarily chosen.

For uniformity of the systems (7) for $k=2, 3$ it is necessary to impose additional restrictions on the molecular parameters of species,

$$c = -\frac{1}{6} \left[n_\alpha \sigma_{\alpha\alpha} a_1^{(\alpha)} + \sum_{(\beta)} {}'n_\beta \sigma_{\alpha\beta} a_1^{(\beta)} (3 - 2\varepsilon_{\alpha\beta}) \varepsilon_{\alpha\beta} \right], \quad (11)$$

$$\alpha = 1, \dots, N.$$

If the conditions (10) and (11) are fulfilled we again obtain the BKW modes (8). In this case the BKW modes will be non-negative for $v_\alpha \rightarrow \infty$ if all the $a^{(\alpha)} \geq 0$, $\alpha = 1, \dots, r$; $\sum_{\alpha=1}^r a^{(\alpha)} n_\alpha < 1$. Correspondingly, for $v_\alpha \rightarrow 0$ they are non-negative if the constant θ_0 varies in the limits $0 \leq \theta_0 \leq \min[\theta_{01}, \theta_{02}]$, where $\theta_{01} = 2/(2 + 3a_M)$, $a_M = \max_{(\alpha)} a^{(\alpha)}$; $\theta_{02} = 2/[2 + 3(1 - \sum_{\alpha=1}^r a^{(\alpha)} n_\alpha) / \sum_{\alpha=r+1}^N n_\alpha]$.

The choice of some $a^{(\alpha)} = 0$ means that the corresponding BKW modes are transformed into unsteady Maxwellian DF with the temperature $T(t)$.

The restrictions (9), (10), and (11), as well as the dependence on the unique constant c [universal temperature function $T(t)$] for the presented BKW solutions (8), are necessary and sufficient conditions, which cannot be weakened (compare Ref. [3]).

The BKW modes obtained keep the same form for any Maxwell molecules with arbitrary dependence on the scattering angle in a differential cross section. In such a general case the restrictions (9), (10), and (11) contain some power moments (functionals) of the cross section.

The mixture of N series of monatomic gases is characterized by a set of $3N$ parameters $\{m_\alpha, n_\alpha, \sigma_{\alpha\alpha}\}_{\alpha=1}^N$. The question naturally arises as to how many of them can be chosen arbitrarily in order to satisfy simultaneously the conditions (9) or (10), (11) to which it is necessary to add the conservation law of concentrations (1). In the case of the BKW modes with $\mathbf{a}_1 = (-1, \dots, -1)$ a complete number of the restrictions is $C = N$, and $2N$ of parameters remain free. For the BKW modes under conditions (10) and (11) a total number of connections is equal to $C = N(r + 1) - r(r + 3)/2$, $0 < r \leq N - 1$. Here, it is possible that $C \geq 3N$ and then it is necessary to consider the solvability of an overdetermined system of the conditions.

For $N = 2$ all the calculations are very simple because the eigenvalues of matrices B_k are explicitly derived. In particular, the restrictions (9) are reduced to the relation $n_1\sigma_{11} + n_2\sigma_{12}\varepsilon_{12}(3 - 2\varepsilon_{12}) = n_2\sigma_{22} + n_1\sigma_{12}\varepsilon(3 - 2\varepsilon_{12})$ obtained in [3]. However, another condition given in [3] does not follow from our results and is really erroneous.

The presented BKW modes allow us to model in an explicit form many physically interesting kinetic processes, even for $N = 2$, that had been previously available only through a very precise numerical computing of the BE.

For example, one can investigate the relaxation in mixtures with disparate species masses such as Lorentz gas or Rayleigh gas. It is interesting to see directly from (8), (10), and (11) that in contrast to the widespread conviction about the relaxation to equilibrium in such mixtures in this case the process has no two-stage character.

Further, it is possible to study the behavior of nonequilibrium impurity in a Maxwellian bath or vice versa of Maxwellian impurity on the nonequilibrium background. On the basis of the BKW modes (8) one can explicitly calculate the rates of certain gas-phase reactions and estimate their deviation from the Arrhenius kinetics. Choosing the BKW mode with $a^{(1)} > 1$ and conditions (10) and (11) one can observe the overpopulation of the far tail of the DF. This phenomenon allows one to model operating by some threshold kinetic processes.

The possibilities of the BKW modes for modeling of the spatially homogeneous gas systems initially not in equilibrium will be discussed in detail elsewhere.

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*Email address: grigor@adm.ict.nsk.su

- [1] A. V. Bobylev, Proc. USSR Acad. Sci. **225**, 1041 (1975).
- [2] M. Krook and T. T. Wu, Phys. Rev. Lett. **36**, 1107 (1976).
- [3] M. Krook and T. T. Wu, Phys. Rev. Lett. **38**, 991 (1977).
- [4] A. V. Bobylev, Proc. USSR Acad. Sci. **250**, 340 (1980).
- [5] A. V. Bobylev and G. Spiga, Riv. Mat. Univ. Parma. **5**, 255 (1992).
- [6] J. H. Ferziger and H. G. Kaper, *Mathematical Theory of Transport Processes in Gases* (North-Holland, Amsterdam, London, 1972).
- [7] Yu. N. Grigoryev and S. V. Meleshko, Proc. USSR Acad. Sci. **297**, 323 (1987).
- [8] *CRC Handbook of Lie Group Analysis of Differential Equations*, edited by M. H. Ibragimov (CRC Press, Boca Raton, FL, New York, London, Tokyo, 1995).