

Kinetic Theory for Mixtures of Dilute Gases of Linear Rotating Molecules in an External Magnetic Field (Formal Theory)

H. H. RAUM and W. E. KÖHLER

Institut für Theoretische Physik der Universität Erlangen-Nürnberg, Erlangen

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A transport theory is developed for mixtures of dilute gases consisting of linear rotating diamagnetic molecules in an external homogeneous magnetic field. This formalism is adequate for a treatment of the Senftleben-Beenakker effects for gas mixtures. Starting point is the system of linearized Waldmann-Snider equations. A complete scheme of orthogonal expansion tensors in velocity and rotational angular momentum is given, up to tensors of third rank and power. The moment method is applied to solve the coupled system of Waldmann-Snider equations and the resulting system of transport relaxation equations (TRE) is stated up to third rank tensor equations. The local conservation laws — linearized in the deviation from thermal equilibrium — are derived from the TRE.

In 1930 SENFTLEBEN¹ first observed that the transport properties of dilute paramagnetic gases are influenced by an applied magnetic field. Since BEENAKKER et al.² in 1962 found that the effect is common to all polyatomic gases, much work on the Senftleben-Beenakker effect has been done experimentally and theoretically³. All calculations performed started with an appropriate Boltzmann equation for rotating molecules; e.g., the classical and somewhat artificial collision model of KAGAN and MAKSIMOV^{4,5} the model of rough spheres⁶ and the more realistic quantum mechanical kinetic equation of WALDMANN and SNIDER^{7,8,9} have been used.

The Waldmann-Snider equation has opened the understanding of the Senftleben-Beenakker effect from the quantum mechanics of molecular collision. Starting from the linearized Waldmann-Snider equation and using a Chapman-Enskog procedure, McCOURT and SNIDER¹⁰ have investigated the change of transport coefficients (heat conductivity and viscosity) in an applied magnetic field for pure gases of rotating molecules. These changes of trans-

port coefficients occur only if the binary molecular scattering amplitude (matrix with respect to magnetic quantum numbers) possesses a nonspherical part, which, in turn is related to the nonspherical part of the intermolecular interaction¹¹. The nonspherical scattering amplitude gives rise to a partial alignment of the rotational angular momenta of the colliding molecules. The saturation values of the changes of the transport coefficients in a magnetic field are related to this collisional alignment via certain collision brackets of the linearized Waldmann-Snider collision term.

There are two reasons mainly why the transport properties of gas mixtures in a magnetic field should be studied. Firstly, it is interesting to study the dependence of the magnetic field effects on the composition of the mixture, especially on the mole fraction. Secondly, the Senftleben-Beenakker effect in gas mixtures is an important tool for obtaining information on the nonspherical interaction between unlike rotating molecules or between rotating molecules and noble gases. Much experimental work is

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¹ H. SENFTLEBEN, *Physik. Z.* **31**, 822, 961 [1930].

² J. J. M. BEENAKKER, G. SCOLES, H. F. P. KNAAP, and R. M. JONKMAN, *Phys. Letters* **2**, 5 [1962].

³ For a survey see J. J. M. BEENAKKER in „Festkörperprobleme VIII“, ed. O. MADELUNG, Vieweg, Braunschweig 1968 and J. J. M. BEENAKKER and F. R. McCOURT, *Ann. Rev. Phys. Chem.* **21**, [1970].

⁴ Y. M. KAGAN and L. A. MAKSIMOV, *Sov. Phys. JETP* **14**, 604 [1962]; **24**, 1272 [1967].

⁵ H. F. P. KNAAP and J. J. M. BEENAKKER, *Physica* **33**, 643 (1967).

⁶ W. M. KLEIN, D. K. HOFFMAN, and J. S. DAHLER, *J. Chem. Phys.* **49**, 2321 [1968]. — F. R. McCOURT,

H. F. P. KNAAP, and H. MORAAL, *Physica* **43**, 485 [1969], — H. MORAAL, F. R. McCOURT, and H. F. P. KNAAP, *Physica* **45**, 455 [1969].

⁷ L. WALDMANN, *Z. Naturforsch.* **12a**, 660 [1957]; **13a**, 609 [1958] and in „Statistical Mechanics of Equilibrium and Nonequilibrium“, ed. Meixner, North Holland 1965, and in “Fundamental Problems in Statistical Mechanics II”, ed. Cohen, North Holland 1968.

⁸ R. F. SNIDER, *J. Chem. Phys.* **32**, 1051 [1960].

⁹ S. HESS, *Z. Naturforsch.* **22a**, 1871 [1967].

¹⁰ F. R. McCOURT and R. F. SNIDER, *J. Chem. Phys.* **41**, 3185 [1964]; **46**, 2387 [1967]; **47**, 4117 [1967].

¹¹ S. HESS and W. E. KÖHLER, *Z. Naturforsch.* **23a**, 1904 [1968]. — W. E. KÖHLER, S. HESS, and L. WALDMANN, *Z. Naturforsch.* **25a**, 336 [1970].



underway on this subject for the heat conductivity and viscosity by the molecular physics group of the Kamerlingh-Onnes Laboratory in Leiden. Measurements of the Senftleben effect (paramagnetic gases) for binary mixtures have been carried out by SENFTLEBEN and coworkers¹². The SENFTLEBEN-BEENAKKER effect of diffusion has been studied by VUGTS, TIP and LOS¹³, but no effect could be found within their accuracy of measurement. Recently, also the influence of a magnetic field on the thermal diffusion has been investigated by HIDALGO et al.¹⁴, but with a negative result, too.

Theoretical treatments of mixtures of dilute gases with internal degrees of freedom have been carried out by WALDMANN and TRÜBENBACHER¹⁵ and by ZHDANOV and ALIEFSKY¹⁶ using the WANG CHANG-UHLENBECK equation¹⁷. But the Wang Chang-Uhlenbeck equation can only be used to study scalar phenomena (e.g. bulk viscosity and sound absorption), i.e. phenomena which are related to collision brackets containing the differential cross section averaged over magnetic quantum numbers. The magnetic field effects are tensorial phenomena and their proper treatment is based on the Waldmann-Snider equation. Theoretical results for the shear viscosity tensor for binary mixtures of diamagnetic gases have been obtained by TIP¹⁸ with a classical treatment.

In the present paper, the quantum mechanical kinetic equation of Waldmann and Snider will be applied to mixtures of dilute gases consisting of linear diamagnetic molecules in an external homogeneous magnetic field. The moment method will be used to obtain the system of linearized (in the deviation from thermal equilibrium) transport relaxation equations. As a preliminary application the local conservation laws are derived. The magnetic field effects will be treated in a following paper, the relevant equations needed appear in this paper.

It should be mentioned that the idea of solving a Boltzmann equation with the moment method dates back to MAXWELL¹⁹. It has been continued by GRAD²⁰ and WALDMANN extended the method to the kinetic theory of particles with internal degrees of freedom, namely to rough spherical molecules²¹ and to spin particles²². A comprehensive treatment of the moment method is presented in a paper of HESS and WALDMANN²³ dealing with spin particles and the present paper may be considered as a generalization for mixtures of rotating molecules. Recently, the 17-moment method has been applied to the polyatomic gas described by the Wang-Chang-Uhlenbeck equation by McCORMACK²⁴. This procedure, however, proves to be a special case of our treatment if an "isotropic" approximation is made, i.e. the rotational angular momentum anisotropy of the one-particle distribution function is neglected. Finally, it should be mentioned that the moment equations are not only useful for the calculation of transport coefficients in external magnetic and electric fields but also for the treatment of Rayleigh light scattering²⁵ and flow birefringence²⁶ in dilute polyatomic gases.

I. General Considerations

1. Single particle description

Consider a non-reacting gas mixture of linear molecules the K components of which are labelled by the subscripts i or j ($i, j = 1, \dots, K$).

A molecule of the species i with mass m_i and internal rotational energy $E_i(J)$ (the molecules are assumed to be in the vibrational and electronic ground states) will be described by its position \mathbf{x} , its velocity \mathbf{c} , and the vector operator of its internal rotational angular momentum $\hbar \mathbf{J}$ which satisfies the commutation relation

$$J_\mu J_\nu - J_\nu J_\mu = i \varepsilon_{\mu\nu\lambda} J_\lambda. \quad (1.1)$$

¹² H. SENFTLEBEN and J. PIETZNER, *Physik. Z.* **34**, 834 [1933]; *Ann. Physik* **30**, 541 [1937].

¹³ H. F. VUGTS, A. TIP, and J. LOS, *Physica* **38**, 579 [1968].

¹⁴ M. A. HIDALGO, J. M. SAVIRON, and D. GONZALEZ, *Physica* **46**, 41 [1970].

¹⁵ L. WALDMANN and E. TRÜBENBACHER, *Z. Naturforsch.* **17a**, 363 [1962].

¹⁶ M. Y. ALIEFSKY and V. M. ZHDANOV, *Zh. Eksper. Teor. Fiz. (USSR)* **55**, 221 [1968].

¹⁷ C. S. WANG CHANG, G. E. UHLENBECK, and J. DE BOER, in "Studies in Statistical Mechanics", Vol II, North Holland, Amsterdam 1964.

¹⁸ A. TIP, *Physica* **37**, 411 [1967].

¹⁹ J. C. MAXWELL, *Scientific Papers*, Dover Publ., New York (first published in 1890).

²⁰ H. GRAD, *Comm. Pure Appl. Math.* **2**, 331 [1949].

²¹ L. WALDMANN, *Z. Naturforsch.* **18a**, 1033 [1963].

²² L. WALDMANN, *Z. Naturforsch.* **15a**, 19 [1960].

²³ S. HESS and L. WALDMANN, *Z. Naturforsch.* **21a**, 1529 [1966]; **23a**, 1893 [1968].

²⁴ F. J. McCORMACK, *Phys. Fluids* **11**, 2533 [1968].

²⁵ S. HESS, *Z. Naturforsch.* **24a**, 1675 [1969]; **25a**, 350 [1970].

²⁶ S. HESS, *Phys. Letters* **30A**, 239 [1969]. *Springer Tracts in Modern Physics* **54**, 136 [1970].

For Greek subscripts (which are exclusively used for the spatial indices of Cartesian tensors) the summation convention is used. The isotropic tensor of third rank, $\varepsilon_{\mu\nu\lambda}$, is totally antisymmetric with $\varepsilon_{123} = 1$.

2. Description of the collision

The gas mixture shall be sufficiently dilute so that we can restrict ourselves to two-particle collisions. The collisions will occur between molecules of the same species as well as with molecules of all other sorts.

The mechanical conservation laws for the collision of two molecules (which, in general, is an energetically inelastic one) are:

$$m_i \mathbf{c}'_I + m_j \mathbf{c}'_{II} = m_i \mathbf{c}_I + m_j \mathbf{c}_{II}, \quad (1.2)$$

$$\begin{aligned} \frac{m_i}{2} c'^2_I + \frac{m_j}{2} c'^2_{II} + E'_{iI} + E'_{jII} \\ = \frac{m_i}{2} c^2_I + \frac{m_j}{2} c^2_{II} + E_{iI} + E_{jII}, \end{aligned} \quad (1.3)$$

where in the case of diatomic rotating molecules

$$E_{iI} = \frac{\hbar^2 J_I(J_I + 1)}{2 \Theta_i} \quad \text{etc.}$$

with Θ_i being the molecular moment of inertia. Here and in the following, primed and unprimed quantities denote the dynamical variables before and after the collision, respectively.

If center of mass and relative velocities are introduced by

$$\tilde{\mathbf{c}} = \frac{m_i}{m_i + m_j} \mathbf{c}_I + \frac{m_j}{m_i + m_j} \mathbf{c}_{II}, \quad (1.4)$$

$$\mathbf{g} = \mathbf{g} \mathbf{e} = \mathbf{c}_I - \mathbf{c}_{II}, \quad (1.5)$$

and analogously for the primed quantities, the energy equation (with $m_{ij} = m_i m_j / (m_i + m_j)$ being the reduced mass) is given by

$$\frac{m_{ij}}{2} g'^2 + E'_{iI} + E'_{jII} = \frac{m_{ij}}{2} g^2 + E_{iI} + E_{jII} \equiv E. \quad (1.6)$$

For the quantum mechanical description of the collision the binary scattering amplitude operator¹¹ is used. If the internal rotational eigenstates of a molecule are denoted by $|JM\rangle$ (J is the magnitude of the rotational angular momentum and M is the magnetic quantum number), the projection operator on the J -subspace is given by

$$P^J = \sum_M |JM\rangle \langle JM|. \quad (1.7)$$

Consider molecule I (II) to be in a rotational level described by $J'_I(J'_{II})$ before the collision and in a rotational level $J_I(J_{II})$ after the collision. Then the single channel scattering amplitude operator (matrix with respect to magnetic quantum numbers) is given by

$$a^{J_I J_{II}, J'_I J'_{II}}_{ij}(\mathbf{e}, \mathbf{e}', E) = P^{J_I} P^{J_{II}} a_{ij}(\mathbf{e}, \mathbf{e}', E) P^{J'_I} P^{J'_{II}}, \quad (1.8)$$

where the binary scattering amplitude a_{ij} is connected with the transition operator T_{ij} (which is connected with the interaction potential via the Lippmann-Schwinger integral equation, cf. Ref. ¹¹) by

$$a_{ij}(\mathbf{k}, \mathbf{k}') = -\frac{m_{ij}}{2\pi\hbar^2} \langle \mathbf{k} | T_{ij} | \mathbf{k}' \rangle, \quad (1.9)$$

where \mathbf{k} and \mathbf{k}' are the relative wave vectors after and before the collision, respectively.

In a more compact notation the abbreviation

$$a^{J_I J_{II}, J'_I J'_{II}}_{ij}(\mathbf{e}, \mathbf{e}', E) = a^{I, II, I', II'}_{ij} \quad (1.10)$$

for the single channel scattering amplitude operator is used. The hermitian adjoint operator $a^{J_I J_{II}, J'_I J'_{II}}_{ij}(\mathbf{e}, \mathbf{e}', E)$ is defined in the usual way used for matrices and is abbreviated with $a^{I, II, I', II'}_{ij}$.

The rotational angular momentum dependence of $a^{I, II, I', II'}_{ij}$ in the case where the nonspherical part of the intermolecular potential is small compared with the spherical part has been discussed in Ref. ¹¹. The single channel scattering amplitude satisfies the optical theorem

$$\begin{aligned} \sum_{J'_I, J'_{II}} \int a^{I, II, I', II'}_{ij} a^{I, II, I', II'}_{ij} g' d^2 e' \\ = \sum_{J'_I, J'_{II}} \int \tilde{a}^{I, II, I', II'}_{ij} \tilde{a}^{I, II, I', II'}_{ij} g' d^2 e' \\ = \frac{\hbar}{i m_{ij}} \{ a^{I, II, I, II}_{ij}(0) - a^{I, II, I, II}_{ij}(0) \}, \end{aligned} \quad (1.11)$$

where $a^{I, II, I, II}_{ij}(0)$ is the single channel scattering amplitude in the forward direction $\mathbf{e} = \mathbf{e}'$ and $\tilde{a}^{I, II, I', II'}_{ij} = a^{I, II, I', II'}_{ij}(\mathbf{e}', \mathbf{e}, E)$.

If \mathbf{J} is the angular momentum operator satisfying (1.1) and $\Phi_i(t, \mathbf{x}, \mathbf{c}, \mathbf{J})$ is any operator function, the following notation, compatible with the definition (1.10) will be used:

$$\begin{aligned} P^{J_I} \Phi_i(t, \mathbf{x}, \mathbf{c}_I, \mathbf{J}) P^{J_I} &\equiv \Phi_i^I; \\ P^{J'_I} \Phi_i(t, \mathbf{x}, \mathbf{c}'_I, \mathbf{J}) P^{J'_I} &\equiv \Phi_i^{I'} \quad \text{etc.} \end{aligned} \quad (1.12)$$

II. Description of the Gas Mixture, Mean Values, Kinetic Equation

For a statistical description of the gas mixture the semi-quantum mechanical distribution opera-

tors (operators with respect to magnetic quantum numbers) are introduced by

$$P^J f_i(t, \mathbf{x}, \mathbf{c}, \mathbf{J}) P^J \equiv f_i^J(t, \mathbf{x}, \mathbf{c}). \quad (2.1)$$

The f_i^J are polynomials in $P^J \mathbf{J} P^J$ with the maximal power $2J$ and they are normalized to give the particle concentration of the i -th component (tr = trace over the $2J+1$ magnetic quantum numbers)

$$n_i(t, \mathbf{x}) = \sum_J \text{tr} \int f_i^J(t, \mathbf{x}, \mathbf{c}) d^3c. \quad (2.2)$$

With $\varrho_i = m_i n_i$ also particle- and mass densities of the mixture are introduced by

$$n = \sum_{i=1}^K n_i, \quad \varrho = \sum_{i=1}^K \varrho_i.$$

The local mean value per particle of some operator function $P^J \Psi_i(t, \mathbf{x}, \mathbf{c}, \mathbf{J}) P^J \equiv \Psi_i^J(t, \mathbf{x}, \mathbf{c})$ results from the well known von Neumann formula

$$\langle \Psi \rangle_i = \sum_J \text{tr} \int \Psi_i^J \frac{f_i^J}{n_i} d^3c, \quad (2.3)$$

and for the whole mixture

$$\langle \Psi \rangle = \frac{1}{n} \sum_{i=1}^K n_i \langle \Psi \rangle_i. \quad (2.4)$$

The change of the distribution matrix f_i^J for the species i with time is governed by the Waldmann-Snider equation for non-reacting gas mixtures

$$\begin{aligned} \mathcal{D}_i(f)^I = & \sum_{j=1}^K \sum_{J_{II}} \text{tr}_{II} \int d^3c_{II} \\ & \cdot \left\{ \sum_{J', I', II'} \int a_{ij}^{II, I', II'} f_i^I f_j^{II'} a_{ij}^{I', II', III} g' d^2e' \right. \\ & \left. - [a_{ij}^{III, III}(0) f_i^I f_j^{II} - f_i^I f_j^{II} a_{ij}^{I, II, III}(0)] \right\}. \end{aligned} \quad (2.5)$$

In Eq. (2.5) the abbreviations $f_i^I \equiv f_i^J(t, \mathbf{x}, \mathbf{c}_I)$ etc. have been used.

The streaming operator $\mathcal{D}_i(f)^I$ is given by

$$\mathcal{D}_i(f)^I = \frac{\partial f_i^I}{\partial t} + \mathbf{c}_I \cdot \frac{\partial f_i^I}{\partial \mathbf{x}} + \frac{\omega_{Hi}}{i} [\mathbf{h} \cdot \mathbf{J}, f_i^I]_-, \quad (2.6)$$

analogously to the pure gas. In Eq. (2.6) \mathbf{h} is a unit vector parallel to the direction of the external magnetic field $\mathbf{H} = H\mathbf{h}$ and ω_{Hi} denotes the frequency of Larmor precession of the diamagnetic moment

$$\mu_i = g_i \mu_N J$$

(μ_N nuclear magneton) of the molecule about \mathbf{h}

$$\omega_{Hi} = \mu_i H / \hbar J = g_i \mu_N H / \hbar. \quad (2.7)$$

III. Discussion of the Linearized Waldmann-Snider Equations

The gas mixture is assumed to be in a state close to thermal equilibrium at temperature T_0 . The equilibrium distribution function is

$$f_i^{(0)}(c, J) = n_i^{(0)} (Q_i)^{-1} \left(\frac{m_i}{2\pi k_B T_0} \right)^{3/2} \cdot \exp \left[-\frac{1}{k_B T_0} \left(\frac{m_i}{2} c^2 + E_i(J) \right) \right], \quad (3.1)$$

where $Q_i = \sum_J (2J+1) \exp(-E_i(J)/k_B T_0)$ is the rotational partition function and k_B is Boltzmann's constant. The temperature and the magnetic field strength are chosen such that a contribution of the magnetic energy $\mu_i \cdot \mathbf{H}/k_B T_0$ in the exponential in (3.1) can be neglected and furthermore the influence of the magnetic field on the collision process has been disregarded in the collision term occurring in Eq. (2.5). For a detailed discussion of these problems see Ref. 9.

The non-equilibrium distribution operator is now written in the form

$$f_i^J(t, \mathbf{x}, \mathbf{c}) = f_i^{(0)}(c, J) (1 + \Phi_i^J(t, \mathbf{x}, \mathbf{c})). \quad (3.2)$$

In Eq. (3.2) and in the following equations, quantities which are matrices with respect to the $(2J+1)$ magnetic quantum numbers have a superscript J while in functions which depend only on J^2 ("classical" functions $\Phi_i(t, \mathbf{x}, \mathbf{c}, J)$) J appears as argument or as subscript in an abbreviating notation, e.g. $\Phi_{iJ} = \Phi_i(t, \mathbf{x}, \mathbf{c}, J)$.

If deviations from thermal equilibrium are small, terms quadratic in Φ_i may be neglected in Eq. (2.5) and one has

$$\mathcal{D}_i(\Phi)^I + \sum_{j=1}^K (\omega_{ij}^I(\Phi)^I + \omega_{ij}^{I \perp}(\Phi)^I) = 0, \quad i = 1, \dots, K, \quad (3.3)$$

where, following WALDMANN²⁷, the collision term has been split into two parts, the first one of which

²⁷ L. WALDMANN, in „Transporterscheinungen in Gasen von mittlerem Druck“ in Handbuch der Physik, Bd. 12, p. 420, ed. S. FLÜGGE, Berlin-Heidelberg 1958; see also in “Molecular Theory of Gases and Liquids” by J. O. HIRSCHFELDER, C. F. CURTISS, and R. B. BIRD, John Wiley, New York 1964.

is a functional of Φ_i , the second one of Φ_j . The two parts are obtained from (2.5) and (3.3) as

$$\omega_{ij}^{\square\square}(\Phi)^I = - \sum_{J_{II}} \text{tr}_{II} \int d^3c_{II} f_{jII}^{(0)} \left\{ \sum_{J'_I, J'_{II}} \int a_{ij}^{II, I' II'} \Phi_i^{I'} a_{ij}^{I' II', II} g' d^2e' - \frac{\hbar}{i m_{ij}} [a_{ij}^{II, II} (0) \Phi_i^I - \Phi_i^I a_{ij}^{II, II} (0)] \right\}, \quad (3.4a)$$

and

$$\omega_{ij}^{\square\square}(\Phi)^I = - \sum_{J_{II}} \text{tr}_{II} \int d^3c_{II} f_{jII}^{(0)} \left\{ \sum_{J'_I, J'_{II}} \int a_{ij}^{II, I' II'} \Phi_j^{II'} a_{ij}^{I' II', II} g' d^2e' - \frac{\hbar}{i m_{ij}} [a_{ij}^{II, II} (0) \Phi_j^{II} - \Phi_j^{II} a_{ij}^{II, II} (0)] \right\}. \quad (3.4b)$$

If $\Phi_i(t, \mathbf{x}, \mathbf{c}, \mathbf{J})$ is a „classical” function (isotropic approximation of the distribution matrix with respect to the orientations of the molecules) the expressions (3.4a, b) reduce to the form

$$\omega_{ij}^{\square\square}(\Phi_{\text{class}})^I = \sum_{J_{II}, J'_I, J'_{II}} \int \int d^3c_{II} f_{jII}^{(0)} (\Phi_{iI} - \Phi_{iI'}) \text{tr}_{II} [a_{ij}^{II, I' II'} a_{ij}^{I' II', II} g' d^2e', \quad (3.5a)$$

$$\omega_{ij}^{\square\square}(\Phi_{\text{class}})^I = \sum_{J_{II}, J'_I, J'_{II}} \int \int d^3c_{II} f_{jII}^{(0)} (\Phi_{jII} - \Phi_{jII'}) \text{tr}_{II} [a_{ij}^{II, I' II'} a_{ij}^{I' II', II} g' d^2e'. \quad (3.5b)$$

The following collision brackets are defined from the collision terms (3.4a) and (3.4b):

$$\langle \Psi \omega(\Phi) \rangle_{ij}^{\square\square} = \sum_{J_I} \text{tr}_I \int \frac{f_i^{(0)}}{n_i^{(0)}} \Psi_i^I \omega_{ij}^{\square\square}(\Phi)^I d^3c_I, \quad (3.6a)$$

and

$$\langle \Psi \omega(\Phi) \rangle_{ij}^{\square\square} = \sum_{J_I} \text{tr}_I \int \frac{f_i^{(0)}}{n_i^{(0)}} \Psi_i^I \omega_{ij}^{\square\square}(\Phi)^I d^3c_I, \quad (3.6b)$$

where Ψ, Φ are arbitrary functions of $t, \mathbf{x}, \mathbf{c}, \mathbf{J}$.

$$\text{The collision brackets} \quad \langle \Psi \omega(\Phi) \rangle_i \equiv \langle \Psi \omega(\Phi) \rangle_{ii}^{\square\square} + \langle \Psi \omega(\Phi) \rangle_{ii}^{\square\square} \quad (3.7)$$

are identical with the collision brackets $\langle \Psi \omega(\Phi) \rangle_0$ for the pure gas of species i which, e.g. have been investigated by HESS and WALDMANN²³ for spin particles and which have also been considered by McCOURT and SNIDER¹⁰.

IV. Application of the Moment Method to the Linearized Boltzmann Equations

1. Expansion tensors

After WALDMANN²² and HESS and WALDMANN²³ the function Φ_i occurring in Eq. (3.2) is expanded into a complete system of orthogonal irreducible tensors built up from velocity \mathbf{c} and rotational angular momentum \mathbf{J}

$$\Phi_i(t, \mathbf{x}, \mathbf{c}, \mathbf{J}) = \sum_{P=\pm 1} \sum_{l'=0}^{\infty} \sum_{k'=1}^{\infty} \Phi_{i\mu_1' \dots \mu_{l'}'}^{(Pk')}(\mathbf{c}, \mathbf{J}) a_{i\mu_1' \dots \mu_{l'}'}^{(Pk')}(t, \mathbf{x}). \quad (4.1)$$

Expansion tensors of the same rank l' and the same parity $P (= \pm 1)$ will be labelled with superscripts $k' = 1, 2, 3, \dots$ with respect to a special scheme of expansion. The time and space dependences of Φ_i are contained in the expansion coefficients $a_{i\mu_1' \dots \mu_{l'}'}^{(Pk')}$. The tensors are normalized in the following way (with respect to the equilibrium distribution function)

$$\langle \Phi_{\mu_1 \dots \mu_{l'}}^{(Pk)} \Phi_{\mu_1' \dots \mu_{l'}'}^{(P'k')} \rangle_i^{(0)} = \delta_{ll'} \delta^{PP'} \delta^{kk'} \Delta_{\mu_1 \dots \mu_{l'}, \mu_1' \dots \mu_{l'}'}^{(l)}. \quad (4.2)$$

The isotropic tensor $\Delta_{\mu_1 \dots \mu_{l'}, \mu_1' \dots \mu_{l'}'}^{(l)}$, when applied to an arbitrary l -th rank tensor, projects out the symmetric irreducible part of this tensor. For further properties of these isotropic tensors see HESS²⁸.

²⁸ S. HESS, Z. Naturforsch. **23a**, 1095 [1968].

Inserting (4.1) in (3.2) and (2.3) shows the physical meaning of the coefficients $a_{i\mu_1\ldots\mu_l}^{(Pk)}$ in consequent linearization (put $n_i \approx n_i^{(0)}$)

$$a_{i\mu_1\ldots\mu_l}^{(Pk)}(t, \mathbf{x}) = \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} \rangle_i, \quad (4.3)$$

with the exception of $\Phi_i^{(+1)} = 1$, where $a_i^{(+1)} = \frac{n_i - n_i^{(0)}}{n_i^{(0)}}$ denotes the deviation of the particle number density of species i from that at thermal equilibrium.

2. The general system of linearized transport relaxation equations

Inserting the expansion (4.1) in the linearized Waldmann-Snider equations (3.3), multiplying (3.3) with an arbitrary expansion tensor $\Phi_{i\mu_1\ldots\mu_l}^{(Pk)}$ and taking the mean values $\langle \cdots \rangle^{(0)}$ with respect to the equilibrium distribution function results in the general transport relaxation equations.

The time derivative in the streaming operator (2.6) just gives $(\partial/\partial t) a_{i\mu_1\ldots\mu_l}^{(Pk)}(t, \mathbf{x})$.

From the convection term $c_\lambda(\partial/\partial x_\lambda)$ three contributions are obtained, namely

$$\begin{aligned} \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} c_\lambda \Phi_{\mu_1'\ldots\mu_{l-1}'}^{(-Pk')} \rangle_i^{(0)} &= \langle Plk | c | -P(l-1)k' \rangle_i^{(0)} \Delta_{\mu_1\ldots\mu_l, \mu_1'\ldots\mu_{l-1}'}^{(l)}, \\ \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} c_\lambda \Phi_{\mu_1'\ldots\mu_{l-1}'}^{(-Pk')} \rangle_i^{(0)} &= \langle Plk | c | -Plk' \rangle_i^{(0)} \square_{\mu_1\ldots\mu_l, \lambda, \mu_1'\ldots\mu_{l-1}'}^{(l)}, \\ \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} c_\lambda \Phi_{\mu_1'\ldots\mu_{l+1}'}^{(-Pk')} \rangle_i^{(0)} &= \langle Plk | c | -P(l+1)k' \rangle_i^{(0)} \Delta_{\mu_1\ldots\mu_l, \lambda, \mu_1'\ldots\mu_{l+1}'}^{(l+1)}. \end{aligned} \quad (4.4)$$

The reduced c -brackets are given by

$$\begin{aligned} \langle Plk | c | -P(l-1)k' \rangle_i^{(0)} &= \langle -P(l-1)k' | c | Plk \rangle_i^{(0)} = \frac{1}{2l+1} \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} c_{\mu_l} \Phi_{\mu_1\ldots\mu_{l-1}}^{(-Pk')} \rangle_i^{(0)}, \\ \langle Plk | c | -Plk' \rangle_i^{(0)} &= -\langle Plk' | c | -Plk \rangle_i^{(0)} = \frac{l}{(l+1)(2l+1)} \varepsilon_{\mu_1\lambda\mu_l'} \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} c_\lambda \Phi_{\mu_1\ldots\mu_{l-1}\mu_l'}^{(-Pk')} \rangle_i^{(0)}, \\ \langle Plk | c | -P(l+1)k' \rangle_i^{(0)} &= \langle -P(l+1)k' | c | Plk \rangle_i^{(0)} = \frac{1}{2l+3} \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} c_\lambda \Phi_{\mu_1\ldots\mu_l\mu_{l+1}'}^{(-Pk')} \rangle_i^{(0)}, \end{aligned} \quad (4.5)$$

where the isotropic tensors $\square_{\mu_1\ldots\mu_l, \lambda, \mu_1'\ldots\mu_{l-1}'}^{(l)}$ occurring in (4.4) are generalizations of the familiar tensor $\varepsilon_{\mu\nu\lambda}$ since they are used for the construction of generalized cross products of a vector with a l -th rank tensor. Their general definition and some of their properties have been discussed in Ref. 28.

Analogous considerations for the precession term $1/i [\mathbf{h} \cdot \mathbf{J}, \Phi_i]_-$ lead to the following non-vanishing J -brackets

$$\begin{aligned} \frac{1}{i} \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} [J_\lambda, \Phi_{\mu_1'\ldots\mu_{l-1}'}^{(Pk')}]_- \rangle_i^{(0)} &= \langle Plk | J | P(l-1)k' \rangle_i^{(0)} \Delta_{\mu_1\ldots\mu_l, \mu_1'\ldots\mu_{l-1}'}^{(l)}, \\ \frac{1}{i} \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} [J_\lambda, \Phi_{\mu_1'\ldots\mu_{l-1}'}^{(Pk')}]_- \rangle_i^{(0)} &= \langle Plk | J | Plk' \rangle_i^{(0)} \square_{\mu_1\ldots\mu_l, \lambda, \mu_1'\ldots\mu_{l-1}'}^{(l)}, \\ \frac{1}{i} \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} [J_\lambda, \Phi_{\mu_1'\ldots\mu_{l+1}'}^{(Pk')}]_- \rangle_i^{(0)} &= \langle Plk | J | P(l+1)k' \rangle_i^{(0)} \Delta_{\mu_1\ldots\mu_l, \lambda, \mu_1'\ldots\mu_{l+1}'}^{(l+1)}. \end{aligned} \quad (4.6)$$

The reduced J -brackets are

$$\begin{aligned} \langle Plk | J | P(l-1)k' \rangle_i^{(0)} &= -\langle P(l-1)k' | J | Plk \rangle_i^{(0)} = \frac{1}{i} \frac{1}{2l+1} \langle \Phi_{\mu_1\ldots\mu_{l-1}\lambda}^{(Pk)} [J_\lambda, \Phi_{\mu_1\ldots\mu_{l-1}}^{(Pk')}]_- \rangle_i^{(0)}, \\ \langle Plk | J | Plk' \rangle_i^{(0)} &= \langle Plk' | J | Plk \rangle_i^{(0)} = \frac{1}{i} \frac{l}{(l+1)(2l+1)} \varepsilon_{\mu_1\lambda\mu_l'} \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} [J_\lambda, \Phi_{\mu_1\ldots\mu_{l-1}\mu_l'}^{(Pk')}]_- \rangle_i^{(0)}, \\ \langle Plk | J | P(l+1)k' \rangle_i^{(0)} &= -\langle P(l+1)k' | J | Plk \rangle_i^{(0)} = \frac{1}{i} \frac{1}{2l+3} \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} [J_\lambda, \Phi_{\mu_1\ldots\mu_l\mu_{l+1}'}^{(Pk')}]_- \rangle_i^{(0)}. \end{aligned} \quad (4.7)$$

As a consequence of the splitting of the collision operator into two parts the one of which $(\omega_{ij}^\top(\Phi))$ is a functional of Φ_i , the other one $(\omega_{ij}^\top(\Phi))$ a functional of Φ_j (cf. Eqs. (3.3), (3.4)) the following form is obtained for the linearized collision term:

$$\sum_j \sum_{P'} \sum_{l'} \sum_{k'} \{ \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} \omega(\Phi_{\mu_1'\ldots\mu_{l-1}'}^{(P'k')}) \rangle_{ij}^\top a_{i\mu_1'\ldots\mu_{l-1}'}^{(P'k')} + \langle \Phi_{\mu_1\ldots\mu_l}^{(Pk)} \omega(\Phi_{\mu_1'\ldots\mu_{l-1}'}^{(P'k')}) \rangle_{ij}^\top a_{j\mu_1'\ldots\mu_{l-1}'}^{(P'k')} \}. \quad (4.8)$$

Since the collision operator is isotropic and conserves parity, the collision brackets can be decomposed into a product of an isotropic tensor and a reduced collision bracket („ ω -matrix element”) which vanishes

unless the tensors $\Phi_{\mu_1 \dots \mu_l}^{(Pk)}$ and $\Phi_{\mu'_1 \dots \mu'_l}^{(P'k')}$ have the same rank and parity, e.g.

$$\langle \Phi_{\mu_1 \dots \mu_l}^{(Pk)} \omega(\Phi_{\mu'_1 \dots \mu'_l}^{(P'k')}) \rangle_{ij}^\top = \delta_{ll'} \delta^{PP'} \Delta_{\mu_1 \dots \mu_l, \mu'_1 \dots \mu'_l}^{(l)} \omega_{ij}^{(kk')\top}. \quad (4.9)$$

A reduced collision bracket, e.g. $Pl\omega_{ij}^{(kk')\top}$, is then given by

$$Pl\omega_{ij}^{(kk')\top} = \frac{1}{2l+1} \langle \Phi_{\mu_1 \dots \mu_l}^{(Pk)} \omega(\Phi_{\mu_1 \dots \mu_l}^{(Pk')}) \rangle_{ij}^\top. \quad (4.10)$$

Thus the collision term (4.8) becomes

$$\sum_j \sum_{k'} \{ Pl\omega_{ij}^{(kk')\top} a_{i\mu_1 \dots \mu_l}^{(Pk')} + Pl\omega_{ij}^{(kk')\top\top} a_{j\mu_1 \dots \mu_l}^{(Pk')} \}. \quad (4.11)$$

By introducing „total” reduced collision brackets

$$Pl\omega_{ij}^{(kk')} = Pl\omega_{ij}^{(kk')\top\top} + \delta_{ij} \sum_{j'} Pl\omega_{ij'}^{(kk')\top}, \quad (4.12)$$

the form $\sum_j \sum_{k'} Pl\omega_{ij}^{(kk')} a_{j\mu_1 \dots \mu_l}^{(Pk')}$ of the collision term is obtained which is more convenient for applications.

Using ((4.4) ... (4.12)) the general system of transport relaxation equations is written in the lucid form:

$$\begin{aligned} \frac{\partial}{\partial t} a_{i\mu_1 \dots \mu_l}^{(Pk)} + \sum_{k'} \left\{ \langle Plk | c | -Pl(l-1)k' \rangle_i^{(0)} \frac{\partial}{\partial x_{\mu_1}} a_{i\mu_1 \dots \mu_{l-1}}^{(-Pk')} \right. \\ + \langle Plk | c | -Plk' \rangle_i^{(0)} \square_{\mu_1 \dots \mu_l, \lambda, v_1 \dots v_l}^{(l)} \frac{\partial}{\partial x_\lambda} a_{iv_1 \dots v_l}^{(-Pk')} + \langle Plk | c | -Pl(l+1)k' \rangle_i^{(0)} \frac{\partial}{\partial x_\lambda} a_{i\mu_1 \dots \mu_l \lambda}^{(-Pk')} \Big\} \\ + \sum_{k'} \omega_{Hi} \{ \langle Plk | J | Pl(l-1)k' \rangle_i^{(0)} \overline{h_{\mu_1} a_{i\mu_1 \dots \mu_{l-1}}^{(Pk')}} + \langle Plk | J | Plk' \rangle_i^{(0)} \square_{\mu_1 \dots \mu_l, \lambda, v_1 \dots v_l}^{(l)} h_\lambda a_{iv_1 \dots v_l}^{(Pk')} \} \\ + \langle Plk | J | Pl(l+1)k' \rangle_i^{(0)} h_\lambda a_{i\mu_1 \dots \mu_l \lambda}^{(Pk')} \} + \sum_{j=1}^K \sum_{k'} Pl\omega_{ij}^{(kk')} a_{j\mu_1 \dots \mu_l}^{(Pk')} = 0. \end{aligned} \quad (4.13)$$

3. General properties of the collision brackets

Rotational invariance and parity invariance of the linearized collision operator have already been used to define reduced collision brackets [cf. Eq. (4.9)]. Another important symmetry, the time reversal invariance of the molecular interaction guarantees the Onsager symmetries of the collision brackets. In the same way as it has been shown in Ref. ²³ it can be shown that for the reduced collision brackets the following symmetries hold

$$n_i^{(0)} Pl\omega_{ij}^{(kk')} = T_k T_{k'} n_j^{(0)} Pl\omega_{ji}^{(k'k)}. \quad (4.14)$$

In Eq. (4.14), T_k and $T_{k'}$ are $+1$ or -1 depending on whether the corresponding expansion tensors are even or odd under time reversal.

Next, some considerations on the positive semidefiniteness of the collision brackets are made. Using Eqs. (3.4a, 3.6a) and both of the forms of the optical theorem (1.11) one gets

$$\langle \Phi \omega(\Phi) \rangle_{ij}^\top \geq 0, \quad (4.15)$$

where Φ is an arbitrary operator function $\Phi(t, \mathbf{x}, \mathbf{c}, \mathbf{J})$. This inequality, e.g., guarantees the positive sign of the binary diffusion coefficient ($D_{12} \propto 1/_{-1}\omega_{12}^{(11)\top}$).

The inequality which guarantees the increase of entropy with time is

$$\sum_i \sum_j n_i^{(0)} \langle \Phi \omega(\Phi) \rangle_{ij} \geq 0, \quad (4.16)$$

where the total collision bracket $\langle \Phi \omega(\Phi) \rangle_{ij}$ is defined according to (4.12). For the proof of (4.16) consider

$$\sum_i \sum_j n_i^{(0)} (\langle \Phi \omega(\Phi) \rangle_{ij}^\top + \langle \Phi \omega(\Phi) \rangle_{ij}^\top{}^\top):$$

Writing down the explicit expressions for the collision brackets after (3.4, 3.6), using the optical theorem and the invariance of the trace against cyclic permutation of operators under the trace, one can show the positive semidefiniteness of this expression. With the use of (4.12) the inequality (4.16) follows.

The equality sign in (4.16) holds if

$$(\Phi_i^I + \Phi_j^II) a_{ij}^{I\text{II}, I'II'} = a_{ij}^{I\text{II}, I'II'} (\Phi_i^{I'} + \Phi_j^{II'}), \quad (4.17)$$

which is only valid if Φ is a collisional invariant.

Finally, collision brackets of collisional invariants, i.e. „classical” quantities with the property

$$\Phi_{i\text{II}} + \Phi_{j\text{II}} - \Phi_{i\text{I}'} - \Phi_{j\text{II}'} = 0, \quad i, j = 1, \dots, K,$$

are considered. From (3.5a) and (3.5b) one infers

$$\langle \Phi \omega (\Phi_{\text{inv}}) \rangle_{ij}^{\top} + \langle \Phi \omega (\Phi_{\text{inv}}) \rangle_{ij}^{\top \top} = 0, \quad (4.18)$$

where Φ_{inv} is a collisional invariant and Φ is an arbitrary operator function. Writing down the corresponding collision brackets with Φ and Φ_{inv} exchanged one also finds after some conversions the following equation

$$n_j^{(0)} \langle \Phi_{\text{inv}} \omega (\Phi) \rangle_{ji}^{\top} + n_i^{(0)} \langle \Phi_{\text{inv}} \omega (\Phi) \rangle_{ij}^{\top \top} = 0. \quad (4.19)$$

From (4.12) and (4.19) one obtains immediately

$$\sum_{i=1}^K n_i^{(0)} \langle \Phi_{\text{inv}} \omega (\Phi) \rangle_{ij} = 0. \quad (4.20)$$

Eq. (4.20) is important for the derivation of the linearized conservation laws from the transport relaxation equations (see Chapter VI).

V. The Truncated System of Transport Relaxation Equations (for a Special Expansion Scheme)

In this section the expansion tensors $\Phi_{i\mu_1 \dots \mu_l}^{(Pk)}(\mathbf{c}, \mathbf{J})$ introduced by Eq. (4.1) will be specified. For this sake it is useful to introduce the dimensionless velocities by

$$\mathbf{C}_i = \sqrt{m_i/2k_B T_0} \mathbf{c}, \quad (5.1)$$

and the dimensionless internal energies by

$$\varepsilon_i(J) = \hbar^2 J(J+1)/2\Theta_i k_B T_0. \quad (5.2)$$

Furthermore, irreducible l^{th} rank tensors built up from the rotational angular momentum vectors \mathbf{J} of Eq. (1.1) are introduced by²⁹

$$S_{i\mu_1 \dots \mu_l}(\mathbf{J}) = \sqrt{\frac{(2l+1)!!}{l!}} \frac{\langle J_0^2 \dots J_{l-1}^2 \rangle_{i0}^{-1/2}}{\overline{J_{\mu_1} \dots J_{\mu_l}}}, \quad (5.3)$$

where $\langle \dots \rangle_0$ denotes an equilibrium mean value. In (5.3), $\overline{J_{\mu_1} \dots J_{\mu_l}}$ is the l^{th} rank irreducible angular momentum tensor used in Ref. 23 and

$$J_{(l)}^2 = J(J+1) - \frac{l}{2} \left(\frac{l}{2} + 1 \right). \quad (5.4)$$

²⁹ Note, that the tensors $S_{i\mu_1 \dots \mu_l}^J$, defined by Eq. (5.3) differ from the corresponding tensors used in Ref. 11 in the sense that the tensors occurring in Ref. 11 are normalized within the J -subspace while the tensors used in the present paper are, similar to the treatment in Ref. 10, normalized with respect to the whole J -variety.

According to (2.1) the angular momentum tensors projected into the J -subspace are

$$S_{i\mu_1 \dots \mu_l}^J = P^J S_{i\mu_1 \dots \mu_l} P^J$$

with $S_{i\mu_1 \dots \mu_l}^J = 0$ for $l \geq 2J$. The $S_{i\mu_1 \dots \mu_l}^J$ -tensors then obey the following normalization property²⁹

$$Q_i^{-1} \sum_J \text{tr} \{ S_{i\mu_1 \dots \mu_l}^J S_{i\nu_1 \dots \nu_l}^J \} \exp(-\varepsilon_i(J)) = \delta_{ll'} \Delta_{\mu_1 \dots \mu_l, \nu_1 \dots \nu_l}^{(l)}, \quad (5.5)$$

where Q_i is the rotational partition function for the species i .

With respect to the dependence on the internal energies or on $\varepsilon_i(J)$ polynomials in $\varepsilon_i(J)$, the so called „Wang Chang-Uhlenbeck polynomials”¹⁷ $P_{il}^{(n)}$ can be constructed using a Schmidt orthogonalization procedure (cf. Ref. 15). The polynomials are orthonormalized according to¹⁰

$$\langle S_{i\mu_1 \dots \mu_l}^J S_{i\nu_1 \dots \nu_l}^J P_{il}^{(n)}(J) P_{il}^{(m)}(J) \rangle = \Delta_{\mu_1 \dots \mu_l, \nu_1 \dots \nu_l}^{(l)} \delta^{mn}. \quad (5.6)$$

A general l -th rank expansion tensor is then constructed from an irreducible tensor in the dimensionless velocity $\overline{C_{i\mu_1} \dots C_{i\mu_l}}$, multiplied by a Sonine polynomial $S_{l+\frac{1}{2}}^{(n)}(C_i^2)$ in C_i^2 where $l', n = 0, 1, 2, \dots$, cf. Ref. 23, which is combined with an irreducible tensor $S_{i\mu_1 \dots \mu_l}^J$ multiplied by a Wang Chang-Uhlenbeck polynomial to give a l^{th} rank irreducible tensor. The tensors obtained in this way must be normalized according to Eq. (4.2). The total power of an expansion tensor is given by the power in C_i plus the rank of the $S_{i\mu_1 \dots \mu_l}^J$ tensor plus twice the power in ε_i of the Wang Chang-Uhlenbeck polynomial.

The first two Wang Chang-Uhlenbeck polynomials are

$$P_{i0}^{(0)} = 1, \quad (5.7a)$$

$$P_{i0}^{(1)} = [\langle \varepsilon^2 \rangle_i^{(0)} - \langle \varepsilon \rangle_i^{(0)2}]^{-1/2} (\varepsilon_i - \langle \varepsilon \rangle_i^{(0)}) = \sqrt{\frac{k_B}{c_{\text{rot},i}^{(0)}}} (\varepsilon_i - \langle \varepsilon \rangle_i^{(0)}), \quad (5.7b)$$

where ε_i is defined in (5.2) and $c_{\text{rot},i}^{(0)}$ is the rotational part of the heat capacity per molecule i at the equilibrium temperature T_0 . For the following treatment only these two Wang Chang-Uhlenbeck polynomials will be needed.

In the first table the complete scheme of expansion tensors up to the third rank and the total power 3 is listed. The symbols $\Phi_{i\mu_1 \dots \mu_l}(\mathbf{c}, \mathbf{J})$ and $\Psi_{i\mu_1 \dots \mu_l}(\mathbf{c}, \mathbf{J})$, respectively, characterize here true and pseudo tensors of rank l . For the treatment of special transport and relaxation phenomena in

Total power	Scalars	PlT	Vectors	PlT	2 nd rank Tensors	PlT	3 rd rank Tensors	PlT
0	$\Phi_i^{(1)} = 1$	+ 0 +						
1			$\Phi_{i\mu}^{(1)} = \sqrt{2} C_{i\mu}$	- 1 -				
1			$\Psi_{i\mu}^{(1)} = S_{i\mu}$	+ 1 -				
2	$\Phi_i^{(2)} = \sqrt{\frac{2}{3}} (C_i^2 - \frac{3}{2})$	+ 0 +			$\Phi_{i\mu\nu}^{(1)} = \sqrt{2} \overline{C_{i\mu} C_{i\nu}}$	+ 2 +		
2	$\Phi_i^{(3)} = N_i (\varepsilon_i - \langle \varepsilon \rangle_i^{(0)})$	+ 0 +						
2					$\Phi_{i\mu\nu}^{(2)} = S_{i\mu\nu}$	+ 2 +		
2	$\Psi_i^{(1)} = \sqrt{\frac{2}{3}} C_{i\mu} S_{i\mu}$	- 0 +	$\Phi_{i\mu}^{(2)} = \varepsilon_{\mu\nu\lambda} C_{i\nu} S_{i\lambda}$	- 1 +	$\Psi_{i\mu\nu}^{(1)} = \sqrt{2} \overline{C_{i\mu} S_{i\nu}}$	- 2 +		
3			$\Phi_{i\mu}^{(3)} = \frac{2}{\sqrt{5}} (C_i^2 - \frac{5}{2}) C_{i\mu}$	- 1 -			$\Phi_{i\mu\nu\lambda}^{(1)} = \frac{2}{3} \overline{C_{i\mu} C_{i\nu} C_{i\lambda}}$	- 3 -
3			$\Phi_{i\mu}^{(4)} = \sqrt{2} N_i (\varepsilon_i - \langle \varepsilon \rangle_i^{(0)}) C_{i\mu}$	- 1 -				
3			$\Psi_{i\mu}^{(2)} = \sqrt{\frac{2}{3}} (C_i^2 - \frac{3}{2}) S_{i\mu}$	+ 1 -				
3			$\Psi_{i\mu}^{(3)} = \tilde{N}_i (\varepsilon_i - \langle \varepsilon^2 \rangle_i^{(0)}) S_{i\mu}$	+ 1 -				
3			$\Phi_{i\mu}^{(5)} = \sqrt{\frac{6}{5}} S_{i\mu\nu} C_{i\nu}$	- 1 -	$\Psi_{i\mu\nu}^{(2)} = \frac{2}{\sqrt{3}} \overline{S_{i\nu\lambda} C_{i\varrho} \varepsilon_{\mu\lambda\varrho}}$	- 2 -	$\Phi_{i\mu\nu\lambda}^{(2)} = \sqrt{2} \overline{C_{i\mu} S_{i\nu\lambda}}$	- 3 -
3			$\Psi_{i\mu}^{(4)} = \sqrt{\frac{6}{5}} \overline{C_{i\mu} C_{i\nu} S_{i\nu}}$	+ 1 -	$\Phi_{i\mu\nu}^{(3)} = \frac{2}{\sqrt{3}} \overline{S_{i\varrho} C_{i\nu} C_{i\lambda} \varepsilon_{\mu\lambda\varrho}}$	+ 2 -	$\Psi_{i\mu\nu\lambda}^{(1)} = \sqrt{2} \overline{C_{i\mu} C_{i\nu} S_{i\lambda}}$	+ 3 -
3							$\Psi_{i\mu\nu\lambda}^{(2)} = S_{i\mu\nu\lambda}$	+ 3 -

Table 1. Special scheme of expansion tensors up to the third rank and total power ≤ 3 (P = parity, l = tensor rank, T = sign under time reversal).The abbreviation $N_i = \sqrt{k_B/c_{\text{rot},i}^{(0)}}$ is used.

Scalars		
$\frac{\partial}{\partial t} a_i^{(1)} + \frac{c_i^{(0)}}{3} \sqrt{3} \operatorname{div} \mathbf{a}_i^{(1)}$		$= 0$
$\frac{\partial}{\partial t} a_i^{(2)} + \frac{c_i^{(0)}}{3} \operatorname{div} (\sqrt{2} \mathbf{a}_i^{(1)} + \sqrt{5} \mathbf{a}_i^{(3)})$	$+\sum_{j=1}^K \sum_{k'=2}^3 +0\omega_{ij}^{(2k')} a_j^{(k')} = 0$	
$\frac{\partial}{\partial t} a_i^{(3)} + \frac{c_i^{(0)}}{3} \sqrt{3} \operatorname{div} \mathbf{a}_i^{(4)}$	$+\sum_{j=1}^K \sum_{k'=2}^3 +0\omega_{ij}^{(3k')} a_j^{(k')} = 0$	
Pseudoscalar		
$\frac{\partial}{\partial t} b_i^{(1)} + \frac{c_i^{(0)}}{3} \operatorname{div} \left(\mathbf{b}_i^{(1)} + \sqrt{\frac{2}{3}} \mathbf{b}_i^{(2)} + \sqrt{\frac{10}{3}} \mathbf{b}_i^{(4)} \right) - \sqrt{\frac{2}{3}} \omega_{Hi} \mathbf{h} \cdot \mathbf{a}_i^{(2)}$	$+\sum_{j=1}^K -0\omega_{ij}^{(11)} b_j^{(1)} = 0$	
Vectors		
$\frac{\partial}{\partial t} a_{i\mu}^{(1)} + \frac{c_i^{(0)}}{3} \operatorname{grad}_\mu (\sqrt{3} a_i^{(1)} + \sqrt{2} a_i^{(2)}) + c_i^{(0)} \left[\frac{2}{3} \frac{\partial}{\partial x_\nu} a_{i\mu\nu}^{(1)} \right.$	$\left. + \sum_{j=1}^K \sum_{k'=1}^5 -1\omega_{ij}^{(1k')} a_{j\mu}^{(k')} = 0 \right.$	
$\frac{\partial}{\partial t} a_{i\mu}^{(2)} + \sqrt{\frac{2}{3}} \omega_{Hi} h_\mu b_i^{(1)} + \frac{1}{2} \omega_{Hi} (\mathbf{h} \times \mathbf{a}_i^{(2)})_\mu + \frac{c_i^{(0)}}{6} \operatorname{rot}_\mu (\sqrt{6} \mathbf{b}_i^{(1)} + 2 \mathbf{b}_i^{(2)} + \sqrt{5} \mathbf{b}_i^{(4)}) + \frac{2}{3} \sqrt{2} c_i^{(0)} \frac{\partial}{\partial x_\nu} a_{i\mu\nu}^{(3)} - \frac{1}{\sqrt{2}} \omega_{Hi} h_\nu b_{i\mu\nu}^{(1)}$	$\left. + \sum_{j=1}^K \sum_{k'=1}^5 -1\omega_{ij}^{(2k')} a_{j\mu}^{(k')} = 0 \right.$	
$\frac{\partial}{\partial t} a_{i\mu}^{(3)} + \frac{c_i^{(0)}}{3} \operatorname{grad}_\mu \sqrt{5} a_i^{(2)} + \frac{c_i^{(0)}}{3} 2 \sqrt{\frac{3}{5}} \frac{\partial}{\partial x_\nu} a_{i\mu\nu}^{(1)}$	$\left. + \sum_{j=1}^K \sum_{k'=1}^5 -1\omega_{ij}^{(3k')} a_{j\mu}^{(k')} = 0 \right.$	
$\frac{\partial}{\partial t} a_{i\mu}^{(4)} + \frac{c_i^{(0)}}{\sqrt{3}} \operatorname{grad}_\mu a_i^{(3)}$	$\left. + \sum_{j=1}^K \sum_{k'=1}^5 -1\omega_{ij}^{(4k')} a_{j\mu}^{(k')} = 0 \right.$	
$\frac{\partial}{\partial t} a_{i\mu}^{(5)} + \frac{2}{3} \omega_{Hi} (\mathbf{h} \times \mathbf{a}_i^{(5)})_\mu + \frac{c_i^{(0)}}{5} \sqrt{5} \frac{\partial}{\partial x_\nu} a_{i\mu\nu}^{(2)} + \frac{3}{\sqrt{10}} \omega_{Hi} h_\nu b_{i\mu\nu}^{(2)}$	$\left. + \sum_{j=1}^K \sum_{k'=1}^5 -1\omega_{ij}^{(5k')} a_{j\mu}^{(k')} = 0 \right.$	
Pseudovectors		
$\frac{\partial}{\partial t} b_{i\mu}^{(1)} + \frac{c_i^{(0)}}{3} \operatorname{grad}_\mu b_i^{(1)} - \frac{c_i^{(0)}}{\sqrt{6}} \operatorname{rot}_\mu \mathbf{a}_i^{(2)} + \omega_{Hi} (\mathbf{h} \times \mathbf{b}_i^{(1)})_\mu + \frac{c_i^{(0)}}{\sqrt{3}} \frac{\partial}{\partial x_\nu} b_{i\mu\nu}^{(1)}$	$\left. + \sum_{j=1}^K \sum_{k'=1}^4 +1\omega_{ij}^{(1k')} b_{j\mu}^{(k')} = 0 \right.$	
$\frac{\partial}{\partial t} b_{i\mu}^{(2)} + \frac{c_i^{(0)}}{3} \operatorname{grad}_\mu \sqrt{\frac{2}{3}} b_i^{(1)} - \frac{c_i^{(0)}}{3} \operatorname{rot}_\mu \mathbf{a}_i^{(2)} + \omega_{Hi} (\mathbf{h} \times \mathbf{b}_i^{(2)})_\mu + \frac{c_i^{(0)}}{3} \sqrt{2} \frac{\partial}{\partial x_\nu} b_{i\mu\nu}^{(1)}$	$\left. + \sum_{j=1}^K \sum_{k'=1}^4 +1\omega_{ij}^{(2k')} b_{j\mu}^{(k')} = 0 \right.$	
$\frac{\partial}{\partial t} b_{i\mu}^{(3)} + \omega_{Hi} (\mathbf{h} \times \mathbf{b}_i^{(3)})_\mu$	$\left. + \sum_{j=1}^K \sum_{k'=1}^4 +1\omega_{ij}^{(3k')} b_{j\mu}^{(k')} = 0 \right.$	
$\frac{\partial}{\partial t} b_{i\mu}^{(4)} + \frac{c_i^{(0)}}{3} \operatorname{grad}_\mu \sqrt{\frac{10}{3}} b_i^{(1)} - \frac{c_i^{(0)}}{6} \operatorname{rot}_\mu \sqrt{5} \mathbf{a}_i^{(2)} - \frac{\omega_{Hi}}{6} (\mathbf{h} \times \mathbf{b}_i^{(4)})_\mu - \omega_{Hi} \frac{3}{5} \sqrt{\frac{5}{2}} h_\nu a_{i\mu\nu}^{(3)} + \frac{c_i^{(0)}}{6} \sqrt{\frac{2}{5}} \frac{\partial}{\partial x_\nu} b_{i\mu\nu}^{(1)}$	$\left. + \sum_{j=1}^K \sum_{k'=1}^4 +1\omega_{ij}^{(4k')} b_{j\mu}^{(k')} = 0 \right.$	

Table 2

Second rank Tensors		
$\frac{\partial}{\partial t} a_{i\mu\nu}^{(1)} + c_i^{(0)} \sqrt{\frac{2}{3}} \frac{\partial}{\partial x_\mu} a_{i\nu}^{(1)} + \frac{2}{3} c_i^{(0)} \sqrt{\frac{3}{5}} \frac{\partial}{\partial x_\mu} a_{i\nu}^{(3)} + c_i^{(0)} \frac{\partial}{\partial x_\lambda} a_{i\mu\nu\lambda}^{(1)}$	$+ \sum_{j=1}^K \sum_{k'=1}^3 +2\omega_{ij}^{(1k')} a_{j\mu\nu}^{(k')} = 0$	
$\frac{\partial}{\partial t} a_{i\mu\nu}^{(2)} + \frac{c_i^{(0)}}{5} \sqrt{5} \frac{\partial}{\partial x_\mu} a_{i\nu}^{(5)} + 2 \omega_{Hi} \square_{\mu\nu, \lambda, \mu' \nu'} h_\lambda a_{i\mu' \nu'}^{(2)} + \frac{c_i^{(0)}}{3} \sqrt{2} \square_{\mu\nu, \lambda, \mu' \nu'} \frac{\partial}{\partial x_\lambda} b_{i\mu' \nu'}^{(2)} + \frac{1}{\sqrt{3}} c_i^{(0)} \frac{\partial}{\partial x_\kappa} a_{i\mu\nu\kappa}^{(2)}$	$+ \sum_{j=1}^K \sum_{k'=1}^3 +2\omega_{ij}^{(2k')} a_{j\mu\nu}^{(k')} = 0$	
$\frac{\partial}{\partial t} a_{i\mu\nu}^{(3)} + \frac{2\sqrt{2}}{3} c_i^{(0)} \frac{\partial}{\partial x_\mu} a_{i\nu}^{(2)} + \frac{3}{5} \sqrt{\frac{5}{2}} \omega_{Hi} h_\mu b_{i\nu}^{(4)} + \frac{3}{2} \omega_{Hi} \square_{\mu\nu, \lambda, \mu' \nu'} h_\lambda a_{i\mu' \nu'}^{(3)} + \frac{c_i^{(0)}}{3} \square_{\mu\nu, \lambda, \mu' \nu'} \frac{\partial}{\partial x_\lambda} b_{i\mu' \nu'}^{(1)} - \sqrt{\frac{2}{3}} \omega_{Hi} h_\kappa b_{i\mu\nu\kappa}^{(1)}$	$+ \sum_{j=1}^K \sum_{k'=1}^3 +2\omega_{ij}^{(3k')} a_{j\mu\nu}^{(k')} = 0$	
Second rank Pseudotensors		
$\frac{\partial}{\partial t} b_{i\mu\nu}^{(1)} + \frac{\omega_{Hi}}{\sqrt{2}} \overline{h_\mu a_{i\nu}^{(2)}} + \frac{c_i^{(0)}}{3} \frac{\partial}{\partial x_\nu} \left(\sqrt{3} b_{i\mu}^{(1)} + \sqrt{2} b_{i\mu}^{(2)} + \frac{1}{\sqrt{10}} b_{i\mu}^{(4)} \right) - \frac{c_i^{(0)}}{3} \square_{\mu\nu, \lambda, \mu' \nu'} \frac{\partial}{\partial x_\lambda} a_{i\mu' \nu'}^{(3)} + \omega_{Hi} \square_{\mu\nu, \lambda, \mu' \nu'} h_\lambda b_{i\mu' \nu'}^{(1)} + \sqrt{\frac{2}{3}} c_i^{(0)} \frac{\partial}{\partial x_\kappa} b_{i\mu\nu\kappa}^{(1)}$	$+ \sum_{j=1}^K \sum_{k'=1}^2 -2\omega_{ij}^{(1k')} b_{j\mu\nu}^{(k')} = 0$	
$\frac{\partial}{\partial t} b_{i\mu\nu}^{(2)} - \frac{3}{\sqrt{10}} \overline{\omega_{Hi} h_\mu a_{i\nu}^{(5)}} - \frac{c_i^{(0)}}{3} \sqrt{2} \square_{\mu\nu, \lambda, \mu' \nu'} \frac{\partial}{\partial x_\lambda} a_{i\mu' \nu'}^{(2)} + \frac{5}{3} \omega_{Hi} \square_{\mu\nu, \lambda, \mu' \nu'} h_\lambda b_{i\mu' \nu'}^{(2)} + \sqrt{\frac{2}{3}} \omega_{Hi} h_\kappa a_{i\mu\nu\kappa}^{(2)}$	$+ \sum_{j=1}^K \sum_{k'=1}^2 -2\omega_{ij}^{(2k')} b_{j\mu\nu}^{(k')} = 0$	
Third rank Tensors		
$\frac{\partial}{\partial t} a_{i\mu\nu\lambda}^{(1)} + c_i^{(0)} \overline{\frac{\partial}{\partial x_\mu} a_{i\nu\lambda}^{(1)}}$	$+ \sum_{j=1}^K \sum_{k'=1}^2 -3\omega_{ij}^{(1k')} a_{j\mu\nu\lambda}^{(k')} = 0$	
$\frac{\partial}{\partial t} a_{i\mu\nu\lambda}^{(2)} + \frac{c_i^{(0)}}{\sqrt{3}} \overline{\frac{\partial}{\partial x_\mu} a_{i\nu\lambda}^{(2)}} - \sqrt{\frac{2}{3}} \omega_{Hi} h_\mu b_{i\nu\lambda}^{(2)} + 2 \omega_{Hi} \square_{\mu\nu\lambda, \kappa, \mu' \nu' \lambda'} h_\kappa a_{i\mu' \nu' \lambda'}^{(2)}$	$+ \sum_{j=1}^K \sum_{k'=1}^2 -3\omega_{ij}^{(2k')} a_{j\mu\nu\lambda}^{(k')} = 0$	
Third rank Pseudotensors		
$\frac{\partial}{\partial t} b_{i\mu\nu\lambda}^{(1)} + \sqrt{\frac{2}{3}} \omega_{Hi} h_\mu a_{i\nu\lambda}^{(3)} + \sqrt{\frac{2}{3}} c_i^{(0)} \overline{\frac{\partial}{\partial x_\mu} b_{i\nu\lambda}^{(1)}} + \frac{2}{3} \omega_{Hi} \square_{\mu\nu\lambda, \kappa, \mu' \nu' \lambda'} h_\kappa b_{i\mu' \nu' \lambda'}^{(1)}$	$+ \sum_{j=1}^K \sum_{k'=1}^2 +3\omega_{ij}^{(1k')} b_{j\mu\nu\lambda}^{(k')} = 0$	
$\frac{\partial}{\partial t} b_{i\mu\nu\lambda}^{(2)} + 3 \omega_{Hi} \square_{\mu\nu\lambda, \kappa, \mu' \nu' \lambda'} h_\kappa b_{i\mu' \nu' \lambda'}^{(2)}$	$+ \sum_{j=1}^K \sum_{k'=1}^2 +3\omega_{ij}^{(2k')} b_{j\mu\nu\lambda}^{(k')} = 0$	

Table 2. Special system of transport relaxation equations

gas mixtures (e.g. the heat conductivity and viscosity in the presence of a magnetic field) only some of these tensors are important.

With the expansion tensors of Table 1, the reduced c -brackets and the reduced J -brackets are calculated. Inserting the results into Eq. (4.12) yields the special truncated system of transport relaxation equations up to third rank expansion tensors with total power ≤ 3 . In Table 2 which shows this special system (which is relevant for the treatment of the various transport and relaxation phenomena like diffusion, thermal diffusion, thermal conductivity and viscosity in gas mixtures in an external magnetic field) l -th rank tensors with parity $(-1)^l$ are denoted by $a_{i\mu_1 \dots \mu_l}$ and l^{th} rank tensors with parity $P = (-1)^{l+1}$ are denoted by $b_{i\mu_1 \dots \mu_l}$ (pseudo tensors). The abbreviation $c_i^{(0)} = \sqrt{3} k_B T_0 / m_i$ is used.

VI. Local Conservation Laws

As a preliminary and simple application of our system of transport relaxation equations the local conservation laws for particle number, energy and linear momentum, linearized in the deviation from thermal equilibrium, are derived in this chapter.

1. Particle number

The first one of the scalar equations of Table 2 is identical with the continuity equation. Since

$$a_i^{(1)} = \frac{n_i - n_i^{(0)}}{n_i^{(0)}}, \quad (6.1a)$$

$$\text{and} \quad a_i^{(1)} \approx \sqrt{3} \frac{\langle \mathbf{c} \rangle_i}{c_i^{(0)}}, \quad (6.1b)$$

one obtains immediately

$$\frac{\partial}{\partial t} n_i + n_i^{(0)} \operatorname{div} \langle \mathbf{c} \rangle_i = 0. \quad (6.2a)$$

Summing (6.2a) over i yields the linearized continuity law

$$\frac{\partial n}{\partial t} + n_0 \operatorname{div} \mathbf{w} = 0, \quad (6.2b)$$

where \mathbf{w} is the mean particle velocity defined by

$$\mathbf{w} = \sum_i n_i^{(0)} \langle \mathbf{c} \rangle_i / n_0. \quad (6.3)$$

At this point also the mean mass velocity is introduced by

$$\mathbf{v} = \sum_i \varrho_i^{(0)} \langle \mathbf{c} \rangle_i / \varrho_0. \quad (6.4)$$

Multiplying (6.2a) with m_i and summing over i then results in the continuity equation for the mass density

$$\partial \varrho / \partial t + \varrho_0 \operatorname{div} \mathbf{v} = 0. \quad (6.5)$$

2. Energy

The second scalar equation of Table 2 is multiplied with $\sqrt{\frac{3}{2}}$ and the third one with $\sqrt{c_{\text{rot},i}^{(0)} / k_B}$ and then both equations are added. The resulting equation is multiplied with $n_i^{(0)}$ and the sum over i is taken. Then theorem (4.20) can be applied, since

$$\sqrt{\frac{3}{2}} \Phi_i^{(2)} + \sqrt{\frac{c_{\text{rot},i}^{(0)}}{k_B}} \Phi_i^{(3)} \propto E_{i,\text{tot}} - \langle E_{i,\text{tot}} \rangle_0$$

is a collisional invariant. Thus, the following equation is obtained:

$$\begin{aligned} \frac{\partial}{\partial t} \sum_i n_i^{(0)} \left\{ \sqrt{\frac{3}{2}} a_i^{(2)} + \sqrt{\frac{c_{\text{rot},i}^{(0)}}{k_B}} a_i^{(3)} + \frac{c_i^{(0)}}{\sqrt{3}} \operatorname{div} a_i^{(1)} \right. \\ \left. + c_i^{(0)} \operatorname{div} \left(\sqrt{\frac{5}{6}} a_i^{(3)} + \sqrt{\frac{c_{\text{rot},i}^{(0)}}{k_B}} a_i^{(4)} \right) \right\} = 0. \end{aligned} \quad (6.6)$$

The scalars $a_i^{(2)}$ and $a_i^{(3)}$ are, in the linearized theory, related to the translational and rotational temperatures which themselves are defined by the corresponding parts of the molecular energy:

$$a_i^{(2)} \approx \sqrt{\frac{3}{2}} \frac{T_{\text{trans},i} - T_0}{T_0}, \quad (6.7a)$$

$$a_i^{(3)} \approx \sqrt{\frac{k_B}{c_{\text{rot},i}^{(0)}}} (\langle \varepsilon \rangle_i - \langle \varepsilon \rangle_i^{(0)}) \approx \sqrt{\frac{c_{\text{rot},i}^{(0)}}{k_B}} \frac{T_{\text{rot},i} - T_0}{T_0}, \quad (6.7b)$$

where $T_{\text{trans},i}$ and $T_{\text{rot},i}$ are the translational and rotational temperatures of species i . Since only small deviations from thermal equilibrium are considered the temperature of the gas mixture can be defined by

$$T \approx \left[\sum_i n_i^{(0)} (c_{\text{rot},i}^{(0)} + \frac{3}{2} k_B) \right]^{-1} \sum_i (c_{\text{rot},i}^{(0)} T_{\text{rot},i} + \frac{3}{2} k_B T_{\text{trans},i}) n_i^{(0)}. \quad (6.8)$$

The total heat flux is given by

$$\mathbf{q} \approx \sum_i n_i^{(0)} c_i^{(0)} k_B T_0 \left[\sqrt{\frac{5}{6}} a_i^{(3)} + \sqrt{\frac{c_{\text{rot},i}^{(0)}}{3 k_B}} a_i^{(4)} \right]. \quad (6.9)$$

Inserting Eqs. (6.7–6.9) into Eq. (6.6) yields the local energy balance (in the linearized form)

$$n_0 \left(\frac{3}{2} k_B + c_{\text{rot}}^{(0)} \right) \partial T / \partial t + n_0 k_B T_0 \operatorname{div} \mathbf{w} + \operatorname{div} \mathbf{q} = 0, \quad (6.10)$$

where

$$c_{\text{rot}}^{(0)} = (1/n_0) \sum_i n_i^{(0)} c_{\text{rot},i}^{(0)}. \quad (6.11)$$

3. Momentum

The first one of the vectorial equations of Table 2 is multiplied with $n_i^{(0)} m_i c_i^{(0)}$ and the summation over i is performed. Since $m_i c_{i\mu} = \frac{1}{\sqrt{3}} m_i c_i^{(0)} \Phi_{i\mu}^{(1)}$ is a collisional invariant, the theorem (4.20) gives

$$\sum_i n_i^{(0)} m_i c_i^{(0)} \omega_{ij}^{(1k)} = 0 \quad \text{for } k = 1 \cdots \infty. \quad (6.12)$$

Now, the symmetric traceless part of the linearized pressure tensor is given by

$$\overline{p}_{\mu\nu} = \sqrt{2} k_B T_0 \sum_i n_i^{(0)} a_{i\mu\nu}^{(1)}, \quad (6.13a)$$

and the linearized isotropic part is

$$p = n_0 k_B T_{\text{trans}} + (n - n_0) k_B T_0. \quad (6.13b)$$

With (6.12), (6.13) the first vector equation of Table 2 yields the local balance of linear momentum

in the familiar form

$$\rho_0 \frac{\partial}{\partial t} v_\mu + \frac{\partial p}{\partial x_\mu} + \frac{\partial \overline{p}_{\mu\nu}}{\partial x_\nu} = 0. \quad (6.14)$$

Because the collision term is local, an antisymmetric part of the pressure tensor does not occur (for a discussion of this problem see Ref.⁹).

The local conservation laws appear as the most simple applications of the special system of transport relaxation equations. Further applications, in particular the treatment of the Senftleben-Beenakker effect of thermal conductivity, viscosity and diffusion for a binary mixture (especially for a mixture of rotating molecules with a noble gas) will be given in a forthcoming paper.

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Oberflächenspannung und Thermodynamik des perfekten Gases

EBERHARD HILF

Physikalisches Institut der Universität Würzburg

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A thermodynamic system of N Fermions or Bosons, bound by an external potential but with almost no additional contribution of the interaction energy between the particles to the binding of the system is called a bound perfect quantum gas. Its single particle energy level density $\rho(\varepsilon)$ depends on the properties of the external potential. This is chosen to be zero inside and infinite outside a given arbitrary simple connected closed shape. Within the leptodermous assumption $N^{1/3} \gg 1$ then $\rho(\varepsilon)$ can be written explicitly as a sum of three terms which are proportional to the volume, surface, curvature tension. Its thermodynamics is developed: 1) one thermodynamic variable can be eliminated, reducing the phase space dimensions; 2) the Gibbs — Duhem relation is disfigured only by surface — and curvature terms, stating that the system is still macroscopically homogenous except in the surface area, where e.g. the particle density falls down to zero smoothly; 3) the Landsberg-definition $p \cdot V = \frac{2}{3} U$ still holds, confirming that our microscopically defined system is macroscopically a perfect gas in the sense of Landsberg, despite the surface phenomena. In the appendix the advantages of an operatorlike shortwriting of the partial derivative notation are demonstrated.

Es wird die Thermodynamik eines räumlich begrenzten perfekten Gases aufgebaut.

In der klassischen Physik wurde ein Gas meist als „ideal“ bezeichnet, wenn es der thermischen Zustandsgleichung $p \cdot v = T$ (Druck p , spezifisches Volumen $v := V/N$. Der Boltzmann-Konstanten ist der Wert 1 zugeordnet. Die Temperatur T kann in erg gemessen werden¹) genügt oder zumindest die mittlere Energie pro Teilchen $u(T) := U/N$ nur von

der Temperatur abhängt. (In der Zuordnung $B := A$ sei die unbekannte Größe A durch die als bekannt angenommene Größe B definiert, $B := A \Leftrightarrow A := B$.) Diese makroskopischen Relationen gelten aber nur für Fermionen- oder Bosonengase hoher Temperatur und großer Verdünnung, falls die thermische Wellenlänge $h/(3mT)^{1/2}$ klein gegen die mittlere Reichweite der Zweiteilchenkräfte geworden ist. Die makroskopische Definitionsrelation $p \cdot v = \frac{2}{3} u$ von

Sonderdruckanforderungen an Dr. E. HILF, Physikalisches Institut der Universität Würzburg, D-8700 Würzburg, Röntgenring 8.

¹ Siehe z. B.: SÜSSMANN, G. u. E. HILF, Thermodynamik, in Vorbereitung.