J Elast (2010) 100: 5–24
DOI 10.1007/s10659-010-9246-9

Translation of Walter Noll's "Derivation of the Fundamental Equations of Continuum Thermodynamics from Statistical Mechanics"*

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Received: 8 March 2009 / Published online: 17 April 2010

Abstract This article represents a translation of the original paper, "Die Herleitung der Grundgleichungen der Thermomechanik der Kontinua aus der Statistischen Mechanik", which was written by Walter Noll and appeared in the *Journal of Rational Mechanics and Analysis* **4** (1955), 627–646. In the original paper, Noll addressed and analyzed the seminal paper of Irving & Kirkwood, published five years earlier, on "The statistical mechanical theory of transport processes. IV, The Equations of Hydrodynamics." Noll gave new interpretations and provided a firm setting for ideas advanced by Irving & Kirkwood that clearly and directly related to the basic principles of continuum mechanics. This translation aims to expose the important contribution of Noll to a wider community of researchers at a time when the atomistic modeling of material behavior is being advanced. Noll's use of elementary mathematics to discover physical effects, to explain physical concepts, and to draw conclusions of a physical nature is exhibited. Noll's paper emerged from a report that he presented in a seminar at Indiana University in the summer of 1954. The seminar was organized by Clifford Truesdell, whose inspiration Noll gratefully acknowledged.

Keywords Continuum mechanical · Statistical mechanical

Mathematics Subject Classification (2000) 82C21 · 82C22 · 35Q82 · 80A17 · 74A15

*Citations of this translation must refer to the original paper. The original paper is available at the digital archives of the Indiana University Mathematics Journal located at http://www.iumj.indiana.edu/IUMJ/FULLTEXT/1955/4/54022. Corrections to the original paper are listed in the Appendix.

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Introduction

Assuming a classical statistical system of particles, the fundamental equations of continuum thermomechanics (continuity equation, equation of motion, and energy equation) are derived exactly. The macroscopic state functions (density, velocity, stress, energy density, and heat flux) are interpreted as expected values.

The system can represent any continuum (gas, liquid, or solid). It is not assumed that the particles are identical. Also, the nature of the interaction forces can be different for different pairs of particles. Therefore it is not necessary that the particles be molecules in the sense of chemistry. The theory is also valid when the continuum is viewed as the system of its atoms (or even elementary particles). It appears to us physically justified to assume that atoms (or at least the elementary particles) are formed of points and rotational and internal degrees of freedom can be neglected. Hence, for the general theory there is no difference between a mixture and a chemical compound. The difference is solely due to the nature of the mutual potentials. The failure of classical mechanics in the atomistic realm and the influence of quantum mechanical effects, however, are not taken into account.

In Sect. 2 we will formulate the problem precisely and summarize the results. By introducing appropriate abbreviations in Sect. 1, cumbersome notation is avoided. In Sect. 3, we provide conditions sufficient to ensure that our subsequent investigations are valid. Derivations of the expected values of the state functions are provided in Sects. 4–5. In Sect. 6 and Sect. 7 we establish the validity of the fundamental equations, first in the absence of external forces. In Sect. 8, we discuss the influence of external forces. Our investigations are crucially based on two mathematical lemmas formulated and proved in Sect. 9.

The problem being treated here was tackled by Irving and Kirkwood [1]. This work differs from that work in the following points:

1) The proofs satisfy all requirements of mathematical rigor and, additionally, should be easier to follow than those in [1].
2) For the stress tensor and the heat flux, we give closed-form integral expressions. In [1], these quantities are presented as infinite series that only make sense if the probability density as a function of the spatial variable is analytic.
3) The interpretations of stress tensor and heat flux as expected values are provided in detail. This is only attempted in [1].
4) The assumption that all particles are identical is not made.
5) The external forces need not arise from a potential and may—apart from space and time—depend on the velocities of the particles.
6) The use of the δ function is avoided. In [1], the delta function serves only technical purposes.

1 Definitions and Assignments

a. Vectors and tensors Vectors and points are described by lower case letters in bold typeface, tensors of higher order are described by capital letters in bold font. The product of two tensors (dyad) is represented by the symbol $\otimes$, the inner product of two vectors or of a vector and a tensor is represented by a dot "$\cdot$", $\nabla_{\mathbf{x}}\mathbf{F}(\mathbf{x})$ represents the gradient of the tensor $\mathbf{F}(\mathbf{x})$, and $\nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathbf{x})$ represents the divergence of $\mathbf{F}(\mathbf{x})$.

b. Probability density We consider a system of particles. The jth particle is (j) and has mass m_j. A state of the system is characterized by the particle locations $\mathbf{x}_1, \ldots, \mathbf{x}_N$ and velocities $\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_N$, i.e., indicated by a "point" $(\mathbf{x}_1, \ldots, \mathbf{x}_N; \boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_N) = (\mathbf{x}_i; \boldsymbol{\xi}_i)$ of $6N$-dimensional phase space Ω. This phase space is the product of $2N$ three-dimensional Euclidean vector spaces[1]. The probability density of the states in Ω at time t is denoted by

$$W = W(\mathbf{x}_1, \ldots, \mathbf{x}_N; \boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_N; t) = W(\mathbf{x}_i; \boldsymbol{\xi}_i; t).$$

c. Potential energy We assume that the force exerted by (j) on (k), $\mathbf{k}_{jk}$, depends only on the locations $\mathbf{x}_j$ and $\mathbf{x}_k$. By invariance, it follows that $\mathbf{k}_{jk}$ must be a central force whose contribution depends only upon the distance $r_{jk} = |\mathbf{x}_j - \mathbf{x}_k|$. Newton's third law states that $\mathbf{k}_{jk} = -\mathbf{k}_{kj}$. The particle pair (j, k) therefore corresponds to a function,

$$V_{jk}(r) = V_{kj}(r), \tag{1.1}$$

such that $V_{jk}(r_{jk})$ yields the potential energy of the pair. Furthermore,

$$\begin{aligned} \mathbf{k}_{jk} &= -\nabla_{\mathbf{x}_j} V_{jk}(r_{jk}) = -V'_{jk}(r_{jk}) \frac{\mathbf{x}_j - \mathbf{x}_k}{r_{jk}} \\ &= -\mathbf{k}_{kj} = -\nabla_{\mathbf{x}_k} V_{jk}(r_{jk}) = V'_{jk}(r_{jk}) \frac{\mathbf{x}_k - \mathbf{x}_j}{r_{jk}}. \end{aligned} \tag{1.2}$$

For the total *internal potential energy* U of the system, this results in

$$U = U(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{j<k} V_{jk}(r_{jk}) = \frac{1}{2} \sum_{j \neq k} V_{jk}(r_{jk}), \tag{1.3}$$

where one has to sum over all those pairs (j, k) for which $j < k$ or $j \neq k$. It follows that the force exerted upon particle (j) by the system is

$$\nabla_{\mathbf{x}_j} U = \sum_{\substack{k=1 \\ k \neq j}}^{N} \nabla_{\mathbf{x}_j} V_{jk}(r_{jk}) = \sum_{\substack{k=1 \\ k \neq j}}^{N} V'_{jk}(r_{jk}) \frac{\mathbf{x}_j - \mathbf{x}_k}{r_{jk}}. \tag{1.4}$$

d. External forces Apart from those forces acting on particle (j) due to other particles, we assume that yet another external force $\mathbf{k}_j$ is exerted that depends only on location $\mathbf{x}_j$ and the velocity $\boldsymbol{\xi}_j$ of the particle at time t,

$$\mathbf{k}_j = \mathbf{k}_j(\mathbf{x}_j, \boldsymbol{\xi}_j, t).$$

Restrictively, we require, however, that the functions $\mathbf{k}_j$ satisfy the equation

$$\sum_{j=1}^{N} \frac{1}{m_j} \nabla_{\boldsymbol{\xi}_j} \cdot \mathbf{k}_j(\mathbf{x}_j, \boldsymbol{\xi}_j, t) = 0 \tag{1.5}$$

identically. In particular, this condition is met if the $\mathbf{k}_j(\mathbf{x}_j, \boldsymbol{\xi}_j, t)$ do not depend on $\boldsymbol{\xi}_j$.

[1] The $\mathbf{x}_i$ and $\boldsymbol{\xi}_i$ vary in the entire, infinite three-dimensional space and not only in a subregion of it.

e. Integrals The $(6N-3)$-dimensional subspace of Ω that arises upon discarding the spatial variable $\mathbf{x}_j$ belonging to (j) is denoted by Ω_j. Analogously, we denote by Ω_{jk} the subspace that arises from discarding both $\mathbf{x}_j$ and $\mathbf{x}_k$. Let F be a scalar, vector, or tensor function defined over Ω. Then, the abbreviations,

$$\langle F|\mathbf{x}_j=\mathbf{x}\rangle, \qquad \langle F|\mathbf{x}_j=\mathbf{x},\mathbf{x}_k=\mathbf{y}\rangle,$$

denote that F is the integral over Ω_j (Ω_{jk}, respectively), where, after performing the integration, the free variable $\mathbf{x}_j$ (or the variables $\mathbf{x}_j$ and $\mathbf{x}_k$, respectively) are to be replaced by $\mathbf{x}$ (or by $\mathbf{x}$ and $\mathbf{y}$), respectively. Generally, we call

$$\int_{\mathbf{y}} f(\mathbf{y})\,d\mathbf{y}$$

the volume integral of $f(\mathbf{y})$ over the infinite three-dimensional space of locations $\mathbf{y}$. Then, apparently, the relation

$$\int_{\mathbf{y}} \langle F|\mathbf{x}_j=\mathbf{x},\mathbf{x}_k=\mathbf{y}\rangle\,d\mathbf{y}=\langle F|\mathbf{x}_j=\mathbf{x}\rangle \tag{1.6}$$

is valid.

2 Posing the Problem

We assume that the probability density, $W(\mathbf{x}_i;\boldsymbol{\xi}_i;t)$, is defined for all $(\mathbf{x}_i,\boldsymbol{\xi}_i)\in\Omega$ and is continuously differentiable with respect to all variables. Under the restriction that the external forces fulfill condition (1.5),[2] the *principle of the conservation of probability* in phase space yields the classical differential equation

$$\frac{\partial W}{\partial t}=\sum_{i=1}^{N}\left\{-\boldsymbol{\xi}_i\cdot\nabla_{\mathbf{x}_i}W+\frac{1}{m_i}(\nabla_{\mathbf{x}_i}U-\mathbf{k}_i)\cdot\nabla_{\boldsymbol{\xi}_i}W\right\}, \tag{2.1}$$

which determines the rate of change of W.

It is the task of this study to derive the fundamental equations of thermomechanics from (2.1) under the regularity requirements to be formulated in Sect. 3. First, in Sects. 6–7, we assume that external forces are absent so that (2.1) simplifies to

$$\frac{\partial W}{\partial t}=\sum_{i=1}^{N}\left\{-\boldsymbol{\xi}_i\cdot\nabla_{\mathbf{x}_i}W+\frac{1}{m_i}\nabla_{\mathbf{x}_i}U\cdot\nabla_{\boldsymbol{\xi}_i}W\right\}. \tag{2.1a}$$

The case of $\mathbf{k}_i\neq\mathbf{0}$ is treated in Sect. 8. For $\mathbf{k}_i=\mathbf{0}$ the fundamental equations are as follows:
A) *Continuity equation*

$$\frac{\partial\rho}{\partial t}+\nabla_{\mathbf{x}}\cdot(\rho\mathbf{u})=0. \tag{2.2}$$

[2] This requirement ensures that phase space is locally volume preserving.

B) *Equation of motion*

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla_{\mathbf{x}}\mathbf{u}\right)=\nabla_{\mathbf{x}}\cdot\mathbf{S}. \tag{2.3}$$

C) *Equation of energy*

$$\frac{\partial \epsilon}{\partial t}+\nabla_{\mathbf{x}}\cdot(\mathbf{q}-\mathbf{S}\cdot\mathbf{u}+\epsilon\mathbf{u})=0. \tag{2.4}$$

These fundamental equations connect the following macroscopic state functions:

$$\begin{aligned}
\rho &= \rho(\mathbf{x},t)=\textit{Mass density},\\
\mathbf{u} &= \mathbf{u}(\mathbf{x},t)=\textit{Velocity},\\
\mathbf{S} &= \mathbf{S}(\mathbf{x},t)=\textit{Stress tensor},\\
\epsilon &= \epsilon(\mathbf{x},t)=\textit{Energy density},\\
\mathbf{q} &= \mathbf{q}(\mathbf{x},t)=\textit{Heat flux density}.
\end{aligned}$$

We prove that these fundamental equations are valid if the aforementioned state functions are interpreted as expected values. In Sects. 4–5, we show that these expected values are given by the following expressions:

$$\rho=\sum_j m_j\langle W\mid \mathbf{x}_j=\mathbf{x}\rangle, \tag{2.5}$$

$$\rho\mathbf{u}=\sum_j m_j\langle \boldsymbol{\xi}_j W\mid \mathbf{x}_j=\mathbf{x}\rangle. \tag{2.6}$$

The stress tensor is symmetric and consists of a *kinetic contribution*, $\mathbf{S}_{\mathrm{K}}$, and an *interaction contribution*, $\mathbf{S}_{\mathrm{V}}$:

$$\mathbf{S}\ \ =\mathbf{S}_{\mathrm{K}}+\mathbf{S}_{\mathrm{V}}, \tag{2.7}$$

$$\mathbf{S}_{\mathrm{K}}=-\sum_j m_j\langle(\boldsymbol{\xi}_j-\mathbf{u})\otimes(\boldsymbol{\xi}_j-\mathbf{u})\,W\mid \mathbf{x}_j=\mathbf{x}\rangle, \tag{2.8}$$

$$\mathbf{S}_{\mathrm{V}}=\frac{1}{2}\sum_{j\neq k}\int_{\mathbf{z}}\left\{\frac{\mathbf{z}\otimes\mathbf{z}}{|\mathbf{z}|}V'_{jk}(|\mathbf{z}|)\int_{\alpha=0}^{1}\langle W\mid \mathbf{x}_j=\mathbf{x}+\alpha\mathbf{z},\mathbf{x}_k=\mathbf{x}-(1-\alpha)\mathbf{z}\rangle d\alpha\right\}d\mathbf{z}. \tag{2.9}$$

The energy density splits into the *kinetic energy density*, ϵ_{K}, and the *interaction energy density*, ϵ_{V}:

$$\epsilon\ \ =\epsilon_{\mathrm{K}}+\epsilon_{\mathrm{V}}, \tag{2.10}$$

$$\epsilon_{\mathrm{K}}=\frac{1}{2}\sum_j m_j\langle\boldsymbol{\xi}_j^2 W\mid \mathbf{x}_j=\mathbf{x}\rangle, \tag{2.11}$$

$$\epsilon_{\mathrm{V}}=\frac{1}{2}\sum_{j\neq k}\langle V_{jk}(|\mathbf{x}_j-\mathbf{x}_k|)\,W\mid \mathbf{x}_j=\mathbf{x}\rangle. \tag{2.12}$$

The heat flux has three terms, the *kinetic contribution*, $\mathbf{q}_{\mathrm{K}}$, the *transport contribution*, $\mathbf{q}_{\mathrm{T}}$, and the *interaction contribution*, $\mathbf{q}_{\mathrm{V}}$:

$$\mathbf{q} = \mathbf{q}_{\mathrm{K}} + \mathbf{q}_{\mathrm{T}} + \mathbf{q}_{\mathrm{V}}, \tag{2.13}$$

$$\mathbf{q}_{\mathrm{K}} = \frac{1}{2}\sum_{j} m_j \langle |\boldsymbol{\xi}_j - \mathbf{u}|^2 (\boldsymbol{\xi}_j - \mathbf{u})\, W \mid \mathbf{x}_j = \mathbf{x}\rangle, \tag{2.14}$$

$$\mathbf{q}_{\mathrm{T}} = \frac{1}{2}\sum_{j\neq k} \langle (\boldsymbol{\xi}_j - \mathbf{u}) V_{jk}(|\mathbf{x}_j - \mathbf{x}_k|)\, W \mid \mathbf{x}_j = \mathbf{x}\rangle, \tag{2.15}$$

$$\mathbf{q}_{\mathrm{V}} = -\frac{1}{2}\sum_{j\neq k} \int_{\mathbf{z}} \Bigg\{ \frac{\mathbf{z}}{|\mathbf{z}|} V'_{jk}(|\mathbf{z}|) \times \mathbf{z} \cdot \int_{\alpha=0}^{1} \Bigg\langle \left(\frac{\boldsymbol{\xi}_j + \boldsymbol{\xi}_k}{2} - \mathbf{u} \right) W \mid \mathbf{x}_j = \mathbf{x} + \alpha \mathbf{z}, \mathbf{x}_k = \mathbf{x} - (1-\alpha)\mathbf{z} \Bigg\rangle d\alpha \Bigg\} d\mathbf{z}. \tag{2.16}$$

3 Regularity Conditions

The expectation expressions occurring in (2.5)–(2.16) are improper integrals containing W and V_{jk}. It is therefore clear that certain regularity conditions must be met for W and V_{jk} if the state functions in (2.5)–(2.16) are to be well-defined and the functions of $\mathbf{x}$ and t are to be continuously differentiable. Already the condition $\int_{\Omega} W d\Omega = 1$ requires that W approaches zero sufficiently fast as $|\mathbf{x}_j| \to \infty$ and $|\boldsymbol{\xi}_j| \to \infty$.

The following three conditions are sufficient for the validity of the results in this work:

A) There is a number $\delta > 0$ such that the function

$$G(\mathbf{x}_i; \boldsymbol{\xi}_i; t) = W(\mathbf{x}_i; \mathbf{x}_i; t) \prod_{j=1}^{N} |\mathbf{x}_j|^{3+\delta} \prod_{k=1}^{N} |\boldsymbol{\xi}_k|^{3+\delta},$$

as well as its derivatives, are restricted by a constant solely dependent on t.

B) The functions $V_{jk}(r)$ are defined for all r, are continuously differentiable, and together with their derivatives, are finite.

C) The functions $\mathbf{k}_j(\mathbf{x}, \boldsymbol{\xi}, t)$ are defined for all values of $\mathbf{x}, \boldsymbol{\xi}, t$, are continuously differentiable, and granted scalars $A(t)$ and $B(t)$, solely dependent on time, and satisfy

$$|\mathbf{k}_j| < A(t)|\boldsymbol{\xi}| + B(t), \qquad |\nabla_{\boldsymbol{\xi}} \mathbf{k}_j| < A(t)|\boldsymbol{\xi}| + B(t).$$

These conditions are sufficient for the convergence of all improper integrals, interchanging the order of integration, and for differentiation and integration, etc.

Furthermore, condition **A** ensures the validity of the following *lemma*, which is proved by partial integration:

Suppose that $F(\mathbf{x}; \boldsymbol{\xi}_i)$ is a continuously differentiable function defined in Ω which, with the constants A and B, satisfies the inequalities

$$|F| < A \prod_{k=1}^{N} |\boldsymbol{\xi}_k|^3 + B, \qquad |\nabla_{\mathbf{x}_j} F| < A \prod_{k=1}^{N} |\boldsymbol{\xi}_k|^3 + B, \qquad |\nabla_{\boldsymbol{\xi}_j} F| < A \prod_{k=1}^{N} |\boldsymbol{\xi}_k|^3 + B.$$

Then, the following formulas are valid:

$$\int F\nabla_{\mathbf{x}_j} W = -\int W\nabla_{\mathbf{x}_j} F, \qquad \int F\nabla_{\boldsymbol{\xi}_j} W = -\int W\nabla_{\boldsymbol{\xi}_j} F, \tag{3.1}$$

where one integrates over a subspace of Ω that contains the space of $\mathbf{x}_j$ or $\boldsymbol{\xi}_j$, respectively, as another subspace (omitting the volume elements). In particular, if F is independent of $\mathbf{x}_j$ or $\boldsymbol{\xi}_j$, one has

$$\int F\nabla_{\mathbf{x}_j} W = 0 \quad \text{or} \quad \int F\nabla_{\boldsymbol{\xi}_j} W = 0, \quad \text{respectively.} \tag{3.2}$$

Note I. The linear partial differential equation (2.1) is of first order in W. According to generally known rules, $W(\mathbf{x}_i; \boldsymbol{\xi}_i; t)$ is therefore uniquely determined for all t if the initial density, $W(\mathbf{x}_i; \boldsymbol{\xi}_i; 0) = W_0(\mathbf{x}_i; \boldsymbol{\xi}_i)$ is prescribed. It would therefore be desirable to apply regularity conditions only to $W_0(\mathbf{x}_i; \boldsymbol{\xi}_i)$ and not to $W(\mathbf{x}_i; \boldsymbol{\xi}_i; t)$, and then prove **A** as a property of W. The author, however, has not yet succeeded in doing so.

Note II. If W is not differentiable for all $(\mathbf{x}_i; \boldsymbol{\xi}_i) \in \Omega$ and t, (2.1) generally loses its meaning. The statistical description, however, is meaningful if W is only integrable over Ω. It is possible to generalize our investigations to this case. Condition **A** can then be replaced by the requirement that $W\prod_{k=1}^{N} |\boldsymbol{\xi}_k|^3$ be integrable for all t over Ω. Then, the expressions (2.5)–(2.16) remain meaningful. The state functions, however, being functions of $\mathbf{x}$ and t, are no longer continuously differentiable for all values of $\mathbf{x}$ and t such that the fundamental equations in the form (2.2)–(2.4) in general, have no meaning. They must be replaced by the laws of conservation of mass, momenta, and energy in finite form.

To carry out this sort of generalization demands considerable formal work. But this can be avoided by understanding all the present differentiations in the sense of Schwartz's [2] theory of distributions. Then, (2.1) is completely equivalent with the principle of conservation of probability. The fundamental equations (2.2)–(2.4) are generally valid in the sense of the theory of distributions and also when the probability density W does not even exist. In this latter case, W and the state functions are to be viewed as measures. The fundamental equations are valid in the conventional sense only for those values of $\mathbf{x}$ and t for which the state functions represent continuously differentiable functions. One can readily derive the transition conditions at discontinuity surfaces (shock and acceleration waves) once (2.2)–(2.4) are understood in the sense of distributions.

4 Expected Values of the State Functions

The value of a physical quantity, F, for the particle (j) is given by a function, $f_j(\mathbf{x}_i; \boldsymbol{\xi}_i)$, defined on Ω. According to the rules of probability calculus, and according to Sect. 1*e*, one has

$$\mathcal{E}_j(F)\, d\mathbf{x} = \langle f_j\, W \mid \mathbf{x}_j = \mathbf{x}\rangle\, d\mathbf{x} \tag{4.1}$$

as the expected value of F for (j) under the condition that (j) is in the volume element $d\mathbf{x}$ at $\mathbf{x}$. Hence, the density $\mathcal{E}(F)$ of the expected value of F for all particles at the position $\mathbf{x}$ is

$$\mathcal{E}(F) = \sum_j \mathcal{E}_j(F) = \sum_j \langle f_j\, W \mid \mathbf{x}_j = \mathbf{x}\rangle. \tag{4.2}$$

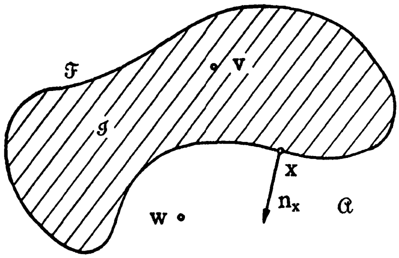

Fig. 1[3]

The expected value of F for (j) under the condition that (j) is in the volume element $d\mathbf{x}$ at $\mathbf{x}$ and (k) in the volume element $d\mathbf{y}$ at $\mathbf{y}$ is given by

$$\mathcal{E}_{jk}(F)\, d\mathbf{x}\, d\mathbf{y} = \langle f_j \; W \mid \mathbf{x}_j = \mathbf{x}, \mathbf{x}_k = \mathbf{y}\rangle \, d\mathbf{x}\, d\mathbf{y}. \tag{4.3}$$

a. Density and velocity It follows immediately from (4.2) that (2.5) and (2.6) represent the expected values for mass and momentum densities.

b. Stress tensor Let $\mathcal{J}$ be a region of three-dimensional space with a continuously differentiable boundary, $\mathcal{F}$. We call $\mathcal{A}$ the exterior of $\mathcal{J}$ with $\mathbf{n}_x$ being the normal unit vector at $\mathbf{x} \in \mathcal{F}$ pointing outwards, and with $d\mathcal{F}_x$ the associated surface element (see Fig. 1).

As generally known, the stress tensor is characterized by the fact that for any part $\mathcal{J}$ of the considered body, the force, $\mathbf{k}$, exerted by $\mathcal{A}$ on $\mathcal{J}$ can be represented in the form

$$\mathbf{k} = \int_{\mathcal{F}} \mathbf{S}(\mathbf{x}) \cdot \mathbf{n}_\mathbf{x} \, d\mathcal{F}_\mathbf{x}. \tag{4.4}$$

One readily sees that according to (2.8),

$$\mathbf{k}_\mathrm{K} = \int_{\mathcal{F}} \mathbf{S}_\mathrm{K} \cdot \mathbf{n}_\mathbf{x} \, d\mathcal{F}_\mathbf{x} \tag{4.5}$$

gives the expected value of the “kinetic” force that corresponds to the momentum per unit time transported from $\mathcal{A}$ to $\mathcal{J}$. Therefore, $\mathcal{J}$ should be thought of moving with the average velocity $\mathbf{u}$. The kinetic contribution (2.8) corresponds to what is normally called “viscous tension” in the kinetic theory of monoatomic gases.

Now, let us assume that the particle (j) is at the position $\mathbf{x}_j = \mathbf{v} \in \mathcal{J}$ and that the particle (k) is at the position $\mathbf{x}_k = \mathbf{w} \in \mathcal{A}$. Then, according to (1.2), (k) exerts the following force on (j):

$$\mathbf{k}_{jk}(\mathbf{v}, \mathbf{w}) = -\nabla_\mathbf{v} V_{jk}(|\mathbf{v} - \mathbf{w}|) = -V'_{jk}(|\mathbf{v} - \mathbf{w}|)\frac{\mathbf{v} - \mathbf{w}}{|\mathbf{v} - \mathbf{w}|}. \tag{4.6}$$

According to (4.3), the expected value of the force exerted by (k) in $\mathcal{A}$ on (j) in $\mathcal{J}$, is therefore given by

$$\int_{\mathbf{v}\in\mathcal{J}} \int_{\mathbf{w}\in\mathcal{A}} \sum_{j \neq k} \mathbf{k}_{jk}(\mathbf{v}, \mathbf{w}) \langle W \mid \mathbf{x}_j = \mathbf{v}, \mathbf{x}_k = \mathbf{w}\rangle \, d\mathbf{v}\, d\mathbf{w}.$$

[3]Translator’s footnote: The image was cropped from a pdf of the original paper. Note the differences in font styles in the figure and in the text.

After summation over j and k, we obtain from the expected value $\mathbf{k}_\mathrm{V}$ of the total force that is exerted by the particles in $\mathcal{A}$ on those in $\mathcal{J}$. With (4.6), this yields

$$\mathbf{k}_\mathrm{V} = -\int_{\mathbf{v}\in\mathcal{J}} \int_{\mathbf{w}\in\mathcal{A}} \sum_{j\neq k} \left\{ \frac{\mathbf{v}-\mathbf{w}}{|\mathbf{v}-\mathbf{w}|} V'_{jk}(|\mathbf{v}-\mathbf{w}|)\langle W \mid \mathbf{x}_j = \mathbf{v}, \mathbf{x}_k = \mathbf{w}\rangle \right\} d\mathbf{w}\, d\mathbf{v}.$$

As one can readily see, the integrand fulfills conditions **A**, **B**, and **C** of Sect. 9. According to Lemma 2, (9.4), and with (2.9), it follows that

$$\mathbf{k}_\mathrm{V} = \int_{\mathcal{F}} \mathbf{S}_\mathrm{V} \cdot \mathbf{n}_\mathbf{x}\, d\mathcal{F}_\mathbf{x}. \tag{4.7}$$

The force $\mathbf{k}$ exerted by $\mathcal{A}$ on $\mathcal{J}$ is composed from the kinetic force $\mathbf{k}_\mathrm{K}$ (4.5) and the interaction force $\mathbf{k}_\mathrm{V}$ (4.7). Because of (2.7), we therefore have

$$\mathbf{k} = \mathbf{k}_\mathrm{K} + \mathbf{k}_\mathrm{V} = \int_{\mathcal{F}} (\mathbf{S}_\mathrm{K} + \mathbf{S}_\mathrm{V}) \cdot \mathbf{n}_\mathbf{x}\, d\mathcal{F}_\mathbf{x} = \int_{\mathcal{F}} \mathbf{S} \cdot \mathbf{n}_\mathbf{x}\, d\mathcal{F}_\mathbf{x}.$$

This equation satisfies (4.4) and so the expected value of the stress tensor is indeed given by (2.7)–(2.9).

c. Energy density Let us think of the kinetic energy, $\frac{1}{2} m_j \boldsymbol{\xi}_j^2$, of particle (j) as being localized at the position $\mathbf{x}_j$ of this particle. Then, according to (4.2) the expected value, $\epsilon_\mathrm{K}(\mathbf{x})$, of the kinetic energy density at position $\mathbf{x}$ is given by (2.11).

The localization of the potential energy demands a certain arbitrariness as it is assigned to particle pairs, and not—as for the kinetic energy—to individual particles. We assume that the potential energy corresponding to the pair (j,k), $V_{jk}(|\mathbf{x}_j - \mathbf{x}_k|)$, is distributed equally at the positions $\mathbf{x}_j$ and $\mathbf{x}_k$. Then, at position $\mathbf{x}_j$, the total potential energy is

$$V_j = V_j(\mathbf{x}_1, \ldots, \mathbf{x}_N) = V_j(\mathbf{x}_i) = \frac{1}{2} \sum_{\substack{k=1\\k\neq j}}^{N} V_{jk}(r_{jk}), \qquad r_{jk} = |\mathbf{x}_j - \mathbf{x}_k|. \tag{4.8}$$

Then, according to (4.2), (2.12) yields the expected value, $\epsilon_\mathrm{V}(\mathbf{x})$, of the density localized according to (4.8).

d. Heat flux (*density*). The heat flux, $\mathbf{q} = \mathbf{q}(\mathbf{x})$, is characterized by the fact that for any part $\mathcal{J}$ of the body, the energy transferred per unit time from $\mathcal{J}$ to $\mathcal{A}$ can be represented in the form

$$Q = \int_{\mathcal{F}} \mathbf{q}(\mathbf{x}) \cdot \mathbf{n}_\mathbf{x}\, d\mathcal{F}_\mathbf{x}, \tag{4.9}$$

(see Fig. 1), where $\mathcal{J}$ travels at the velocity $\mathbf{u}$.

One is readily convinced that, with (2.14), the expected value of the kinetic energy flowing per unit time from $\mathcal{J}$ to $\mathcal{A}$ is represented by the expression

$$Q_\mathrm{K} = \int_{\mathcal{F}} \mathbf{q}_\mathrm{K} \cdot \mathbf{n}_\mathbf{x}\, d\mathcal{F}_\mathbf{x}. \tag{4.10}$$

Therefore, $\mathbf{q}_\mathrm{K}$, given by (2.14), is indeed the kinetic contribution of the heat flux. This is well known from the kinetic theory of monoatomic gases.

Let us consider the expression

$$\mathbf{q}_{\mathrm{T}}^{*} = \mathbf{q}_{\mathrm{T}} + \epsilon_{\mathrm{V}}\mathbf{u} = \frac{1}{2}\sum_{j\neq k}\langle \boldsymbol{\xi}_j\, V_{jk}(|\mathbf{x}_j - \mathbf{x}_k|)\, W \mid \mathbf{x}_j = \mathbf{x}\rangle \tag{4.11}$$

and compare to (2.12) and (2.15). According to (4.8), we have

$$\mathbf{q}_{\mathrm{T}}^{*} = \sum_{j}\langle \boldsymbol{\xi}_j V_j W \mid \mathbf{x}_j = \mathbf{x}\rangle. \tag{4.12}$$

The expression $\boldsymbol{\xi}_j V_j(\mathbf{x}_j)$ indicates the flow of potential energy, localized according to (4.8) at $\mathbf{x}_j$. Therefore, with (4.12) and because of (4.2), we have

$$Q_{\mathrm{T}}^{*} = \int_{\mathcal{F}} \mathbf{q}_{\mathrm{T}}^{*}\cdot \mathbf{n}_{\mathbf{x}}\, d\mathcal{F}_{\mathbf{x}}$$

as the potential energy that must be transferred per time unit through $\mathcal{F}$. However, $\mathcal{J}$ has to be seen as fixed in time. To obtain the potential energy Q_{T} that is transported per time unit via the moving surface $\mathcal{F}$ one has to subtract the macroscopic convection contribution

$$Q_{\mathrm{T}}^{0} = \int_{\mathcal{F}} \epsilon_{\mathrm{V}}\, \mathbf{u}\cdot \mathbf{n}_{\mathbf{x}}\, d\mathcal{F}_{\mathbf{x}}.$$

So, because of (4.11), one finds

$$Q_{\mathrm{T}} = Q_{\mathrm{T}}^{*} - Q_{\mathrm{T}}^{0} = \int_{\mathcal{F}} \mathbf{q}_{\mathrm{T}}\cdot \mathbf{n}_{\mathbf{x}} d\mathcal{F}_{\mathbf{x}}. \tag{4.13}$$

Therefore, the $\mathbf{q}_{\mathrm{T}}$ given in (2.15) is indeed the contribution of the heat flux that stems from the transport of the potential energy.

Finally, let us consider

$$\begin{aligned}\mathbf{q}_{\mathrm{V}}^{*} &= \mathbf{q}_{\mathrm{V}} - \mathbf{S}_{\mathrm{V}}\cdot\mathbf{u}\\ &= -\frac{1}{2}\sum_{j\neq k}\int_{\mathbf{z}}\Bigg\{\frac{\mathbf{z}}{|\mathbf{z}|}V_{jk}'(|\mathbf{z}|)\\ &\quad\times \mathbf{z}\cdot\int_{\alpha=0}^{1}\Bigg\langle\frac{\boldsymbol{\xi}_j+\boldsymbol{\xi}_k}{2}\, W \mid \mathbf{x}_j = \mathbf{x}+\alpha\mathbf{z}, \mathbf{x}_k = \mathbf{x}-(1-\alpha)\mathbf{z}\Bigg\rangle d\alpha\Bigg\}\, d\mathbf{z}\end{aligned} \tag{4.14}$$

(compare to (2.9) and (2.16)). In Sect. 5, we show that

$$Q_{\mathrm{V}}^{*} = \int_{\mathcal{F}} \mathbf{q}_{\mathrm{V}}^{*}\cdot \mathbf{n}_{\mathbf{x}}\, d\mathcal{F}_{\mathbf{x}} \tag{4.15}$$

represents the expected value of the potential energy, transferred per unit time from $\mathcal{J}$ to $\mathcal{A}$, which stems from particles in $\mathcal{A}$ performing work on particles in $\mathcal{J}$. Here, $\mathcal{J}$ can be viewed as fixed in time. To obtain the interaction energy, Q_{V}, transferred from $\mathcal{A}$ to the moving $\mathcal{J}$, one has to subtract from Q_{V}^{*} the macroscopic interaction work performed by $\mathcal{J}$ on $\mathcal{A}$ per unit time

$$Q_{\mathrm{V}}^{0} = -\int_{\mathcal{F}} (\mathbf{S}_{\mathrm{V}}\cdot\mathbf{u})\cdot \mathbf{n}_{\mathbf{x}}\, d\mathcal{F}_{\mathbf{x}}.$$

So, according to (4.14) one finds that

$$Q_{\mathrm{V}} = Q_{\mathrm{V}}^{*} - Q_{\mathrm{V}}^{0} = \int_{\mathcal{F}} (\mathbf{q}_{\mathrm{V}}^{*} + \mathbf{S}_{\mathrm{V}} \cdot \mathbf{u}) \cdot \mathbf{n}_{\mathbf{x}} \, d\mathcal{F}_{\mathbf{x}} = \int_{\mathcal{F}} \mathbf{q}_{\mathrm{V}} \cdot \mathbf{n}_{\mathbf{x}} \, d\mathcal{F}_{\mathbf{x}}. \tag{4.16}$$

Consequently, (2.16) indeed gives the interaction contribution to the heat flux. Therefore $Q = Q_{\mathrm{K}} + Q_{\mathrm{T}} + Q_{\mathrm{V}}$ is the total energy per unit time transferred from the moving $\mathcal{J}$ to $\mathcal{A}$, and (4.9) is satisfied because of (4.10), (4.13), (4.16), and (2.13). It has therefore been shown that the expected value of the heat flux is indeed given by (2.13)–(2.16).

5 Interaction Contribution to the Heat Flux

We wish to prove the validity of (4.15), replacing expression (4.14) by $\mathbf{q}_{\mathrm{V}}^{*}$. To this end, we investigate the mechanical system $\mathcal{S}$ composed solely from particles in $\mathcal{J}$. For this system, the forces exerted by the particles in $\mathcal{A}$ on the particles in $\mathcal{J}$ are considered to be external forces. These forces have the time dependent variable potential

$$\psi(\mathbf{x}_i \in \mathcal{J}; t) = \sum_{\mathbf{x}_j \in \mathcal{J}} \sum_{\mathbf{x}_k \in \mathcal{A}} V_{jk}(|\mathbf{x}_j - \mathbf{x}_k(t)|). \tag{5.1}$$

Here, $\mathbf{x}_j \in \mathcal{J}$ is to be viewed as the independent variable while $\mathbf{x}_k(t)$ are those functions that describe the trajectories of the particles $\mathbf{x}_k \in \mathcal{A}$. The internal energy of the system $\mathcal{S}$ is E_I. Then, the total energy E with respect to the external potential (5.1) is given by

$$E = E_I + \psi(\mathbf{x}_i \in \mathcal{J}; t). \tag{5.2}$$

According to the energy law in particle mechanics,

$$\dot{E} = \frac{\partial}{\partial t} \psi(\mathbf{x}_i \in \mathcal{J}, t),$$

which, along with (5.1), yields

$$\dot{E} = \sum_{\mathbf{x}_j \in \mathcal{J}} \sum_{\mathbf{x}_k \in \mathcal{A}} V'_{jk}(|\mathbf{x}_j - \mathbf{x}_k(t)|) \, \frac{\mathbf{x}_j - \mathbf{x}_k(t)}{|\mathbf{x}_j - \mathbf{x}_k(t)|} \cdot (-\dot{\mathbf{x}}_k(t))$$

and, because $\dot{\mathbf{x}}_k = \boldsymbol{\xi}_k$,

$$\dot{E} = -\sum_{\mathbf{x}_j \in \mathcal{J}} \sum_{\mathbf{x}_k \in \mathcal{A}} V'_{jk}(r_{jk}) \frac{\mathbf{x}_j - \mathbf{x}_k}{r_{jk}} \cdot \boldsymbol{\xi}_k, \quad r_{jk} = |\mathbf{x}_j - \mathbf{x}_k|. \tag{5.3}$$

The energy, E, however, does not equal the energy that is localized in $\mathcal{J}$ according to (4.8). The energy E^* localized in $\mathcal{J}$ according to that expression is composed from the internal energy E_I and half of the potential energy that corresponds to all those particle pairs (j, k) for which $\mathbf{x}_j \in \mathcal{J}$ and $\mathbf{x}_k \in \mathcal{A}$. Therefore, we have:

$$E^* = E_I + \frac{1}{2} \sum_{\mathbf{x}_j \in \mathcal{J}} \sum_{\mathbf{x}_k \in \mathcal{A}} V_{jk}(r_{jk}). \tag{5.4}$$

From this, (5.1), and (5.2) results

$$E^* = E - \frac{1}{2} \sum_{\mathbf{x}_j \in \mathcal{J}} \sum_{\mathbf{x}_k \in \mathcal{A}} V_{jk}(r_{jk}).$$

Differentiation with respect to t yields

$$\dot{E}^* = \dot{E} - \frac{1}{2} \sum_{\mathbf{x}_j \in \mathcal{J}} \sum_{\mathbf{x}_k \in \mathcal{A}} V'_{jk}(r_{jk}) \frac{\mathbf{x}_j - \mathbf{x}_k}{r_{jk}} \cdot (\boldsymbol{\xi}_j - \boldsymbol{\xi}_k), \tag{5.5}$$

where $\dot{\mathbf{x}}_j$ and $\dot{\mathbf{x}}_k$ have been replaced by $\boldsymbol{\xi}_j$ and $\boldsymbol{\xi}_k$, respectively. Insertion of (5.3) into (5.5) results in

$$\dot{E}^* = - \sum_{\mathbf{x}_j \in \mathcal{J}} \sum_{\mathbf{x}_k \in \mathcal{A}} V'_{jk}(r_{jk}) \frac{\mathbf{x}_j - \mathbf{x}_k}{r_{jk}} \cdot \frac{\boldsymbol{\xi}_j + \boldsymbol{\xi}_k}{2}.$$

This expression indicates how much the energy, localized by expression (4.8) in $\mathcal{J}$, varies per unit time and due to the interaction between the particles. The energy flux contribution directed from $\mathcal{J}$ to $\mathcal{A}$ is therefore given by $-\dot{E}^*$. According to (4.3), the expected value of this contribution has the form,

$$Q^*_{\mathrm{V}} = \int_{\mathbf{v} \in \mathcal{J}} \int_{\mathbf{w} \in \mathcal{A}} \sum_{j \neq k} V'_{jk}(|\mathbf{v} - \mathbf{w}|) \frac{\mathbf{v} - \mathbf{w}}{|\mathbf{v} - \mathbf{w}|} \cdot \left\langle \frac{\boldsymbol{\xi}_j + \boldsymbol{\xi}_k}{2} W \mid \mathbf{x}_j = \mathbf{v}, \mathbf{x}_k = \mathbf{w} \right\rangle d\mathbf{v}\, d\mathbf{w}.$$

The integrand fulfills the conditions **A**, **B**, **C** in Sect. 9. With (4.14), this results, according to Lemma 2, (9.4), in

$$Q^*_{\mathrm{V}} = \int_{\mathcal{F}} \mathbf{q}^*_{\mathrm{V}} \cdot \mathbf{n}_{\mathbf{x}}\, d\mathcal{F}_{\mathbf{x}}.$$

6 Continuity Equation and Equation of Motion

The proof of the continuity equation (2.2) is extremely easy. Multiply (2.1a) by m_j, integrate over Ω_j, replace $\mathbf{x}_j$ by $\mathbf{x}$ and sum over j. Because of (3.2), various terms cancel. Eventually, one obtains equation (2.2) with (2.5) and (2.6).

We multiply (2.1a) by $m_j \boldsymbol{\xi}_j$, integrate over Ω_j, replace the free variable $\mathbf{x}_j$ by $\mathbf{x}$ and finally sum over j. Then, taking (3.2) and (2.6) into account, we obtain the equation

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) = \mathbf{v}_1 + \mathbf{v}_2, \tag{6.1}$$

where

$$\mathbf{v}_1 = -\sum_j m_j \langle \boldsymbol{\xi}_j (\boldsymbol{\xi}_j \cdot \nabla_{\mathbf{x}_j} W) \mid \mathbf{x}_j = \mathbf{x} \rangle, \tag{6.2}$$

$$\mathbf{v}_2 = \sum_j \langle (\nabla_{\mathbf{x}_j} U \cdot \nabla_{\boldsymbol{\xi}_j} W) \boldsymbol{\xi}_j \mid \mathbf{x}_j = \mathbf{x} \rangle. \tag{6.3}$$

Exchanging integration and differentiation with respect to $\mathbf{x}_j$ in (6.2) yields

$$\mathbf{v}_1 = \nabla_{\mathbf{x}} \cdot \left\{ -\sum_j m_j \langle (\boldsymbol{\xi}_j \otimes \boldsymbol{\xi}_j) W \mid \mathbf{x}_j = \mathbf{x} \rangle \right\}.$$

Since

$$\boldsymbol{\xi}_j \otimes \boldsymbol{\xi}_j = (\boldsymbol{\xi}_j - \mathbf{u}) \otimes (\boldsymbol{\xi}_j - \mathbf{u}) + \mathbf{u} \otimes \boldsymbol{\xi}_j + \boldsymbol{\xi}_j \otimes \mathbf{u} - \mathbf{u} \otimes \mathbf{u},$$

and taking (2.5), (2.6), and (2.8) into account, it follows that

$$\mathbf{v}_1 = \nabla_{\mathbf{x}} \cdot \left\{ \mathbf{S}_{\mathrm{K}} - \mathbf{u} \otimes \rho \mathbf{u} \right\} = \nabla_{\mathbf{x}} \cdot \mathbf{S}_{\mathrm{K}} - \mathbf{u} \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u}) - \rho \mathbf{u} \cdot \nabla_{\mathbf{x}} \mathbf{u}. \tag{6.4}$$

Inserting (3.1) in (6.3) yields

$$\mathbf{v}_2 = -\sum_j \langle \nabla_{\mathbf{x}_j} U \, W \mid \mathbf{x}_j = \mathbf{x} \rangle.$$

If we replace $\nabla_{\mathbf{x}_j} U$ by expression (1.4) we find

$$\mathbf{v}_2 = -\sum_{j \neq k} \left\langle V'_{jk}(r_{jk}) \, \frac{\mathbf{x}_j - \mathbf{x}_k}{r_{jk}} \, W \mid \mathbf{x}_j = \mathbf{x} \right\rangle, \quad r_{jk} = |\mathbf{x}_j - \mathbf{x}_k|.$$

Thus, with (1.6),

$$\mathbf{v}_2 = -\int_{\mathbf{y}} \left\{ \frac{\mathbf{x} - \mathbf{y}}{r} \sum_{j \neq k} V'_{jk}(r) \langle W \mid \mathbf{x}_j = \mathbf{x}, \mathbf{x}_k = \mathbf{y} \rangle \right\} d\mathbf{y}, \quad r = |\mathbf{x} - \mathbf{y}|. \tag{6.5}$$

One can easily see that the integrand fulfills the conditions **A**, **B**, and **C** in Sect. 9. In particular, the validity of (9.1) follows if the summation indices j and k are exchanged in (6.5). According to Lemma 1, (9.2), it follows from (2.9) that

$$\mathbf{v}_2 = \nabla_{\mathbf{x}} \cdot \mathbf{S}_{\mathrm{V}}.$$

We insert this and (6.4) into (6.1) and obtain

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) = \mathbf{u} \frac{\partial \rho}{\partial t} + \rho \frac{\partial \mathbf{u}}{\partial t} = -\mathbf{u} \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u}) - \rho \mathbf{u} \cdot \nabla_{\mathbf{x}} \mathbf{u} + \nabla_{\mathbf{x}} \cdot (\mathbf{S}_{\mathrm{K}} + \mathbf{S}_{\mathrm{V}}).$$

Bearing in mind the continuity equation (2.2), the equation of motion (2.3) indeed follows.

7 Energy Equation

We multiply (2.1a) with $(m_j \boldsymbol{\xi}_j^2/2 + V_j)$ (see (4.8)), integrate over Ω_j, subsequently replace $\mathbf{x}_j$ by $\mathbf{x}$ and sum over j. Because of (3.2) various terms cancel. Eventually, with (2.10)–(2.12) we obtain

$$\frac{\partial \epsilon}{\partial t} = q_1 + q_2 + q_3, \tag{7.1}$$

where

$$q_1 = -\frac{1}{2} \sum_j m_j \langle \boldsymbol{\xi}_j^2 \boldsymbol{\xi}_j \cdot \nabla_{\mathbf{x}_j} W \mid \mathbf{x}_j = \mathbf{x} \rangle, \tag{7.2}$$

$$q_2 = -\sum_j \sum_l \langle V_j \boldsymbol{\xi}_l \cdot \nabla_{\mathbf{x}_j} W \mid \mathbf{x}_j = \mathbf{x} \rangle, \tag{7.3}$$

$$q_3 = \frac{1}{2} \sum_j \langle \boldsymbol{\xi}_j^2 \nabla_{\mathbf{x}_j} U \cdot \nabla_{\boldsymbol{\xi}_j} W \mid \mathbf{x}_j = \mathbf{x} \rangle + \sum_j \sum_l \langle V_j \nabla_{\mathbf{x}_l} U \cdot \nabla_{\boldsymbol{\xi}_j} W \mid \mathbf{x}_j = \mathbf{x} \rangle. \tag{7.4}$$

Exchanging integration and differentiation with respect to $\mathbf{x}_j$ in (7.2) yields

$$q_1 = -\nabla_{\mathbf{x}} \cdot \left\{ \frac{1}{2} \sum_j m_j \langle \boldsymbol{\xi}_j^2 \boldsymbol{\xi}_j W \mid \mathbf{x}_j = \mathbf{x} \rangle \right\}.$$

Because

$$\boldsymbol{\xi}_j^2 \boldsymbol{\xi}_j = |\boldsymbol{\xi}_j - \mathbf{u}|^2 (\boldsymbol{\xi}_j - \mathbf{u}) + 2\left[(\boldsymbol{\xi}_j - \mathbf{u}) \otimes (\boldsymbol{\xi}_j - \mathbf{u})\right] \cdot \mathbf{u} + |\boldsymbol{\xi}|^2 \mathbf{u} + |\mathbf{u}|^2 (\boldsymbol{\xi}_j - \mathbf{u}),$$

and taking (2.5), (2.6), (2.8), (2.11) and (2.14) into account, it follows that

$$q_1 = -\nabla_{\mathbf{x}} \cdot (\mathbf{q}_{\mathrm{K}} - \mathbf{u} \cdot \mathbf{S}_{\mathrm{K}} + \mathbf{u} \epsilon_{\mathrm{K}}). \tag{7.5}$$

Inserting (4.8) into (7.3) and using (3.2), we obtain

$$q_2 = -\frac{1}{2} \sum_{j \neq k} \{ \langle V_{jk}(r_{jk}) \boldsymbol{\xi}_j \cdot \nabla_{\mathbf{x}_j} W \mid \mathbf{x}_j = \mathbf{x} \rangle + \langle V_{jk}(r_{jk}) \boldsymbol{\xi}_k \cdot \nabla_{\mathbf{x}_k} W \mid \mathbf{x}_j = \mathbf{x} \rangle \}. \tag{7.6}$$

According to the product rule,

$$V_{jk}(r_{jk}) \nabla_{\mathbf{x}_j} W = \nabla_{\mathbf{x}_j} (V_{jk}(r_{jk})\, W) - \nabla_{\mathbf{x}_j} V_{jk}(r_{jk})\, W.$$

If one inserts this into the first term on the right-hand side of (7.6) and rearranges the second term according to (3.1), this yields

$$\begin{aligned} q_2 = \frac{1}{2} \sum_{j \neq k} \{ & -\nabla_{\mathbf{x}} \langle \boldsymbol{\xi}_j V_{jk}(r_{jk})\, W \mid \mathbf{x}_j = \mathbf{x} \rangle \\ & + \langle \boldsymbol{\xi}_j \cdot \nabla_{\mathbf{x}_j} V_{jk}(r_{jk})\, W \mid \mathbf{x}_j = \mathbf{x} \rangle + \langle \boldsymbol{\xi}_k \cdot \nabla_{\mathbf{x}_k} V_{jk}(r_{jk})\, W \mid \mathbf{x}_j = \mathbf{x} \rangle \}. \end{aligned} \tag{7.7}$$

Equation (3.1), applied to (7.4), yields

$$q_3 = -\sum_j \langle \boldsymbol{\xi}_j \cdot \nabla_{\mathbf{x}_j} U\, W \mid \mathbf{x}_j = \mathbf{x} \rangle = -\sum_{j \neq k} \langle \boldsymbol{\xi}_j \cdot \nabla_{\mathbf{x}_j} V_{jk}(r_{jk})\, W \mid \mathbf{x}_j = \mathbf{x} \rangle, \tag{7.8}$$

where (1.4) has been employed. Adding (7.7) and (7.8), and use of (1.2) results in

$$q_2 + q_3 = -\nabla_{\mathbf{x}} \cdot \mathbf{q}_{\mathrm{T}}^* - q_0, \tag{7.9}$$

where $\mathbf{q}_{\mathrm{T}}^*$ is given by (4.11), and so

$$q_0 = \frac{1}{2} \sum_{j \neq k} \left\langle V'_{jk}(r_{jk}) \frac{\mathbf{x}_j - \mathbf{x}_k}{r_{jk}} \cdot (\boldsymbol{\xi}_j + \boldsymbol{\xi}_k)\, W \mid \mathbf{x}_j = \mathbf{x} \right\rangle.$$

Because of (1.6), we can write q_0 in the form

$$q_0 = \int_{\mathbf{y}} \left\{ \frac{\mathbf{x} - \mathbf{y}}{r} \cdot \sum_{j \neq k} V'_{jk}(r) \cdot \left\langle \frac{\boldsymbol{\xi}_j + \boldsymbol{\xi}_k}{2} W \mid \mathbf{x}_j = \mathbf{x}, \mathbf{x}_k = \mathbf{y} \right\rangle \right\} d\mathbf{y}, \quad r = |\mathbf{x} - \mathbf{y}|.$$

In the same way as for (6.5) one easily sees also here that the conditions **A**, **B**, and **C** in Sect. 9 are fulfilled for this integrand. Therefore it follows from Lemma 1, (9.2), that

$$q_0 = -\nabla_{\mathbf{x}} \cdot \mathbf{q}_{\mathrm{V}}^*$$

is valid when $\mathbf{q}_\mathrm{V}^*$ is given by (4.14). Inserting this into (7.9), it follows with (7.5), (7.1), (4.11), and (4.14) that

$$\begin{aligned}\frac{\partial \epsilon}{\partial t} &= -\nabla_\mathbf{x} \cdot \{\mathbf{q}_\mathrm{K} - \mathbf{u} \cdot \mathbf{S}_\mathrm{K} + \mathbf{u}\epsilon_\mathrm{K} + \mathbf{q}_\mathrm{T}^* + \mathbf{q}_\mathrm{V}^*\} \\ &= -\nabla_\mathbf{x} \cdot \{\mathbf{q}_\mathrm{K} + \mathbf{q}_\mathrm{T} + \mathbf{q}_\mathrm{V} - \mathbf{u} \cdot (\mathbf{S}_\mathrm{K} + \mathbf{S}_\mathrm{V}) + \mathbf{u}(\epsilon_\mathrm{K} + \epsilon_\mathrm{V})\},\end{aligned}$$

i.e., the energy equation (2.4).

8 External Forces

When the external forces $\mathbf{k}_j$ are different from zero and provided that (1.5) is fulfilled, the following situation emerges:

a. The *Continuity Equation* (2.2) remains valid.

b. According to

$$\mathbf{f} = \mathbf{f}(\mathbf{x}, t) = \sum_j \langle \mathbf{k}_j\, W \mid \mathbf{x}_j = \mathbf{x} \rangle, \tag{8.1}$$

the *Equation of Motion* (2.3) transforms into

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla_\mathbf{x} \mathbf{u} \right) = \nabla_\mathbf{x} \cdot \mathbf{S} + \mathbf{f}. \tag{8.2}$$

According to (4.2), $\mathbf{f}(\mathbf{x}, t)$ represents the expected value of the external force density.

c. With

$$A = A(\mathbf{x}, t) = \sum_j \langle \boldsymbol{\xi}_j \cdot \mathbf{k}_j\, W | \mathbf{x}_j = \mathbf{x} \rangle, \tag{8.3}$$

the *Energy Equation* (2.4) becomes

$$\frac{\partial \epsilon}{\partial t} + \nabla_\mathbf{x} \cdot (\mathbf{q} - \mathbf{S} \cdot \mathbf{u} + \epsilon \mathbf{u}) = A. \tag{8.4}$$

According to (4.2), $A(\mathbf{x}, t)$ corresponds to the expected value of the work performed by the external forces per unit volume, per unit time.

To prove **a**, we bear in mind that (2.1) is obtained by adding the term

$$-\sum_{l=1}^{N} \frac{1}{m_l} \mathbf{k}_l \cdot \nabla_{\xi_l} W$$

to the right-hand side of (2.1a). According to the explanations in Sect. 6, one must add to the right-hand side of (2.2) the term

$$-\sum_j \sum_l \frac{m_j}{m_l} \langle \mathbf{k}_l \cdot \nabla_{\xi_l} W \mid \mathbf{x}_j = \mathbf{x} \rangle.$$

Rearranging with the help of (3.1), we obtain

$$\sum_j m_j \left\langle \left(\sum_l \frac{1}{m_l} \nabla_{\xi_l} \cdot \mathbf{k}_l \right) W \mid \mathbf{x}_j = \mathbf{x} \right\rangle = 0.$$

This, however, entirely disappears according to (1.5), whereby we have established claim **a**. Completely analogous calculations establish claims **b** and **c**.

From (8.1) and (8.3), one can see that the functional forms of $\mathbf{f}(\mathbf{x}, t)$ and $A(\mathbf{x}, t)$ do not only depend on the external forces $\mathbf{k}_j$ but also on W, i.e., the respective microscopic state of the system. In certain cases, knowledge of certain macroscopic averages over W is sufficient to determine $\mathbf{f}$ and A. We will treat two such cases:

A) *Electrical and gravitational fields.* If the external forces stem from an electric field of strength $\mathbf{e}(\mathbf{x}, t)$, we have

$$\mathbf{k}_j(\mathbf{x}, \xi, t) = e_j \mathbf{e}(\mathbf{x}, t), \tag{8.5}$$

where e_j is the charge of particle (j). For the expected value of the charge density λ and the electric current density $\mathbf{i}$, we obtain, according to (4.2),

$$\lambda = \lambda(\mathbf{x}, t) = \sum_j e_j \langle W \mid \mathbf{x}_j = \mathbf{x} \rangle, \tag{8.6}$$

$$\mathbf{i} = \mathbf{i}(\mathbf{x}, t) = \sum_j e_j \langle \boldsymbol{\xi}_j \, W \mid \mathbf{x}_j = \mathbf{x} \rangle. \tag{8.7}$$

With (8.5)–(8.7), (8.1) and (8.3) yield:

$$\mathbf{f} = \lambda \mathbf{e}, \qquad A = \mathbf{i} \cdot \mathbf{e}. \tag{8.8}$$

For the case of a gravitational field, $\mathbf{g}(\mathbf{x}, t)$, we set $e_j = m_j$ and obtain, because of (2.5) and (2.6),

$$\mathbf{f} = \rho \mathbf{e}, \qquad A = \rho \mathbf{u} \cdot \mathbf{g}. \tag{8.9}$$

B) *Magnetic field.* In this case

$$\mathbf{k}_j(\mathbf{x}, \boldsymbol{\xi}, t) = e_j \boldsymbol{\xi} \times \mathbf{b}(\mathbf{x}, t), \tag{8.10}$$

where $\mathbf{b}$ is the magnetic field strength. Because of

$$\nabla_{\xi} \cdot \mathbf{k}_j(\mathbf{x}, \boldsymbol{\xi}, t) = e_j (\mathrm{rot}_{\xi} \boldsymbol{\xi}) \cdot \mathbf{b} = 0,$$

condition (1.5) is fulfilled. For a restricted/limited $\mathbf{b}(\mathbf{x}, t)$, the $\mathbf{k}_j$ satisfies the regularity condition **C** in Sect. 3. Inserting (8.10) in (8.1) and (8.3), and with (8.7) borne in mind, we obtain

$$\mathbf{f} = \mathbf{b} \times \mathbf{i}, \qquad A = 0. \tag{8.11}$$

9 Two Lemmas

Let $f(\mathbf{v}, \mathbf{w})$ be a scalar, vector, or tensor function of the two vector variables $\mathbf{v}$ and $\mathbf{w}$ that satisfies the following conditions:

A) $f(\mathbf{v}, \mathbf{w})$ is defined and continuously differentiable for all $\mathbf{v}$ and $\mathbf{w}$.

B) There exists a $\delta > 0$ such that the function

$$g(\mathbf{v},\mathbf{w}) = f(\mathbf{v},\mathbf{w})|\mathbf{v}|^{3+\delta}|\mathbf{w}|^{3+\delta},$$

as well as its derivatives are bounded.

C) The functional relation

$$f(\mathbf{v},\mathbf{w}) = -f(\mathbf{w},\mathbf{v}) \tag{9.1}$$

holds.

Under these circumstances, the following two lemmas are valid.

Lemma 1

$$\int_{\mathbf{y}} f(\mathbf{x},\mathbf{y})d\mathbf{y} = -\frac{1}{2}\nabla_{\mathbf{x}}\cdot\int_{\mathbf{z}}\left\{\mathbf{z}\otimes\int_{\alpha=0}^{1} f(\mathbf{x}+\alpha\mathbf{z},\mathbf{x}-(1-\alpha)\mathbf{z})\,d\alpha\right\}d\mathbf{z}. \tag{9.2}$$

Proof The conditions **A** and **B** ensure the absolute convergence of the improper integrals, occurring in the following, as well as the validity of the anticipated exchanges of integration etc. According to (9.1), we have

$$\int_{\mathbf{y}} f(\mathbf{x},\mathbf{y})\,d\mathbf{y} = -\int_{\mathbf{y}} f(\mathbf{y},\mathbf{x})\,d\mathbf{y}.$$

If we introduce the new integration variable $\mathbf{z} = \mathbf{x}-\mathbf{y}$ into the left-hand integral, and $\mathbf{z} = \mathbf{y}-\mathbf{x}$ into the right-hand integral, we find

$$\begin{aligned}\int_{\mathbf{y}} f(\mathbf{x},\mathbf{y})\,d\mathbf{y} = \int_{\mathbf{z}} f(\mathbf{x},\mathbf{x}-\mathbf{z})\,d\mathbf{z} &= -\int_{\mathbf{z}} f(\mathbf{x}+\mathbf{z},\mathbf{x})\,d\mathbf{z}\\ &= \frac{1}{2}\int_{\mathbf{z}}[f(\mathbf{x},\mathbf{x}-\mathbf{z}) - f(\mathbf{x}+\mathbf{z},\mathbf{x})]\,d\mathbf{z}.\end{aligned} \tag{9.3}$$

According to the chain rule, this gives

$$\nabla_{\mathbf{x}} f(\mathbf{x}+\alpha\mathbf{z},\mathbf{x}-(1-\alpha)\mathbf{z}) = \nabla_{\mathbf{v}} f + \nabla_{\mathbf{w}} f$$

and

$$\frac{d}{d\alpha} f(\mathbf{x}+\alpha\mathbf{z},\mathbf{x}-(1-\alpha)\mathbf{z}) = \mathbf{z}\cdot(\nabla_{\mathbf{v}} f + \nabla_{\mathbf{w}} f),$$

where we must insert on the right-hand sides $\mathbf{v} = \mathbf{x}+\alpha\mathbf{z}$ and $\mathbf{w} = \mathbf{x}-(1-\alpha)\mathbf{z}$ as arguments of $\nabla_{\mathbf{v}} f$ and $\nabla_{\mathbf{w}} f$. Therefore, we have

$$\mathbf{z}\cdot\nabla_{\mathbf{x}} f(\mathbf{x}+\alpha\mathbf{z},\mathbf{x}-(1-\alpha)\mathbf{z}) = \frac{d}{d\alpha} f(\mathbf{x}+\alpha\mathbf{z},\mathbf{x}-(1-\alpha)\mathbf{z}).$$

Integration of this equation with respect to α from $\alpha = 0$ to $\alpha = 1$ yields

$$\mathbf{z}\cdot\nabla_{\mathbf{x}}\int_{\alpha=0}^{1} f(\mathbf{x}+\alpha\mathbf{z},\mathbf{x}-(1-\alpha)\mathbf{z})\,d\alpha = f(\mathbf{x}+\mathbf{z},\mathbf{x}) - f(\mathbf{x},\mathbf{x}-\mathbf{z}).$$

Insertion into (9.3) yields (9.2). □

Lemma 2 *Let $\mathcal{J}$ be any region in space with piece-wise smooth bounding surface $\mathcal{F}$. Let $\mathcal{A}$ be the exterior of $\mathcal{J}$ and $\mathbf{n_x}$ the outward normal unit vector at point $\mathbf{x}$ on $\mathcal{F}$* (see Fig. 1). *Then,*

$$\int_{\mathbf{v}\in\mathcal{J}}\int_{\mathbf{w}\in\mathcal{A}} f(\mathbf{v},\mathbf{w})\,d\mathbf{w}\,d\mathbf{v} = -\frac{1}{2}\int_{\mathcal{F}}\int_{\mathbf{z}}\int_{\alpha=0}^{1} f(\mathbf{x}+\alpha\mathbf{z},\mathbf{x}-(1-\alpha)\mathbf{z})(\mathbf{z}\cdot\mathbf{n_x})\,d\alpha\,d\mathbf{z}\,d\mathcal{F}_{\mathbf{x}}. \quad (9.4)$$

Proof First, one sees immediately that, because of the antisymmetry of $f(\mathbf{v},\mathbf{w})$ in (9.1),

$$\int_{\mathbf{v}\in\mathcal{J}}\int_{\mathbf{w}\in\mathcal{J}} f(\mathbf{v},\mathbf{w})\,d\mathbf{v}\,d\mathbf{w} = 0.$$

Therefore, we see that

$$\int_{\mathbf{v}\in\mathcal{J}}\int_{\mathbf{w}\in\mathcal{A}} f(\mathbf{v},\mathbf{w})\,d\mathbf{v}\,d\mathbf{w} = \int_{\mathbf{v}\in\mathcal{J}}\int_{\mathbf{w}} f(\mathbf{v},\mathbf{w})\,d\mathbf{w}\,d\mathbf{v}. \quad (9.5)$$

Now, according to Lemma 1,

$$\int_{\mathbf{w}} f(\mathbf{v},\mathbf{w})\,d\mathbf{w} = \nabla_{\mathbf{v}}\cdot\mathbf{g}(\mathbf{v}), \quad (9.6)$$

where

$$\mathbf{g}(\mathbf{v}) = -\frac{1}{2}\int_{\mathbf{z}}\left\{\mathbf{z}\otimes\int_{\alpha=0}^{1} f(\mathbf{v}+\alpha\mathbf{z},\mathbf{v}-(1-\alpha)\mathbf{z}\,d\alpha\right\}\,d\mathbf{z}. \quad (9.7)$$

According to Gauss' theorem,

$$\int_{\mathbf{v}\in\mathcal{J}} \nabla_{\mathbf{v}}\cdot\mathbf{g}(\mathbf{v})\,d\mathbf{v} = \int_{\mathcal{F}} \mathbf{g}(\mathbf{x})\cdot\mathbf{n_x}\,d\mathcal{F}_{\mathbf{x}}.$$

From this and from (9.5)–(9.7), we find the relation (9.4) as claimed. □

References

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2. Schwartz, L.: Théorie des distributions. Hermann, Paris (1950)

Author's Acknowledgment The first translator would like to thank his co-translator Anatole Von Lilienfeld-Toal for the preliminary translation into English from German. The first translator also thanks Professors Eliot Fried and Roger Fosdick for their interest in this translation and their careful readings, and he also thanks Professor Paolo Podio-Guidugli for comments on the translation. Mistakes in the translation and/or corrections are the responsibility of the two translators. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

Appendix

The following changes were made to equations in the original manuscript.

1. Equation (1.4): replaced $\nabla\mathbf{x}_j$ with $\nabla_{\mathbf{x}_j}$.

2. Equation (2.14): replaced $(\boldsymbol{\xi}_j - \mathbf{u})((\boldsymbol{\xi}_j - \mathbf{u})^2$ with $|\boldsymbol{\xi}_j - \mathbf{u}|^2(\boldsymbol{\xi}_j - \mathbf{u})$.
3. Equation (2.16): replaced

$$\frac{\mathbf{z}}{|\mathbf{z}|}\mathbf{z} \cdot V'_{jk}(|\mathbf{z}|) \quad \text{with} \quad \frac{\mathbf{z}}{|\mathbf{z}|} V'_{jk}(|\mathbf{z}|)\,\mathbf{z}\cdot$$

   to improve clarity.
4. Section 3: replaced

$$G(\mathbf{x}_i; \boldsymbol{\xi}_i; t) = W(\mathbf{x}_i; \mathbf{x}_i; t) \prod_{j=1}^{N} |\mathbf{x}_j|^{3+\delta} \prod_{k=1}^{N} |\boldsymbol{\xi}_k|^{6+\delta}$$

   with

$$G(\mathbf{x}_i; \boldsymbol{\xi}_i; t) = W(\mathbf{x}_i; \mathbf{x}_i; t) \prod_{j=1}^{N} |\mathbf{x}_j|^{3+\delta} \prod_{k=1}^{N} |\boldsymbol{\xi}_k|^{3+\delta}.$$

5. Equation $(3.2)_1$: replaced $F\nabla_{\mathbf{x}_j} W = 0$ with $\int F\nabla_{\mathbf{x}_j} W = 0$.
6. Equation (7.3): replaced $\nabla_{\mathbf{x}_2}$ with $\nabla_{\mathbf{x}_j}$.
7. Equation (7.4): replaced

$$-\frac{1}{2}\sum_j \langle \boldsymbol{\xi}_j^2 \nabla_{\mathbf{x}_j} U \cdot \nabla_{\boldsymbol{\xi}_j} W \mid \mathbf{x}_j = \mathbf{x}\rangle$$

   with

$$\frac{1}{2}\sum_j \langle \boldsymbol{\xi}_j^2 \nabla_{\mathbf{x}_j} U \cdot \nabla_{\boldsymbol{\xi}_j} W \mid \mathbf{x}_j = \mathbf{x}\rangle + \sum_j \sum_l \langle V_j \nabla_{\mathbf{x}_i} U \cdot \nabla_{\boldsymbol{\xi}_j} W \mid \mathbf{x}_j = \mathbf{x}\rangle.$$

8. Equation (7.5); replaced q_{K} with $\mathbf{q}_{\mathrm{K}}$.
9. Section 8: replaced

$$\sum_j m_j \left\langle \left(\sum_l \frac{1}{m_l} \nabla_{\boldsymbol{\xi}_l} \cdot \mathbf{k}_l \right) W \mid \mathbf{x}_j = \mathbf{x} \right\rangle$$

   with

$$\sum_j m_j \left\langle \left(\sum_l \frac{1}{m_l} \nabla_{\boldsymbol{\xi}_l} \cdot \mathbf{k}_l \right) W \mid \mathbf{x}_j = \mathbf{x} \right\rangle = 0.$$

10. Proof of Lemma 2: replaced

$$\int_{\mathbf{v}\in\mathcal{J}} \int_{\mathbf{w}\in\mathcal{A}} f(\mathbf{v}, \mathbf{w})\, d\mathbf{v}\, d\mathbf{w} = 0$$

   with

$$\int_{\mathbf{v}\in\mathcal{J}} \int_{\mathbf{w}\in\mathcal{J}} f(\mathbf{v}, \mathbf{w})\, d\mathbf{v}\, d\mathbf{w} = 0.$$

11. Equation (9.5)$_2$: replaced

$$\int_{\mathbf{v}\in\mathcal{J}} \int_{\mathbf{w}\in\mathcal{A}} f(\mathbf{v}, \mathbf{w})\, d\mathbf{w}\, d\mathbf{v}$$

with

$$\int_{\mathbf{v}\in\mathcal{J}} \int_{\mathbf{w}} f(\mathbf{v}, \mathbf{w})\, d\mathbf{w}\, d\mathbf{v}.$$