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2003 J. Phys. A: Math. Gen. 36 6019

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On the definition of Burnett transport coefficients of the dense multi-element charged matter

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Received 9 October 2002, in final form 31 March 2003

Published 22 May 2003

Online at stacks.iop.org/JPhysA/36/6019

Abstract

To determine the Burnett transport coefficients of non-ideal multi-element charged matter the representations of conservation equations of matter as generalized Langevin equations are used. Mori's algorithm is revised to derive the equation of motion of a dynamical value operator of a system in the form of the generalized nonlinear Langevin equation. After transformation, using necessary variational derivatives, these equations are compared with the Burnett hydrodynamical conservation equations. In consequence, the response function expressions of transport coefficients corresponding to second-order derivatives of thermal disturbances are found in the long-wavelength and low-frequency limits. To establish a link between the results of the executed investigations and hydrodynamical problems the properties of the high derivative coefficients matrix of the set of conservation equations in the linearized Burnett approximation are discussed.

PACS numbers: 52.25.Fi, 05.70.Ln

1. Introduction

The transport processes in the Burnett approximation define, for example, the following hydrodynamical phenomena: thermal-stress convection, sound propagation, the structure of weak shock waves and so on. The investigation of the problem of propagation of supersonic waves in a gas shows the strong dependence of the corresponding dispersion relations on taking into account Burnett transport processes. The asymmetrical parameters of the density and temperature profiles of a weak shock wave also depend on these processes. The well-known approximations for investigations of the corresponding transport coefficients of weak coupled matter are based on the Boltzmann kinetic equation, which is solved by the second-order Chapman–Enskog method [1, 2]. At the same time the definition of the Burnett transport coefficients of the dense matter is a difficult problem of the response theory.

The traditional linear transport relations are in the main studied within the framework of the response theory to the thermal disturbances (see, for example, [3]). Transport equations for a non-Newtonian fluid with a complex rheology were derived by the method of nonequilibrium statistical operator. The procedure permitted the study, in principle, of the transport relations for complex liquids [4, 5]. Nevertheless the attempts to construct a nonlinear response theory to thermal disturbances did not lead to the appearance of the method of determination of the nonlinear disturbance transport coefficients and also of the coefficients in the corresponding linearized current relations. Therefore, in the paper for the definition of these coefficients the procedure of the comparison of the conservation equations of a continuous charged medium and the microscopic equations for dynamical variables is applied. In this case information about phenomenological forms of the conservation equations, mass, heat and other currents is used. This information, in the known sense, sets the microscopic expressions for transport coefficients in the conservation equations.

The representations of conservation equations of matter as generalized Langevin equations are used for the determination of the Burnett transport coefficients of non-ideal multi-element charged matter. The equation of motion of a dynamical value operator of a system in the form of the generalized nonlinear Langevin equation is derived by Mori's algorithm in section 2. In the next section these equations are compared with the Burnett hydrodynamical conservation equations after transformation, using necessary variational derivatives. The response function expressions of transport coefficients which correspond to the second-order derivatives of thermal disturbances are found in section 4 in the long-wavelength and low-frequency limits. The properties of the high derivative coefficient matrix of the set of conservation equations in the linearized Burnett approximation are discussed to establish a link between the results of the executed investigations and hydrodynamical problems.

2. Thermal disturbances. Nonlinear generalized Langevin equations

In the majority of problems of the quantum response theory to thermal disturbances it is impossible to use the perturbation theory and the known Kubo's method, in particular, because the corresponding corrections to the Hamiltonian of the system (H) due to these disturbances cannot be formulated in the general form. Therefore, in this case the more appropriate approach is Mori's algorithm according to which the equation of motion of the operator for a dynamical value can be presented in a form of generalized Langevin equations. For the linear case this equation was derived in [6]. The given method was used in [7] to get the same equation in the nonlinear case for the mechanical disturbances situation. The analogous derivation is briefly discussed here to describe the response to thermal disturbances. Let us define a scalar product of operators in the Heisenberg representation, where $\rho(t)$ is the density matrix of the system,

$$\langle A(t); B(t_0) \rangle = \text{Tr} \rho(t_0) \int_0^\beta d\lambda e^{\lambda H} A(t) e^{-\lambda H} B(t_0). \quad (1)$$

The projection operator is

$$\begin{aligned} PG(t) &= \frac{\langle G(t); B(t_0) \rangle}{\langle B(t_0); B(t_0) \rangle} \cdot B(t_0) \\ B(t) &= \sum(t; t_0) \cdot B(t_0) + B'(t_0) \quad \sum(t; t_0) = \langle B(t); B(t_0) \rangle / \langle B(t_0); B(t_0) \rangle \\ B'(t) &= (1 - P)B(t) \\ B(t_0) &= i\omega B(t_0) + K(t_0) \quad i\omega = \left[\frac{d}{dt} \Sigma(t; t_0) \right]_{t=t_0} \quad K(t_0) = (1 - P)\dot{B}(t_0). \end{aligned} \quad (2)$$

We obtain the equation of motion for $B'(t)$

$$\frac{d}{dt}B'(t) = (1 - P)i[H, B'(t)] + \Sigma(t; t_0)K(t_0)$$

which has the solution of the form

$$B'(t) = \int_{t_0}^t dt' \Sigma(t'; t_0) f(t - t'; t_0) \quad f(t) = \exp[t(1 - P)iL]K(t_0).$$

After transformation similar to that performed above we get the equation for $\Sigma(t; t_0)$,

$$\frac{d}{dt}\Sigma(t; t_0) = i\omega\Sigma(t; t_0) + \langle K(t); B(t_0) \rangle / \langle B(t_0); B(t_0) \rangle$$

where $K(t)$ is the Heisenberg operator; using $B(t)$ decomposition and solution for $B'(t)$, $\langle K(t); B(t_0) \rangle$ becomes

$$\begin{aligned} \langle K(t); B(t_0) \rangle &= \text{Tr} \rho(t) \int_0^\beta d\lambda e^{\lambda H} B(t_0 - t) e^{-\lambda H} K(t_0) \\ &= \text{Tr} \rho(t) \int_0^\beta d\lambda e^{\lambda H} B(t_0) e^{-\lambda H} K(t_0) \cdot \Sigma(t_0 - t; t) \\ &\quad - \int_{t_0}^t dt' \Sigma(t'; t_0) \text{Tr} \rho(t) \int_0^\beta d\lambda e^{-\lambda H} f(t - t'; t_0) e^{\lambda H} K(t_0). \end{aligned}$$

Hence, the equation for $\Sigma(t; t_0)$ is the following:

$$\begin{aligned} \frac{d}{dt}\Sigma(t; t_0) &= i\omega\Sigma(t; t_0) - \int_{t_0}^t dt' \varphi(t', t_0) \Sigma(t - t'; t_0) + r(t, t_0) \\ \varphi(t; t_0) &= \text{Tr} \rho(t) \int_0^\beta d\lambda e^{\lambda H} f(t; t_0) e^{-\lambda H} f(t_0; t_0) / \langle B(t_0); B(t_0) \rangle \\ r(t; t_0) &= \text{Tr} \rho(t) \int_0^\beta d\lambda e^{\lambda H} B(t_0) e^{-\lambda H} K(t_0) \cdot \Sigma(t_0 - t; t_0) / \langle B(t_0); B(t_0) \rangle \end{aligned}$$

where $r(t; t_0) = 0$ in the linear approximation. Thus, the generalized Langevin equation for $B(t)$ has the nonlinear form

$$\frac{d}{dt}B(t) - i\omega B(t) + \int_{t_0}^t dt' \varphi(t - t'; t_0) B(t') = f(t; t_0) + r(t; t_0) B(t_0) \quad (3)$$

where

$$\text{Tr} \rho(t) \int_0^\beta d\lambda e^{\lambda H} f(t; t_0) e^{-\lambda H} B(t_0) = 0. \quad (3')$$

The nonlinearity of the generalized Langevin equation (3) follows from the dependences of the density matrix of the system and consequently ‘frequency’, ‘transport coefficient’ and ‘random force’ in this equation on operators of dynamical variables $\{B(t)\}$ [5]. Nonequilibrium density matrix $\rho(t)$ can be determined, for example, by Zubarev’s method [4, 5].

3. Decomposition of the nonlinear generalized Langevin equations. Burnett phenomenological kinetic coefficients

To rewrite the generalized Langevin equation in a form convenient for the definition of the Burnett transport coefficient we use a decomposition of the equation [8]. Let us write the

nonlinear generalized Langevin equation in the form

$$\frac{d}{dt}B(t) = F[B(t)] + f(t; t_0)$$

$$F[B(t)] = i\omega B(t) - \int_{t_0}^t dt' \varphi(t - t'; t_0) B(t') + r(t; t_0) B(t_0)$$

where $F[B(t)]$ is the analytical functional and $B(t)$ is a vector

$$F[B(t)] = \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^t d\tau_1 \dots \int_0^{\tau_1} d\tau_n \Theta_n(t - \tau_1, \dots, t - \tau_n) B(\tau_1) \dots B(\tau_n)$$

$$F[B(t)] \cong \int_0^t d\tau \Theta_1(t - \tau) B(\tau) + \frac{1}{2} \int_0^t \int_0^{\tau} d\tau_1 d\tau_2 \Theta_2(t - \tau_1, t - \tau_2) B(\tau_1) B(\tau_2)$$

where Θ_n is the n -order functional derivative. We take into account the coordinate dependences of the operators, use the local approximation for the Θ_2 , multiply the equations by $B(\mathbf{r})$, average over a density matrix $\rho(t)$ and then by Fourier–Laplace transformation receive the matrix equation for correlation functions of two and three orders, which has, in general, the following form

$$z \langle B(\mathbf{k}, z) B(-\mathbf{k}, 0) \rangle - \langle B(\mathbf{k}) B(-\mathbf{k}) \rangle = \Theta_1 \langle B(\mathbf{k}, z) B(-\mathbf{k}, 0) \rangle + \Theta_2 M \quad (4)$$

where $\langle \dots \rangle$ means averaging over a nonequilibrium density matrix, z -complex variable, $B(\mathbf{r}, t)$ -operators in the Heisenberg representation; Θ_2 , M are three-index objects which correspond to Burnett phenomenological kinetic coefficients and three order correlation functions; Θ_1 , $\langle BB \rangle$ -matrices, which correspond to ordinary phenomenological kinetic coefficients and correlation functions.

Following a scheme of approach we write a continuity equation, the equations for the diffusion of chemical elements, a dynamical equation and energy conservation equation. We reduce the system of differential conservation equations to a system of algebraic equations by Fourier–Laplace transformation, multiply the equations by $B(-\mathbf{k})$, average over a density matrix $\rho(t)$ and receive the matrix equation for correlation functions of two and three orders

$$z \langle B(\mathbf{k}, z) B(-\mathbf{k}, 0) \rangle - \langle B(\mathbf{k}) B(-\mathbf{k}) \rangle = -k^2 M_1 R_{BX}^{-1} \langle B(\mathbf{k}, z) B(-\mathbf{k}, 0) \rangle - ik^3 M_2 R_{BX}^{-1} R_{BX}^{-1} M$$

$${}^t B = [Q(k, z), \{\rho_m c_a(k, z)\}, \rho_m(k, z), v_l(k, z), v_t(k, z)]$$

$$Q(k, z) = u(k, z) - \rho_m(k, z)(u + p)/\rho_m \quad (5)$$

$${}^t X = [T(k, z), \{\rho_m c_a(k, z)\}, \rho_m(k, z), v_l(k, z), v_t(k, z)]$$

$$B = R_{BX} X.$$

To find the Burnett kinetic coefficient definitions over Θ_2 -elements, we can equate the $\sim k^3$ -members of equations (4) and (5). On the other hand the definitions of the Burnett kinetic coefficients follow from the last equation, if we use the object, reverse of M . These procedures are cumbersome. The relations get simplified by using some variants of the density matrix $\rho(t)$, in particular, an undisturbed density matrix ρ_0 . Besides that, it takes into account the fact that the vector and tensor currents (J_i) in the conservation laws have different definitions, which are governed by nonlinear irreversible thermodynamics [9, 10], by the Chapman–Enskog method of the second order [1] and by some phenomenological rheology laws [11]. Let us write the corresponding definitions in the schematic form

1. $J_i = L_{ik}X_k + L_{ijk}X_jX_k$
2. $J_i = J_i[\nabla T \nabla \cdot \mathbf{u}, \nabla(T \nabla \cdot \mathbf{u}), \nabla \mathbf{u} \cdot \nabla T, (\nabla p + \nabla T) \cdot \mathbf{e}, \mathbf{d} \nabla \cdot \mathbf{u}, \nabla \mathbf{u} \cdot \mathbf{d}, \nabla \nabla \cdot \mathbf{u}, \mathbf{d} \cdot \mathbf{e}]$
 $J_i = J_i[\mathbf{e} \nabla \cdot \mathbf{u}, \{\nabla \nabla p + \nabla \mathbf{u} \cdot \mathbf{e} + \nabla \mathbf{u} \cdot \nabla \mathbf{u}\}, \{\mathbf{e} \cdot \mathbf{e}\}, \{\nabla \nabla T\}, \{\nabla T \nabla T\}, \dots]$
 $\{N_{\alpha\beta}\} = \frac{1}{2}(N_{\alpha\beta} + N_{\beta\alpha}) - \frac{1}{3}\delta_{\alpha\beta}N_{\gamma\gamma}$

(Rheology relation types: generalized Newton, Bingham, Reiner–Rivlin, etc).

Here X_k are the usual thermodynamical forces; L_{ik}, L_{ikl} are the phenomenological kinetic coefficients; definition 2 corresponds to vector currents and tensor currents, respectively. Obviously, the coincidence of definitions 1 and 2 is not perfect and second-order kinetic coefficients depend on the form of current which is used. The coincidence takes place for the linearized Burnett approximation.

4. Linearized Burnett approximation

Let us consider the linearized Burnett approximation. The corresponding set of conservation equations can be reduced to a system of algebraic equation by Fourier–Laplace transformation. In writing the algebraic system we use phenomenological kinetic coefficients (α, β) taking the non-locality of spatial and time dependences of currents from thermodynamical forces into account. The system has the following form (compare with [3])

$$z\mathcal{Q}(k, z) - \mathcal{Q}(k) = -k^2[\alpha_{11}(k, z)T(k, z) + T\alpha_{1b}(k, z)L_b(k, z) + ik\alpha_{1v}(k, z)v_l(k, z)]$$

$$z\rho_m c_a(k, z) - \rho_m c_a(k) = -k^2[\alpha_{a1}(k, z)T(k, z) + \alpha_{ab}(k, z)L_b(k, z) + ik\alpha_{av}(k, z)v_l(k, z)]$$

$$z\rho_m(k, z) - \rho_m(k, z) = -k^2\rho_m \frac{ik}{k^2}v_l(k, z)$$

$$zv_l(k, z) - v_l(k, z) = -k^2 \frac{1}{ik\rho_m} [k^2\beta_{v1}(k, z)T(k, z) + k^2\beta_{vb}(k, z)L_b(k, z) + p(k, z) + ikb(k, z)v_l(k, z)]$$

$$zv_t(k, z) - v_t(k) = -k^2 \frac{1}{\rho_m} \eta(k, z)v_t(k, z)$$

where $L_b(k, z) = T(\mu_b/T)(k, z) + (4\pi e^2/k^2)c_\rho(k, z)\delta_{b\rho}\rho_m/(m_b m_e)$; we shall write the set of equations in matrix form because $\mu_b, p = \mu_b, p(T, \rho_m c_a, \rho_m)$

$$zB(\mathbf{k}, z) - B(\mathbf{k}) = -k^2 M_1(\mathbf{k}, z)X(\mathbf{k}, z). \tag{6}$$

Following a scheme of approach we multiply the equations by $B(-\mathbf{k})$, average over a density matrix $\rho(t)$ and obtain the matrix equation for correlation functions of two orders

$$J_{BB}(\mathbf{k}, z) - \Phi(\mathbf{k}) = \left[1 + \frac{k^2}{z} M_1(\mathbf{k}, z) R_{BX}^{-1} \right]^{-1} M_1(\mathbf{k}, z) R_{BX}^{-1} \langle B(\mathbf{k}) B(-\mathbf{k}) \rangle / (V k_B T)$$

$$\Phi(\mathbf{k}) = (V k_B T k^2)^{-1} \left(\frac{d}{dt} \langle B(\mathbf{k}) B(-\mathbf{k}) \rangle \right).$$

After the calculation of the matrix inverse to the matrix in square brackets in the long-wavelength limit and the multiplications we obtain for the linearized Burnett kinetic coefficients of dense charged matter

$$\tilde{\alpha}_{1v}(k, z) = ik[\alpha_{1v}(k, z) + (\varepsilon^{-1} - 1)\alpha_{1\rho}\alpha_{\rho v}/\alpha_{\rho\rho}] \tag{7}$$

where $\tilde{\alpha}_{ab}$ is an element of the J_{BB} matrix. Note that the polarization effects, which correspond to the second term on the right-hand side of (7), do not arise for the tensor kinetic coefficients in this approximation.

The properties of the high derivative coefficients matrix of the set of conservation equations in the linearized Burnett approximation are necessary to establish a link between the results of the executed investigations and hydrodynamical problems. For this purpose we consider the entropy production of the multi-element condensed matter. The compatibility of principles of irreversible thermodynamics with the linearized Burnett approximation was shown under the condition that the collection of phenomenological relations for currents and thermodynamical forces is extended. Consequently, the entropy production has the following form (see, for example, [12])

$$\begin{aligned} \sigma = & -(1/T)[(\mathbf{J}'_q \cdot \nabla) \ln T + \hat{\pi} \otimes \{\nabla \mathbf{u}\} + p \sum_{a=1}^{N_a-1} (\mathbf{w}_a - \mathbf{w}_e) \cdot \mathbf{d}_a + (1/T) \hat{\mathbf{J}}^T \otimes \{\nabla \nabla\} T \\ & + \hat{\mathbf{J}}^u \otimes \{\nabla \nabla \mathbf{u}\} + \mathbf{J}^v \cdot \nabla^2 \mathbf{u} + \sum_{a=1}^{N_a-1} (\hat{\mathbf{J}}_a^D - \hat{\mathbf{J}}_e^D) \otimes \{\nabla \mathbf{d}_a\}. \end{aligned} \quad (8)$$

This expression contains the ‘physical’ currents, the first three currents, which are used in the set of hydrodynamical conservation equations, and the ‘non-physical’ currents. We can write the currents according to the Curie principle

$$\begin{aligned} \mathbf{w}_a - \mathbf{w}_e &= - \sum_{a=1}^{N_a-1} \alpha_{ab} \mathbf{d}_b - \alpha_{aq} \nabla \ln T - \alpha_{au} \nabla^2 \mathbf{u} \\ \mathbf{J}'_q &= - \sum_{a=1}^{N_a-1} \alpha_{qa} \mathbf{d}_a - \alpha_{qq} \nabla \ln T - \alpha_{qu} \nabla^2 \mathbf{u} \\ \mathbf{J}^v &= - \sum_{b=1}^{N-1} \alpha_{ub} \mathbf{d}_b - \alpha_{uq} \nabla \ln T - \alpha_{uu} \nabla^2 \mathbf{u}; \end{aligned} \quad (9)$$

other tensor currents are written in the same manner. Rewrite the currents in the matrix form

$$\begin{bmatrix} \mathbf{w}_a - \mathbf{w}_e \\ \mathbf{J}'_q \\ \mathbf{J}^v \\ \hat{\mathbf{J}}_a^D - \hat{\mathbf{J}}_e^D \\ \hat{\pi} \\ \hat{\mathbf{J}}^T \\ \hat{\mathbf{J}}^u \end{bmatrix} = \begin{bmatrix} \alpha_{ab} & \alpha_{aq} & \alpha_{au} & 0 & 0 & 0 & 0 \\ \alpha_{qa} & \alpha_{qq} & \alpha_{qu} & 0 & 0 & 0 & 0 \\ \alpha_{ua} & \alpha_{uq} & \alpha_{uu} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \beta_{ab} & \beta_{au} & \beta_{aq} & 0 \\ 0 & 0 & 0 & \beta_{ua} & \beta_{uu} & \beta_{uq} & 0 \\ 0 & 0 & 0 & \beta_{qa} & \beta_{qu} & \beta_{qq} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \beta_{vv} \end{bmatrix} \cdot \begin{bmatrix} \nabla \ln T \\ \mathbf{d}_b \\ \nabla^2 \mathbf{u} \\ \{\nabla \mathbf{d}_b\} \\ \{\nabla \mathbf{u}\} \\ \{\nabla \nabla\} T \\ \{\nabla \nabla \mathbf{u}\} \end{bmatrix}. \quad (10)$$

According to the Curie principle matrix (10) is decomposed; submatrices 3×3 and 4×4 are symmetrical. But the submatrices properties do not define the properties of the high derivative coefficient matrix of the set of conservation equations (for example, its parabolicity [3]) in the linearized Burnett approximation, because part of the coefficients of the submatrices includes the ‘physical’ and part the ‘non-physical’ currents. In other words the properties of the high derivative coefficients matrix are governed by calculation algorithms with the aid of which the corresponding linearized Burnett transport coefficients are defined. This circumstance produces the difficulties in the corresponding hydrodynamical problems.

5. Conclusions

Mori’s algorithm is used to derive the equation of motion of an operator of a dynamical value in the form of nonlinear generalized Langevin equations. This derivation is produced for

the system under the thermal disturbances situation. A convenient form of the generalized Langevin equation is defined by the decomposition method for the determination of Burnett transport coefficients. The determinations of the local phenomenological Burnett coefficients, which correspond to thermal disturbances of dense charged matter, are discussed. The corresponding linearized Burnett approximations are described.

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