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Nonlinear transport properties of non-ideal systems

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Abstract
The theory of nonlinear transport is elaborated to determine the Burnett transport properties of non-ideal multi-element plasma and neutral systems. The procedure for the comparison of the phenomenological conservation equations of a continuous dense medium and the microscopic equations for dynamical variable operators is used for the definition of these properties. The Mori algorithm is developed to derive the equations of motion of dynamical value operators of a non-ideal system in the form of the generalized nonlinear Langevin equations. In consequence, the microscopic expressions of transport coefficients corresponding to second-order thermal disturbances (temperature, mass velocity, etc) have been found in the long wavelength and low frequency limits.

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1. Introduction

The investigations of nonlinear transport in non-ideal Coulomb and neutral systems (i.e., systems with significant intercharge interaction in comparison with temperature) can be performed in the framework of the nonlinear response theory. The response theory implements notions of mechanical and thermal disturbances. The mechanical disturbances of a system are the result of the action of external fields; the total Hamiltonian is the sum of an unperturbed system's Hamiltonian and a Hamiltonian of the interaction of a system with an external field. For the description of nonlinear response for mechanical disturbances of non-ideal charged matter we can use the Kubo approach (see, e.g., [1]), but this approach does not fit the thermal disturbances (disturbances of temperature, medium mass velocity, etc).

Nonlinear response theory for thermal disturbances is elaborated below to determine the Burnett transport properties of a non-ideal multi-element plasma. The analysis can also be used for other condensed charged media—one- and two-component Coulomb systems, electrolytes, liquid metals, nuclear matter, etc—and for dense neutral isotropic matter. The transport processes in the Burnett approximations define, for example, the following hydrodynamic phenomena: thermal-stress convection, sound propagation, the structure of weak shock waves and so on. The well-known approximation for investigations of the corresponding transport coefficients of a weak coupled matter (e.g., gas and plasma with weak inter-particle interaction) is based on the Boltzmann kinetic equation, which is solved by the second-order Chapman–Enskog method [2, 3]. At the same time, the definition of Burnett transport coefficients of a dense matter is a difficult problem of the response theory. The traditional linear or generalized transport relations are mainly studied within the framework of the response theory for thermal disturbances (see, e.g., [4, 5]). Therefore, in this paper, for the definition of Burnett coefficients we discuss a procedure [6] for the comparison of the phenomenological conservation equations of a continuous charged medium and the equations for operators of dynamical variables. The generalized Langevin equations are used as the operator equations for dynamical variables of non-ideal multi-element charged matter. In this approach the information about forms of conservation equations, currents of mass, heat and others is used. This information, in the known sense, defines the microscopic expressions for transport coefficients in the flux relations.

2. Nonlinear transport in non-ideal matter

2.1. The description of the nonlinear transport cannot be performed by the known Kubo's method (see, e.g., [1, 4]). This situation takes place because the corresponding corrections to the Hamiltonian of the system (H^{ext}) due to thermal disturbances cannot be formulated in the general form. The characteristic times of transport processes correspond to the hydrodynamical description of a system. In the nonlinear case, the transport processes induced by fields are not separated from processes induced by gradients of concentration of components or temperature. Therefore, it is necessary to create the general description of nonlinear reaction of a matter to these thermal disturbances. In this case, the more appropriate approach to the definition of Burnett transport coefficients is the procedure in [6]. This procedure uses the density matrix ($\rho(t)$) equation [7] and phenomenological definitions of transport processes. According to the given procedure, the microscopic definition of nonlinear transport properties is made by the comparison of the Burnett phenomenological conservation equations of a continuous charged medium and the operator equations for dynamical variables in the form of the generalized Langevin equations. The equations of motion of the operators for dynamical values can be presented in the form of GLE by the Mori algorithm. For the linear case these equations were derived in [8]. The given method was used in [9] to get the microscopic equations in the nonlinear case to describe the response to mechanical disturbances. The analogous derivation can be used to describe the response to thermal disturbances [6].

In general, the GLE can be presented in the following form with ($B(t)$ being the operator of dynamical variables, ω being the frequency, $\varphi(t; t_0)$ being the transport coefficient, $f(t; t_0)$ being the random force and $r(t; t_0)$ are defined in [6, 9], $r(t; t_0) = 0$ for $\rho = \rho_0$, the undisturbed density matrix):

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t}B(t) = \mathrm{i}\,\omega B(t) + F[B(t)] + f(t; t_0); \\ &F[B(t)] = -\int_{t_0}^{t} \mathrm{d}t'\varphi(t - t'; t_0)B(t') + r(t; t_0)B(t_0), \\ &\mathrm{Tr}\,\rho(t)\int_0^{\beta} \mathrm{d}\lambda\, \mathrm{e}^{\lambda H} f(t; t_0)\, \mathrm{e}^{-\lambda H} B(t_0) = 0. \end{aligned} \tag{1}$$

Note that the GLE can be considered as a form of the nonlinear fluctuation–dissipation theorem for thermal disturbance response functions. Let $F[B(t)]$ be an analytical functional (with F being the square matrix and $B(t)$ being the vector), then the functional $F[B(t)]$ has the following form [10]:

$$F[B(t)] \cong \int_0^t \mathrm{d}\tau\,\vartheta_1(t-\tau)B(\tau) + \frac{1}{2}\int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\vartheta_2(t-\tau_1, t-\tau_2)B(\tau_1)B(\tau_2) + \cdots, \tag{2}$$

where ϑ_1, ϑ_2 are the first and second functional derivatives, definitions of which depend on the concrete form of density matrix (for $\rho(t)$ definitions see [5, 7]). We rewrite (1) using (2) with two members, take into account the coordinate dependences of the operators, use the local approximation for ϑ_2, multiply the equations by $B(\mathbf{r})$, average over a density matrix (see (1)) and then by Fourier–Laplace transformation receive the microscopic matrix equation for correlation functions of second and third orders, which has, in general, the form ($\Gamma(k,z)$, $\Gamma_2(k,z)$ are Fourier–Laplace transformations of ϑ_1, ϑ_2)

$$\begin{aligned} &zC_{BB}(k,z) - C_{BB}(k) = S(k)C_{BB}(k,z) - \Gamma(k,z)C_{BB}(k,z) - \Gamma_2(k,z) : C_{BBB}(k,z) \\ &A\frac{k^2 J_{BB}}{z^2} = -C_{BB}(k,z) + z^{-1}C_{BB}(k) - z^{-2}S(k)C_{BB}(k). \end{aligned} \tag{3}$$

In (3), the second equation follows from the relation $zB(\mathbf{k},z) - B(\mathbf{k}) = -i\mathbf{k}\cdot\mathbf{J}_B$; $\mathrm{A} = Vk_BT$; $C_{BBB}(k,z)$, $C_{BB}(k,z)$, $C_{BB}(k)$, $J_{BB}(k,z)$ are the triple and pair correlation functions of densities and currents, $S(k) = [(\mathrm{d}/\mathrm{d}t)C_{BB}(k)]C_{BB}^{-1}(k)$. We can equate expressions for $C_{BB}(k,z)$ from first and second equations (3). The corresponding relation is split and then the correlation function definitions of $\{\Gamma\}$ are

$$\begin{aligned} &Vk_BT\frac{k^2 J_{BB}(\sim k^0)}{z^2} - \frac{[z - S(k)]C_{BB}(k)}{z^2} = \frac{C_{BB}(k)}{z - S(k) + \Gamma(k,z)} \\ &Vk_BT\frac{k^2 J_{BB}}{z^2} = \frac{\Gamma_2(k,z) : C_{BBB}(k,z)}{z - S(k) + \Gamma(k,z)}. \end{aligned} \tag{4}$$

The first equation in (4) was used in [4, 6] for linear and linearized Burnett transport process investigations, and the second equation in (4) is considered here to get the microscopic definitions of nonlinear Burnett coefficients.

2.2. According to the scheme of approach we have to use the set of the Burnett phenomenological conservation equations relative to densities $\{B(\mathbf{r},t)\}$ and compare these sets with (1) and (2) to find from *(4)* the microscopic definitions of nonlinear coefficients. The set of the phenomenological differential conservation equations—an energy conservation equation (with density Q), equations for the diffusion of chemical elements ($\rho_m c_a$), a continuity equation (ρ_m) and a dynamical equation (v_l, v_t)—is known (see, e.g., [2, 3]; definitions in [6]). This set is reduced to a system of algebraic equations by Fourier–Laplace transformation (cf [4]), and its matrix form (using the local approximation for the nonlinear kinetic coefficients) is as follows:

$$\begin{aligned} &zB(k,z) - B(k) = \cdots - \mathrm{i}\,k^3\mathrm{M}_2(k,z) : XX \\ &{}^tB = [Q(k,z), \{\rho_m c_a(k,z)\}, \rho_m(k,z), v_l(k,z), v_t(k,z)]; \\ &Q(k,z) = u(k,z) - \rho_m(k,z)(u+p)/\rho_m; \\ &{}^tX = [T(k,z), \{\rho_m c_a(k,z)\}, \rho_m(k,z), v_l(k,z), v_t(k,z)]. \end{aligned} \tag{5}$$

In (5), ρ_m, T, v, p, u, c_a are the density, temperature, mass velocity, pressure, internal energy, part of 'chemical element a' of a matter, respectively; ordinary transport coefficients are omitted, and M_2 is a cubic matrix with Burnett transport coefficients. Then we can compare equations (5) with (1) and (2). This comparison shows

$$\mathrm{i}\,k^3\mathrm{M}_2(k,z):\left[R_{BX}^{-1}R_{BX}^{-1}\right]=\Gamma_2(k,z). \tag{6}$$

Therefore, using (4) we can get the relations which allow one to find the microscopic definitions of Burnett kinetic coefficients ($\tilde{M}_2 = M_2 : [R^{-1}R^{-1}]$, $B = RX$):

$$Vk_BT\frac{k^2J_{BB}}{z^2}=\frac{\mathrm{i}k^3\tilde{M}_2(k,z):C_{BBB}(k,z)}{z-S(k)+\Gamma(k,z)}. \tag{7}$$

This formula is convenient to determine the nonlinear kinetic coefficients as the long-wavelength and low frequency limits of the corresponding relation for each layer of cubic matrix $\tilde{M}_2$ (for each conservation equation); that is, the Burnett kinetic coefficients are found from the solution of the linear algebraic equation system using the Cramer rule. Nonlinear kinetic coefficients are expressed over double and triple correlation functions (see (3)) and thermodynamic derivatives. In this case, the investigations of long-wavelength limits of correlation functions by analytical or calculation methods are especially important (cf [4]). The linearized Burnett kinetic coefficients were investigated in [6, 11] and depend on double correlation functions.

3. Conclusions

The approach is offered for the microscopic definition of nonlinear transport properties for the dense multi-element system under thermal disturbances. This approach together with the results from [6, 11] determines the total set of Burnett kinetic coefficients. Given approaches can be applied to different dense charged and neutral isotropic media. It is important to provide the calculation of Burnett kinetic coefficients of non-ideal matter, for instance, by computer modeling. The properties of the set of Burnett coefficients and the corresponding matrix of coefficients of higher order derivatives in the system of conservation equations (5) (which are significant for hydrodynamic applications) cannot be investigated in a general form (in contrast to that for the linear case [4]). These properties are determined, as a matter of fact, by these coefficient calculation algorithms. The given circumstance may give rise to unjustified difficulties and non-adequate solutions in the corresponding hydrodynamic problems when an incorrect Burnett coefficient calculation algorithm is used. Therefore, the comprehensive investigations of Burnett coefficients have to accompany the use of these coefficients in non-ideal matter hydrodynamic problems.

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