

A Consideration on the Nonlocal Continuum Theory by Using the Kinetic Theory

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The concepts of stress and energy density of the material with long-range interaction are examined explicitly by using the kinetic theory in connection with nonlocal continuum theory. It is also examined that how these concepts are modified when we construct the continuum theory with long-range interaction.

1. Introduction

Up to now, many continuum theories have been developed under the assumption that the range of the mutual interactions between the constituent particles of the material considered can be taken as infinitesimal. Recently, however, *nonlocal continuum theory* has been developed by taking into consideration of the *finite* range of the mutual interactions between the constituent particles (i.e., long-range interaction). About these theories, refer to Eringen and Edelen¹⁾ and others cited in this reference 1).

In this paper, fundamental points, that is, reexamination of the concepts of the stress, energy density, etc., will be considered explicitly by using the *kinetic theory*. Since these concepts have been used only for materials with short-range interaction, it is necessary to reexamine them when we construct the continuum theory governing the behaviors of materials with long-range interaction. Here materials with long-range interaction is defined as follows: Let λ be the longest characteristic length of the interactions in the material considered. And let l be the characteristic length depending on one's measuring instruments. Then, if $\lambda \geq l$, materials are defined as these with long-range interaction.

2. On the operations of averages, the Liouville equation, and some definitions

In this section fundamental equations and definitions necessary in the following discussions are presented.²⁾

Following after the consideration of Irving and Kirkwood,²⁾ we mean *macroscopic quantities* as those obtained by the operation of the following three averages simultaneously:

- (1) Statistical average over the system of an ensemble.
- (2) Spatial average over a small domain depending on one's measuring instrument.
- (3) Time average over an interval depending on one's measuring instrument.

We consider a system with N particles. We denote the probability distribution function by $f(R_1, \dots, R_N; p_1, \dots, p_N; t)$ satisfying the normalization condition

$$\int \dots \int f dR_1 \dots dR_N dp_1 \dots dp_N = 1, \quad (2.1)$$

where R_i and p_i are, respectively, position vector and momentum of the i -th particle. (Here for simplicity, internal degrees of freedom are not considered.) f changes in time according to the well-known Liouville equation

$$\frac{\partial f}{\partial t} = \sum_{k=1}^N \left[-\frac{p_k}{m_k} \cdot \frac{\partial}{\partial R_k} f + \frac{\partial}{\partial R_k} U \cdot \frac{\partial}{\partial p_k} f \right], \quad (2.2)$$

where U is the potential of the entire system, and m_k denotes mass of the k -th particle. Any dynamic variable $\alpha(R_1, \dots, R_N; p_1, \dots, p_N)$ has an expectation value given at time t by

$$\langle \alpha; f \rangle \equiv \int \cdots \int \alpha(R_1, \dots, R_N; p_1, \dots, p_N) f(R_1, \dots, R_N; p_1, \dots, p_N; t) dR_1 \cdots dR_N dp_1 \cdots dp_N, \quad (2.3)$$

and by using (2.2) and Green's theorem, changes in time as follows

$$\frac{\partial}{\partial t} \langle \alpha; f \rangle = \sum_{k=1}^N \left\langle \frac{p_k}{m_k} \cdot \frac{\partial}{\partial R_k} \alpha - \frac{\partial}{\partial R_k} U \cdot \frac{\partial}{\partial p_k} \alpha; f \right\rangle. \quad (2.4)$$

Next, we consider, for simplicity, the ideal situation in which measuring instrument indicates the values averaged in the sphere S (whose center is located at r and its radius is l). This corresponds to the operation of (2). For this purpose, function S_k is defined by

$$S_k \equiv S(|R_k - r|) = \begin{cases} 1 & \text{for } |R_k - r| \leq l, \\ 0 & \text{for } |R_k - r| > l, \end{cases} \quad (2.5)$$

(Average operation of (3) will not be considered explicitly in the following discussions.) The mass density $\rho(r, t)$ at r at time t is given by

$$\rho(r, t) = \frac{1}{V} \sum_{k=1}^N m_k \langle S_k; f \rangle, \quad (2.6)$$

where

$$V \equiv \frac{4\pi}{3} l^3. \quad (2.7)$$

The mean velocity $u(r, t)$ at r at time t is given by

$$u(r, t) = \frac{1}{V} \frac{1}{\rho(r, t)} \sum_{k=1}^N \langle p_k S_k; f \rangle. \quad (2.8)$$

The kinetic energy density $E_K(r, t)$ at r at time t is given by

$$E_K(r, t) = \frac{1}{V} \sum_{j=1}^N \left\langle \frac{p_j^2}{2m_j} S_j; f \right\rangle. \quad (2.9)$$

The potential energy density $E_\phi(r, t)$ at r associated with the interaction of particles with the external field is given by

$$E_\phi(r, t) = \frac{1}{V} \sum_{j=1}^N \langle \phi_j(R_j) S_j; f \rangle, \quad (2.10)$$

where ϕ is the potential energy of the particle in an external field of force and we will limit the potential U to the form such as

$$U = \sum_{k=1}^N \phi_k(R_k) + \frac{1}{2} \sum_{j \neq k} V_{jk}, \quad (2.11)$$

where V_{jk} is the mutual potential between j -th and k -th particles. The external force (body force) per unit volume $X(r, t)$ at r is given by

$$X(r, t) = -\frac{1}{V} \sum_{k=1}^N \left\langle \left[\frac{\partial}{\partial R_k} \phi_k(R_k) \right] S_k; f \right\rangle. \quad (2.12)$$

The pair density $\phi^{(2)}(r, r', t)$ and the current density

$j_1^{(2)}(r, r', t)$ of r are, respectively, given by

$$\phi^{(2)}(r, r', t) = \sum_{j \neq k} \langle \delta(R_j - r) \delta(R_k - r'); f \rangle, \quad (2.13)$$

$$j_1^{(2)}(r, r', t) = \sum_{j \neq k} \left\langle \frac{p_k}{m_k} \delta(R_k - r) \delta(R_j - r'); f \right\rangle. \quad (2.14)$$

Finally, it must be noted that we have not employed the Maxwell-Boltzmann integro-differential equation obtained by using many assumptions but N-particle distribution function and Liouville equation as the starting point.

3. On the concepts of stress and energy density

When we use the concept of stress, we consider the following situations: (see for example reference 3)) "We can say that the forces which causes the internal stresses are, as regards the theory of elasticity, "near-action" forces, which act from any point only to neighboring points. But the above assertion is not valid in cases where the deformation of the body results in macroscopic electric field in it (pyroelectric and piezoelectric bodies)." This situation means that the stress at r must be determined by the conditions at the same point r . In other words, principle of determinism must be imposed.⁴⁾ So that there arises the new problem, i.e., how we can consider the concept of stress in the material with long-range interaction. This will be considered in section 4.

Next, let us consider the concept of energy density. The concept of energy density is connected with the fact that the energy is additive quantity. Thus, rigorously speaking, as energy is not additive quantity because of the long-range interaction, the concept of energy density can not be adopted. In the rest of this section let us examine to what extent the concept of energy density is available in the materials with short-range interaction.

We adopt

$$E_V(r, t) \equiv \frac{1}{2V} \sum_{i \neq j} \langle V_{ij}(R_{ij}) S_i S_j; f \rangle, \quad R_{ij} \equiv |R_j - R_i| \quad (3.1)$$

as one of the energy density. As is seen, this energy density contains mutual interactions only in region S . The difference from the real total energy E_0 is, in the first order approximation, given by

$$\begin{aligned} & \iint \int (E_K + E_\phi + E_V) dr - E_0 \\ & \sim -\frac{1}{\rho} \sum_{i \neq j} \langle V_{ij}(R_{ij}) R_{ij}; f \rangle. \end{aligned} \quad (3.2)$$

From this equation, we can see that the right hand side is the order λ/l in the first order approximation if we put the the zero order approximation as the order 1, where λ is the characteristic length of the short-range interaction. On the other hand, when we adopt

$$\begin{aligned} \varepsilon_V(r, t) = & \frac{1}{2V} \sum_{j \neq k} \langle V_{kj}(R_{kj}) S_k S_j; f \rangle \\ & + \frac{1}{2V} \sum_{j \neq k} \langle V_{kj}(R_{kj}) \{S_k(1-S_j) + S_j(1-S_k)\}; f \rangle \end{aligned} \quad (3.3)$$

as the other energy density, the difference from E_0 is given by

$$\begin{aligned} & \iint (E_K + E_\phi + \varepsilon_V) dr - E_0 \\ & \sim \frac{1}{\rho} \sum_{i \neq j} \langle V_{ij}(R_{ij}) R_{ij}; f \rangle. \end{aligned} \quad (3.4)$$

Thus, so long as $\lambda \ll l$, it is equivalent whether ε_V or E_V is adopted as the energy density in the zero order approximation.

4. Transport phenomena for the construction of the macroscopic constitutive equations

In this section, we consider the simple case such that all particles are identical and mutual interactions depend only on its distance. When we take into account the long-range interaction we will see how this interaction changes the situation in which only short-range interactions are considered by use of the results in section 2 and 3.

i) The equation of continuity.

From (2.4), (2.6) and (2.8), the equation of continuity is given by

$$\frac{\partial}{\partial t} \rho(r, t) + \frac{\partial}{\partial r} \cdot [\rho(r, t) u(r, t)] = 0. \quad (4.1)$$

Thus the equation of continuity is not affected by the long-range interaction as was expected.

ii) The equation of motion.

From (2.4), (2.6), (2.8), (2.11)-(2.13), the equation of motion is given by

$$\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial r} \cdot (\rho u u) = X + \frac{\partial}{\partial r} \cdot \sigma, \quad (4.2)$$

where

$$\sigma(r, t) = \sigma_K(r, t) + \sigma_V(r, t), \quad (4.3)$$

$$\sigma_K = -\frac{1}{V} \sum_{k=1}^N \langle m \left(\frac{p_k}{m} - u \right) \left(\frac{p_k}{m} - u \right) S_k; f \rangle, \quad (4.4)$$

$$\begin{aligned} \sigma_V = & \frac{1}{2V} \sum_{j \neq k} \langle \frac{R_{jk} R_{jk}}{R_{jk}} V'(R_{jk}) S_j S_k; f \rangle \\ & + \frac{1}{4V} \sum_{j \neq k} \langle \frac{R_{jk} R_{jk}}{R_{jk}} V'(R_{jk}) \{S_k(1-S_j) \} \end{aligned}$$

$$\begin{aligned} & + S_j(1-S_k)\}; f \rangle \\ & + \frac{1}{2V} \iint \frac{RR}{R} V'(R) \left(R \cdot \frac{l}{l} \right) \left\{ \frac{1}{2} + \dots \right. \\ & \left. + \frac{1}{n!} \left(-R \cdot \frac{\partial}{\partial r} \right)^{n-2} + \dots \right\} \\ & \times \phi^{(2)}(r+l, r+l+R) dR d\Omega, \end{aligned} \quad (4.5)$$

$$V'(R) \equiv -\frac{d}{dR} V(R),$$

l : Any vector oriented from r with length l .

$d\Omega$: Surface element of the sphere with center r and radius l .

From these equations, we find the following results:

(1) External force X , which is a macroscopic quantity, is obtained by taking the averages over the particles. Since the sphere S is considered to be very small compared with the macroscopic characteristic length, X is given by in the first order approximation

$$X(r, t) \sim -\left(\frac{\partial}{\partial r} \phi(r) \right) n(r, t), \quad (4.6)$$

where $n(r, t)$ is the number density.

(2) Stress tensor σ can be split into two parts, i.e., one of them, σ_K , is the kinetic contribution and the other part σ_V is the intermolecular force contribution. σ_K is the dominant term for gases, but is negligibly small compared with σ_V for liquids and solids.

Furthermore, σ_V can be split into three parts:

1°. The first part is determined by the particles only in the region S .

2°. The second part is determined by the interactions between the particle in the region S and the one in the outer region of S .

3°. The last part is determined by the interactions between the particle on the fringe of the region S and the one which is not on it. In the materials with short-range interaction, the part 1° is dominant compared with the part 2°, but in the materials with long-range interaction, the parts 1° and 2° are of comparable order. The part 3° is, however, negligibly small in the first order approximation so far as the boundary of the material is not considered. So that the principle of determinism can be imposed only on the case of materials with short-range interaction where part 1° is dominant.

(3) From the above considerations we can conclude that the concept of stress at r in the material with long-range interaction has its meaning in the generalized sense of the term, that is, it depends not only on the conditions at r but also on the conditions at other places.

iii) Law of conservation of energy.

The quantities $E_K(r, t)$ and $E_\phi(r, t)$ in (2.9) and (2.10), respectively, are the well-defined ones as the densities. But the quantity $\varepsilon_V(r, t)$ can approximately be considered as the density only in the materials with short-range interaction as is seen in section 3.

In what follows, we will calculate the change in time of the measurable quantity $E_K + E_\phi + \varepsilon_V$ which is not the energy density in the materials with long-range interaction. From (2.4), (2.8) - (2.10), (2.13), (2.14), (3.3), (4.3) - (4.5), the equation of conservation of energy is given by

$$\begin{aligned} & \frac{\partial}{\partial t} (E_K + E_\phi + \varepsilon_V) + \frac{\partial}{\partial r} \cdot \left\{ (E_K + E_\phi + \varepsilon_V) u \right\} \\ & - \frac{\partial}{\partial r} \cdot (u \cdot \sigma) \\ = & -\frac{1}{V} \frac{\partial}{\partial r} \cdot \left[\sum_{k=1}^N \langle \psi(R_k) \left(\frac{p_k}{m} - u \right) S_k; f \rangle \right. \\ & + \sum_{k=1}^N \langle \frac{m}{2} \left| \frac{p_k}{m} - u \right|^2 \left(\frac{p_k}{m} - u \right) S_k; f \rangle \\ & + \frac{1}{2} \sum_{j \neq k} \langle V_{jk} \left(\frac{p_k}{m} - u \right) S_j S_k; f \rangle \\ & + \sum_{j \neq k} \langle V_{jk} \left(\frac{p_k}{m} - u \right) S_k (1 - S_j); f \rangle \\ & - \frac{1}{2} \sum_{j \neq k} \langle \frac{R_{jk} R_{jk}}{R_{jk}} V'(R_{jk}) \left(\frac{p_k}{m} - u \right) S_j S_k; f \rangle \\ & - \frac{1}{2} \sum_{j \neq k} \langle \frac{R_{jk} R_{jk}}{R_{jk}} V'(R_{jk}) \left(\frac{p_k}{m} - u \right) S_k (1 - S_j); f \rangle \\ & - \frac{1}{2} \int \int \frac{RR}{R} V'(R) \left(R \cdot \frac{l}{l} \right) \left\{ \frac{1}{2} + \dots \right. \\ & \left. + \frac{1}{n!} \left(-R \cdot \frac{\partial}{\partial r} \right)^{n-2} + \dots \right\} \left\{ j_1^{(2)}(r+l, r+l+R) \right. \\ & \left. - u \phi^{(2)}(r+l, r+l+R) dR d\Omega \right\} \\ & + \frac{1}{V} \sum_{j \neq k} \langle \left(\frac{\partial}{\partial R_k} V_{jk} \right) \cdot \frac{p_k}{m} \left\{ \frac{1}{2} (S_j + S_k) - S_j S_k \right\}; f \rangle \\ & + \frac{1}{2V} \sum_{j \neq k} \langle \int \langle V_{jk} \frac{p_k}{m} \cdot \frac{l}{l} \left\{ \delta(|R_j - r| - l) S_k \right. \right. \\ & \left. \left. - \delta(|R_k - r| - l) S_j \right\}; f \rangle d\Omega \right. \end{aligned} \tag{4.7}$$

From this equation we find the following results:

(1) There are two terms not expressed in the divergence form, i.e., they are the last two terms in (4.7). The last term but one is dominant compared with the last one. These two terms are negligibly small in the materials with short-range interaction, but are not so in those with long-range interaction.

(2) The term expressing heat supply from the external field is of comparable order with the other terms when characteristic length of the spatial change of the external field is of comparable order with or smaller than that of the characteristic length of one's measuring instruments. In the other cases this term is

negligible.

(3) The terms in the divergence operator in (4.7) can be split into two parts, i.e., one is the heat flux due to the transport of thermal kinetic energy q_K and the other is the heat flux by molecular interaction q_V . The relations of the order of magnitude between q_K and q_V in the different materials are the same as those of the stresses σ_K and σ_V .

Furthermore we can split q_V into three parts and the discussions for each part are the same as those of the σ_V stated above.

(4) From the above considerations we can conclude that the total heat flux $q \equiv q_K + q_V$ at r depends not only on the conditions at r but also on the conditions at other places.

5. Conclusions

The concepts of stress and energy density of the material with long-range interaction are reexamined. It is found that the concept of stress is valid in the broad sense of the term. And it is also pointed out that the expression of the law of conservation of energy is not the same as those for the materials with short-range interactions. One possible expression for this is considered in section 4.

Finally, it must be said that some important discussions such as boundary conditions, second law of thermodynamics, etc., which are necessary to complete the continuum theory, are not considered here.

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