POSSIBLE DEFINITIONS OF THE CONCEPTS OF STRESS AND STRAIN IN A SYSTEM OF INTERACTING PARTICLES

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We examine a system of a large number or interacting particles. We assume that the interaction force between two particles can be expressed in terms of a potential of pair-wise interaction. In this case the force $F(t, x)$ acting on each particle under the action of the given external field $a(t, x)$ can be defined in the form [1]

$$F(t, x) = \alpha(t, x) + \frac{1}{P(t, x)} \int p(t, x, \xi) \operatorname{grad}_x Q(|x - \xi|)\, d\xi, \quad d\xi = d\xi_1\, d\xi_2\, d\xi_3$$

$$(Q(r) \neq 0 \quad \text{for} \quad 0 < r < R, \qquad Q(r) = 0 \quad \text{for} \quad r \geqslant R)$$

Here $Q(r)$ is the potential of pair-wise interaction between two particles, $p(t, x, \xi)$ is the joint density distribution of two particles, $P(t, x)$ is the density distribution of a single particle

$$P(t, x) = \int p(t, x, \xi)\, d\xi$$

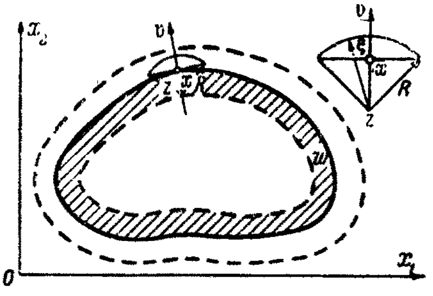

Fig. 1.

We isolate a certain volume V from this system of interacting particles. The force $F(t, x)$ acts on each particle of this volume. If surface forces $f_\nu(t, x)$ are introduced, that is, if the particles not lying in the volume V are discarded and the sum of their action is replaced by the mean stress $f_\nu(t, x) A_\nu(t, x)$ ($A(t, x)$ is the particle density on the surface), then the equations of motion of the volume can, by use of the force $F(t, x)$, be represented in the form

$$\int_V \mathbf{F}(t,\,\mathbf{x})\,P(t,\,\mathbf{x})\,dx = \int_\Sigma \mathbf{f}_\nu(t,\,\mathbf{x})\,A_\nu(t,\,\mathbf{x})\,ds \qquad (dx = dx_1\,dx_2\,dx_3) \tag{1}$$

The equations of the projections of the principal moment of momentum are

$$\int_V P(t,\,\mathbf{x})\,[\mathbf{x}\times\mathbf{F}(t,\,\mathbf{x})]\,dx = \int_\Sigma A_\nu(t,\,\mathbf{x})\,[\mathbf{x}\times\mathbf{f}_\nu(t,\,\mathbf{x})]\,ds \tag{2}$$

Making use of the expression of the force $\mathbf{F}(t,\,\mathbf{x})$ in terms of the potential of pair-wise interaction $Q(r)$ and, assuming $a(t,\,\mathbf{x}) \equiv 0$, the volume integral in Equation (1) can be transformed to the surface (Fig. 1)

$$\int_V \mathbf{F}(t,\,\mathbf{x})\,P(t,\,\mathbf{x})\,dx = \int_W dx \int_{w(\mathbf{x})} p(t,\,\mathbf{x},\,\xi)\,\mathrm{grad}_x\, Q(|\mathbf{x}-\xi|)\,d\xi =$$

$$= \int_\Sigma ds \int_0^R dh \int_{R_1}^R r^2\,\mathrm{grad}\,Q(r)\,dr \int_0^\vartheta \sin\theta\,d\theta \times$$

$$\times \int_0^{2\pi} p\,[t,\,x_1 - hl_1,\,x_2 - hl_2,\,x_3 - hl_3;\,(r,\,\theta,\,\varphi)]\,d\varphi$$

$$\nu\mathbf{x}_1{}^\circ = l_1, \qquad \nu\mathbf{x}_2{}^\circ = l_2, \qquad \nu\mathbf{x}_3{}^\circ = l_3, \qquad R_1 = \frac{h}{\cos\theta}$$

$$\vartheta = \cos^{-1}\frac{h}{R} \qquad (0 \leqslant h \leqslant R) \tag{3}$$

Here $ds = ds_1 ds_2$ is a surface element; $w(\mathbf{z})$ is the volume of a segment which a tangent plane introduced at the point $\mathbf{x}$ cuts off of a sphere of radius R with center at the point $\mathbf{z}$; the volume W is a layer of the volume V of the thickness R.

Hence the mean stress at the point $\mathbf{x}$ may be defined in the following way by the use of (3):

$$\mathbf{f}_\nu(t,\,x)\,A_\nu(t,\,\mathbf{x}) = \int_0^R dh \int_{R_1}^R r^2\,\mathrm{grad}\,Q(r)\,dr \int_0^\vartheta \sin\theta\,d\theta \times$$

$$\times \int_0^{2\pi} p\,[t,\,x_1 - hl_1,\,x_2 - hl_2,\,x_3 - hl_3;\,(r,\,\theta,\,\varphi)]\,d\varphi \tag{4}$$

It is easy to verify that the stress so defined satisfies the system of equations (2).

For the complete definition of the stress at the point $\mathbf{x}$ it is necessary to define the surface density $A_\nu(t, \mathbf{x})$. This clearly must be a certain functional of the volume density $P(t, \mathbf{x})$. This density can be defined in the following way:

$$A_\nu(t, \mathbf{x}) = \int_0^R dh \int_{R_1}^R r^2\, dr \int_0^\theta \sin\theta\, d\theta \times$$
$$\times \int_0^{2\pi} p\,[t,\ x_1 - hl_1,\ x_2 - hl_2,\ x_3 - hl_3;\ (r,\ \theta,\ \varphi)]\, d\varphi$$

In the given definition of the mean stress it was necessary to take the volume $w(\mathbf{z})$ that is cut out by the surface Σ which bounds the volume V from the sphere of radius R with center at the point $\mathbf{z}$ belonging to the volume W. The mean stress is rigorously defined in this case for a surface with normal ν.

As is easily seen, if the joint density distribution of the particles $p(t, \mathbf{x}, \xi)$ is assumed uniform, then the force $\mathbf{F}(t, \mathbf{x}) \equiv 0$ at all points of the volume occupied by the system of interacting particles; the mean stress will be identical at all points and will be directed along the normal to the surface for which it is defined. Hence the force $\mathbf{F}(t, \mathbf{x})$ and the shear component of the stress in the system of interacting particles arise as a consequence of the nonuniformity of the particle distribution.

Cauchy was the first to use central forces for the definition of stress [2-3]. If the mean stress is defined as suggested by Cauchy, then in the example being considered (Fig. 2) we have

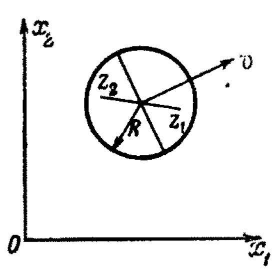

Fig. 2.

$$\mathbf{f}_\nu(t, \mathbf{x})\, A_\nu(t, \mathbf{x}) = \int_0^R dr_1 \int_0^R \operatorname{grad} Q\,(r_1 + r_2)\, dr_2 \int_0^{\pi/2} r_2^2 \sin\theta\, d\theta$$
$$\int_0^{2\pi} p\,[t,\ x + (r_1,\ \theta,\ \varphi);\ x + (r_2,\ \theta + \pi,\ \varphi + \pi)]\, d\varphi$$

Thus, the definition of the mean stress according to Cauchy differs from the definition of the mean stress in the form (4) only by the summation over $\mathbf{z}_2$. In the latter case $\mathbf{z}_2$ can change only along the normal ν; in the case of Cauchy's definition $\mathbf{z}_2$ changes in the interior of a hemisphere of radius R.

It can be shown that to obtain the mean pressure in an ideal gas it is necessary to compute the sum of the change in the momentum as a result of the impact of the particles distributed on the positive side of the normal with those lying on the negative side. In this computation the line of impact must pass through the point x at which the mean pressure is defined [4]. In the definition of the mean stress according to Cauchy there occurs a similar computation of the change of momentum.

It is easy to verify that the change of momentum of Cauchy does not satisfy the equations of equilibrium (1) and of moment of momentum (2).

In Cauchy's work [2,3] the existence of an elastic potential was shown. Repeating completely Cauchy's reasoning, we try next to obtain an elastic potential. We shall carry out the reasoning for fictitious particles z_1 and z_2. In the case under consideration each of the particles moves, therefore the geometric point x must be placed to conform to the physically defined particle.

We examine some surface at the point x, with the position of the surface defining the normal ν. The stress will be defined according to Cauchy. We examine the stationary state of particles, defined by the condition $dP(t,\mathbf{x})/dt = 0$. We take the stationary state as the initial state and we call the mean stress computed for this state the mean initial stress

$$\sigma_{\nu_0}(\mathbf{x}) = \mathbf{f}_\nu{}^\circ(\mathbf{x})\, A_\nu{}^\circ(\mathbf{x}) = \int p(\mathbf{x}, \xi)\, \Phi(r)\, \mathbf{b}^\circ\, d\xi\, dr_1$$

$$\Phi(r) = \frac{\partial Q(r)}{\partial r}, \quad r = r_1 + r_2 = |\mathbf{x} - \xi|, \quad \mathbf{b}^\circ = \frac{\mathbf{x} - \xi}{|\mathbf{x} - \xi|}$$

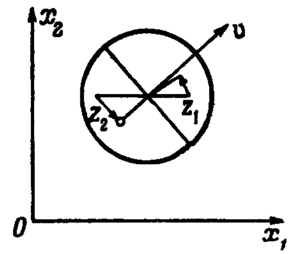

Fig. 3.

Let an external field act on the given system of interacting particles and let these fictitious particles take on some displacements, the displacements having to satisfy the condition that the particles lie at all times on a straight line passing through the point x. If such fictitious displacements are introduced, then the mean stress at the point x and time t for the given surface with direction ν is defined in the form

$$\sigma_\nu(t, \mathbf{x}) \equiv \int \Phi(r)\, p(t, \mathbf{x}, \xi)\, \mathbf{b}^\circ\, d\xi\, dr_1 = \int \Phi(r + \delta r)\, p(\mathbf{x}, \xi)\, (\mathbf{b}^\circ + \delta\mathbf{b}^\circ)\, d\xi\, dr_1. \tag{5}$$

Thus, for every direction ν at the given point x we obtain three equations for the determination of four quantities: δr, δa_1, δa_2, δa_3, where the δa_i are increments in the direction cosines of the vector $\mathbf{b}^\circ$. From the well-known relation for direction cosines

$$(\alpha_1 + \delta\alpha_1)^2 + (\alpha_2 + \delta\alpha_2)^2 + (\alpha_3 + \delta\alpha_3)^3 = 1,$$

we obtain, under the assumption that the δa_i are all sufficiently small, the additional equation

$$\alpha_1\, \delta\alpha_1 + \alpha_2 \delta\alpha_2 + \alpha_3\, \delta\alpha_3 = 0 \tag{6}$$

Making the assumption that δr, δa_1, δa_2, δa_3 are sufficiently small, Equation (5) can be transformed to the form

$$\sigma_\nu(t, \mathbf{x}) = \sigma_{\nu_0}(\mathbf{x}) + \int \Phi'(r)\, \delta r \mathbf{b}^\circ p(\mathbf{x}, \xi)\, d\xi\, dr_1 + \int \Phi(r)\, p(\mathbf{x}, \xi)\, \delta \mathbf{b}^\circ\, d\xi\, dr_1 \tag{7}$$

Since, as a result of displacements, $\mathbf{z}_1$ and $\mathbf{z}_2$ remain on the same line, passing through the point $\mathbf{x}$, the introduction of the finite deformation tensor $\epsilon_{ij}(t, \mathbf{x})$ at the point $\mathbf{x}$ makes it is easy to obtain

$$\delta r = r \sum_{i,\, j=1}^{3} \alpha_i \alpha_j \varepsilon_{ij}(t, \mathbf{x}), \quad \varepsilon(t, \mathbf{x}) = \sum_{i,\, j=1}^{3} \alpha_i \alpha_j \varepsilon_{ij}(t, \mathbf{x}) \tag{8}$$

$$\delta\alpha_i = \sum_{j=1}^{3} \alpha_j \frac{\partial u_i(t, \mathbf{x})}{\partial x_j} - \alpha_i \varepsilon(t, \mathbf{x}) - \varepsilon(t, \mathbf{x}) \sum_{j=1}^{3} \alpha_j \frac{\partial u_i(t, \mathbf{x})}{\partial x_j} + \frac{r^2}{4} \sum_{j,\, k=1}^{3} \frac{\partial^2 u_i(t, \mathbf{x})}{\partial x_j\, \partial x_k} \alpha_j \alpha_k$$

Here $u_i(t, \mathbf{x})$ are the components of the fictitious displacement vector.

In the case of small deformations, relations (8) change to the relations

$$\delta r = r \sum_{i,\, j=1}^{3} \alpha_i \alpha_j e_{ij}(t, \mathbf{x}), \qquad e_{ij}(t, \mathbf{x}) = \frac{1}{2}\left(\frac{\partial u_i(t, \mathbf{x})}{\partial x_j} + \frac{\partial u_j(t, \mathbf{x})}{\partial x_i}\right) \tag{9}$$

$$\delta\alpha_i = \sum_{j=1}^{3} \alpha_j \frac{\partial u_i(t, \mathbf{x})}{\partial x_j} - \alpha_i e(t, \mathbf{x}), \; e(t, \mathbf{x}) = \sum_{i,\, j=1}^{3} \alpha_i \alpha_j e_{ij}(t, \mathbf{x})$$

Equation (6), as is easily verified, will be satisfied for small displacements.

Using (9), the relation (7) can be transformed to a form analogous to the expression for an elastic potential

$$\mathbf{A}_\nu(t, \mathbf{x}, \nu) = \sum_{i=1}^{3} a_i(\mathbf{x}, \nu) \frac{\partial \mathbf{u}(t, \mathbf{x})}{\partial x_i} + \frac{1}{2} \sum_{i,\, j=1}^{3} \mathbf{b}_{ij}(\mathbf{x}, \nu) \left(\frac{\partial u_i(t, \mathbf{x})}{\partial x_j} + \frac{\partial u_j(t, \mathbf{x})}{\partial x_i}\right)$$

$$\mathbf{A}_\nu(t, \mathbf{x}, \nu) = \int \Phi(r)\, \mathbf{b}^\circ [p(t, \mathbf{x}, \xi) - p(\mathbf{x}, \xi)]\, d\xi\, dr_1$$

$$a_i(\mathbf{x}, \nu) = \int \Phi(r)\, \alpha_i\, p(\mathbf{x}, \xi)\, d\xi\, dr_1$$

$$\mathbf{b}_{ij}(\mathbf{x}, \nu) = \int [r\Phi'(r) - \Phi(r)]\, \mathbf{b}^\circ \alpha_i \alpha_j\, p(\mathbf{x}, \xi)\, d\xi\, dr_1 \tag{10}$$

Thus from the three equations (10) it is necessary to obtain three functions of the displacements $u_1(t, \mathbf{x})$, $u_2(t, \mathbf{x})$, $u_3(t, \mathbf{x})$. But since the displacements do not have to depend on the normal ν, Equations (10) will not always be valid. The question as to what conditions must be applied to the potential of pair-wise interaction $Q(r)$, the joint density distribution $p(x, \xi)$, and the external field $a(t, x)$ in order for Equations (10) to be valid still remains open.

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