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LOCAL INHOMOGENEITIES IN AN ELASTIC MEDIUM

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A method for investigating the perturbations of the external field due to a system of local inhomogeneities (defects) in an elastic medium is proposed. The method is based on a certain special representation of Green's tensor for a medium with defects in terms of the interaction energy operator which is convenient for describing the asymptotic behavior of perturbed fields. If the defects are small compared with the distances between them this representation makes it possible to construct effective solutions and to find expressions for the energy and for the interaction forces between the defects.

Section 1 introduces the interaction energy operator and deals with the construction of the asymptotic representation of Green's tensor for a homogeneous medium containing a single defect. The procedure for calculating the coefficients of the expansion is presented in Sect. 2 by way of an example (an ellipsoidal inhomogeneity). Section 3 concerns the general case of interaction of a defect system. Section 4 contains sample calculations for two ellipsoidal inhomogeneities. An explicit expression for the asymptotic behavior of the interaction energy is derived and special cases considered.

1. We begin with the general scheme. Let L_0 be a linear operator associated with a known Green's function G_0 satisfying certain boundary conditions, namely $L_0 G_0 = I$, where I is an identity operator. If L_1 is a perturbation of the operator L_0 such that there exists a Green's function G of the operator $L = L_0 + L_1$, we can show that G is given by the representation

$$G = G_0 - G_0 P G_0 \quad (1.1)$$

where the operator P is defined by the expression

$$P = L_1 (L_1 + L_1 G_0 L_1)^{-1} L_1 \quad (1.2)$$

In fact, substituting P into (1.1) and applying L from the left side, we obtain

$$LG = (L_0 + L_1) [G_0 - G_0 L_1 (L_1 + L_1 G_0 L_1)^{-1} L_1 G_0] = \\ = I + [I - (L_1 + L_1 G_0 L_1) (L_1 + L_1 G_0 L_1)^{-1}] L_1 G_0 = I$$

Thus, construction of G reduces to finding P from Eq. (1.2); this is more convenient in the defect problem, since the kernel of the operator L_1 is localized in a bounded domain which can usually be assumed small. We note that when the operator L_1^{-1} has meaning, expression (1.2) can also be written as

$$P = (L_1^{-1} + G_0)^{-1} \quad (1.3)$$

Now let us consider a homogeneous elastic medium with a single defect. The operator L is defined by equations relating the displacement $u_\mu(x)$ and the external forces $q^\beta(x)$.

$$\partial_\alpha [c^{\alpha\beta\lambda\mu}(x) \partial_\lambda u_\mu(x)] = -q^\beta(x) \quad (1.4)$$

Let us suppose that the tensor of elastic moduli is of the form

$$c^{\alpha\beta\lambda\mu}(x) = c_0^{\alpha\beta\lambda\mu} + c_1^{\alpha\beta\lambda\mu}(x) \quad (1.5)$$

Here $c_0^{\alpha\beta\lambda\mu}$ is the tensor of elastic constants of the homogeneous medium; $c_1^{\alpha\beta\lambda\mu}(x)$ is the perturbation produced by the defect localized in the (small) domain V . The case $c_1 \rightarrow \infty$ corresponds to a rigid inclusion and $c_1 = -c_0$ to a cavity.

Assuming that the Green's tensor $G_{\alpha\beta}^\circ(x, x')$ for the homogeneous medium is known and applying the above scheme, we can write the Green's tensor $G_{\alpha\beta}(x, x')$ for the defective medium,

$$G_{\alpha\beta}(x, x') = G_{\alpha\beta}^\circ(x, x') - \\ - \iint G_{\alpha\nu}^\circ(x, y) \partial_\lambda P^{\lambda\nu\sigma\tau}(y, y') \partial_{(\sigma} G_{\tau)\beta}^\circ(y', x') dy dy' \quad (1.6)$$

Rewritten in operator form this becomes

$$G = G^\circ - G^\circ \nabla P \nabla G^\circ \quad (1.7)$$

where (as is easy to show) P satisfies the following integral equation in the domain V :

$$P(x, x') - c_1(x) \int_V \nabla G^\circ(x, y) \nabla P(y, x') dy = -c_1(x) \delta(x-x'), \quad x \in V, x' \in V' \quad (1.8)$$

Its solution can be expressed symbolically in a form similar to that of (1.2),

$$P = c_1 (c_1 \nabla G^\circ \nabla c_1 - c_1)^{-1} c_1 = c_1 Q^{-1} c_1 \quad (1.9)$$

$$Q(y, y') = -c_1(y) \nabla \nabla' G^\circ(y, y') c_1(y') - c_1(y) \delta(y - y') \\ y \in V, y' \in V' \quad (1.10)$$

If the operator c_1^{-1} has meaning, then P can be written as

$$P = (\nabla G^\circ \nabla - c_1^{-1})^{-1} = R^{-1} \quad (1.11)$$

$$R(y, y') = -\nabla \nabla' G^\circ(y, y') - c_1^{-1}(y) \delta(y - y'), \quad y \in V, y' \in V' \quad (1.12)$$

It is clear that the operator P is selfadjoint and that its kernel satisfies the symmetry conditions

$$P^{\lambda\nu\sigma\tau}(y, y') = P^{\nu\lambda\sigma\tau}(y, y') = P^{\sigma\tau\lambda\nu}(y', y) \quad (1.13)$$

and is concentrated in the (small) domain $V \times V'$.

The solution of Eqs. (1.4) now becomes

$$u_\alpha(x) = u_\alpha^\circ(x) - \int G_{\alpha\nu}^\circ(x, y) \partial_\lambda P^{\lambda\nu\sigma\tau}(y, y') \varepsilon_{\sigma\tau}(y') dy dy' \quad (1.14)$$

where $u_{\alpha}^{\circ}(\mathbf{x})$ and $\varepsilon_{\alpha\beta}^{\circ}(\mathbf{x})$ are the displacement and strain in the defect-free medium. The operator P also enables us to write the expression for $u_{\alpha}(\mathbf{x})$ in explicit form provided the forces and moments acting on the defect are given.

The energy of interaction between the defect and the external field $\varepsilon_{\alpha\beta}(\mathbf{x})$ turns out to be

$$\Phi = \frac{1}{2} \iint_{V, V'} \varepsilon_{\alpha\beta}^{\circ}(y) P^{\alpha\beta\lambda\mu}(y, y') \varepsilon_{\lambda\mu}^{\circ}(y') dy dy' \quad (1.15)$$

which means that P can be regarded as the operator of the energy of interaction between the defect and the external field.

In some problems (e.g. in the case where a local inhomogeneity models a vacancy or a foreign atom in the crystal) it is interesting to determine the force acting on the defect [1]. This force can be found by assuming that the defect is capable of translational motion through the medium. The kernel of the operator P and therefore the interaction energy Φ then depend on the coordinates x_0^{ν} of the center of mass of the defect, and the force acting on the defect is given by

$$f_{\nu} = - \frac{\partial \Phi(x_0)}{\partial x_0^{\nu}} = - \frac{1}{2} \iint_{V, V'} \varepsilon_{\alpha\beta}^{\circ}(y) \frac{\partial}{\partial x_0^{\nu}} P^{\alpha\beta\lambda\mu}(y, y', x_0) \varepsilon_{\lambda\mu}^{\circ}(y') dy dy' \quad (1.16)$$

The same method can be used to find the resultant moment exerted on the defect by the external field.

In general the kernel $P^{\alpha\beta\lambda\mu}(y, y')$ of the interaction energy operator can be found numerically. This is facilitated by the fact that unlike $G_{\alpha\beta}(\mathbf{x}, \mathbf{x}')$, the kernel $P^{\alpha\beta\lambda\mu}(y, y')$ is concentrated in a bounded domain.

The problem becomes much simpler (and in some cases solvable analytically) if we are interested merely in the asymptotic behavior of the perturbed field. This is equivalent to the assumption that the defect is small compared with the distances from the defect, or (which is the same thing) to the approximation of P by the first terms of the expansion in multipoles.

The expansion of P in a multipole series at the point x_0 is of the form

$$P^{\alpha\beta\lambda\mu}(y, y') = \sum_{mn} (-1)^{m+n} P^{\alpha\beta\lambda\mu\lambda_1 \dots \lambda_m \mu_1 \dots \mu_n} \delta_{\lambda_1 \dots \lambda_m}(y - x_0) \delta_{\mu_1 \dots \mu_n}(y' - x_0) \quad (1.17)$$

$$P^{\alpha\beta\lambda\mu\lambda_1 \dots \lambda_m \mu_1 \dots \mu_n} = \frac{1}{m!n!} \iint P^{\alpha\beta\lambda\mu}(y + x_0, y' + x_0) y^{\lambda_1} \dots y^{\lambda_m} y'^{\mu_1} \dots y'^{\mu_n} dy dy'$$

which can be abbreviated as

$$P(y, y') = \sum_{mn} (-1)^{m+n} P_{mn} \delta_{(m)}(y - x_0) \delta_{(n)}(y' - x_0) \quad (1.18)$$

Substituting this expansion into (1.8), we eventually arrive at a linear system of equations for determining the coefficients P_{mn} .

Expression (1.14) implies that to obtain the asymptotics of $u_{\alpha}(\mathbf{x})$ of order $|\mathbf{x} - \mathbf{x}_0|^{-l}$ we must retain terms up to the order $m + n = l - 2$, inclusively, in expansion (1.17). In the zero-th approximation we are left with one term with the coefficient P_{00} . It can be shown that this approximation corresponds to the model of a point defect in an elastic quasicontinuum considered in [2].

In the case of a homogeneous external field $\varepsilon_{\alpha\beta}^{\circ} = \text{const}$ the energy of defect-field interaction is given by the exact formula

$$\Phi = 1/2 \varepsilon_{\alpha\beta} \circ P_{00}^{\alpha\beta\lambda\mu} \varepsilon_{\lambda\mu} \circ \tag{1.19}$$

which makes possible a physical interpretation of P_{00} .

As we shall show, the asymptotic behavior of the solution for a defective system can be constructed provided the first coefficients P_{mn} for each defect are known.

2. Let us consider in more detail the independently interesting case of an ellipsoidal anisotropic inhomogeneity in an infinite isotropic homogeneous medium. Let

$$c_1^{\alpha\beta\lambda\mu}(x) = c_1^{\alpha\beta\lambda\mu} V(x) \tag{2.1}$$

where $c_1^{\alpha\beta\lambda\mu}$ is a constant tensor and $V(x)$ is the characteristic function of the ellipsoid defined by the canonical equation

$$\frac{(x^1)^2}{a_1^2} + \frac{(x^2)^2}{a_2^2} + \frac{(x^3)^2}{a_3^2} = 1 \tag{2.2}$$

It can be shown that the system of equations for P_{mn} breaks down in this case into independent equations for each of the coefficients P_{m0} and P_{m1} . The remaining coefficients are related by recursion formulas. Thus, the expressions for the coefficients are obtainable in closed form (in quadratures).

From now on we shall confine our attention to the principal terms of the asymptotics of the perturbed fields, which will enable us to limit ourselves to the explicit expression for the coefficient P_{00} . Omitting the cumbersome intervening expressions, we state the final result $P_{00} = -v c_1 (c_1 + c_1 A c_1)^{-1} c_1 = -v (c_1^{-1} + A)^{-1}$ (2.3)

where v is the volume of the ellipsoid and A is a constant tensor with the symmetry of $c^{\alpha\beta\lambda\mu}$ over its indices; this tensor depends on the geometric characteristics of the ellipsoid, the shear modulus μ_0 , and the Poisson's ratio ν_0 of the external medium. We infer from this that A must have ellipsoidal symmetry and be defined by nine essential components. In the chosen coordinate system attached to the principal axes of the ellipsoid we have

$$A_{1111} = \kappa_0 [3I_{11} + (1-4\nu_0)I_1], \quad A_{1122} = \kappa_0 [I_{21} - I_1] \tag{2.4}$$

$$A_{1212} = 1/2 \kappa_0 [I_{21} + I_{12} + (1-2\nu_0)(I_1 + I_2)], \quad \kappa_0 = 1/16 [\pi \mu_0 (1-\nu_0)]^{-1}$$

The quantities

$$I_p = \frac{3}{2} v \int_0^\infty \frac{d\xi}{(a_p^2 + \xi) \Delta(\xi)}, \quad I_{pq} = \frac{3}{2} v a_p^2 \int_0^\infty \frac{d\xi}{(a_p^2 + \xi)(a_q^2 + \xi) \Delta(\xi)}$$

$$(\Delta(\xi) = \sqrt{(a_1^2 + \xi)(a_2^2 + \xi)(a_3^2 + \xi)}) \tag{2.5}$$

can be expressed in terms of elliptic integrals.

The remaining six nonzero components of the tensor $A_{\alpha\beta\lambda\mu}$ are obtainable from (2.4) by cyclic permutation of the indices 1, 2, 3.

The resulting expression for P_{00} enables us to use relation (1.14) to obtain the principal term of the asymptotic expression for the perturbed field in an arbitrary external field. As already noted, expression (1.19) is exact for a homogeneous external field, and the asymptotic behavior of the perturbed field in the particular case of isotropic ellipsoidal inhomogeneity coincides with the asymptotic expression previously obtained by a different method by Eshelby [1].

3. Now let us consider a homogeneous elastic medium containing a system of defects.

The operator L is defined by Eq. (1.4) as before, but the tensor of elastic moduli is of the form

$$c^{\alpha\beta\lambda\mu}(x) = c_0^{\alpha\beta\lambda\mu} + \sum_i c_i^{\alpha\beta\lambda\mu}(x) \tag{3.1}$$

where $c_i^{\alpha\beta\lambda\mu}(x)$ is the perturbation produced by a defect localized in the (small) domain V_i .

It is clear that the Green's tensor $G_{\alpha\beta}(x, x')$ for a medium containing a defect system is of the form (1.6). However, in contrast to the case of a single defect the interaction energy operator is given by the operator sum

$$P = \sum_{ij} P^{ij} \tag{3.2}$$

where P^{ij} has a kernel concentrated in the domain $V_i \times V_j'$ and is expressible in a form similar to that of (1.9),

$$P^{ij} = c_i (c_j \nabla G^\circ \nabla c_i - c_j \delta_{ij})^{-1} c_j = (\nabla G^\circ \nabla - c_i^{-1} \delta_{ij})^{-1} = R_{ij}^{-1} \tag{3.3}$$

$$R_{ij}(y, y') = -\nabla \nabla' G^\circ(y, y') - c_i^{-1}(y) \delta(y - y') \delta_{ij} \tag{3.4}$$

$y \in V_i, y' \in V_j'$

We see from this that the operator P is selfadjoint and that its kernel satisfies symmetry conditions (1.13) and is concentrated in the domain $\bigcup_{ij} V_i \times V_j$.

Expressions (1.14) and (1.15) are valid for the displacement due to defects and for the interaction energy; the force exerted on the k th defect by the external field and by the external defects can be determined from formula (1.16), where x_0^α must be replaced by the coordinates x_k^α of the center of mass of the k th defect.

The components of the matrix P^{ij} depend on the distances $r_{ij} = |x_i - x_j|$ between defects. Let us consider the case where the distances between defects are large compared with the sizes of the defects and find the principal term of the expansion of the matrix P^{ij} in distances. In the zero-th approximation the defects do not interact and $P^{ij} = P^i \delta^{ij}$, where P^i is the operator of the i th defect. It can be shown that the problem reduces to paired interactions in the first approximation. It is therefore sufficient to consider the case of two defects.

In this case P^{ij} is a second-order matrix and according to (3.3) we have

$$R_{ij} = \left\| \begin{matrix} (P^1)^{-1} & \nabla G^\circ \nabla \\ \nabla G^\circ \nabla & (P^2)^{-1} \end{matrix} \right\| \quad (i, j = 1, 2) \tag{3.5}$$

It can be verified directly that the operator components P^{ij} are given by the formulas (no summation!)

$$P^{ii} = (R_{ii} - R_{ij} R_{jj}^{-1} R_{ji})^{-1}, \quad P^{ij} = (R_{ji} - R_{jj} R_{ij}^{-1} R_{ii})^{-1} \quad (i \neq j) \tag{3.6}$$

Retaining the principal terms in $r_{12} = |x_1 - x_2|$ in these expressions, we obtain

$$P^{ij} = \begin{pmatrix} P^1 & -P^1 \nabla G^\circ \nabla P^2 \\ -P^2 \nabla G^\circ \nabla P^1 & P^2 \end{pmatrix} + O(r_{12}^{-6}) \tag{3.7}$$

i. e. the principal term in r_{12} of the matrix P^{ij} can be expressed explicitly in terms of the operators P^i of the individual defects.

If, as in the case of a single defect, we are interested only in the asymptotics of the perturbed field and in the defect interaction energy, we can approximate the kernel $P(y, y')$ by the first terms of its expansion in multipoles in the neighborhood of each defect,

$$P(y, y') = \sum_{mn} (-1)^{m+n} \sum_{ij} P_{mn}^{ij}(r_{ij}) \delta_{(m)}(y - x_i) \delta_{(n)}(y' - x_j), \quad x_i \in V_i, \quad x_j \in V_j' \quad (3.8)$$

It is important to note that the principal terms in r_{ij} of the first coefficients of the expansion are obtainable in explicit form provided the first coefficients P_{mn} for each defect in the absence of other defects are known.

In the case of a homogeneous external field the energy of interaction between the defects and the external field is given by the formula

$$\Phi = 1/2 \varepsilon^\circ P_{00}(r_{12}) \varepsilon^\circ, \quad P_{00}(r_{12}) = \sum_{ij} P_{00}^{ij}(r_{12}) \quad (3.9)$$

which is exact for any r_{12} .

It follows from this that the asymptotic expression of the matrix $P_{00}^{ij}(r_{12})$ is the sole contributor to the principal term of the asymptotic expression of Φ in r_{12} in a homogeneous field. In the case of an arbitrary external field it is also necessary to take into account the contributions made to the asymptotic expression of Φ by the asymptotics of the diagonal components of the matrices $P_{01}^{ij}(r_{12})$ and $P_{10}^{ij}(r_{12})$. This contribution is equal to zero if the defects have central symmetry or if the external field varies slowly at distances on the order of defect sizes.

4. To illustrate our method let us find the principal term of the asymptotic expression of the interaction energy Φ of two ellipsoidal inhomogeneities in an unbounded elastic medium.

The principal term P_{00}^i of the expansion of the kernel of the operator P^i for each ellipsoid considered as an isolated defect is known,

$$P_{00}^i = -v_i (A_i + c_i^{-1})^{-1} \quad (4.1)$$

The tensors A_i have structure (2.4) in the coordinate systems attached to the ellipsoids. Recalling (3.7), we can obtain the components of the matrix

$$P_{00}^{ij}(r_{12}) = \left\| \begin{array}{cc} P_{00}^1 & P_{00}^1 \nabla \nabla G^\circ(x_1 - x_2) P_{00}^2 \\ P_{00}^2 \nabla \nabla G^\circ(x_2 - x_1) P_{00}^1 & P_{00}^2 \end{array} \right\| \quad (4.2)$$

in the approximation under consideration.

As already noted the matrices P_{01}^{ij} and P_{10}^{ij} need not be considered by virtue of the central symmetry of the ellipsoids.

Substituting $P_{00}^{ij}(r_{12})$ into (3.9), we obtain

$$\Phi = \Phi_0^1 + \Phi_0^2 + \Phi_1 r_{12}^{-3} + O(r_{12}^{-4}) \quad (4.3)$$

$$\Phi_0^i = 1/2 \varepsilon^\circ P_{00}^i \varepsilon^\circ, \quad \Phi_1 r_{12}^{-3} = \varepsilon^\circ P_{00}^1 \nabla \nabla G^\circ(x_1 - x_2) P_{00}^2 \varepsilon^\circ \quad (4.4)$$

Here Φ_0^i is the intrinsic energy of the i th defect and Φ_1 is a quadratic function of the external field which also depends on the elastic constants of the medium and on the defect parameters.

Let us write out the explicit expressions for Φ_0^i and Φ_1 for the case where the external field is purely dilatational,

$$\varepsilon_{\alpha\beta}^* = \varepsilon_0 \delta_{\alpha\beta} \quad (4.5)$$

and where the inclusions take the form of two spheroids with the common axis of rotation x^2 and isotropic elastic constants,

$$\Phi_0^i = - \frac{\nu_i \varepsilon_0^2}{2\kappa_0 \Delta_1} (3p_1^i + p_2^i) \quad (4.6)$$

$$\Phi_1 = \frac{4\nu_1 \nu_2 \varepsilon_0^2}{\kappa_0 \Delta_1 \Delta_2} [(1 - 2\nu_0)(p_1^1 p_2^2 + p_2^1 p_1^2) + 2(1 - \nu_0)p_2^1 p_2^2] \quad (4.7)$$

$$p_1^i = (5 - 4\nu_0)I_2^i - 3I_{12}^i + 8\pi(1 - \nu_0)\mu_0/\mu_i, \quad p_2^i = 2(1 - 2\nu_0)(I_1^i - I_2^i) \quad (4.8)$$

$$\Delta_i = \left[4(1 - \nu_0)I_2^i - 2I_{12}^i - 8\pi(1 - \nu_0)\frac{\mu_0}{\mu_i} \frac{1}{1 + \nu_i} \right] \left[(3 - 4\nu_0)I_1^i - I_{21}^i - \right. \\ \left. - 8\pi(1 - \nu_0)\frac{\mu_0}{\mu_i} \frac{1 - \nu_i}{1 + \nu_i} \right] - 2 \left[-I_2^i + I_{12}^i + 8\pi(1 - \nu_0)\frac{\mu_0}{\mu_i} \frac{\nu_i}{1 + \nu_i} \right]^2$$

Here the index i is the number of the defect and the subscript in the quantities p_q^i denotes the principal axes of the ellipsoids (assuming only the values 1, 2 by virtue of rotational symmetry).

The limiting case of a rigid inclusion results if we let $\mu_i \rightarrow \infty$ in (4.8); the case of a cavity results if we set $\mu_i = -\mu_0$, $\nu_i = \nu_0$.

If one of the ellipsoids (e. g. the second one) is a sphere, then $p_2^2 = 0$ and the expression for Φ_1 becomes much simpler,

$$\Phi_1 = \frac{3\nu_1 \nu_2 \varepsilon_0^2}{\pi \kappa_0} \left[1 + 3 \frac{\mu_0}{\mu_2} \frac{1 - \nu_0}{1 - 2\nu_0} \frac{1 - 2\nu_2}{1 + \nu_2} \right]^{-1} \frac{I_1^1 - I_2^1}{\Delta_1} (1 - 2\nu_0) \quad (4.9)$$

If both ellipsoids are spheres, then $p_2^1 = p_2^2 = 0$ and $\Phi_1 = 0$. This agrees with the familiar result of [3] whereby the interaction energy for isotropic spherical inclusions is $\sim r^{-6}$.

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