

STRESS-STRAIN DEPENDENCE IN THE NONLINEAR THEORY OF ELASTICITY

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It is proved in a simple way that all components of the stress tensor are to be received straightforward by differentiating the free energy function with respect to the components of the tensor of natural strain. Some consequences of this fact are discussed. As an example a derivation of approximate equations of elastic equilibrium is given for a case of near hydrostatically strained body.

Stress-strain correlation under a finite deformation was discussed by many authors^{1,7-9}. It was established that the result of differentiation of the free energy function with respect to the distortion tensor¹ or to the strain tensor⁷⁻⁹ is some tensor, which is connected, more or less simply, with the stress tensor.

In this work it is shown that the stress tensor is to be received by differentiation the free energy function with respect to the so called tensor of natural strain, the principal values of which were introduced by Hencky³ and were discussed by many authors⁷.

§1. Let x_i and ξ_i be the Cartesian coordinates of a point of a solid under a deformation and in nondeformed state correspondingly. They differ by the displacement vector u_i ;

$$x_i = \varphi_i(\{\xi_\alpha\}) = \xi_i + u_i. \quad \dots(1)$$

The work done by external forces of density f_i and of surface density $P_i = \sigma_{ij} n_j$ through the virtual displacement δx_i is

$$\delta R = \int dV f_i \delta x_i + \phi \delta S_j \sigma_{ij} \delta x_i. \quad \dots(2)$$

Integration here is performed over the real volume of strained body and over its surface (in the second term), σ_{ij} is the stress tensor, $dS_j = dS n_j$ the vector of infinitesimal area of the surface; all the terms are functions of x_i .

After transforming the second term at volume integral⁵ and taking into account the equilibrium equations

$$\frac{\partial \sigma_{ij}}{\partial x_j} + f_i = 0 \quad \dots(3)$$

we have

$$\delta R = \int dV \sigma_{ij} \frac{\partial \delta x_i}{\partial x_j} \quad \dots(2a)$$

Here

$$\delta x_i = \bar{x}_i - x_i$$

and

$$\bar{x}_i = \bar{\varphi}(\{\xi_\alpha\}) \quad \dots(1a)$$

are the coordinates of a point $\{x_i\}$ of a body after the virtual deformation. Set

$$\lambda_{i\alpha} = \frac{\partial x_i}{\partial \xi_\alpha}, \mu_{\alpha i} = \frac{\partial \xi_\alpha}{\partial x_i} (\mu = \lambda^{-1}) \quad \dots(4)$$

then

$$\frac{\partial \delta x_i}{\partial x_j} = \frac{\partial \bar{x}_i}{\partial \xi_\alpha} \frac{\partial \xi_\alpha}{\partial x_j} - \delta_{ij} = (\bar{\lambda}_{i\alpha} - \lambda_{i\alpha}) \mu_{\alpha j} = \delta \lambda_{i\alpha} \mu_{\alpha j}$$

and

$$\delta R = \int dV S_p (\sigma \delta \lambda \mu) \quad \dots(2b)$$

where $S_p a$ is a trace of matrix a .

If $\delta \lambda$ is expressed through distortion tensor $\partial u_i / \partial x_j$ (2b) leads or to Finger's result¹.

Let γ be the tensor

$$\gamma = \mu^T \mu \quad \dots(5)$$

(the symbol T indicates forming of the transposed matrix). γ_{ij} are the coefficients of quadratic form

$$dl_0^2 = d\xi_\alpha d\xi_\alpha = \mu_{\alpha i} \mu_{\alpha j} dx_i dx_j = \gamma_{ij} dx_i dx_j \quad \dots(5a)$$

Now we introduce tensor of natural strain

$$z = -\frac{1}{2} \ln \gamma = -\frac{1}{2} \ln \mu^T \mu \quad \dots(6)$$

As γ is the only symmetric tensor which defines the strained state of a body, we can assume, that σ and γ have the same principal axes and so are permuttable matrices. Under this assumption

$$S_p(\sigma \delta \gamma^n) = \sum_{k=1}^n S_p[\sigma \gamma^{n-k} (\delta \gamma) \gamma^{k-1}] = n S_p[\sigma (\delta \gamma) \gamma^{n-1}]$$

hence

$$S_p[\sigma \delta F(\gamma)] = S_p[\sigma \delta \gamma f(\gamma)]$$

where $f(x) = F'(x)$ and $f(\gamma)$, $F(\gamma)$ are functions of matrix γ [ref. 2], therefore

$$\begin{aligned} S_p(\sigma \delta s) &= -\frac{1}{2} S_p[\delta (\delta \gamma) \gamma^{-1}] = -\frac{1}{2} S_p[\sigma (\delta \mu^T) \mu \gamma^{-1}] \\ &\quad -\frac{1}{2} S_p[\sigma \mu^T (\delta \mu) \gamma^{-1}]. \end{aligned}$$

By using again commutability of σ and γ^{-1} , symmetry of σ and the next identity (following from (4))

$$\delta \mu = \delta \gamma^{-1} = -\mu (\delta \lambda) \mu$$

we have

$$S_p(\sigma \delta s) = S_p[\sigma (\delta \lambda) \mu]. \quad \dots(7)$$

From (2b) it is clear⁶ that the thermodynamical identity for free energy f per unit mass, defined as

$$F = \int \rho dV f$$

(F is the full free energy of a body) may be written in a form :

$$df = -\eta dT + \frac{1}{\rho} S_p(\sigma ds). \quad \dots(8)$$

(η is the entropy per unit mass, T the temperature, ρ the mass density) and therefore

$$\sigma_{ij} = \rho \left(\frac{\partial f}{\partial s_{ij}} \right)_T \quad \dots(8a)$$

or briefly (σ and s are the matrices)

$$\sigma = \rho \left(\frac{\partial f}{\partial s} \right)_T. \quad \dots(8b)$$

From (1) and (4) it follows that

$$\mu_{\alpha i} = \delta_{\alpha i} - \partial U_{\alpha} / \partial x_i = \delta_{\alpha i} - \beta_{i\alpha}$$

where β is a distortion tensor⁴, hence (E is a matrix unit)

$$\gamma = E - 2u \tag{9}$$

where

$$u = \frac{1}{2} (\beta + \beta^T - \beta \beta^T) \tag{9a}$$

is a strain tensor in Eulerian variables⁷ which are used here.

Hence the connection of u with s is as follows :

$$u = 1/2 [E - \exp (- 2s)]$$

and it is clear that $u \approx s$ as $u \rightarrow 0$.

Under the transformations of coordinates for which the form (5a) is invariable, the next quantity is invariant¹⁰:

$$\sqrt{\det \gamma} \, d x_1 \, d x_2 \, d x_3 = d \xi_1 \, d \xi_2 \, d \xi_3 = d V_0.$$

On the other hand, at a strained state x_i are the Cartesian coordinates and

$$d x_1 \, d x_2 \, d x_3 = d V$$

then from (6)

$$I_1^s = S_p s = - \frac{1}{2} \ln (\det \gamma) = \ln (d V / d V_0) = \ln (\rho_0 / \rho). \tag{10}$$

(ρ_0 and ρ are mass densities of the same point of a body at unstrained and strained states accordingly).

§ 2. If a solid is elastically isotropic, its free energy f is a function of a temperature and of a set of any three independent invariants of tensor s (or γ). Our choice of such a set will be I_1^s, k_2^s, k_3^s (a definition of invariants is in Appendix). Under such a choice

(A. 4a) gives*)

$$\sigma = -pE + 2\mu \Delta_s + \nu \Delta_{2s} = -pE + \tau$$

where functions p, μ, ν of the variables I_1^s, k_2^s, k_3^s are

$$p = -\rho \frac{\partial f}{\partial I_1^s}, \quad \mu = \rho \frac{\partial f}{\partial k_2^s}, \quad \nu = \rho \frac{\partial f}{\partial k_3^s}$$

$$p = p_0 \exp \left(-I_1^s \right). \quad \dots(11a)$$

As Δ_s and Δ_{2s} are traceless, $p = -\frac{1}{3} S_p \sigma$ is pressure at a given point of a body. It is also clear that in a limit of infinitesimal distortion μ is a shear modulus of linear theory.

From (11a) it follows that next identities hold:

$$\frac{\partial p}{\partial k_2^s} = -2\rho \frac{\partial}{\partial I_1^s} \frac{\mu}{\rho} = -2 \frac{\partial \mu}{\partial I_1^s} - 2\mu. \quad \dots(11b)$$

$$\frac{\partial p}{\partial k_3^s} = -\frac{\partial \nu}{\partial I_1^s} - \nu, \quad 2 \frac{\partial \mu}{\partial k_3^s} = \frac{\partial \nu}{\partial k_1^s}.$$

If stress is a hydrostatic one, without shear parts of stress and distortion, let us represent the isothermal bulk modulus K

$$K = \rho \frac{\partial p}{\partial \rho} = \frac{\partial p}{\partial \ln \rho} = -\frac{\partial p}{\partial I_1^s} \quad \dots(12)$$

as a series expansion in powers¹⁰ of I_1^s

$$K \left(I_1^s \right) = \sum_{n=0}^{\infty} \frac{\alpha_n}{n!} \left(I_1^s \right)^n \quad \dots(13)$$

*As

$$\frac{\partial k_p^\lambda}{\partial s} = -2 \exp(-2ps) = -2\gamma^p = -2\gamma \frac{\partial K^\lambda}{\partial \gamma}$$

when differentiating any isotropic function f one can set

$$-\frac{\partial}{\partial s} = -2\gamma \frac{\partial}{\partial \gamma} = \frac{\partial}{\partial u} - 2u \frac{\partial}{\partial u}.$$

Therefore (8b) gives rise to Murnaghan's equation in Birch's form⁸.

the equation of state is

$$-p \left(I_1^s \right) = \int_0^{I_1^s} dx K(x) = \sum_{n=0}^{\infty} \frac{\alpha_n}{(n+1)!} \left(I_1^s \right)^{n+1} \quad \dots(13a)$$

and from (11a), (10) we obtain an expression for elastic part of f

$$\begin{aligned} f - f_0 &= - \int_0^{I_1^s} p_p d I_1^s = \frac{1}{\rho_0} \sum_{n=0}^{\infty} \frac{\alpha_n}{(n+1)!} \int_0^{I_1^s} dx e^x x^{n+1} \\ &= \frac{1}{\rho_0} \sum_{n=1}^{\infty} \frac{(-1)^n \alpha_n}{(n+1)!} \gamma(n+2, -I_1^s) \\ &= \frac{1}{\rho_0} \sum_{m=0}^{\infty} \frac{\left(I_1^s \right)^{m+2}}{m+2} \sum_{n=0}^{\infty} \frac{\alpha_n}{(n+1)! (m-n)!} \end{aligned} \quad \dots(13b)$$

where $\gamma(\alpha, x)$ is a noncomplete gamma-function

$$\gamma(\alpha, x) = \int_0^x dt t^{\alpha-1} e^{-t}$$

(at compressed state $I_1^s < 0$).

If a bulk modulus is regarded as function of pressure

$$\frac{1}{K(p)} = \sum_{n=0}^{\infty} \frac{\beta_n}{n!} p^n \quad \dots(14)$$

from

$$\frac{1}{K(p)} = - \frac{\partial I_1^s}{\partial p} \quad \dots(14a)$$

equation of state has a form

$$-I_1^s - \int_0^p \frac{dp}{K(p)} = \sum_{n=0}^{\infty} \frac{\beta_n}{(n+1)!} p^{n+1} \quad \dots(14b)$$

and from (13a) we have

$$\beta_0 = 1/\alpha_0, \beta_1 = \alpha_1/\alpha_0^3 \quad \dots(15)$$

$$\beta_2 = \frac{1}{\alpha_0^3} \left[3 \left(\frac{\alpha_1}{\alpha_0} \right)^2 - \frac{\alpha_2}{\alpha_0} \right]$$

$$\beta_3 = \frac{1}{\alpha_0^4} \left[\frac{\alpha_3}{\alpha_0} + 15 \left(\frac{\alpha_1}{\alpha_0} \right)^3 - 10 \frac{\alpha_1 \alpha_2}{\alpha_0^2} \right]$$

etc. and vice versa $\{\alpha_n\}$ may be expressed through $\{\beta_n\}$ by these identities serially.

§3. For solving problems of stress and strain distribution the equation of state in which σ is expressed through tensor γ instead of s may be found more useful than (11).

After substituting at (11) the functions

$$\Delta_s = -\frac{1}{2} \ln \left[\gamma / \left(I_3^Y \right)^{1/3} \right], \Delta_s^2 = \frac{1}{4} \ln^2 \left[\gamma / \left(I_3^Y \right)^{1/3} \right] \quad \dots(16)$$

which are expressed through γ by (A. 6a), (A. 9) – (A. 12a), we have

$$\sigma = -pE - \mu\gamma \Delta\gamma + (\nu\gamma/4) \Delta_2\gamma = -pE + 2\mu\gamma \Delta_u + \gamma \Delta_{2u} \quad \dots(17)$$

where

$$\mu\gamma = \left(\mu + (\nu/6) \ln I_3^Y \right) \sum_{k=1}^3 \psi_k^Y \ln \gamma_k - (\nu/4) \sum_{k=1}^3 \psi_k^Y \ln^2 \gamma_k \dots(17a)$$

$$\nu\gamma = \nu \sum_{k=1}^3 \omega_k^Y \ln^2 \gamma_k - 4 \left(\mu + (\nu/6) \ln I_3^Y \right) \sum_{k=1}^3 \omega_k^Y \ln \gamma_k$$

and the dependence of p, μ, ν on invariants of tensor may be found from (16), (A.9) – (A. 13b), (10) and (A.3);

$$k_2^s = \frac{1}{8} \sum_{k=1}^3 \ln^2 \left[\gamma_k / \left(I_3^Y \right)^{1/3} \right]$$

$$k_3^s = - \frac{1}{24} \sum_{k=1}^3 \ln^3 \left[\gamma_{kl} \left(I_3^Y \right)^{1/3} \right] \quad \dots(18a)$$

$$I_1^s = - \frac{1}{2} \ln I_3^Y.$$

Substitution of (17) at (3) gives us three equations of elastic equilibrium which determine three unknown functions

$$\xi_\alpha ((\bar{x}_i)) \text{ [see (4), (5)].}$$

Differentiation of invariants of tensor s is to be accomplished by means of (A.3), (A.4) and an identity

$$\frac{\partial I}{\partial x_i} = Sp \left(\frac{\partial I}{\partial \gamma} \frac{\partial \gamma}{\partial x_i} \right) = \frac{\partial I}{\partial \gamma_{km}} \frac{\partial \gamma_{km}}{\partial \bar{x}_i} \quad \dots(19)$$

If we want to determine tensor γ from (3), it is necessary to take into account also the so-called compatibility relations, which are, as it is clear from (5a), necessary and sufficient conditions for three dimensional space to be Euclidean^{9,10}.

$$R_{ij} = 0 \quad \dots(20)$$

where R_{ij} is a Ricci tensor of a space with metric tensor γ_{ij} :

$$R_{ij} = \frac{\partial \Gamma_{ij}^m}{\partial x_m} - \frac{\partial \Gamma_{im}^m}{\partial x_j} + \Gamma_{ij}^m \Gamma_{mn}^n - \Gamma_{in}^m \Gamma_{jm}^n \quad \dots(20a)$$

and Γ_{ij}^k are the Christoffel's symbols

$$\Gamma_{ij}^k = \frac{1}{2} (\gamma^{-1})_{km} \left(\frac{\partial \gamma_{mi}}{\partial x_j} + \frac{\partial \gamma_{mj}}{\partial x_i} - \frac{\partial \gamma_{ij}}{\partial x_m} \right)$$

$$\Gamma_{im}^m = \partial \ln \sqrt{I_3^Y} / \partial x_i = - \partial I_1^s / \partial x_i.$$

After substituting at (20a) γ which is expressed through s :

$$\gamma = \frac{E}{3} \sum_{k=1}^3 \exp(-2s_k) + \Delta_s \sum_{k=1}^3 \psi_k^s \exp(-2s_k) \quad \dots(21)$$

(equation continued on p. 572)

$$+ \Delta_{2s} \sum_{k=1}^3 \omega_k^s \exp(-2s_k)$$

it becomes possible to determine tensor s from (3), (11) and (20).

§ 4. As an example of application of obtained here formulas let us write down an equation of state (see below (24)) and equations of equilibrium (see (30)) of nearly hydrostatically compressed sample in a high pressure cell: This means that dilatation is of arbitrary magnitude but shear distortion is small. The equations will be written down up to the second power of shear distortion.

An approximate equation of state may be found from exact formulas (17), (17a), (18) by using (A. 13) — (A. 13b) but it is instructive to expand (11) straight forward in powers of small shear part of s . Set

$$\gamma = \alpha \epsilon \quad \dots(22)$$

where $\alpha > 1$ is an arbitrary quantity.

From (3) (see also (11))

$$-\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} = 0$$

it is clear that change of pressure along a sample is not more than yield stress (under pressure there is no crack destruction as all the σ_{ij} components are negative). so if we set

$$\epsilon = E - 2\nu \quad \dots(22a)$$

then ν may be considered as a small quantity ($Sp \nu \ll 1$).

As from (6) it follows that

$$s = - (E/2) \ln \alpha + \nu + \nu^2 + O(\nu^3)$$

next expressions hold with a needed accuracy (up to a second order of ν in (24));

$$I_1^s \approx - (3/2) \ln \alpha + I_1^\nu + J_2^\nu$$

$$\Delta_s \approx \nu - \left(I_1^\nu / 3 \right) E + \nu^2 - \left(J_2^\nu / 3 \right) E$$

$$\begin{aligned} \Delta_{23} &\cong v^2 - \left(J_2^v / 3 \right) E - \left(2I_1^v / 3 \right) v + \left(2 \left(I_1^v \right)^2 / 9 \right) E \\ k_2^s &\cong k_2^{v'} , v \left(I_1^s , k_2^s , k_3^s \right) \cong v \quad \dots(23a) \\ \mu \left(I_1^s , k_2^s , k_3^s \right) &\mu + \mu' I_1^v \\ p \left(I_1^s , k_2^s , k_3^s \right) &\cong p - K I_1^v - (K + \mu + \mu') J_2^v \\ &+ ((\mu + \mu')/3 - K'/2) \left(I_1^v \right)^2. \end{aligned}$$

Thermodynamic quantities (moduli and their derivatives) with omitted arguments are taken to the point $\left(I_1^s , k_2^s , k_3^s \right) = \left(-(3/2) \ln \alpha , \theta , 0 \right)$ and by ψ' is marked any quantity

$$\psi' = \partial \psi \left(I_1^s , 0 , 0 \right) / \partial I_1^s \Big|_{I_1^s} = - (3/2) \ln \alpha = - K \partial \psi / \partial p \quad \dots(23b)$$

where p and $I_1^s = - (3/2) \ln \alpha$ are connected by the equation of state (13a) or (14b). The derivative $\partial p / \partial k_2^s$ is expressed through μ and μ' by (11b).

By substituting (23a) at (11) we have :

$$\begin{aligned} \sigma &\cong - pE + K I_1^v E + 2\mu \left(v - \left(I_1^v / 3 \right) E \right) + K + \mu' \\ &+ (\mu - v)/3 J_2^v E + (K'/2 - \mu' + (2v - \mu)/3) \left(I_1^v \right)^2 E \\ &+ 2 (\mu' - v/3) I_1^v v + (2\mu + v) v^2. \quad \dots(24) \end{aligned}$$

Excluding the finite rigid-body rotations we can relate to any v the corresponding small tensor of distortion θ and the displacement vector η :

$$\begin{aligned} v &= \frac{1}{2} (\theta + \theta^T - \theta \theta^T) \\ \theta_{ij} &= \partial \eta_j / \partial \bar{x}_i. \quad \dots(25) \end{aligned}$$

In linear approximation

$$\begin{aligned}\sigma &= -d E + \sigma^{(1)}(\eta) \\ \sigma^{(1)}(\eta) &= \left(K - \frac{2\mu}{3}\right) (\nabla \eta) E + \mu (\theta + \theta^T) \quad \dots (26)\end{aligned}$$

and an equation of equilibrium is

$$L(\eta) = \left(K + \frac{\mu}{3}\right) \nabla (\nabla \eta) + \mu \Delta \eta = 0 \quad \dots (27)$$

set

$$\eta = \eta_1 + \eta_2 \quad (|\eta_2| \ll |\eta_1|) \quad \dots (28)$$

with η_1 satisfying (27) and boundary condition

$$P_i = \sigma_{ij}^{(i)}(\eta_i) n_j \quad (\forall \{x_i\}) (\{x_i\} \in S_0). \quad \dots (27a)$$

Here S_0 is a surface of the initially unstrained sample that is compressed α times. Now from (24) it is easy to see that

$$\sigma \approx -p E + \sigma^{(1)}(\eta_1) + \sigma^{(1)}(\eta_2) + \sigma^{(2)}(\eta_1) \quad \dots (29)$$

where

$$\begin{aligned}\sigma^{(2)}(\eta) &= \frac{1}{2} \left(\mu + \mu' - \frac{\nu}{3}\right) S p (\theta \theta^T) E \\ &+ \frac{1}{2} \left(K + \mu' + \frac{\mu - \nu}{3}\right) J_2^{\theta} E + \left(\frac{K}{2} - \mu'\right) \\ &+ \frac{2\nu - \mu}{3} (\nabla \eta)^2 E + \left(\mu' - \frac{\nu}{3}\right) (\nabla \eta) (\theta + \theta^T) \\ &+ \frac{\mu}{2} (\theta^2 + \theta^{T^2} + \theta^T \theta - \theta \theta^T) + \frac{\nu}{4} (\theta^2 + \theta^{T^2} \\ &+ \theta^T \theta + \theta \theta^T) \\ J_2^{\theta} &= S p \theta^2 = \frac{\partial \eta_i}{\partial x_j} \frac{\partial \eta_j}{\partial x_i}, \quad S p (\theta \theta^T) = \frac{\partial \eta_i}{\partial x_j} \frac{\partial \eta_i}{\partial x_j}\end{aligned}$$

and an equation of equilibrium in a second order approximation is

$$L(\eta_2) + \lambda(\eta_1) = 0 \quad \dots (30)$$

with

$$[\lambda(\eta)]_I = \partial \sigma_{ij}^{(2)}(\eta) / \partial x_j \quad \dots(30a)$$

A boundary condition (on a surface S_1 which is received from S_0 by displacement of all its points by vector η_i on S_0) is to be set in a different way for each problem: a force P_i is taken to a real surface of a body and when its variation under the displacement of surface is no less than of order $P_i |\eta_2| / |\eta_1| \sim P_i |\eta_i| / l$ (l is a size of a sample) it must be taken into consideration.

Coordinates ξ_i of a point x_i before deformation are

$$\xi_i = \sqrt{\alpha} (x_i - \eta_i) \quad \dots(31)$$

and the displacement vector u_i

$$u_i = -(\sqrt{\alpha} - 1) x_i + \sqrt{\alpha} \eta_i = -(1 - 1/\sqrt{\alpha}) \xi_i + \eta_i \quad \dots(31a)$$

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APPENDIX

1. We want to consider the following invariants of a 3×3 matrix a :

$$J_p^a = S p a^p, \quad K_p^a = \frac{1}{p} J_p^a, \quad p = 1, 2, 3 \quad \dots(A.1)$$

coefficients I_p^a of its characteristic polynomial $D^a(\lambda) = \det |\lambda E - a| = \lambda^3 - I_1^a \lambda^2 + I_2^a \lambda - I_3^a$ and "Small" invariants

$$J_p^a = J_p^\Delta, k_p^a = K_p^1, i_p^a = I_p^\Delta \tag{A.1a}$$

where Δ is a deviator of a

$$\Delta = \Delta_a = a - \left(I_1^a / 3 \right) E \tag{A.2}$$

All the formulas through the appendix are related to a certain matrix a , that is way the superscript a is further omitted.

Only three of these invariants are independent. The identities used in this work are :

$$\begin{aligned} I_1 &= J_1, i_2 = -\frac{1}{2} j_2 = -k_2, i_3 = \frac{1}{3} j_3 = k_3 \\ j_2 &= J_2 - \frac{1}{3} J_1^2, j_3 = J_3 - J_1 J_2 + \frac{2}{9} J_1^3 \\ I_3 &= \left(\frac{I_1}{3} \right)^3 + \frac{I_1}{3} i_2 + i_3. \end{aligned} \tag{A.3}$$

As from (A. 1) it follows that

$$\partial J_p / \partial a^T = p a^{p-1}, \partial K_p / \partial a^T = a^{p-1} \tag{A.4}$$

(A. 3) leads to

$$\partial k_2 / \partial a^T = \Delta, \partial k_3 / \partial a^T = \Delta^2 - (j_2/3) E \equiv \Delta_2. \tag{A.4a}$$

The Hamilton-Cayley theorem states that

$$D^\Delta(\Delta) = \Delta^3 + i_2 \Delta - i_3 E = 0. \tag{A.5}$$

2. It is well known² that the matrix valued function of matrix may be presented in a form

$$f(a) = \sum_k \sum_{m=0}^{p_k-1} f^{(m)}(a_k) Z_{km} \tag{A.6}$$

where p_k is a multiplicity of an eigenvalue a_k , $f^{(m)}$ is the m th derivative of f , and the component matrices Z_{km} depend only on matrix a but not on function f .

Introducing a matrix $W(a)$ with elements

$$W_{kl} = a_i^{k-l} = \partial K_k / \partial a_l \tag{A.7}$$

we can easily see from the representation of $f(a)$ by Lagrange-Sylvester's interpolating polynomial² that if all roots a_k are nondegenerate then

$$Z_k = \sum_{l=1}^3 W_{kl}^{-1}(a) a^{l-1}. \tag{A.8}$$

As from (A.7)

$$W_{kl}^{-1} = \partial a_k / \partial K_l. \tag{A.7a}$$

(A.8) and (A.4) imply

$$Z_k = \partial a_k / \partial a^T.$$

An expression (A. 6) with Z_k from (A.8)

$$f(a) = \sum_k f(a_k) Z_k \tag{A.6a}$$

holds also for degenerate eigenvalues after the corresponding limiting transition (that leads to (A.6)) though (A.8) loses meaning as $\det W$ becomes a zero

3. The eigenvalues of matrix a are

$$a_k = \frac{I_1}{3} + \Delta_k \tag{A.9}$$

where Δ_k are the eigenvalues of deviator Δ of a and satisfy an equation

$$\Delta_k^3 + i_2 \Delta_k - i_3 = 0. \tag{A.5a}$$

For symmetric matrix Δ all the roots of this equation are real.

This is possible if⁴

$$d = -4 i_2^3 - 27 i_3^2 \geq 0.$$

Taking into account an obvious relation $k_2 = -i_2 > 0$ we have

$$|\kappa| \leq 2/3 \sqrt{2} \approx 0.385 \tag{A10}$$

with

$$\kappa = i_3 / |i_2|^{3/2} = k_3/k_2^{3/2}. \tag{A.10a}$$

The roots of (A.5a) are Kurosch⁴

$$\Delta_k = 2 \sqrt{k_2/3} \cos \chi_k \tag{A.11}$$

where

$$\chi_k = (\varphi + 2\pi k)/3, \varphi = \arccos(\kappa \sqrt{3/2}). \tag{A.11a}$$

Now from (A.8a), (A.9), (A.11), (A.10a) and (A.4), (A.4a) it follows that

$$Z_k = E/3 + \psi_k \Delta + \omega_k \Delta_2 \tag{A.12}$$

where

$$\psi_k = \frac{\sin(\varphi - \chi_k)}{\sqrt{3k_2} \sin \varphi}, \omega_k = \frac{\sin \chi_k}{k_2 \sin \varphi}. \tag{A12a}$$

4. In order to get an explicit expansion of analytical function of matrix in powers of its "small" invariants let's take the trace of Taylor series of $F(a) = F(I_1/3E + \Delta)$:

$$\begin{aligned} J = SpF(a) &= Sp F(I_1/3E + \Delta) = \sum_{n=0}^{\infty} \frac{F^{(n)}(I_1/3)}{n!} Sp \Delta^n \\ &= 3F(I_1/3) + \sum_{2m+3n>0} \frac{(m+n-1)! k_2^m k_3^n}{(2m+3n-1)! m! n!} F^{(2m+3n)}(I_1/3). \end{aligned}$$

We used here a well known in the theory of symmetric polynomials expression for $\sum_k \Delta_k^n$ (Waring's formula) which is in our notation :

$$\frac{I}{n} \sum_{k=1}^3 \Delta_k^n = \sum_{2\lambda+3\mu=n} \frac{(1)^{n-\mu} (\lambda + \mu - 1)!}{\lambda! \mu!} k_2^\lambda k_3^\mu.$$

If $f(x) \doteq F'(x)$

$$f(a) = \partial J / \partial a^T = (\partial J / \partial I_1) E + (\partial J / \partial k_2) \Delta + (\partial J / \partial k_3) \Delta_2. \quad \dots(A.12b)$$

Therefore from (A.12), (A.6a), (A.13) we have

$$\left| \sum_k \psi_k f(a_k) = \partial J / \partial k_1 = \sum_{n^*m=0}^{\infty} \frac{(m+n)! f^{(2m+3n+1)}(I_1/3)}{(2m+3n+1)! m! n^*} k_2^m k_3^n \right. \\ \left. \dots(A.13a) \right.$$

$$\sum_k \omega_k f(a_k) = \partial J / \partial k_3 = \sum_{n^*m=0}^{\infty} \frac{(m+n)! f^{(2m+3n+2)}(I_1/3)}{(2m+3n+2)! m! n!} k_2^m k_3^n. \\ \dots(A.13b)$$

As for $\Sigma f(a_k) = Spf(a) = \partial J / \partial I_1$, it may be received from (A.13) with F substituted by f .