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A NOTE TO THE SIMPLIFICATION IN DESCRIPTION OF SOME MOLECULAR-BASED POLYMER MODELS

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Summary: *One type of integral is frequently met in various description of behaviour of polymer materials through molecular-based models starting with the classical Doi-Edwards one. The integrand in this integral for which an integrated region represents a solid angle is formed by a product of a unit vector (pointed at an element of this region) with a deformation gradient tensor. This product is raised to an exponent that is not usually an integer. The aim of this contribution is to derive substantially simplified expression for this integral respecting high accuracy of an approximation.*

1. Introduction

In derivation of some basic rheological models the following integral has regularly appeared

$$H(s) = \oiint_{\Omega'} \left| \underline{u}' \cdot \underline{\underline{F}}^{-1} \right|^{2s} \mathrm{d}^2\Omega' , \tag{1}$$

where $\underline{u}'$ is a unit vector pointing at element $\mathrm{d}^2\Omega'$, $\underline{\underline{F}}^{-1}$ is a deformation gradient tensor that preserves volume, integration is taken over a solid angle Ω'. An exponent s attains usually non-integer values.

As the examples of appearance of this integral it is possible to mention

- for s=1/2 this integral is involved in the expression for a damping function in the classical monograph by Doi & Edwards (1978) where it corresponds to an average increase of the length of a molecule under affine deformation;
- in Mhetar & Archer (1999) the Partial Strand Extension model is considered, and based on molecular considerations we again run across the integral (1) with s=1/4;
- in a model with partial retraction in Larson (1988) this integral with non-integer s appears as well.

2. Analysis

The integral (1) is related with central moments of a distorted normal distribution

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$$\Psi_d(\underline{R}') = \left(\frac{\beta}{\pi}\right)^3 \mathrm{e}^{-\beta^2 \left|\underline{R}'\cdot\underline{\underline{F}}^{-1}\right|^2}, \tag{2}$$

through a term 'distorted Gaussian function' introduced in Boue et al. (1985)

$$\left\langle R'^{s-2}\right\rangle \equiv \iiint R'^{s-2}\Psi_d(\underline{R}')\,\mathrm{d}^3\underline{R}' = \frac{\beta^{2-s}}{2\pi^{3/2}}\Gamma\left(\frac{s+1}{2}\right)H\left(-\frac{s+1}{2}\right), \tag{3}$$

where Γ represents the gamma function. The last equation is obtained by integrating over $R'\in(0,\infty)$.

As far as the authors are aware the analytical form of the integral $H(s)$ is known only for s=1 for which it can be found as convolution of an expression for stress for rubber elasticity, Eq. (8.B.1) in Lin (2003).

The function $H(s)$ is a scalar function of the Finger tensor

$$\underline{\underline{C}}^{-1} = \left(\underline{\underline{F}}^{-1}\right)^{\mathrm{T}}\cdot\underline{\underline{F}}^{-1}, \tag{4}$$

hence it can be expressed as a function of its invariants

$$I_1 = \mathrm{trace}\,\underline{\underline{C}}^{-1}, \quad I_2 = \frac{1}{2}\left[\left(\mathrm{trace}\,\underline{\underline{C}}^{-1}\right)^2 - \mathrm{trace}\,\underline{\underline{C}}^{-2}\right], \quad I_3 = \det\underline{\underline{C}}^{-1}, \tag{5}$$

and a scalar s. For the sake of generality we consider that the deformation does not have to preserve volume, thus both possibilities I_3=1 and $I_3\neq 1$ are taken into account.

Function $H(s)$ can be calculated in a straightforward way for all natural values (including zero), e.g. for s=0 and s=1 we obtain

$$H(0)=4\pi, \;\; H(1)=4\pi I_1/3 \;\; . \tag{6}$$

For this it is convenient to use a coordinate system in which the Finger tensor $\underline{\underline{C}}^{-1}$ is diagonal (with a^2, b^2, c^2 as the elements on the diagonal), though the results are valid for any $\underline{\underline{C}}^{-1}$. The unit vector can be written as u' = (cosα•cosβ, cosα•sinβ, sinα), then the differential equals $\mathrm{d}^2\Omega'$ = cosαdαdβ, and integration is carried out over $\alpha\in[-\pi/2,\pi/2]$, $\beta\in[0,2\pi]$.

Changing variable $\underline{R}' = \underline{R}\cdot\underline{\underline{F}}$ (where $\underline{\underline{F}}$ is the inverse deformation gradient tensor) in the first integral in rel.(3) it is possible to determine $H(s)$ for some negative s.

Let us consider a function that reflects asymptotical trend of $H(s)$

$$K(s) \equiv a^{2s} + b^{2s} + c^{2s}. \tag{7}$$

Asymptotically it behaves as a power function and for two given values $K(s)$ and $K(s+1)$ with an integer $|s| \gg 1$ there is possible to find $K(s+\xi)$ for $0 \le \xi \le 1$

$$K(s+\xi) = K(s+1)^{\xi} K(s)^{1-\xi}. \qquad (8)$$

As can be seen in Fig.1 the function $H(\xi)$ in the interval [0,1] is still close to linear (in semi-log scale). Hence, using rels. (6) and (8) in this interval we can determine an approximate relation for $H(\xi)$

$$H(\xi) \simeq 4\pi (I_1/3)^{\xi}. \qquad (9)$$

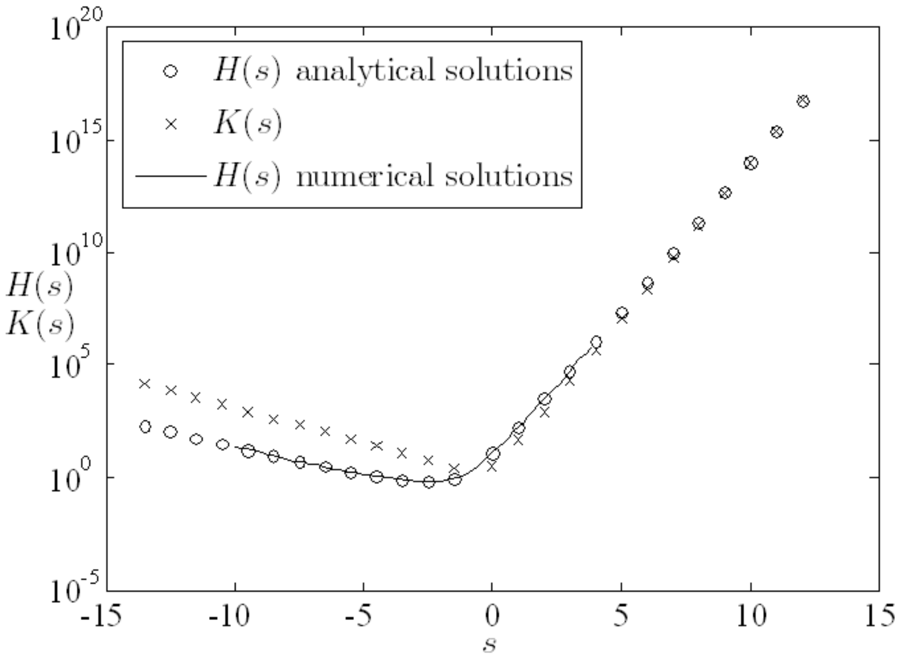

Figure 1 Behaviour of the functions $H(s)$ and $K(s)$.

3. Conclusions

The approximate relation to the integral $H(s)$ in rel.(1) was derived. This approximation depends only on the first invariant I_1 of the Finger tensor $\underline{\underline{C}}^{-1}$.

Numerical tests have shown that deviation of the approximate relation (8) from the exact one is 6% on the average. As the error has systematic tendency, it can be substantially reduced by an introduction of a correction coefficient.

4. Acknowledgment

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5. References

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