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EXACT EVALUATION OF THE INTEGRAL INVOLVED IN DOI-EDWARDS CONSTITUTIVE EQUATIONS

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Abstract. A basic two-dimensional integral, used for establishment of a connection between the stress and the strain tensor, is evaluated exactly and in closed form in terms of elliptic integrals of the first and the second kind. This integral has not been evaluated before. Our result will allow exact analysis of entangled polymeric systems. A generalization of the basic integral is presented in the last section.

Introduction. The Doi-Edwards model (Doi and Edwards, 1986), describing dynamics of entangled polymeric systems, was introduced many years ago. Since then, numerous approximating schemes were proposed for the analysis of such systems (Hassager and Hansen, [5]; Marin and Rasmussen, [6], etc.). To the best of my knowledge, nobody has managed so far to compute the basic integral exactly. This is done for the first time here. The problem was brought to my attention by A. Kharlamov.

Procedure of evaluation. We need to compute the following integral:

$$I = \frac{1}{4\pi}\int_0^{2\pi}\left[\int_{-\pi/2}^{\pi/2}\sqrt{(\lambda_1\cos[\alpha]\cos[\beta])^2+(\lambda_2\cos[\alpha]\sin[\beta])^2+(\lambda_3\sin[\alpha])^2}\cos[\alpha]\mathrm{d}\alpha\right]\mathrm{d}\beta. \quad (1)$$

The integral (1) gives the weighted average of a unit vector with components $(\cos[\alpha]\cos[\beta], \cos[\alpha]\sin[\beta], \sin[\alpha])$ over the whole sphere. The parameters $\lambda_1, \lambda_2, \lambda_3$, are the eigenvalues of the strain tensor. We may presume without loss of generality that $\lambda_1 > \lambda_2 > \lambda_3$.

The first integration with respect to α can be performed in an elementary manner, and the result is

$$I = \frac{1}{4\pi}\left[2\pi\lambda_3 + \int_0^{2\pi}\frac{r^2(\beta)}{\sqrt{r^2(\beta)-\lambda_3^2}}\sin^{-1}\left[\frac{\sqrt{r^2(\beta)-\lambda_3^2}}{r(\beta)}\right]\mathrm{d}\beta\right], \quad (2)$$

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where

$$r(\beta)=\sqrt{\lambda_1^2\cos^2[\beta]+\lambda_2^2\sin^2[\beta]}. \tag{3}$$

Now we need to compute the integral

$$I_1=\int_0^{2\pi}\frac{r^2(\beta)}{\sqrt{r^2(\beta)-\lambda_3^2}}\sin^{-1}\left[\frac{\sqrt{r^2(\beta)-\lambda_3^2}}{r(\beta)}\right]\mathrm{d}\beta. \tag{4}$$

We use first formula 9.121.26 from (Gradshteyn and Ryzhik, [4]) to get

$$\frac{r(\beta)}{\sqrt{r^2(\beta)-\lambda_3^2}}\sin^{-1}\left[\frac{\sqrt{r^2(\beta)-\lambda_3^2}}{r(\beta)}\right]=F\left(\frac{1}{2},\frac{1}{2};\frac{3}{2};1-\frac{\lambda_3^2}{r^2(\beta)}\right). \tag{5}$$

Here F is the Gaussian hypergeometric function. Now an application of formula 9.131.2 from (Gradshteyn and Ryzhik, [4]) to (5) yields

$$F\left(\frac{1}{2},\frac{1}{2};\frac{3}{2};1-\frac{\lambda_3^2}{r^2(\beta)}\right)=\frac{\pi}{2}\frac{r(\beta)}{\sqrt{r^2(\beta)-\lambda_3^2}}-\frac{\lambda_3}{r(\beta)}F\left(1,1;\frac{3}{2};\frac{\lambda_3^2}{r^2(\beta)}\right). \tag{6}$$

Now the integral in (4) can be presented as

$$I_1=I_2-I_3, \tag{7}$$

with

$$I_2=\frac{\pi}{2}\int_0^{2\pi}\frac{r^2(\beta)\mathrm{d}\beta}{\sqrt{r^2(\beta)-\lambda_3^2}}, \tag{8}$$

$$I_3=\lambda_3\int_0^{2\pi}F\left(1,1;\frac{3}{2};\frac{\lambda_3^2}{r^2(\beta)}\right)\mathrm{d}\beta. \tag{9}$$

The integral in (8) can be computed in an elementary fashion to give

$$I_2=2\pi\left[\boldsymbol{E}(p)\sqrt{\lambda_1^2-\lambda_3^2}+\boldsymbol{K}(p)\frac{\lambda_3^2}{\sqrt{\lambda_1^2-\lambda_3^2}}\right], \tag{10}$$

where $\boldsymbol{K}(\bullet)$ and $\boldsymbol{E}(\bullet)$ are the complete elliptic integrals of the first and the second kind respectively, and

$$p=\sqrt{\frac{\lambda_1^2-\lambda_2^2}{\lambda_1^2-\lambda_3^2}}. \tag{11}$$

The hypergeometric function in (9) can be represented as

$$F\left(1,1;\frac{3}{2};\frac{\lambda_3^2}{r^2(\beta)}\right)=\frac{\sqrt{\pi}}{2}\sum_{m=0}^{\infty}\frac{\Gamma(m+1)}{\Gamma(m+3/2)}\left(\frac{\lambda_3^2}{r^2(\beta)}\right)^m. \tag{12}$$

Now we make use of the formula

$$\int_0^{2\pi}\frac{\mathrm{d}\varphi}{\left(a^2\sin^2[\varphi]+b^2\cos^2[\varphi]\right)^n}=\frac{2\sqrt{\pi}}{a^{2n}}\left[\left(\frac{a}{b}\right)^{2n-1}\frac{\Gamma(n-1/2)}{\Gamma(n)}F\left(\frac{1}{2},1-n;\frac{3}{2}-n;\frac{b^2}{a^2}\right)\right.$$
$$\left.+\frac{\Gamma(1/2-n)}{\Gamma(1-n)}F\left(\frac{1}{2},n;n+\frac{1}{2};\frac{b^2}{a^2}\right)\right], \tag{13}$$

which in the case of n positive and integer simplifies as

$$\int_0^{2\pi} \frac{\mathrm{d}\varphi}{\left(a^2 \sin^2[\varphi] + b^2 \cos^2[\varphi]\right)^n} = \frac{2}{b^{2n}} \sum_{k=0}^{n-1} \frac{\Gamma(n-k-1/2)\Gamma(k+1/2)}{\Gamma(n-k)\Gamma(k+1)} \left(\frac{b}{a}\right)^{2k+1}. \tag{14}$$

Formula (14) is valid for $n \geq 1$; it is not valid for $n = 0$, where the result is trivial and equal to 2π.

Utilization of (12) and (14) in (9) allows us to compute the integral as

$$I_3 = \lambda_3 \left[2\pi + \sqrt{\pi} \sum_{m=1}^{\infty} \frac{\Gamma(m+1)}{\Gamma(m+3/2)} \frac{\lambda_3^{2m}}{\lambda_2^{2m}} \sum_{k=0}^{m-1} \frac{\Gamma(m-k-1/2)\Gamma(k+1/2)}{\Gamma(m-k)\Gamma(k+1)} \left(\frac{\lambda_2}{\lambda_1}\right)^{2k+1} \right]. \tag{15}$$

Formal replacement of m by $j+1$ and interchange of the order of summation yields

$$I_3 = \lambda_3 \left[2\pi + \sqrt{\pi} \sum_{k=0}^{\infty} \frac{\Gamma(k+1/2)}{\Gamma(k+1)} \left(\frac{\lambda_2}{\lambda_1}\right)^{2k+1} \sum_{j=k}^{\infty} \frac{\Gamma(j-k+1/2)\Gamma(j+2)}{\Gamma(j+5/2)\Gamma(j-k+1)} \frac{\lambda_3^{2j+2}}{\lambda_2^{2j+2}} \right]. \tag{16}$$

Yet another formal replacement of j by $m+k$ gives us

$$I_3 = \lambda_3 \left[2\pi + \sqrt{\pi} \sum_{k=0}^{\infty} \frac{\Gamma(k+1/2)}{\Gamma(k+1)} \left(\frac{\lambda_3}{\lambda_1}\right)^{2k+1} \sum_{m=0}^{\infty} \frac{\Gamma(m+1/2)\Gamma(m+k+2)}{\Gamma(m+k+5/2)\Gamma(m+1)} \left(\frac{\lambda_3}{\lambda_2}\right)^{2m+1} \right]. \tag{17}$$

If we look at the definition of the hypergeometric function F_1 of 2 variables (formula 9.180.1 of Gradshteyn and Ryzhik, [4]), we may conclude that

$$I_3 = \lambda_3 \left[2\pi + \frac{4\pi}{3} \frac{\lambda_3^2}{\lambda_1 \lambda_2} F_1 \left(2, \frac{1}{2}, \frac{1}{2}; \frac{5}{2}; \frac{\lambda_3^2}{\lambda_1^2}, \frac{\lambda_3^2}{\lambda_2^2} \right) \right]. \tag{18}$$

We use the following integral representation of F_1 (Bateman and Erdélyi, [1], Vol. 1, formula 5.8.5):

$$F_1(a, b, c, d; x, y) = \frac{\Gamma(d)}{\Gamma(a)\Gamma(d-a)} \int_0^1 \frac{u^{a-1}(1-u)^{d-a-1}\mathrm{du}}{(1-ux)^b (1-uy)^c}. \tag{19}$$

We get then

$$F_1 \left(2, \frac{1}{2}, \frac{1}{2}; \frac{5}{2}; \frac{\lambda_3^2}{\lambda_1^2}, \frac{\lambda_3^2}{\lambda_2^2} \right) = \frac{3}{4} \frac{\lambda_1 \lambda_2}{\lambda_3^2} \int_0^1 \frac{u\mathrm{du}}{\sqrt{1-u}\sqrt{(\lambda_1^2/\lambda_3^2) - u}\sqrt{(\lambda_2^2/\lambda_3^2) - u}}. \tag{20}$$

The integral in (20) can be computed following formula 3.132.1 of (Gradshteyn and Ryzhik, 1994) as

$$\int_0^1 \frac{u\mathrm{du}}{\sqrt{1-u}\sqrt{(\lambda_1^2/\lambda_3^2) - u}\sqrt{(\lambda_2^2/\lambda_3^2) - u}} = 2 \left[\frac{\lambda_3}{\sqrt{\lambda_1^2 - \lambda_3^2}} \left(F(q,p) + \frac{\lambda_1^2 - \lambda_3^2}{\lambda_3^2} E(q,p) \right) - \frac{\lambda_1}{\lambda_2} \right], \tag{21}$$

where $F(\bullet,\bullet)$ and $E(\bullet,\bullet)$ are the incomplete elliptic integrals of the first and the second kind respectively, with p defined by (11) and

$$q = \sin^{-1}\left[\lambda_3/\lambda_2\right]. \tag{22}$$

Utlilization of (21) and (20) all the way up to (4) yields

$$I_1 = 2\pi \left[[\boldsymbol{E}(p) - E(q,p)]\sqrt{\lambda_1^2 - \lambda_3^2} + [\boldsymbol{K}(p) - F(q,p)]\frac{\lambda_3^2}{\sqrt{\lambda_1^2 - \lambda_3^2}} + \lambda_3\left(\frac{\lambda_1}{\lambda_2} - 1\right)\right] \tag{23}$$

and

$$I = \frac{1}{2}\left[[\boldsymbol{E}(p) - E(q,p)]\sqrt{\lambda_1^2 - \lambda_3^2} + [\boldsymbol{K}(p) - F(q,p)]\frac{\lambda_3^2}{\sqrt{\lambda_1^2 - \lambda_3^2}} + \lambda_3\frac{\lambda_1}{\lambda_2}\right]. \tag{24}$$

Further simplification can be achieved by the use of the addition theorem for elliptic integrals (Bateman and Erdélyi, [2], Vol. 3, formulae 13.7.4-13.7.6) which in this particular case will take the form

$$\boldsymbol{K}(p) - F(q,p) = F\left(q_1, p\right), \ \boldsymbol{E}(p) - E(q,p) = E\left(q_1, p\right) - p^2\frac{\lambda_3}{\lambda_2}\frac{\sqrt{\lambda_1^2 - \lambda_3^2}}{\lambda_1}, \tag{25}$$

with

$$q_1 = \sin^{-1}\left[\frac{\sqrt{\lambda_1^2 - \lambda_3^2}}{\lambda_1}\right]. \tag{26}$$

The back substitution of (25) in (24) gives us the final result:

$$\begin{aligned}\frac{1}{4\pi}\int_0^{2\pi}\left[\int_{-\pi/2}^{\pi/2}\sqrt{(\lambda_1\cos[\alpha]\cos[\beta])^2 + (\lambda_2\cos[\alpha]\sin[\beta])^2 + (\lambda_3\sin[\alpha])^2}\cos[\alpha]\mathrm{d}\alpha\right]\mathrm{d}\beta \\ = \frac{1}{2}\left[\sqrt{\lambda_1^2 - \lambda_3^2}E\left(q_1,p\right) + \frac{\lambda_3^2}{\sqrt{\lambda_1^2 - \lambda_3^2}}F\left(q_1,p\right) + \lambda_3\frac{\lambda_2}{\lambda_1}\right],\end{aligned} \tag{27}$$

with q_1 defined by (26) and p defined by (11).

Discussion. It might be of interest to generalize the basic integral (1) to an arbitrary power n as follows:

$$I = \frac{1}{4\pi}\int_0^{2\pi}\left[\int_{-\pi/2}^{\pi/2}\left((\lambda_1\cos[\alpha]\cos[\beta])^2 + (\lambda_2\cos[\alpha]\sin[\beta])^2 + (\lambda_3\sin[\alpha])^2\right)^n\cos[\alpha]\mathrm{d}\alpha\right]\mathrm{d}\beta. \tag{28}$$

In this case, the substitution $x = \sin[\alpha]$ allows us to compute the integral with respect to α as follows:

$$I = \frac{1}{2\pi}\int_0^{2\pi} r^{2n}(\beta)F\left(-n, \frac{1}{2}; \frac{3}{2}; 1 - \frac{\lambda_3^2}{r^2(\beta)}\right)\mathrm{d}\beta. \tag{29}$$

We transform the hypergeometric function using formula 9.131.2 from (Gradshteyn and Ryzhik, [4]) as

$$\begin{aligned}F\left(-n, \frac{1}{2}; \frac{3}{2}; 1 - \frac{\lambda_3^2}{r^2(\beta)}\right) = \frac{\sqrt{\pi}\Gamma(1+n)}{2\Gamma(n+3/2)}\left(1 - \frac{\lambda_3^2}{r^2(\beta)}\right)^{-1/2} \\ -\frac{1}{2(n+1)}\left(\frac{\lambda_3^2}{r^2(\beta)}\right)^{n+1}F\left(\frac{3}{2}+n, 1; 2+n; \frac{\lambda_3^2}{r^2(\beta)}\right).\end{aligned} \tag{30}$$

Now we have 2 single integrals to compute:

$$J_1 = \frac{\Gamma(1+n)}{4\sqrt{\pi}\Gamma(n+3/2)}\int_0^{2\pi}\frac{r^{2n+1}(\beta)}{\sqrt{r^2(\beta)-\lambda_3^2}}\mathrm{d}\beta \tag{31}$$

and

$$J_2 = \frac{\lambda_3^{2(n+1)}}{4\pi(n+1)}\int_0^{2\pi}F\left(\frac{3}{2}+n,1;2+n;\frac{\lambda_3^2}{r^2(\beta)}\right)\frac{\mathrm{d}\beta}{r^2(\beta)}. \tag{32}$$

Using the substitution $u=\sin^2[\beta]$, the integral (31) can be presented as

$$J_1 = \frac{\Gamma(1+n)}{2\sqrt{\pi}\Gamma(n+3/2)}\left(\lambda_1^2-\lambda_2^2\right)^n\int_0^1\frac{\left[\lambda_1^2/\left(\lambda_1^2-\lambda_2^2\right)-u\right]^{n+1/2}}{\sqrt{u(1-u)}\sqrt{\left(\lambda_1^2-\lambda_3^2\right)/\left(\lambda_1^2-\lambda_2^2\right)-u}}\mathrm{d}u. \tag{33}$$

It can be evaluated through an Appel hypergeometric function F_1 of 2 variables as

$$J_1 = \frac{\sqrt{\pi}\Gamma(1+n)}{2\Gamma(n+3/2)}\frac{\lambda_1^{2n+1}}{\sqrt{\lambda_1^2-\lambda_3^2}}F_1\left(\frac{1}{2},\frac{1}{2},-n-\frac{1}{2},1;\frac{\lambda_1^2-\lambda_2^2}{\lambda_1^2-\lambda_3^2},\frac{\lambda_1^2-\lambda_2^2}{\lambda_1^2}\right). \tag{34}$$

By using the expansion

$$F\left(\frac{3}{2}+n,1;2+n;\frac{\lambda_3^2}{r^2(\beta)}\right) = \frac{\Gamma(n+2)}{\Gamma(n+3/2)}\sum_{m=0}^{\infty}\frac{\Gamma(n+m+3/2)\Gamma(m+1)}{\Gamma(m+n+2)\Gamma(m+1)}\left(\frac{\lambda_3^2}{r^2(\beta)}\right)^m, \tag{35}$$

the integral (32) can be computed as

$$J_2 = \frac{\Gamma(n+1)}{\Gamma(n+3/2)}\frac{\lambda_3^{2(n+1)}}{2\pi\lambda_1\lambda_2}\sum_{k=0}^{\infty}\frac{\Gamma(j+1/2)\Gamma(k+1/2)}{\Gamma(j+1)\Gamma(k+1)}\left(\frac{\lambda_3^2}{\lambda_1^2}\right)^k\sum_{j=0}^{\infty}\frac{\Gamma(n+k+j+3/2)}{\Gamma(n+k+j+2)}\frac{\lambda_3^{2j}}{\lambda_2^{2j}}. \tag{36}$$

This result is also an Appel hypergeometric function, namely,

$$J_2 = \frac{\lambda_3^{2(n+1)}}{2\lambda_1\lambda_2(n+1)}F_1\left(n+\frac{3}{2},\frac{1}{2},\frac{1}{2};n+2;\frac{\lambda_3^2}{\lambda_1^2},\frac{\lambda_3^2}{\lambda_2^2}\right). \tag{37}$$

It can be presented as an integral of elementary functions:

$$J_2 = \frac{\Gamma(n+1)}{2\sqrt{\pi}\Gamma(n+3/2)}\lambda_3^{2n}\int_0^1\frac{u^{n+1/2}(1-u)^{-1/2}\mathrm{d}u}{\left[(\lambda_1^2/\lambda_3^2)-u\right]^{1/2}\left[(\lambda_2^2/\lambda_3^2)-u\right]^{1/2}}. \tag{38}$$

Finally, the generalized integral (28) can be presented as

$$\begin{aligned}\frac{1}{4\pi}\int_0^{2\pi}&\left[\int_{-\pi/2}^{\pi/2}\left((\lambda_1\cos[\alpha]\cos[\beta])^2+(\lambda_2\cos[\alpha]\sin[\beta])^2+(\lambda_3\sin[\alpha])^2\right)^n\cos[\alpha]\mathrm{d}\alpha\right]\mathrm{d}\beta\\ &= \frac{\sqrt{\pi}\Gamma(1+n)}{2\Gamma(n+3/2)}\frac{\lambda_1^{2n+1}}{\sqrt{\lambda_1^2-\lambda_3^2}}F_1\left(\frac{1}{2},\frac{1}{2},-n-\frac{1}{2},1;\frac{\lambda_1^2-\lambda_2^2}{\lambda_1^2-\lambda_3^2},\frac{\lambda_1^2-\lambda_2^2}{\lambda_1^2}\right)\\ &\quad -\frac{\lambda_3^{2(n+1)}}{2\lambda_1\lambda_2(n+1)}F_1\left(n+\frac{3}{2},\frac{1}{2},\frac{1}{2};n+2;\frac{\lambda_3^2}{\lambda_1^2},\frac{\lambda_3^2}{\lambda_2^2}\right)\end{aligned} \tag{39}$$

or as

$$\frac{1}{4\pi}\int_0^{2\pi}\left[\int_{-\pi/2}^{\pi/2}\left((\lambda_1\cos[\alpha]\cos[\beta])^{\,2}+(\lambda_2\cos[\alpha]\sin[\beta])^{\,2}+(\lambda_3\sin[\alpha])^{\,2}\right)^n\cos[\alpha]\mathrm{d}\alpha\right]\mathrm{d}\beta$$
$$=\frac{\Gamma(1+n)}{2\sqrt{\pi}\Gamma(n+3/2)}\left[\left(\lambda_1^2-\lambda_2^2\right)^n\int_0^1\frac{\left[\lambda_1^2/\left(\lambda_1^2-\lambda_2^2\right)-u\right]^{\,n+1/2}}{\sqrt{u(1-u)}\sqrt{\left(\lambda_1^2-\lambda_3^2\right)/\left(\lambda_1^2-\lambda_2^2\right)-u}}\mathrm{du}\right.$$
$$\left.-\lambda_3^{2n}\int_0^1\frac{u^{n+1/2}\mathrm{du}}{\sqrt{(1-u)\left[(\lambda_1^2/\lambda_3^2)-u\right]\left[(\lambda_2^2/\lambda_3^2)-u\right]}}\right]. \tag{40}$$

The last expression by proper change of variables can be presented in a more elegant form, namely,

$$\frac{1}{4\pi}\int_0^{2\pi}\left[\int_{-\pi/2}^{\pi/2}\left((\lambda_1\cos[\alpha]\cos[\beta])^{\,2}+(\lambda_2\cos[\alpha]\sin[\beta])^{\,2}+(\lambda_3\sin[\alpha])^{\,2}\right)^n\cos[\alpha]\mathrm{d}\alpha\right]\mathrm{d}\beta$$
$$=\frac{\Gamma(1+n)}{2\sqrt{\pi}\Gamma(n+3/2)}\lambda_1^{2n}\left(\int_{\lambda_2^2/\lambda_1^2}^1-\int_0^{\lambda_3^2/\lambda_1^2}\right)\frac{u^{n+1/2}\mathrm{du}}{\sqrt{(1-u)\left(\lambda_2^2/\lambda_1^2-u\right)\left(\lambda_3^2/\lambda_1^2-u\right)}}. \tag{41}$$

One can see that in the particular case of $n = 1/2$, the integral in (40) can be easily computed as elliptic integrals, which is in agreement with (27).

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