JOURNAL OF RHEOLOGY

On the eigenfunctions for Hookean and FENE dumbbell models

Michael Renardy

Citation: Journal of Rheology (1978-present) **57**, 1311 (2013); doi: 10.1122/1.4816631
View online: http://dx.doi.org/10.1122/1.4816631
View Table of Contents: http://scitation.aip.org/content/sor/journal/jor2/57/5?ver=pdfcov
Published by the The Society of Rheology

On the eigenfunctions for Hookean and FENE dumbbell models

Michael Renardy[a)]

Department of Mathematics, Virginia Tech, Blacksburg, Virginia 24061-0123

(Received 8 April 2013; final revision received 8 July 2013; published 29 July 2013)

Synopsis

We study the linear eigenvalue problem for the distribution function associated with Hookean and FENE dumbbell models. For Hookean dumbbells, the eigenfunctions can be expressed by generalized Laguerre polynomials. The eigenvalue problem for the FENE dumbbell leads to a confluent Heun equation. The first few eigenvalues are calculated numerically. We also calculate these eigenvalues using perturbation of the Hookean case. We show how the knowledge of the eigenvalues and eigenfunctions can be used to construct the stress relaxation modulus. © *2013 The Society of Rheology*. [http://dx.doi.org/10.1122/1.4816631]

I. INTRODUCTION

Dumbbell models for dilute polymer solutions lead to a diffusion equation for the configurational distribution function. For stress relaxation in absence of flow, the diffusion equation has the form [Bird *et al.* (1977)]

$$\frac{\partial \psi}{\partial t} = \frac{2kT}{\zeta}\Delta\psi + \frac{2}{\zeta}\nabla\cdot(\mathbf{F}\psi). \tag{1}$$

Here, ζ is a drag coefficient, and $\mathbf{F}$ is the connector force which, for Hookean dumbbells, has the form

$$\mathbf{F} = H\mathbf{R}, \tag{2}$$

while for FENE dumbbells, we have

$$\mathbf{F} = \frac{H\mathbf{R}}{1-(|\mathbf{R}|/R_0)^2}. \tag{3}$$

We may write Eq. (1) in the schematic form

$$\frac{\partial \psi}{\partial t} = \mathcal{L}\psi. \tag{4}$$

a)Electronic mail: mrenardy@math.vt.edu

The operator $\mathcal{L}$ is self-adjoint in the weighted Hilbert space

$$\left\{\psi \mid \int \exp(U/kT)\psi^2 < \infty\right\}, \tag{5}$$

where U is the potential associated with $\mathbf{F}$, i.e., $\nabla U = \mathbf{F}$. We can, therefore, obtain a general solution of Eq. (1) by a superposition of eigenfunctions of $\mathcal{L}$.

Notwithstanding the fundamental role of these eigenfunctions, I have not been able to find them in the literature. For Hookean dumbbells, it may be that the problem has attracted little attention, since the distribution function in an arbitrary flow was found by Lodge and Wu (1971). (Even so, there may be a flow history leading to an initial condition that is not given by the Lodge–Wu solution if the past evolution of the distribution function was affected by something other than flow, e.g., molecular diffusion, electromagnetic effects, etc.) For FENE dumbbells, on the other hand, the eigenvalues and eigenfunctions are needed to determine the stress relaxation function for linear viscoelasticity. Ilg *et al*. (2000) consider a one-dimensional version of a finitely extensible dumbbell model, but with a force law different from the usual FENE dumbbell, and determine eigenvalues and eigenfunctions. Vincenzi and Bodenschatz (2006) consider a one-dimensional approximation of the FENE model in a strong steady elongational flow. Their analysis leads to the confluent Heun equation, which will also play a role in our analysis below.

We shall use a dimensionless form of the equations. We scale length with $\sqrt{kT/H}$ and time with $\zeta/(2H)$. As is well known, this length scale represents the radius of gyration and the time scale is twice the relaxation time of a Hookean dumbbell. We obtain the dimensionless equation

$$\frac{\partial\psi}{\partial t} = \Delta\psi + \nabla\cdot(\mathbf{R}\psi) \tag{6}$$

for Hookean dumbbells, and

$$\frac{\partial\psi}{\partial t} = \Delta\psi + \nabla\cdot\left(\frac{\mathbf{R}}{1-(|\mathbf{R}|/L)^2}\psi\right) \tag{7}$$

for FENE dumbbells, where $L = R_0/\sqrt{kT/H}$.

We remark that, for the FENE dumbbell model, there is a difference between the cases $L^2 \geq 6$ and $L^2 < 6$. If $L^2 < 6$, a zero flux boundary condition

$$\lim_{R\to L}\left(\frac{\partial\psi}{\partial R} + \frac{HR\psi}{1-(|\mathbf{R}|/L)^2}\right) = 0 \tag{8}$$

needs to be imposed. If $L^2 \geq 6$, the weight in Eq. (5) grows strongly enough as $R \to L$ to automatically ensure this boundary condition. The distinction is not important for the discussion of eigenfunctions below, and in any case, only $L^2 > 6$ is physically relevant.

II. THE HOOKEAN CASE

We consider the eigenvalue problem associated with Eq. (6), i.e.,

$$\lambda\psi = \Delta\psi + \nabla\cdot(\mathbf{R}\psi). \tag{9}$$

We use spherical harmonics to separate variables, i.e., we set

$$\psi = \chi(r) Y_l^m(\theta, \phi). \tag{10}$$

The resulting eigenvalue problem is

$$\lambda\chi(r) = \chi''(r) + \frac{2}{r}\chi'(r) - \frac{l(l+1)\chi(r)}{r^2} + r\chi'(r) + 3\chi(r). \tag{11}$$

The substitution $\chi(r) = \exp(-r^2/2) r^l v(r)$ leads to the equation

$$\lambda v(r) = v''(r) + \frac{2+2l}{r} v'(r) - rv'(r) - lv(r) = 0. \tag{12}$$

This is a confluent hypergeometric equation, and the solution which is regular at the origin is given by

$$v(r) = {}_1F_1\left(\frac{\lambda + l}{2}, l + \frac{3}{2}, \frac{r^2}{2}\right). \tag{13}$$

For large r, we have [Abramowitz and Stegun (1965)] the asymptotic behavior

$$v(r) \sim \frac{\Gamma\left(l + \frac{3}{2}\right)}{\Gamma\left(\frac{\lambda + l}{2}\right)} \exp(r^2/2) r^{(\lambda - l - 3)/2}, \tag{14}$$

unless $\lambda + l$ is an even nonpositive integer, in which case v is a polynomial. Except in this specific case, the behavior at infinity is inconsistent with membership in the weighted Hilbert space defined by Eq. (5). Therefore, the condition that v is a polynomial identifies the eigenvalues.

Therefore, the eigenvalues are given by $\lambda = -l - 2n$, where n is an non-negative integer. In this case, the corresponding eigenfunction is

$$v(r) = {}_1F_1(-n, l + \frac{3}{2}, \frac{r^2}{2}) = \frac{n!}{(l + 3/2)_n} L_n^{(l+1/2)}\left(\frac{r^2}{2}\right). \tag{15}$$

Here,

$$\left(l + \frac{3}{2}\right)_n = \left(l + \frac{3}{2} + n - 1\right)\left(l + \frac{3}{2} + n - 2\right) \dots \left(l + \frac{3}{2}\right) \tag{16}$$

and $L_n^{(\alpha)}$ is the generalized Laguerre polynomial.

Above we have used spherical coordinates because we want to consider the FENE case later. For the Hookean dumbbell, separation of variables in Cartesian coordinates actually yields a simpler representation of the eigenfunctions. By separating variables in Cartesian coordinates, we find eigenfunctions of the form $\psi = \psi_1(x)\psi_2(y)\psi_3(z)$, where $\mathbf{R} = (x, y, z)$, the function ψ_i satisfies

$$\lambda_i \psi_i = \psi_i'' + x\psi_i' + \psi_i \tag{17}$$

and the eigenvalue is $\lambda = \lambda_1 + \lambda_2 + \lambda_3$. The solution for this eigenvalue problem is $\lambda_i = -n$, where n is a non-negative integer, and

$$\psi_i(x) = e^{-x^2/2} H_n(x/\sqrt{2}), \tag{18}$$

where H_n is the Hermite polynomial of order n. In summary, we find the eigenfunctions

$$\psi = e^{-r^2/2} H_l(x/\sqrt{2}) H_m(y/\sqrt{2}) H_n(z/\sqrt{2}), \tag{19}$$

with associated eigenvalue $\lambda = -(l + m + n)$.

It is instructive to see how the Lodge–Wu solution fits in with this. The Lodge–Wu solution is of the form

$$\psi = \exp(-\mathbf{R} \cdot \mathbf{A}(t) \cdot \mathbf{R} - \beta(t)), \tag{20}$$

where $\mathbf{A}$ is a symmetric matrix. By inserting this into the governing equation, we find that in the absence of a flow, we have

$$\begin{aligned} \dot{\mathbf{A}} &= -4\mathbf{A}^2 + 2\mathbf{A}, \\ \dot{\beta} &= 2\mathrm{tr}\,\mathbf{A} - 3. \end{aligned} \tag{21}$$

Thus if there is no flow, the principal axes of $\mathbf{A}$ remain invariant, and we may assume they are aligned with the coordinate axes. Moreover, in equilibrium, we have $\mathbf{A} = \frac{1}{2}\mathbf{I}$. We, therefore, set

$$\mathbf{A} = \begin{pmatrix} \frac{1}{2} + c_1 & 0 & 0 \\ 0 & \frac{1}{2} + c_2 & 0 \\ 0 & 0 & \frac{1}{2} + c_3 \end{pmatrix} \tag{22}$$

and

$$\beta = \beta_1 + \beta_2 + \beta_3 \tag{23}$$

and we obtain the set of equations

$$\begin{aligned} \dot{c}_i &= -4c_i^2 - 2c_i, \\ \dot{\beta}_i &= 2c_i. \end{aligned} \tag{24}$$

The solution of this set of equation can be given as

$$\begin{aligned} c_i &= \frac{\tau}{2(1-\tau)}, \\ \beta_i &= C + \frac{1}{2}\ln(1-\tau). \end{aligned} \tag{25}$$

Here, C is a constant and $\tau = K\exp(-2t)$, where $K < 1$ is another constant. We now find that, up to a constant factor,

$$\exp(-c_i x_i^2 - \beta_i) = \exp\left(-\frac{x_i^2}{2}\frac{\tau}{1-\tau}\right)(1-\tau)^{-1/2}. \tag{26}$$

By the well-known formula for the generating function of the generalized Laguerre polynomials, this equals

$$\sum_{k=0}^{\infty} \tau^k L_k^{(-1/2)}(x_i^2/2) = \sum_{k=0}^{\infty} \frac{\tau^k}{(-4)^k k!} H_{2k}(x_i/\sqrt{2}). \tag{27}$$

This last expression shows how the Lodge–Wu solution can be expressed as a superposition of eigenmodes.

III. THE FENE CASE

We now turn to the FENE dumbbell. We again use spherical harmonics to separate variables, and the eigenvalue problem for Eq. (7) becomes

$$\lambda\chi(r) = \chi''(r) + \frac{2}{r}\chi'(r) - \frac{l(l+1)}{r^2}\chi(r) + r\frac{d}{dr}\left(\frac{\chi(r)}{1 - r^2/L^2}\right) + 3\frac{\chi(r)}{1 - r^2/L^2}. \tag{28}$$

We substitute $\chi(r) = r^l v(r^2/L^2)$, substitute $s = r^2/L^2$, and obtain the equation

$$\begin{aligned} &4s(s-1)^2 v''(s) + (s-1)(-6 + 4l(s-1) - 2s(L^2-3))v'(s) \\ &\quad + L^2(3 - l(s-1) - \lambda(s-1)^2 - s)v(s) = 0. \end{aligned} \tag{29}$$

This equation has regular singular points at $s=0$ and $s=1$ and an irregular singular point of rank 1 at infinity; hence it is a confluent Heun equation. We can transform it to standard form by setting $v(s) = (1-s)^{L^2/2} w(s)$. The new equation is

$$4s(s-1)w''(s) + (-6 + 4l(s-1) + 2(3+L^2)s)w'(s) + L^2(l - \lambda(s-1))w(s) = 0. \tag{30}$$

Equation (30) can be put in the form

$$w''(s) + \left(\frac{\gamma}{s} + \frac{\delta}{s-1}\right)w'(s) + \frac{\alpha s - \sigma}{s(s-1)}w(s) = 0, \tag{31}$$

where

$$\gamma = l + \frac{3}{2}, \qquad \delta = \frac{L^2}{2}, \qquad \alpha = -\frac{\lambda L^2}{4}, \qquad \sigma = -\frac{L^2(\lambda + l)}{4}. \tag{32}$$

This is the nonsymmetrical canonical form given as (1.2.27) in Ronveaux (1995), p. 94. In the notation of Maple, the solution of Eq. (31) which is regular at $s=0$ is given by

$$w(s) = \mathrm{HeunC}(0, b, c, d, e, s), \tag{33}$$

where

$$\begin{aligned} b &= \gamma - 1 = l + \frac{1}{2}, \\ c &= \delta - 1 = \frac{L^2 - 2}{2}, \\ d &= \alpha = -\frac{\lambda L^2}{4}, \\ e &= -\sigma + \frac{1}{2}(1 - \gamma\delta) = \frac{1}{2} + L^2\left(\frac{\lambda}{4} - \frac{3}{8}\right). \end{aligned} \tag{34}$$

Maple has the capability of evaluating the function HeunC. This is used for computing the eigenvalues below.

The eigenvalues λ are determined by the requirement that w must be analytic at $s = 1$. As long as $L^2 > 2$, nonanalytic solutions of Eq. (30) are infinite at $s = 1$, and we can obtain a quite accurate approximation to the eigenvalues by a numerical solution of the equation $w(1-\epsilon) = 0$, where ϵ is a small number. In this fashion, we computed the first few eigenvalues for the case $L^2 = 10$ and $L^2 = 20$. We used $\epsilon = 0.001$ for $L^2 = 10$ and $\epsilon = 0.01$ for $L^2 = 20$. We have verified that the results do not change if ϵ is decreased further. Table I shows the computed eigenvalues λ; the Hookean case ($L^2 = \infty$) is also included for reference. It is apparent from the numbers that the eigenvalues for $L^2 = 10$ differ approximately twice as much from the Hookean ones as those for $L^2 = 20$, i.e., the difference is approximately proportional to $1/L^2$. We shall return to this point later. We note that a proportionality to $1/L^2$ is also predicted for the FENE-P dumbbell. The relaxation time for the FENE-P model should be compared with the reciprocal of the first eigenvalue for $l = 2$. As is well known [see e.g., Herrchen and Öttinger (1997)], the relaxation time for the FENE-P dumbbell decreases by a factor $L^2/(L^2+3)$ compared to the Hookean case, i.e., the relaxation rate increases by a factor of $1 + 3/L^2$. For the first eigenvalue for $l = 2$, this would predict -2.6 for $L^2 = 10$ and -2.3 for $L^2 = 20$. As we can see, this does not compare well with the actual FENE model. Of course, if L^2 is really large, the eigenvalue will be close to the Hookean one, regardless if we use FENE or FENE-P. But as far as predicting the difference from the Hookean case, the FENE-P underpredicts it by more than a factor of 2! If we consider the evolution of the full distribution function rather than just the stress, the agreement is even worse, since the FENE-P model would predict that all the eigenvalues other than those for $l = 0$ should simply be the Hookean ones multiplied by $(L^2+3)/L^2$.

While the method of calculation described above yields accurate eigenvalues, it is not very suitable for the calculation of the eigenfunctions, since the Heun function will blow up at $s = 1$ if the value of λ is just a little bit off. To get better approximations of the eigenfunctions, we can take advantage of the fact that the solution of Eq. (31) which is analytic at $s = 1$ is given by

$$w(s) = \mathrm{HeunC}(0, c, b, -d, e+d, 1-s). \tag{35}$$

This can be seen by substituting $s = 1 - \tau$ in Eq. (31). Therefore, our eigenfunction is, on the one hand, given by $\mathrm{HeunC}(0, b, c, d, e, s)$, but it must also be a multiple of $\mathrm{HeunC}(0, c, b, -d, e+d, 1-s)$. The former expression becomes numerically inaccurate

TABLE I. Eigenvalues for the FENE dumbbell.

L^2	10	20	∞
$l = 0$	0	0	0
	−3.976	−2.989	−2
	−10.069	−7.072	−4
	−18.210	−12.205	−6
$l = 1$	−1.473	−1.241	−1
	−6.542	−4.789	−3
	−13.672	−9.403	−5
$l = 2$	−3.269	−2.656	−2
	−9.410	−6.749	−4
	−17.571	−11.888	−6

near $s=1$, but the latter expression is accurate precisely near $s=1$. Hence a suitably accurate eigenfunction can be constructed as

$$w(s)=\begin{cases}\mathrm{HeunC}(0,b,c,d,e,s), & \text{if } s\le a\\ \mu\mathrm{HeunC}(0,c,b,-d,e+d,1-s), & \text{if } s>a\end{cases} \tag{36}$$

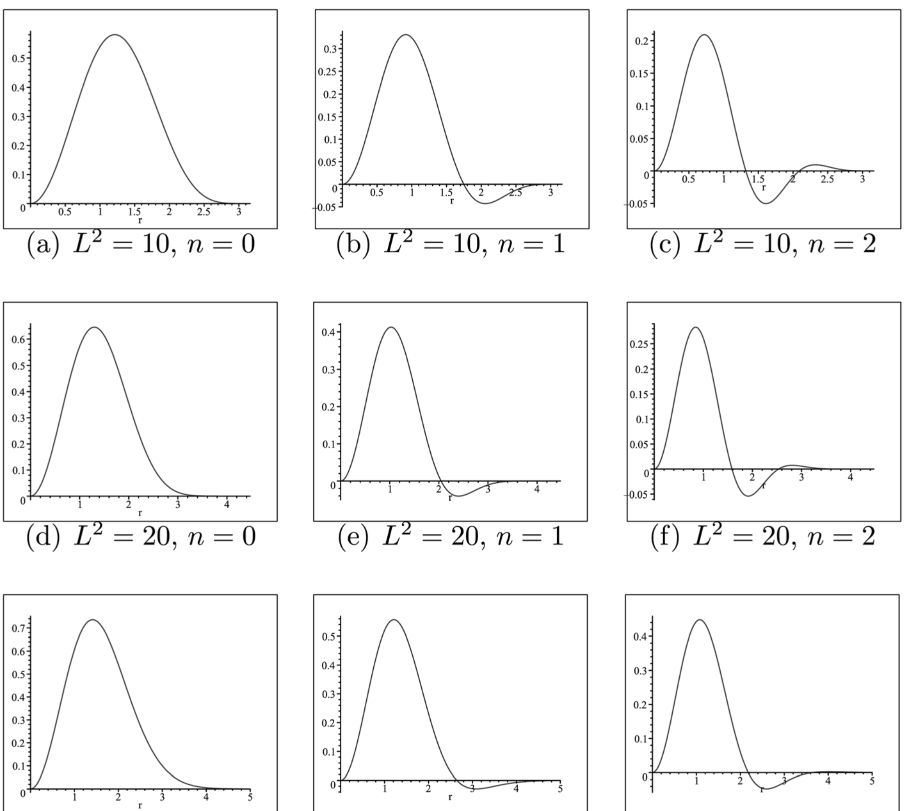
and the constant μ is determined by the requirement of continuity at $s=a$. The number a can in principle be anything between 0 and 1; the choice which is numerically optimal depends on L^2.

In Fig. 1, we have plotted the first three eigenfunctions $\chi(r)$ for $l=2$. We have chosen $l=2$ since this is the value of l which is relevant for linear viscoelasticity (see Sec. VI). The eigenfunction as plotted has not been normalized. In generating these plots, we have used $a=0.8$.

We can use the method of matched asymptotics to determine the behavior of large eigenvalues. We set $-\lambda L^2/4=k^2$ and rewrite Eq. (31) in the form

$$w''+\left(\frac{\gamma}{s}+\frac{\delta}{s-1}\right)w'+\frac{k^2}{s}w+\frac{L^2 l}{4s(s-1)}w=0. \tag{37}$$

We assume k is large. Near $s=0$, we set $s=\tau/k^2$, $w(s)=w_1(\tau)$. At leading order, we obtain the equation



(a) $L^2=10$, $n=0$ (b) $L^2=10$, $n=1$ (c) $L^2=10$, $n=2$

(d) $L^2=20$, $n=0$ (e) $L^2=20$, $n=1$ (f) $L^2=20$, $n=2$

(g) Hookean, $n=0$ (h) Hookean, $n=1$ (i) Hookean, $n=2$

FIG. 1. Radial part of the eigenfunctions for the FENE model with $l=2$.

$$w_1''(\tau) + \frac{\gamma}{\tau} w_1'(\tau) + \frac{1}{\tau} w_1 = 0. \tag{38}$$

The solution of this which is analytic and equal to 1 at the origin is given by

$$w_1(\tau) = \Gamma(\gamma) \tau^{(1-\gamma)/2} J_{\gamma-1}(2\sqrt{\tau}). \tag{39}$$

Near $s = 1$, we set $1 - s = \rho/k$, $w(s) = w_2(\rho)$, and at leading order, we obtain

$$w_2''(\rho) + \frac{\delta}{\rho} w_2'(\rho) + w_2(\rho) = 0. \tag{40}$$

From this equation and the requirement of regularity at $\rho = 0$, we find the solution

$$w_2(\rho) = C \rho^{(1-\delta)/2} J_{(\delta-1)/2}(\rho). \tag{41}$$

Away from the boundaries, we use a Wentzel-Kramers-Brillouin approximation. We set

$$w(s) = e^{ik\phi(s)} y(s), \tag{42}$$

which, at leading orders, leads to the equations

$$-\phi'(s)^2 + \frac{1}{s} = 0, \qquad \phi''(s)y(s) + 2\phi'(s)y'(s) + \left(\frac{\delta}{s-1} + \frac{\gamma}{s}\right)\phi'(s)y(s) = 0. \tag{43}$$

This leads to

$$\phi(s) = \pm 2\sqrt{s} \tag{44}$$

and

$$y(s) = C(1-s)^{-\delta/2} s^{1/4-\gamma/2}. \tag{45}$$

Thus, we find the approximate solution

$$w_3(s) = (1-s)^{-\delta/2} s^{1/4-\gamma/2} (C_1 e^{2ik\sqrt{s}} + C_2 e^{-2ik\sqrt{s}}). \tag{46}$$

For $\tau \to \infty$, we find [Abramowitz and Stegun (1965)]

$$w_1(\tau) \sim \Gamma(\gamma) \sqrt{\frac{1}{\pi}} \tau^{1/4-\gamma/2} \cos\left(2\sqrt{\tau} - \frac{\pi}{4} - \frac{\gamma - 1}{2}\pi\right). \tag{47}$$

By matching this with Eq. (46), we obtain

$$C_1 = \bar{C}_2 = \frac{1}{2} k^{1/2-\gamma} \Gamma(\gamma) \sqrt{\frac{1}{\pi}} \exp\left(i\pi\left(\frac{1}{4} - \frac{\gamma}{2}\right)\right). \tag{48}$$

In a similar fashion, we can set $\sqrt{s} \sim 1 - \rho/(2k)$ in Eq. (46) and then match with the solution for w_2 above. In this way, we obtain the relationship

$$k \sim \pi\left(n + \frac{\gamma}{4} + \frac{\delta - 1}{8}\right), \tag{49}$$

where n is an integer. At leading order, k is therefore proportional to πn, and λ is proportional to $-4\pi^2 n^2/L^2$. We note that this behavior contrasts with the Hookean case, where λ is proportional to n. We note that eigenvalues proportional to n^2 were also found in Ilg *et al.* (2000).

IV. THE COHEN–PADÉ SPRING LAW

Instead of the Warner spring law (3), the Cohen–Padé law [Cohen (1991)]

$$\mathbf{F}(\mathbf{R}) = \frac{H(1 - |\mathbf{R}|^2/(3R_0^2))\mathbf{R}}{(1 - (|\mathbf{R}|/R_0)^2)} \tag{50}$$

is sometimes used as an improved approximation to an inverse Langevin function. In this case, we can go through the exact same manipulations and transformations as above for the Warner law, except that we set $v(s) = (1-s)^{L^2/3} w(s)$ instead of $v(s) = (1-s)^{L^2/2} w(s)$. We end up with the confluent Heun equation

$$w''(s) + \left(\frac{\gamma}{s} + \frac{\delta}{s-1} + \epsilon\right) w'(s) + \frac{\alpha s - \sigma}{s(s-1)}(s) = 0, \tag{51}$$

where

$$\begin{gathered} \gamma = \frac{3}{2} + l, \qquad \delta = \frac{L^2}{3}, \qquad \epsilon = \frac{L^2}{6}, \\ \alpha = \frac{L^2}{36}(9 + 3l + 2L^2 - 9\lambda), \qquad \sigma = \frac{L^2}{12}(3 - l - 3\lambda). \end{gathered} \tag{52}$$

The solution which is regular at $s = 0$ is now

$$w(s) = \mathrm{HeunC}(a, b, c, d, e, s), \tag{53}$$

where

$$\begin{aligned} a = \epsilon = \frac{L^2}{6}, \qquad b = \gamma - 1 = l + \frac{1}{2}, \qquad c = \delta - 1 = \frac{L^2}{3} - 1, \\ d = \alpha - \frac{1}{2}(\gamma + \delta)\epsilon = \frac{L^2}{72}(9 + 2L^2 - 18\lambda), \\ e = -\sigma + \frac{1}{2}(1 + \gamma\epsilon - \gamma\delta) = \frac{4 - 3L^2 + 6L^2\lambda}{8}. \end{aligned} \tag{54}$$

We recomputed the eigenvalues of Table I for the Cohen–Padé spring law. The results are given in Table II. Generally, the eigenvalues are somewhat closer to the Hookean ones, as would be expected.

V. PERTURBATION ANALYSIS FOR LARGE L^2

If L^2 is large, we may attempt a perturbation expansion. Expansion of Eq. (7) to the leading order leads to

TABLE II. Eigenvalues for the Cohen dumbbell.

L^2	**10**	**20**	∞
$l=0$	0	0	0
	−3.608	−2.751	−2
	−9.187	−6.448	−4
	−16.742	−11.111	−6
$l=1$	−1.372	−1.178	−1
	−5.956	−4.392	−3
	−12.521	−8.567	−5
$l=2$	−3.021	−2.495	−2
	−8.594	−6.179	−4
	−16.146	−10.834	−6

$$\frac{\partial \psi}{\partial t} = \Delta\psi + \nabla \cdot (\mathbf{R}(1 + |\mathbf{R}|^2/L^2)\psi). \tag{55}$$

Separating variables in spherical coordinates as before, we obtain the eigenvalue problem

$$\lambda\chi = \chi'' + 2\frac{\chi'}{r} - l(l+1)\frac{\chi}{r^2} + r\chi' + \frac{r^3}{L^2}\chi' + \left(3 + 5\frac{r^2}{L^2}\right)\chi. \tag{56}$$

Again, we set $\chi = \exp(-r^2/2)r^l v$, which leads us to

$$\lambda v = v'' + \frac{2+2l}{r}v' - rv' - lv + \frac{1}{L^2}((5+l)r^2 v - r^4 v + r^3 v'). \tag{57}$$

We now make the perturbation *ansatz*

$$v = v_0 + \frac{v_1}{L^2} + \cdots, \qquad \lambda = -l - 2n + \frac{\lambda_1}{L^2} + \cdots. \tag{58}$$

Then v_0 is given by Eq. (15) above, and v_1 must satisfy

$$\lambda_1 v_0 + (-l-2n)v_1 = v_1'' + \frac{2+2l}{r}v_1' - rv_1' - lv_1 + (5+l)r^2 v_0 - r^4 v_0 + r^3 v_0'. \tag{59}$$

The solution of this differential equation is in general quite complicated, but we can take advantage of the fact that v_0 is an even polynomial of degree $2n$. We may therefore look for a solution v_1 that is also an even polynomial of degree $2n+4$. We can then derive the expression for λ_1 by equating the coefficients of r^{2n+4}, r^{2n+2}, and r^{2n} in Eq. (59). We omit the algebra and give the result

$$\lambda_1 = -3l - 2l^2 - 8n - 12ln - 12n^2. \tag{60}$$

Table III gives the approximations for the eigenvalues in Table I computed using $\lambda = -l - 2n + \lambda_1/L^2$. We see that the approximation is quite good, even though the perturbation of the eigenvalues is not small.

For the Cohen spring, the perturbation is simply 2/3 of that for the Warner spring. The analogue of Table III is given below as Table IV.

TABLE III. Approximations for the eigenvalues in Table I computed by perturbation theory.

L^2	10	20	∞
$l=0$	0	0	0
	−4	−3	−2
	−10.4	−7.2	−4
	−19.2	−12.6	−6
$l=1$	−1.5	−1.25	−1
	−6.7	−4.85	−3
	−14.3	−9.65	−5
$l=2$	−3.4	−2.7	−2
	−9.8	−6.9	−4
	−18.6	−12.3	−6

VI. STRESS RELAXATION AND LINEAR VISCOELASTICITY

In this section, we discuss how the eigenfunctions determined above are used to obtain rheological information. Throughout, we shall use the dimensionless form of the equation. The spring force is given by $\mathbf{F} = q(r)\mathbf{R}$, where

$$q(r) = \begin{cases} \dfrac{1}{1 - r^2/L^2} & \text{for FENE,} \\ \dfrac{1 - r^2/(3L^2)}{1 - r^2/L^2} & \text{for Cohen} - \text{Pade.} \end{cases} \tag{61}$$

Moreover, $U(r)$ will denote the potential associated with the spring force, i.e., $\mathbf{F} = \nabla U$.

For each spherical harmonic Y_l^m, we have a sequence of eigenvalues λ_{ln} and corresponding eigenfunctions $\chi_{ln}(r)$. We shall count n starting from 0 to be consistent with our notation for the Hookean case. If there is no flow, then, in general, the distribution function ψ is a superposition of these eigenmodes

$$\psi(\mathbf{R}, t) = \sum_{l,m,n} c_{lmn}\chi_{ln}(r)Y_l^m(\theta, \phi)\exp(\lambda_{ln}t). \tag{62}$$

The functions χ_{ln} satisfy the orthogonality relation

TABLE IV. Approximations for the eigenvalues in Table II computed by perturbation theory.

L^2	10	20	∞
$l=0$	0	0	0
	−3.333	−2.667	−2
	−8.267	−6.133	−4
	−14.8	−10.4	−6
$l=1$	−1.333	−1.1675	−1
	−5.467	−4.233	−3
	−11.2	−8.1	−5
$l=2$	−2.933	−2.467	−2
	−7.867	−5.933	−4
	−14.4	−10.2	−6

$$\int_0^L r^2 \exp(U(r))\chi_{ln}(r)\chi_{lp}(r)\,dr = 0 \tag{63}$$

for $p \neq n$. We choose the χ_{ln} to be normalized so that

$$\int_0^L r^2 \exp(U(r))\chi_{ln}(r)^2\,dr = 1 \tag{64}$$

and we shall also choose the spherical harmonics to be normalized with respect to integration over the sphere ("standard" conventions in this regard vary according to discipline). If ψ satisfies the initial condition $\psi(\mathbf{R},0) = \psi_0(\mathbf{R})$, then we can determine the coefficients in Eq. (62) as

$$c_{lmn} = \int_0^L r^2 \exp(U(r))\chi_{ln}(r)\int_0^\pi \sin\theta \int_0^{2\pi} \psi_0(\mathbf{R})Y_l^m(\theta,\phi)\,d\phi\,d\theta\,dr. \tag{65}$$

Stress relaxation refers to the relaxation of stresses to equilibrium after the cessation of flow. Clearly, in this situation, ψ is given by an expression of the form [Eq. (62)]. The stress tensor is given by

$$\mathbf{T} = \int \mathbf{R}\mathbf{F}(\mathbf{R})\psi(\mathbf{R},t)\,d\mathbf{R}. \tag{66}$$

The dyadic product $\mathbf{RF}(\mathbf{R})$ is given by $r^2 q(r)\mathbf{M}(\theta,\phi)$, and the matrix $\mathbf{M}(\theta,\phi)$ involves only spherical harmonics of orders $l = 0$ and $l = 2$. Specifically,

$$\mathbf{M}(\theta,\phi) = \begin{pmatrix} \sin^2\theta\cos^2\phi & \sin^2\theta\cos\phi\sin\phi & \sin\theta\cos\theta\cos\phi \\ \sin^2\theta\cos\phi\sin\phi & \sin^2\theta\sin^2\phi & \sin\theta\cos\theta\sin\phi \\ \sin\theta\cos\theta\cos\phi & \sin\theta\cos\theta\sin\phi & \cos^2\theta \end{pmatrix}. \tag{67}$$

We consequently find, up to an isotropic term,

$$\mathbf{T} = \sum_{n=0}^{\infty}\sum_{m=-2}^{2} c_{2mn}\mathbf{M}_m \exp(\lambda_{2n}t)\int_0^L r^4 q(r)\chi_{ln}(r)\,dr, \tag{68}$$

where

$$\mathbf{M}_m = \int_0^\pi \sin\theta \int_0^{2\pi} \mathbf{M}(\theta,\phi)Y_2^m(\theta,\phi)\,d\phi\,d\theta. \tag{69}$$

The relaxation function for linear viscoelasticity can also be determined from the eigenfunctions. In the presence of a flow, the diffusion equation becomes

$$\frac{\partial\psi}{\partial t} = \Delta\psi + \nabla\cdot(\mathbf{F}(\mathbf{R})\psi) - \nabla\cdot((\nabla\mathbf{v})\mathbf{R}\psi). \tag{70}$$

To determine the linear viscoelastic response, we assume $\nabla\mathbf{v}$ is small, say of order ϵ, and then expand ψ up to first order in ϵ. We shall assume a shear flow of the form

$$\nabla\mathbf{v} = \epsilon\kappa(t)\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{71}$$

This leads to

$$\nabla \cdot ((\nabla \mathbf{v})\mathbf{R}\psi) = \epsilon\kappa(t)y\frac{\partial\psi}{\partial x}. \tag{72}$$

We now expand ψ as $\psi = \psi_0 + \epsilon\psi_1 + O(\epsilon^2)$. ψ_0 is simply the equilibrium distribution given by $\psi_0 = K\exp(-U(r))$, where K is a normalization constant. At the next order, ψ_1 satisfies the equation

$$\begin{aligned}-\frac{\partial\psi_1}{\partial t} + \Delta\psi_1 + \nabla\cdot(\mathbf{F}(\mathbf{R})\psi_1) &= \kappa(t)y\frac{\partial\psi_0}{\partial x} = \kappa(t)\frac{xy}{r}\frac{\partial\psi_0}{\partial r}\\ &= \kappa(t)r\sin^2\theta\sin\phi\cos\phi\frac{\partial\psi_0}{\partial r}.\end{aligned} \tag{73}$$

Next, we note that

$$\begin{aligned}\sin^2\theta\sin\phi\cos\phi &= \frac{1}{2}\sin^2\theta\sin(2\phi) = \frac{1}{4i}\sin^2\theta(e^{2i\phi} - e^{-2i\phi})\\ &= i\sqrt{2\pi/15}(Y_2^{-2}(\theta,\phi) - Y_2^2(\theta,\phi).\end{aligned} \tag{74}$$

The solution of Eq. (73) is now given by

$$\psi_1 = \sum_n (a_n(t)Y_2^2(\theta,\phi) + \overline{a_n(t)}Y_2^{-2}(\theta,\phi))\chi_{2n}(r), \tag{75}$$

where

$$-\dot{a}_n + \lambda_{2n}a_n = \kappa(t)b_n, \tag{76}$$

and

$$b_n = -i\sqrt{2\pi/15}\int_0^L \exp(U(r))r^3\frac{\partial\psi_0}{\partial r}\chi_{2n}(r)\,dr. \tag{77}$$

Consequently, we find

$$a_n(t) = -b_n\int_{-\infty}^t \exp(\lambda_{2n}(t-s))\kappa(s)\,ds. \tag{78}$$

The shear stress T_{12} is given by

$$\begin{aligned}T_{12}(t) &= \int r^2 q(r)\sin^2\theta\cos\phi\sin\phi\psi(\mathbf{R},t)\,d\mathbf{R}\\ &= i\sqrt{2\pi/15}\int r^2 q(r)(Y_2^{-2}(\theta,\phi) - Y_2^2(\theta,\phi))\psi(\mathbf{R},t)\,d\mathbf{R}\\ &= i\sqrt{2\pi/15}(\overline{a_n(t)} - a_n(t))\int_0^L r^4\chi_{2n}(r)q(r)\,dr.\end{aligned} \tag{79}$$

This finally yields the stress relaxation modulus

$$G(t) = \sum_n g_n\exp(\lambda_{2n}t), \tag{80}$$

where

$$g_n = -\frac{4\pi}{15}\int_0^L \exp(U(r))r^3 \frac{\partial \psi_0}{\partial r}\chi_{2n}(r)\,dr \int_0^L r^4 \chi_{2n}(r) q(r)\,dr$$
$$= \frac{4\pi}{15} K\left(\int_0^L r^4 \chi_{2n}(r) q(r)\,dr\right)^2. \tag{81}$$

For the Hookean case, the integrals can be evaluated analytically. We recover the well-known result that $g_0 = 1$ and $g_n = 0$ for all $n > 0$.

VII. CONCLUSIONS

We have examined the eigenvalue problem associated with the Fokker–Planck equation for FENE dumbbells. The eigenfunctions can be determined in terms of confluent Heun functions for the Warner spring as well as the Cohen–Padé spring. A perturbation solution for large L^2 has also been derived and has been found to do surprisingly well, especially for the Warner spring. On the other hand, the relaxation time predicted by the FENE-P model compares rather poorly with that of the full FENE model. The stress relaxation modulus for linear viscoelasticity has been expressed in terms of the eigenvalues and eigenfunctions. This provides an analytic procedure to determine the stress relaxation modulus without any need for Brownian dynamics simulations [see, e.g., Herrchen and Öttinger (1997)].

ACKNOWLEDGMENT

This research was supported by the National Science Foundation under Grant DMS-1008426.

References

Abramowitz, M., and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).

Bird, R. B., O. Hassager, R. C. Armstrong, and C. F. Curtiss, *Dynamics of Polymeric Liquids, Vol. 2: Kinetic Theory* (Wiley, New York, 1977).

Cohen, A., "A Padé approximant to the inverse Langevin function," Rheol. Acta **30**, 270–273 (1991).

Herrchen, M., and H. C. Öttinger, "A detailed comparison of various FENE dumbbell models," J. Non-Newtonian Fluid Mech. **68**, 17–42 (1997).

Ilg, P., I. V. Karlin, and S. Succi, "Supersymmetry solution for finitely extensible dumbbell model," Europhys. Lett. **51**, 355–360 (2000).

Lodge, A. S., and Y. Wu, "Constitutive equations for polymer solutions derived from the bead/spring model of Rouse and Zimm," Rheol. Acta **10**, 539–553 (1971).

Ronveaux, A., *Heun's Differential Equations* (Oxford University Press, Oxford, 1995).

Vincenzi, D., and E. Bodenschatz, "Single polymer dynamics in elongational flow and the confluent Heun equation," J. Phys. A **39**, 10691–10701 (2006).