

On the existence and uniqueness of solutions of the configurational probability diffusion equation for the generalized rigid dumbbell polymer model

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ABSTRACT. Kinetic phase-space theories (see [3]) have long been associated with successfully predicting the rheological properties of a variety of macromolecular fluids. Their cornerstone is the configurational probability density, essential to calculating the stress tensor. This function is a solution to the probability diffusion equation. In Section 2 we prove the existence and uniqueness of solutions to the corresponding evolutionary diffusion equation, in Section 3 to the stationary (time independent) equation; these problems, within the context of polymer dynamics theory, did not receive attention until now.

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1. Introduction

The macroscopic flow behavior of elastic liquids is strongly related to the fluid microscopic architecture and molecular interactions. This has been recognized since the early days of modern rheology. Consequently, scientists took on to obtaining constitutive relationships relating the stress tensor to molecular complexity. A very successful theory dealing with this difficult task is the kinetic (phase-space) one developed by Bird, Curtiss, Armstrong and Hassager and their collaborators in [3]

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(for some early kinetic model fundamentals see Kirkwood's [9]; for other accounts on this topic and related molecular theories see e.g. [1], [8], [10], [11], [12], [13], [14] and [15]). It has been applied to model and predict rheological properties of both polymer solutions and undiluted (including mixtures of) polymers.

The polymer chains are modeled either as spring-bead or rod-bead mechanical systems subjected to hydrodynamic, Brownian, intra-molecular interactions in the phase space. Statistical mechanics techniques (averages and projections) reduce the problem of the multi-chain liquid to the configuration space of a single macromolecule.

One of the salient ingredients in the polymer mean-field theories is the configuration (probability) distribution function, with the help of which the stress tensor is calculated. This function is actually the solution to diffusion equations (see equation 19.3-26 on page 322 and equation 19.5-1 on page 328 in [3]) pertaining to the (large) family of Fokker-Planck-Smoluchowski partial differential equations (PDEs). In [3] series expansion solutions are obtained.

We undertake to proving the existence and uniqueness of solutions to the fore-mentioned PDEs obeying physically meaningful initial boundary conditions, an issue that has not been addressed as yet. This work consists of two parts. Section 2 is devoted to the evolutionary (i.e. time dependent) boundary value problem and a procedure based on the Galerkin approximation is used. In Section 3 we prove the existence, uniqueness and positivity of a stationary solution. The proof uses the Krein-Rutman theory (see also [5] and [4] for related works on a diluted polymer FENE model and a neuroscience model respectively).

2. Evolutionary boundary value problems

2.1. The boundary value problems. The problems we study describe the configurational dynamics of polymer melts made up of Kramers chains. Specifically, each macromolecule is assimilated to a finite succession of freely jointed rods; the orientation of each rod is given by the unitary vector $x \in \mathbb{R}^3$. The macromolecule mass is concentrated on "beads" located at the joints. For full details see Chap. 19 in [3].

Let the unit sphere be denoted $S_2 := \{x \in \mathbb{R}^3 \text{ s.t. } \|x\|_2 = 1\}$. In the following we denote by "∇" the gradient on the sphere S_2 .

The first boundary value problem (referred to subsequently as P-1) reads:

Problem 1

Find $\tilde{\psi} : S_2 \times [0, +\infty[\rightarrow \mathbb{R}$, with $\tilde{\psi}(x, t)$ solution to

$$(2.1) \quad \frac{\partial \tilde{\psi}}{\partial t} - \alpha \nabla \cdot (\nabla \tilde{\psi}) + \nabla \cdot (\tilde{a}(x) \tilde{\psi}) = 0, \quad x \in S_2, \quad t > 0$$

$$(2.2) \quad \tilde{\psi} \geq 0$$

$$(2.3) \quad \int_{S_2} \tilde{\psi}(x, t) dx = 1, \quad \forall t \geq 0$$

$$(2.4) \quad \tilde{\psi}(x, 0) = \tilde{\psi}_0(x)$$

where $\alpha > 0$ is a given, fluid related, parameter, and $\tilde{a} : \mathbb{R}^3 \rightarrow \mathbb{R}^3$, $\tilde{\psi}_0 : S_2 \rightarrow \mathbb{R}$, $\tilde{\psi}_0 \geq 0$, are known functions (the later being an initial - or equilibrium - probability distribution). Moreover, $\int_{S_2} \tilde{\psi}_0(x) dx = 1$. With our notations, this problem is

basically equation 19.5-1 on page 328 in [3].

The second boundary value problem (referred to subsequently as P-2) reads:

Problem 2

Find $\tilde{\psi} : S_2 \times]0, 1[\times]0, +\infty[\rightarrow \mathbb{R}$, with $\tilde{\psi}(x, \sigma, t)$ solution to

$$(2.5) \quad \frac{\partial \tilde{\psi}}{\partial t} - \alpha_1 \frac{\partial^2 \tilde{\psi}}{\partial \sigma^2} - \alpha_2 \nabla \cdot (\nabla \tilde{\psi}) + \nabla \cdot (\tilde{a}(x) \tilde{\psi}) = 0, \quad x \in S_2, \quad \sigma \in]0, 1[, \quad t > 0$$

$$(2.6) \quad \tilde{\psi} \geq 0$$

$$(2.7) \quad \int_{S_2} \tilde{\psi}(x, \sigma, t) dx = 1, \quad \forall \sigma \in]0, 1[, \quad \forall t > 0$$

$$(2.8) \quad \tilde{\psi}|_{\sigma \in \{0,1\}} = \frac{1}{4\pi}$$

$$(2.9) \quad \tilde{\psi}(x, \sigma, 0) = \tilde{\psi}_0^\sigma(x, \sigma), \quad \forall x \in S_2, \quad \forall \sigma \in]0, 1[$$

where $\alpha_1, \alpha_2 > 0$ are given, fluid related, parameters and $\tilde{a} : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is a known function. Next, $\tilde{\psi}_0^\sigma : S_2 \times]0, 1[\rightarrow \mathbb{R}$, $\tilde{\psi}_0^\sigma \geq 0$, is the known initial configurational probability; it is such that $\int_{\Omega_2} \tilde{\psi}_0^\sigma(x) dx = 1$, $\forall \sigma \in]0, 1[$. With our notations, this problem is basically equation 19.3-26 on page 322 in [3].

In the following, for both P-1 and P-2, we assume that the following general hypothesis holds true:

(H): $\tilde{a} \in \mathcal{C}^\infty(V)$ and $\tilde{a} \cdot x = 0$ for all $x \in S_2$, where $V \subset \mathbb{R}^3$ is a neighborhood of S_2 .

We shall make use of the short hand notation $xx = x \otimes x$. As customary in engineering/applied mathematics literature, a dot “ \cdot ” stands for summation over one repeated (dummy) index, “ $:$ ” for summation over two repeated indices. For rigid dumbbell molecules, $\tilde{a} = A \cdot x - A : xxx$, where A is a 3×3 matrix, henceforth compliance with hypothesis (H) is ensured.

From [2] we observe, in the case of spherical coordinates, that:

$$\nabla := e_\theta \frac{\partial}{\partial \theta} + e_\phi \frac{1}{\sin \theta} \frac{\partial}{\partial \phi}$$

$$\nabla \cdot \nabla = \Delta := \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

Moreover, for any vector \tilde{b} such that $\tilde{b} \cdot x = 0$, denoting $b_1 = \tilde{b} \cdot e_\theta$ and $b_2 = \tilde{b} \cdot e_\phi$, one has

$$\nabla \cdot (\tilde{b}f) = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (b_1 f \sin \theta) + \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} (b_2 f)$$

Let us now denote

$$D =]0, \pi[\times]0, 2\pi[$$

and

$$D_\sigma = D \times]0, 1[.$$

Making use of the above results, one may now re-state problems P-1 and P-2 in the following way:

Problem 1

Search for solutions $\psi : D \times [0, +\infty[\rightarrow \mathbb{R}$ to the following initial-boundary value problem:

$$(2.10) \quad \frac{\partial \psi}{\partial t} - \alpha \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (a_1 \sin \theta \psi) + \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} (a_2 \psi) = 0, \quad (\theta, \phi) \in D, t > 0$$

$$(2.11) \quad \psi \text{ is a } \phi - \text{periodic function, of period } 2\pi$$

$$(2.12) \quad \psi \geq 0$$

$$(2.13) \quad \int_D \psi \sin \theta d\theta d\phi = 1, \quad \forall t > 0$$

$$(2.14) \quad \psi(\theta, \phi, 0) = \psi_0(\theta, \phi)$$

where ψ_0 satisfies

$$(2.15) \quad \psi_0 \geq 0, \quad \int_D \psi_0 \sin \theta d\theta d\phi = 1$$

Problem 2

Search for solutions $\psi : D_\sigma \times [0, +\infty[\rightarrow \mathbb{R}$ to the following initial-boundary value problem:

$$(2.16) \quad \frac{\partial \psi}{\partial t} - \alpha_1 \frac{\partial^2 \psi}{\partial \sigma^2} - \alpha_2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (a_1 \sin \theta \psi) + \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} (a_2 \psi) = 0, \quad (\theta, \phi) \in D, t > 0$$

$$(2.17) \quad \psi \text{ is a } \phi - \text{periodic function, of period } 2\pi$$

$$(2.18) \quad \psi \geq 0$$

$$(2.19) \quad \int_D \psi \sin \theta d\theta d\phi = 1, \quad \forall t > 0, \forall \sigma \in]0, 1[$$

$$(2.20) \quad \psi|_{\sigma \in \{0,1\}} = \frac{1}{4\pi}$$

$$(2.21) \quad \psi(\theta, \phi, t = 0) = \psi_0^\sigma(\theta, \phi, \sigma)$$

where ψ_0^σ satisfies

$$(2.22) \quad \psi_0^\sigma \geq 0, \quad \int_D \psi_0^\sigma \sin \theta d\theta d\phi = 1$$

In the above we made use of the following notations: $a_1 = a \cdot e_\theta$, $a_2 = a \cdot e_\phi$.

2.2. Functional spaces framework.

2.2.1. *Functional spaces for problem P-1.* Let the following Hilbert spaces:

$$L_s^2(D) := \left\{ v \in L_{\text{loc}}^1(D) \text{ s.t. } \int_D v^2 \sin \theta d\theta d\phi < \infty \right\},$$

$$H_s^1(D) := \left\{ v \in L_{\text{loc}}^1(D) \text{ s.t. } v \text{ periodic w.r.t. } \phi, \int_D \left(\sin \theta \left| \frac{\partial v}{\partial \theta} \right|^2 + \frac{1}{\sin \theta} \left| \frac{\partial v}{\partial \phi} \right|^2 + v^2 \sin \theta \right) d\theta d\phi < \infty \right\}$$

Notice the continuous, dense inclusions:

$$H_s^1(D) \underset{\text{cont.}}{\subset} L_s^2(D) = (L_s^2(D))' \underset{\text{cont.}}{\subset} (H_s^1(D))'$$

Let now the linear operators be defined as following: $A_1 : H_s^1(D) \rightarrow (H_s^1(D))'$, such that $\langle A_1 u, v \rangle = \alpha \int_D \left(\sin \theta \frac{\partial u}{\partial \theta} \frac{\partial v}{\partial \theta} + \frac{1}{\sin \theta} \frac{\partial u}{\partial \phi} \frac{\partial v}{\partial \phi} \right) d\theta d\phi$, $\forall u, v \in H_s^1$, and $B_1 : L_s^2(D) \rightarrow (H_s^1(D))'$, such that $\langle B_1 u, v \rangle = - \int_D \left(\sin \theta u \frac{\partial v}{\partial \theta} + a_2 u \frac{\partial v}{\partial \phi} \right) d\theta d\phi$. Then, multiplying formally (2.10) by $v \sin \theta$, with v arbitrary in $H_s^1(D)$, and integrating on D we deduce that P-1 can be written in variational form as

$$(2.23) \quad \frac{d\psi}{dt} + A_1 \psi + B_1 \psi = 0$$

$$(2.24) \quad \psi(t = 0) = \psi_0$$

In the above, ψ must be positive, $\psi \geq 0$, and such that $\int_D \psi \sin \theta d\theta d\phi = 1$.

2.2.2. *Functional spaces for problem P-2.* Let the following Hilbert spaces $L_s^2(D_\sigma)$ and $H_{s0}^2(D_\sigma)$ be defined as (with $dD_\sigma = d\theta d\phi d\sigma$)

$$L_s^2(D_\sigma) := \left\{ v \in L_{\text{loc}}^1(D_\sigma) \text{ s.t. } \int_{D_\sigma} v^2 \sin \theta dD_\sigma < \infty \right\}$$

$$H_{s0}^1(D_\sigma) := \left\{ v \in L_{\text{loc}}^1(D_\sigma) \text{ s.t. } v \text{ periodic w.r.t. } \phi, v(\sigma = 0) = v(\sigma = 1) = 0, \int_{D_\sigma} \left[\sin \theta \left(\frac{\partial v}{\partial \sigma} \right)^2 + \sin \theta \left(\frac{\partial v}{\partial \theta} \right)^2 + \frac{1}{\sin \theta} \left(\frac{\partial v}{\partial \phi} \right)^2 + v^2 \sin \theta \right] dD_\sigma < \infty \right\}$$

Notice the continuous, dense inclusions:

$$H_{s0}^1(D_\sigma) \underset{\text{cont.}}{\subset} L_s^2(D_\sigma) = (L_s^2(D_\sigma))' \underset{\text{cont.}}{\subset} (H_{s0}^1(D_\sigma))'$$

Let now the linear operators be defined as following:

$$A_2 : H_{s0}^1(D_\sigma) \rightarrow (H_{s0}^1(D_\sigma))'$$

such that

$$\langle A_2 u, v \rangle = \alpha_1 \int_{D_\sigma} \left(\sin \theta \frac{\partial u}{\partial \theta} \frac{\partial v}{\partial \theta} + \frac{1}{\sin \theta} \frac{\partial u}{\partial \phi} \frac{\partial v}{\partial \phi} \right) dD_\sigma + \alpha_2 \int_{D_\sigma} \sin \theta \frac{\partial u}{\partial \sigma} \frac{\partial v}{\partial \sigma} dD_\sigma,$$

and

$$B_2 : L_s^2(D_\sigma) \rightarrow (H_{s0}^1(D_\sigma))'$$

such that

$$\langle B_2 u, v \rangle = - \int_{D_\sigma} \left(\sin \theta u \frac{\partial v}{\partial \theta} + a_2 u \frac{\partial v}{\partial \phi} \right) d\theta d\phi.$$

Next, let

$$(2.25) \quad \psi = \frac{1}{4\pi} + \bar{\psi}$$

Then, P-2 can be stated as: find $\bar{\psi} : [0, +\infty[\rightarrow H_{s0}^1(D_\sigma)$ solution to the variational problem expressed as

$$(2.26) \quad \frac{d\bar{\psi}}{dt} + A_2\bar{\psi} + B_2\bar{\psi} = f$$

$$(2.27) \quad \bar{\psi}(t=0) = \psi_0^\sigma - \frac{1}{4\pi}$$

$$(2.28) \quad \frac{1}{4\pi} + \bar{\psi} \geq 0$$

$$(2.29) \quad \int_D \bar{\psi} \sin \theta d\theta d\phi = 0, \forall \sigma \in [0, 1], \forall t$$

where $\langle f, v \rangle = \frac{1}{4\pi} \int_D \left(a_1 \sin \theta \frac{\partial v}{\partial \theta} + a_2 \frac{\partial v}{\partial \phi} \right) dD_\sigma, \forall v \in H_{s0}^1(D_\sigma)$. Moreover, with r, θ, ϕ being the spherical coordinates of a position vector x , denote

$$\Omega := \{x \in \mathbb{R}^3, 1 < r < 2\},$$

and Ω_σ the 4-dimensional domain

$$\Omega_\sigma := \{(x, \sigma) \in \mathbb{R}^3 \times]0, 1[, 1 < r < 2\},$$

and

$$V_\sigma := \{u \in H^1(\Omega_\sigma), u(\sigma=0) = u(\sigma=1) = 0\}.$$

REMARK 2.1. Any function $u(\theta, \Phi)$ defined in D can be viewed as a function defined in Ω independent on r .

Let us now prove the first result of this Section.

PROPOSITION 2.1. (i) $u \in L_s^2(D) \Leftrightarrow u \in L^2(\Omega)$ and u independent of r ; moreover

$$\|u\|_{L_s^2(D)} \leq \|u\|_{L^2(\Omega)} \leq 2\|u\|_{L_s^2(D)}.$$

(ii) $u \in H_s^1(D) \Leftrightarrow u \in H^1(\Omega)$ and u independent of r ; moreover

$$\frac{1}{2}\|u\|_{H_s^1(D)} \leq \|u\|_{H^1(\Omega)} \leq 2\|u\|_{H^1(\Omega)}.$$

(iii) $u \in L_s^2(D_\sigma) \Leftrightarrow u \in L^2(\Omega_\sigma)$ and u independent of r ; moreover

$$\|u\|_{L^2(D_\sigma)} \leq \|u\|_{L^2(\Omega_\sigma)} \leq 2\|u\|_{L^2(D_\sigma)}.$$

(iv) $u \in H_{s0}^1(D_\sigma) \Leftrightarrow u \in V_\sigma$ and u independent of r ; moreover

$$\frac{1}{2}\|u\|_{H_{s0}^1(D_\sigma)} \leq \|u\|_{H^1(\Omega_\sigma)} \leq 2\|u\|_{H_{s0}^1(D_\sigma)}.$$

PROOF. The proof of the above statements is a direct consequence of the following formulae

$$\|u\|_{L^2(\Omega)}^2 = \int_D \int_0^1 |u|^2 r^2 \sin \theta dr d\theta d\phi$$

$$\|u\|_{H^1(\Omega)}^2 = \int_D \int_0^1 \left[\frac{1}{r^2} \left(\frac{\partial u}{\partial \theta} \right)^2 + \frac{1}{r^2 \sin^2 \theta} \left(\frac{\partial u}{\partial \phi} \right)^2 + u^2 \right] r^2 \sin \theta dr d\theta d\phi$$

$$\begin{aligned} \|u\|_{L^2(\Omega_\sigma)}^2 &= \int_D \int_0^1 \int_0^1 |u|^2 r^2 \sin \theta dr d\theta d\phi d\sigma \\ \|u\|_{H^1(\Omega_\sigma)}^2 &= \int_D \int_0^1 \int_0^1 \left[\left(\frac{\partial u}{\partial \sigma} \right)^2 + \frac{1}{r^2} \left(\frac{\partial u}{\partial \theta} \right)^2 + \frac{1}{r^2 \sin^2 \theta} \left(\frac{\partial u}{\partial \phi} \right)^2 + u^2 \right] \\ &\quad r^2 \sin \theta dr d\theta d\phi d\sigma \end{aligned}$$

□

Before ending this Section, we prove the following:

PROPOSITION 2.2. *The inclusions $H_s^1(D) \subset L_s^2(D)$ and $H_{s_0}^1(D_\sigma) \subset L_s^2(D_\sigma)$ are compact.*

PROOF. We focus on proving the first inclusion as the proof for the second one is similar in nature.

Let u_n be a bounded sequence of elements of $H_s^1(D)$, then u_n is bounded in $H^1(\Omega)$. Invoking the compact inclusion $H^1(\Omega) \subset L^2(\Omega)$, we get the existence of an element $u \in H^1(\Omega)$ and of a sub-sequence of u_n - for convenience also denoted u_n - such that $u_n \xrightarrow{n \rightarrow \infty} u$ in $H^1(\Omega)$, and $u_n \xrightarrow{n \rightarrow \infty} u$ in $L^2(\Omega)$. Moreover $\frac{\partial u_n}{\partial r} \xrightarrow{n \rightarrow \infty} \frac{\partial u}{\partial r}$ in $L^2(\Omega)$. As $\frac{\partial u_n}{\partial r} = 0$, this gives $\frac{\partial u}{\partial r} = 0$, henceforth $u = u(\theta, \phi)$. Then $u \in L_s^2(D)$ and $u_n \xrightarrow{n \rightarrow \infty} u$ in $L^2(\Omega)$.

□

2.3. Evolutionary boundary value problems: existence and uniqueness results. Observe first that for any $\beta > 0$ the operator $A_1 + \beta \text{Id}$ is invertible and its inverse maps $(H_s^1(D))'$ onto $H_s^1(D)$.

As the inclusion $H_s^1(D) \subset L_s^2(D)$ is compact, one deduces the existence of a sequence of eigenvectors of A_1 , i.e. $0 \leq \lambda_1^1 \leq \lambda_2^1 \leq \dots \leq \lambda_k^1 \leq \dots \rightarrow +\infty$, and that of an orthonormal basis for the space $L_s^2(D)$ consisting of eigenvectors $\varphi_1^1, \varphi_2^1 \dots \varphi_k^1 \dots$. Invoking arguments similar in nature one deduces the existence of a sequence of eigenvectors of A_2 , i.e. $0 \leq \lambda_1^2 \leq \lambda_2^2 \leq \dots \leq \lambda_k^2 \leq \dots \rightarrow +\infty$, and that of an orthonormal basis for the space $L_s^2(D_\sigma)$ consisting of eigenvectors $\varphi_1^2, \varphi_2^2 \dots \varphi_k^2 \dots$.

One has the following result:

THEOREM 2.1. *Let $\psi_0 \in L_s^2(D)$, $T > 0$. There exists a unique solution ψ to equations (2.23)-(2.24), s.t. $\psi \in L^2(0, T; H_s^1(D)) \cap \mathcal{C}^0(0, T; L_s^2(D))$ and $\frac{d\psi}{dt} \in L^2(0, T; (H_s^1(D))')$. In addition, whenever ψ_0 obeys (2.15), ψ also solves (2.12)-(2.13).*

PROOF. Multiply (2.10) by $\psi \sin(\theta)$ and integrate on D . It entails:

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\psi\|_{L_s^2}^2 + \alpha \int_D \left[\left(\frac{\partial \psi}{\partial \theta} \right)^2 \sin \theta + \frac{1}{\sin \theta} \left(\frac{\partial \psi}{\partial \phi} \right)^2 \right] d\theta d\phi \\ - \int_D \left(a_1 \psi \frac{\partial \psi}{\partial \theta} \sin \theta + a_2 \psi \frac{\partial \psi}{\partial \phi} \right) d\theta d\phi = 0 \end{aligned}$$

Since:

$$(2.30) \quad \int_D a_1 \psi \frac{\partial \psi}{\partial \theta} \sin \theta d\theta d\phi \leq \frac{\alpha}{2} \int_D \left(\frac{\partial \psi}{\partial \theta} \right)^2 \sin \theta d\theta d\phi + \frac{1}{2\alpha} \int_D a_1^2 \psi^2 \sin \theta d\theta d\phi$$

$$(2.31) \quad \int_D a_2 \psi \frac{\partial \psi}{\partial \phi} d\theta d\phi \leq \frac{\alpha}{2} \int_D \frac{1}{\sin \theta} \left(\frac{\partial \psi}{\partial \phi} \right)^2 d\theta d\phi + \frac{1}{2\alpha} \int_D a_2^2 \psi^2 \sin \theta d\theta d\phi$$

as $a_1, a_2 \in L^\infty(D)$, the above estimates lead to:

$$(2.32) \quad \frac{d}{dt} \|\psi\|_{L_s^2}^2 + \alpha \|\psi\|_{H_s^1}^2 \leq c \|\psi\|_{L_s^2}^2$$

where $c > 0$. Further on, making use of Gronwall's inequality, one gets:

$$(2.33) \quad \|\psi(t)\|_{L_s^2} \leq \|\psi_0\|_{L_s^2} e^{cT/2}, \quad \forall t \in [0, T]$$

$$(2.34) \quad \|\psi(t)\|_{L^2(0, T; H_s^1)} \leq \frac{1}{\alpha} \left(\|\psi_0\|_{L_s^2}^2 + cT \|\psi_0\|_{L_s^2}^2 e^{cT} \right)$$

The rest of the proof is classical in the sense we use the Galerkin's method to obtain an approximate solution $\psi^n = \sum_{k=1}^n \gamma_k(t) \varphi_k^1$. Next, estimates similar in nature to those in equations (2.33)-(2.34) can be easily obtained. Letting $n \rightarrow +\infty$ leads to the result.

Taking now as test function $\varphi = 1$ in (2.23), invoking $\langle A_1 \psi, 1 \rangle = 0$, $\langle B_1 \psi, 1 \rangle = 0$, leads to

$$(2.35) \quad \frac{d}{dt} \int_D \psi \sin \theta d\theta d\phi = 0$$

from which one infers $\int_D \psi \sin \theta d\theta d\phi = \int_D \psi_0 \sin \theta d\theta d\phi = 1$.

Next, denote $\psi^+ = \max\{\psi, 0\}$, $\psi^- = -\min\{\psi, 0\}$, $\psi = \psi^+ - \psi^-$. Apply (2.23) to ψ^- . It gives $-\frac{1}{2} \frac{d}{dt} |\psi^-|^2 - \langle A_1 \psi^-, \psi^- \rangle + \langle B_1 \psi^-, \psi^- \rangle = 0$. We easily obtain (2.33) with ψ^- in the place of ψ . As $\psi_0^- = 0$, it follows $\psi^- = 0$, and hence $\psi \geq 0$. \square

For P-2 we have the following existence and uniqueness result:

THEOREM 2.2. *Let $\psi_0 \in L_s^2(D_\sigma)$, $T > 0$. Then there exists a unique solution $\bar{\psi}$ to equations (2.25)-(2.26) s.t. $\bar{\psi} \in L^2(0, T; H_{s_0}^1(D_\sigma)) \cap \mathcal{C}([0, T]; L_s^2(D_\sigma))$ and $\frac{d\bar{\psi}}{dt} \in L^2(0, T; (H_{s_0}^1(D_\sigma))')$. In addition, whenever ψ_0^σ solves (2.22), $\bar{\psi}$ solves (2.28)-(2.29).*

PROOF. The proof of the existence and uniqueness result is similar to that of Theorem 2.1.

Let us now prove that $\psi \equiv \frac{1}{4\pi} + \bar{\psi} \geq 0$. Applying (2.26) to

$$\psi^- \in L^2(0, T; H_{s_0}^1(D_\sigma))$$

we obtain

$$\left\langle \frac{d\psi}{dt}, \psi^- \right\rangle + \alpha_1 \int_{D_\sigma} \left(\frac{\partial\psi}{\partial\theta} \frac{\partial\psi^-}{\partial\theta} \sin\theta + \frac{1}{\sin\theta} \frac{\partial\psi}{\partial\phi} \frac{\partial\psi^-}{\partial\phi} \right) dD_\sigma + \alpha_2 \int_{D_\sigma} \frac{\partial\psi}{\partial\sigma} \frac{\partial\psi^-}{\partial\sigma} \sin\theta dD_\sigma - \int_{D_\sigma} \left(a_1\psi \frac{\partial\psi^-}{\partial\theta} \sin\theta + a_2\psi \frac{\partial\psi^-}{\partial\phi} \right) dD_\sigma = 0.$$

The above leads, as in Theorem 2.1, to $\psi^- = 0$, that is $\psi \geq 0$.

In order to prove (2.29), consider in (2.26) an arbitrary test function $\varphi \in H_0^1(]0, 1[)$, with φ depending uniquely on σ . Denote $\tilde{\psi} := \int_D \bar{\psi} \sin\theta d\theta d\phi$. Then $\left\langle \frac{d\tilde{\psi}}{dt}, \varphi \right\rangle + \alpha_2 \int_0^1 \frac{\partial\tilde{\psi}}{\partial\sigma} \frac{\partial\varphi}{\partial\sigma} d\sigma = 0$, where $\tilde{\psi} \in L^2(0, T; H_0^1(]0, 1[))$, $\tilde{\psi}(t = 0) = 0$. This eventually gives $\tilde{\psi} = 0$ and (2.29) is proved. □

2.4. Connection between the two probability configuration equations.

Denote ψ the solution to problem P-1, and ψ_σ the solution to problem P-2. Let also $\psi_\sigma = \frac{1}{4\pi} + \bar{\psi}_\sigma$. From now on we take $\alpha = \alpha_2$.

We shall prove in the following that $\bar{\psi}_\sigma$ can be Fourier expanded as following:

$$(2.36) \quad \bar{\psi}_\sigma(t, \theta, \phi, \sigma) = \sum_{n=1}^{\infty} \sin(n\pi\sigma) g_n(t, \theta, \phi)$$

where g_n is to be found.

Observe that $1 = \sum_{n=1}^{\infty} d_n \sin(n\pi\sigma)$, with $d_n = 2 \int_0^1 \sin(n\pi\sigma) d\sigma$. Moreover, $d_n = 0$ for n even, and $d_n = \frac{4}{n\pi}$ for n odd.

Let $\bar{\psi}_\sigma^n$ given by

$$(2.37) \quad \bar{\psi}_\sigma^n = \sum_{k=1}^n \sin(k\pi\sigma) g_k(t, \theta, \phi)$$

denote an approximation for $\bar{\psi}_\sigma$ for n large enough, where $\bar{\psi}_\sigma^n$ solves

$$(2.38) \quad \frac{d}{dt} \bar{\psi}_\sigma^n + A_2 \bar{\psi}_\sigma^n + B_2 \bar{\psi}_\sigma^n = f \sum_{k=1}^n d_k \sin(k\pi\sigma)$$

$$(2.39) \quad \bar{\psi}_\sigma^n(t = 0) = \sum_{k=1}^n g_{0k} \sin(k\pi\sigma)$$

where g_{0k} is given in equation (2.44) below.

Remark that

$$(2.40) \quad A_2 \bar{\psi}_\sigma^n = \alpha_1 \sum_{k=1}^n k^2 \pi^2 \sin(k\pi\sigma) g_k(t, \theta, \phi) + \sum_{k=1}^n \sin(k\pi\sigma) A_1(g_k)$$

$$(2.41) \quad B_2 \overline{\psi_\sigma^n} = \sum_{k=1}^n \sin(k\pi\sigma) B_1(g_k)$$

From equations (2.38)-(2.41) above one concludes the g_k functions are solutions to the following problem: find $g_k \in L^2(0, T; H_s^1(D)) \cap \mathcal{C}^0([0, T]; L_s^2(D))$ s.t.

$$(2.42) \quad \frac{\partial g_k}{\partial t} + \alpha_1 k^2 \pi^2 g_k + A_1(g_k) + B_1(g_k) = d_k f$$

$$(2.43) \quad g_k(0) = g_{0k}$$

$$(2.44) \quad g_{0k} = 2 \int_0^1 \left(\overline{\psi_0^\sigma} - \frac{1}{4\pi} \right) \sin(k\pi\sigma) d\sigma$$

We now prove the following result:

THEOREM 2.3. *Let $T > 0$. Assume the initial data $\overline{\psi_0^\sigma}$ is such that $\|g_{0k}\|_{L_s^2} \leq \frac{c}{k^2}$, with c independent of k . Then $\overline{\psi_\sigma^n} \xrightarrow{n \rightarrow \infty} \overline{\psi_\sigma}$ in*

$$L^2(0, T; H_{s0}^1(D_\sigma)) \cap L^\infty(0, T; L_s^2(D_\sigma)).$$

PROOF. Existence and uniqueness of solutions to the problem given in equations (2.42)-(2.43) is easily proved as in Theorem 2.1. Applying (2.42) to g_k one gets:

$$(2.45) \quad \frac{1}{2} \frac{d}{dt} \|g_k\|_{L_s^2}^2 + \alpha_1 k^2 \pi^2 \|g_k\|_{L_s^2}^2 + \langle A_1 g_k, g_k \rangle + \langle B_1 g_k, g_k \rangle = d_k \langle f, g_k \rangle$$

However, there exists $\gamma > 0$ s.t.

$$(2.46) \quad \langle A_1 g_k, g_k \rangle + \langle B_1 g_k, g_k \rangle + \gamma \|g_k\|_{L_s^2}^2 \geq \alpha_2 \|g_k\|_{H_s^1}^2$$

from which one infers

$$(2.47) \quad \frac{1}{2} \frac{d}{dt} \|g_k\|_{L_s^2}^2 + (\alpha_1 k^2 \pi^2 - \gamma) \|g_k\|_{L_s^2}^2 + \alpha_2 \|g_k\|_{H_s^1}^2 \leq d_k \langle f, g_k \rangle$$

Further on, using the result for d_n previously obtained, we give for k large enough:

$$(2.48) \quad d_k \langle f, g_k \rangle \leq \frac{4}{k\pi} \|f\|_{L_s^2}^2 \|g_k\|_{L_s^2}^2 \leq \frac{1}{2} (\alpha_1 k^2 \pi^2 - \gamma) \|g_k\|_{L_s^2}^2 + \frac{8 \|f\|_{L_s^2}^2}{2k^2 \pi^2 (\alpha_1 k^2 \pi^2 - \gamma)}$$

From (2.47) one deduces there exists $c > 0$ s.t.

$$(2.49) \quad \frac{d}{dt} \|g_k\|_{L_s^2}^2 + (\alpha_1 k^2 \pi^2 - \gamma) \|g_k\|_{L_s^2}^2 + 2\alpha_2 \|g_k\|_{H_s^1}^2 \leq \frac{c}{k^4}$$

from which, upon integration from 0 to T , it gives

$$(2.50) \quad \|g_k\|_{L^\infty(0,T;L_s^2)}^2 + \|g_k\|_{L^2(0,T;H_s^1)}^2 \leq \frac{c}{k^4}$$

$$(2.51) \quad \|g_k\|_{L^\infty(0,T;L_s^2)}^2 \leq \frac{c}{k^6}$$

Next, from equation (2.37) one gets:

$$(2.52) \quad \|\overline{\psi_\sigma^n}\|_{L_s^2(D_\sigma)}^2 = \frac{1}{2} \int_{D_\sigma} \int_0^1 \left| \sum_{k=1}^n \sin(k\pi\sigma) g_k(t, \theta, \phi) \right|^2 \sin \theta d\sigma d\theta d\phi = \frac{1}{2} \sum_{k=1}^n \|g_k\|_{L_s^2(D)}^2$$

In a similar way one obtains that

$$(2.53) \quad \left\| \frac{\partial}{\partial \sigma} \overline{\psi_\sigma^n} \right\|_{L_s^2(D_\sigma)}^2 = \frac{\pi^2}{2} \sum_{k=1}^n k^2 \|g_k\|_{L_s^2(D)}^2$$

Therefore

$$(2.54) \quad \|\overline{\psi_\sigma^n}\|_{H_{s0}^1(D_\sigma)}^2 \leq c \sum_{k=1}^n k^2 \|g_k\|_{L_s^2(D)}^2$$

As $\sum_{k=1}^{+\infty} \frac{1}{k^2}$ is convergent, invoking equations (2.50)-(2.51) one observes that $\|\overline{\psi_\sigma^n}\|_{L^\infty(0,T;L_s^2(D_\sigma))}$ and $\|\overline{\psi_\sigma^n}\|_{L^2(0,T;H_{s0}^1(D_\sigma))}$ are bounded and independent of n . Therefore, there exists $\xi \in L^\infty(0,T;L_s^2(D_\sigma)) \cap L^2(0,T;H_{s0}^1(D_\sigma))$ s.t. $\overline{\psi_\sigma^n} \xrightarrow{n \rightarrow +\infty} \xi$ weakly.

Taking the limit $n \rightarrow +\infty$ in equation (2.38) and using the uniqueness of the solution to the problem P-2 leads to $\overline{\psi_\sigma} = \xi$. □

One can now state that

$$(2.55) \quad \overline{\psi_\sigma} = \sum_{k=1}^{\infty} g_n \sin(n\pi\sigma)$$

Before ending this Section we shall establish several connections between this work results and those in Section 19.5 in [3].

Let us first notice that $f = -\frac{B_1(1)}{4\pi}$. Let $\eta_k = g_k + \frac{d_k}{4\pi}$. From equations (2.42)-(2.43) it follows that η_k solves

$$\frac{\partial \eta_k}{\partial t} + \alpha_1 k^2 \pi^2 \left(\eta_k - \frac{d_k}{4\pi} \right) + A_1 \eta_k + B_1 \eta_k = 0$$

$$\eta_k(0) = g_{k0} + \frac{d_k}{4\pi}$$

Therefore one has:

$$(2.56) \quad \frac{\partial \eta_k}{\partial t} + \alpha_1 k^2 \pi^2 \eta_k + A_1 \eta_k + B_1 \eta_k = \frac{\alpha_1 k^2 \pi d_k}{4}$$

$$(2.57) \quad \eta_k(0) = \eta_{0k} = 2 \int_0^1 \psi_0^\sigma \sin(k\pi\sigma) d\sigma$$

Since $\sum_{k=1}^{\infty} \frac{d_k}{4\pi} \sin(k\pi\sigma) = \frac{1}{4\pi}$, by equation (2.55) one obtains

$$(2.58) \quad \psi_\sigma = \sum_{n=1}^{\infty} \eta_n \sin(n\pi\sigma)$$

We must now calculate η_k . To do so we first carry out the function change $z_k(t, \theta, \phi) = e^{\alpha_1 k^2 \pi^2 t} \eta_k(t, \theta, \phi)$ which, after some calculations, gives

$$(2.59) \quad \frac{\partial z_k}{\partial t} + A_1 z_k + B_1 z_k = \frac{\alpha_1 k^2 \pi d_k}{4} e^{\alpha_1 k^2 \pi^2 t}$$

$$(2.60) \quad z_k(t=0) = \eta_{0k}$$

The solution to the above given problem may be obtained using Duhamel's formula and written in the following form:

$$(2.61) \quad z_k = e^{-(A_1+B_1)t} \eta_{0k} + \int_0^t e^{-(A_1+B_1)(t-t')} e^{\alpha_1 k^2 \pi^2 t'} \frac{\alpha_1 k^2 \pi d_k}{4} dt'$$

Now η_k can be calculated: assuming $\psi_0^\sigma = \frac{1}{4\pi}$ (in which case $\eta_{0k} = \frac{d_k}{4\pi}$), it looks

$$(2.62) \quad \eta_k = d_k e^{-\alpha_1 k^2 \pi^2 t} F(u, t, 0) + \alpha_1 k^2 \pi^2 d_k \int_0^t e^{-\alpha_1 k^2 \pi^2 (t-t')} F(u, t, t') dt'$$

where, in the above, u stands for (θ, ϕ) , and $F(u, t, t') = \frac{1}{4\pi} e^{-(A_1+B_1)(t-t')}$. $F(u, t, t')$ is a notation first employed on page 328 in [3].

Next, making use of equations (2.58) and (2.62) and using the fact that $d_n = 0$ for n even, leads to

$$(2.63) \quad \psi_\sigma = F(u, t, 0) \sum_{\substack{n=1 \\ n \text{ odd}}}^{\infty} e^{-\alpha_1 n^2 \pi^2 t} d_n \sin(n\pi\sigma) + \int_0^t \tilde{P}(\sigma, t-t') F(u, t, t') dt'$$

where

$$(2.64) \quad \tilde{P}(\sigma, s) = \sum_{\substack{n=1 \\ n \text{ odd}}}^{\infty} 4\alpha_1 n \pi e^{-\alpha_1 n^2 \pi^2 s} \sin(n\pi\sigma)$$

Notice the above \tilde{P} is basically function P obtained on page 328 in [3]. Also, taking $F(u, 0, 0) = \frac{1}{4\pi}$, from our equation (2.63) one gets

$$\psi_\sigma(t = 0) = F(u, 0, 0) \sum_{\substack{n=1 \\ n \text{ odd}}}^{\infty} d_n \sin(n\pi\sigma) = \frac{1}{4\pi},$$

as expected. Moreover, in this case $g_{0k} = 0$ (see equation (2.42)), and the constitutive assumption in Theorem 2.3 is obeyed.

3. Stationary boundary value problems

The corresponding stationary boundary value problems (referred to as SP-1 and SP-2) are:

Stationary Problem 1 (SP-1): Find $\psi_s \in H_s^1(D)$ that solves

$$(3.1) \quad A_1\psi_s + B_1\psi_s = 0$$

$$(3.2) \quad \psi_s \geq 0, \quad \int_D \psi_s \sin \theta d\theta d\phi = 1$$

Stationary Problem 2 (SP-2): Find $\overline{\psi}_s \in H_{s0}^1(D)$ that solves

$$(3.3) \quad A_2\overline{\psi}_s + B_2\overline{\psi}_s = -\frac{1}{4\pi}B_2(1)$$

$$(3.4) \quad \frac{1}{4\pi} + \overline{\psi}_s \geq 0, \quad \int_D \overline{\psi}_s \sin \theta d\theta d\phi = 0, \quad \forall \sigma \in]0, 1[.$$

For convenience we recall operators $A_{1,2}$, $B_{1,2}$ have been defined in Sections 2.2.1 and 2.2.2. Moreover, r, θ, ϕ are the spherical coordinates of a position vector x ; denote $\Omega := \{x \in \mathbb{R}^3, 1 < r < 2\}$, Ω_σ the 4-dimensional domain $\Omega_\sigma := \{(x, \sigma) \in \mathbb{R}^3 \times]0, 1[, 1 < r < 2\}$, and $V_\sigma := \{u \in H^1(\Omega_\sigma), u(\sigma = 0) = u(\sigma = 1) = 0\}$.

We solve the above presented problems using, in each case, a specific method.

It is clear that any function $u(\theta, \Phi)$ defined in D can be viewed as a function defined in Ω independent on r .

3.1. Existence and uniqueness of solutions for the problem SP-1.

Solving problem SP-1 boils down to proving $\lambda = 0$ is an eigenvalue for the operator $A_1 + B_1$. Use fo the Krein-Rutman's Theorem is made in the same way as in [5].

To begin with, by virtue of Lax-Milgram's Theorem one sees that there exists a large enough $\beta > 0$ such that $A_1 + B_1 + \beta\text{Id}$ is invertible, with the inverse operator mapping $H_s^1(D)$ onto $(H_s^1(D))'$. Denote $L_\beta = (A_1 + B_1 + \beta\text{Id})^{-1}$, $L_\beta \in \mathcal{L}((H_s^1(D))', H_s^1(D))$. Then, for any $g \in (H_s^1(D))'$, one has $L_\beta u = g$ iff u solves

$$(3.5) \quad a_\beta(u, v) = \langle g, v \rangle, \quad \forall v \in H_s^1(D)$$

where

$$\begin{aligned}
a_\beta(u, v) &= \alpha \int_D \left(\frac{\partial u}{\partial \theta} \frac{\partial v}{\partial \theta} \sin \theta + \frac{1}{\sin \theta} \frac{\partial u}{\partial \phi} \frac{\partial v}{\partial \phi} \right) d\theta d\phi \\
(3.6) \quad &- \int_D \left(a_1 u \frac{\partial v}{\partial \theta} \sin \theta + a_2 u \frac{\partial v}{\partial \phi} \right) d\theta d\phi + \beta \int_D uv \sin \theta d\theta d\phi
\end{aligned}$$

We now prove the following result:

LEMMA 3.1. *Let $g \in L^2_s(D)$ and $u = L_\beta(g)$. Then $u \in H^1(\Omega)$ is the unique solution to the problem*

$$(3.7) \quad \alpha \int_\Omega \nabla_x u \cdot \nabla_x \hat{v} d\Omega - \int_\Omega \hat{a} u \cdot \nabla_x \hat{v} d\Omega + \int_\Omega \hat{\beta} u \hat{v} d\Omega = \int_\Omega \hat{g} \hat{v} d\Omega, \quad \forall \hat{v} \in H^1(\Omega)$$

where: $\hat{a} : \Omega \rightarrow \mathbb{R}^3$, $\hat{\beta} : \Omega \rightarrow \mathbb{R}$ and $\hat{g} : \Omega \rightarrow \mathbb{R}$ are such that $\hat{a} \cdot e_r = 0$, $\hat{a} \cdot e_\theta = \frac{a_1}{r}$, $\hat{a} \cdot e_\phi = \frac{a_2}{r}$, $\hat{\beta} = \frac{\beta}{r^2}$, $\hat{g} = \frac{g}{r^2}$.

PROOF. Equality (3.7), written in spherical coordinates, looks:

$$\begin{aligned}
&\int_D \int_1^2 \left(\frac{1}{r^2} \frac{\partial u}{\partial \theta} \frac{\partial \hat{v}}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial u}{\partial \phi} \frac{\partial \hat{v}}{\partial \phi} \right) r^2 \sin \theta dr d\theta d\phi \\
&- \int_D \int_1^2 u \left(\frac{1}{r} \hat{a} \cdot e_\theta \frac{\partial \hat{v}}{\partial \theta} + \frac{1}{r \sin \theta} \hat{a} \cdot e_\phi \frac{\partial \hat{v}}{\partial \phi} \right) r^2 \sin \theta dr d\theta d\phi \\
(3.8) \quad &+ \int_D \int_1^2 \hat{\beta} u \hat{v} r^2 \sin \theta d\theta d\phi = \int_D \int_1^2 \hat{g} \hat{v} r^2 \sin \theta dr d\theta d\phi
\end{aligned}$$

Therefore, one must show that, for any $\hat{v} \in H^1(\Omega)$, the following holds true:

$$\begin{aligned}
&\int_D \int_1^2 \left(\frac{\partial u}{\partial \theta} \frac{\partial \hat{v}}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial u}{\partial \phi} \frac{\partial \hat{v}}{\partial \phi} \right) \sin \theta d\theta d\phi \\
&- \int_D \int_1^2 u \left(a_1 \frac{\partial \hat{v}}{\partial \theta} + \frac{1}{\sin \theta} a_2 \frac{\partial \hat{v}}{\partial \phi} \right) \sin \theta d\theta d\phi \\
(3.9) \quad &+ \beta \int_D \int_1^2 u \hat{v} \sin \theta d\theta d\phi = \int_D \int_1^2 g \hat{v} \sin \theta d\theta d\phi
\end{aligned}$$

Let $v = \int_1^2 \hat{v} dr$ in (3.5), with $\hat{v} \in H^1(\Omega)$ arbitrary. It follows that u solves (3.9). □

REMARK 3.1. *Observe that equality (3.7) is the weak (variational) formulation of the following problem:*

$$\begin{aligned}
(3.10) \quad &-\alpha \Delta_x u + \nabla_x(\hat{a}u) + \beta u = \hat{g}, \quad \text{on } \Omega \\
&-\alpha \frac{\partial u}{\partial \nu} + \hat{a} \cdot \nu u = 0, \quad \text{on } \partial\Omega
\end{aligned}$$

LEMMA 3.2 (Maximum Principle). *Let $f \in L^2_s(D)$, $u = L_\beta(g)$. Then:*

- (i) *whenever $g \geq 0$, we have $u \geq 0$ (weak maximum principle)*
- (ii) *whenever $g \geq 0$, $g \neq 0$, we have $u > 0$ (strong maximum principle)*

PROOF. (i) it follows immediately by taking $v = u^-$ in (3.5)

(ii) Denote $D_0 := \{(\theta, \phi) \in D, u(\theta, \phi) = 0\}$. The proof is by contradiction: assume $D_0 \neq \emptyset$. Then $D - D_0 \neq \emptyset$ as well. Let now $(\theta_0, \phi_0) \in \partial D_0$. Let $x^0 := \frac{3}{2}(\sin \theta_0 \cos \phi_0, \sin \theta_0 \sin \phi_0, \cos \theta_0)$, $x^0 \in \Omega$. One can find an $y^0 \in \Omega$ and a $r > 0$ such that $x^0 \in \partial B(y^0, r)$, which $B(y^0, r) \subset \{x \in \Omega, u(x) > 0\}$. Since u satisfies the problem (3.10) in Ω , one deduces by the strong maximum principle (see e.g. [6]) that $\frac{\partial u}{\partial \nu_B}(x^0) < 0$, where ν_B denotes the outward normal to $B(y^0, r)$. On the other hand, since x^0 is a minimum point for u on Ω we have $\nabla u(x^0) = 0$, a contradiction. □

Denote by $C_{\text{per}}(\overline{D})$ the set of continuous functions on D and periodic w.r.t. variable ϕ , endowed with the usual sup norm. Observe the following continuous inclusion: $C_{\text{per}}(\overline{D}) \hookrightarrow L^2_s$. One has the following result:

LEMMA 3.3 (Compactness). *One has $L_\beta \in \mathcal{L}(C_{\text{per}}(\overline{D}), C_{\text{per}}(\overline{D}))$, and L_β is compact.*

PROOF. Let $g \in C_{\text{per}}(\overline{D})$ and $u = L_\beta(g)$. Then u solves equation (3.7). Clearly $g \in L^p(\Omega)$, for any $p > 1$, and by the interior smoothness property, it follows that $u \in W^{2,p}(\Omega')$ for any open set Ω' s.t. $\overline{\Omega'} \subset \Omega$.

Next, there exists $c = c(\Omega', p)$ s.t. $\|u\|_{W^{2,p}(\Omega')} \leq c\|g\|_{L^p(\Omega)} \leq c\|g\|_{C_{\text{per}}(\overline{D})}$, for any $g \in C_{\text{per}}(\overline{D})$. However, the following Sobolev continuous inclusion $W^{2,p}(\Omega') \hookrightarrow \mathcal{C}^0(\Omega')$ is compact for large enough $p > 1$. Then choose an open set Ω' so that it contains the set $\{x \in \Omega, r = 3/2\}$; the proof is over. □

We are now in a position allowing us to state Section 3.1 main result:

THEOREM 3.1. *The boundary value problem SP-1 given in equations (3.1)-(3.2) has a unique solution $\psi_s \in C_{\text{per}}(\overline{D})$, $\psi_s > 0$. Moreover, any eigenvalue $\lambda \in \mathbb{C}$ of $A_1 + B_1$ is s.t. $\text{Re}(\lambda) \geq 0$.*

PROOF. Let the cone of non-negative functions be defined as $P := \{u \in C_{\text{per}}(\overline{D}), u \geq 0\}$. Clearly its interior is given by $\overset{\circ}{P} := \{u \in C_{\text{per}}(\overline{D}), u > 0\}$. By Lemma 3.3 and part (ii) in Lemma 3.2 one sees the strong version of Krein-Rutman's theorem can be applied to operator L_β . Then there exists a simple eigenvalue $\mu > 0$ of L_β , and denote $\psi_s \in \overset{\circ}{P}$ the corresponding eigenvector. Also observe that $\psi_s \in H^1_s(D)$. Next, $\lambda = \frac{1}{\mu} - \beta$ is a simple eigenvalue of $A_1 + B_1$, and $(A_1 + B_1)\psi_s = \lambda\psi_s$. Therefore, ψ_s solves, for any $v \in H^1_s(D)$,:

$$(3.11) \quad \alpha \int_D \left(\frac{\partial \psi_s}{\partial \theta} \frac{\partial v}{\partial \theta} \sin \theta + \frac{1}{\sin \theta} \frac{\partial \psi_s}{\partial \phi} \frac{\partial v}{\partial \phi} \right) d\theta d\phi - \int_D \left(a_1 \psi_s \frac{\partial v}{\partial \theta} \sin \theta + a_2 \psi_s \frac{\partial v}{\partial \phi} \right) d\theta d\phi = \lambda \int_D \psi_s v \sin \theta d\theta d\phi$$

Let $v = 1$ in (3.11); as $\psi_s > 0$, it results that $\lambda = 0$. Therefore $\lambda = 0$ is a simple eigenvalue for $A_1 + B_1$, which ends the proof. □

REMARK 3.2. *One can also prove, using the strong version of the Krein-Rutman’s Theorem as done above, that ψ_s granted by Theorem 3.1 is, up to a multiplicative constant, the unique solution to the problem:*

$$(3.12) \quad \begin{aligned} -\alpha \Delta_x \psi_s + \nabla_x(\hat{a}\psi_s) &= 0, \quad \text{on } \Omega \\ -\alpha \frac{\partial \psi_s}{\partial \nu} + \hat{a} \cdot \nu \psi_s &= 0, \quad \text{on } \partial\Omega \end{aligned}$$

3.2. Existence and uniqueness of solutions for the problem SP-2. We first take on proving the following Poincaré inequality:

PROPOSITION 3.1. *There exists $c > 0$ such that, for any $v \in H_{s_0}^1(D_\sigma)$,*

$$(3.13) \quad \|v\|_{L_s^2(D_\sigma)}^2 \leq c \int_{D_\sigma} \left[\left(\frac{\partial v}{\partial \sigma} \right)^2 \sin \theta + \left(\frac{\partial v}{\partial \theta} \right)^2 \sin \theta + \frac{1}{\sin \theta} \left(\frac{\partial v}{\partial \phi} \right)^2 \right] d\theta d\phi$$

PROOF. The above stated result is a straightforward consequence of part (iii) and part (iv) in Proposition 2.1 and of the classical Poincaré inequality:

$$(3.14) \quad \|v\|_{L^2(\Omega_\sigma)}^2 \leq c \int_{\Omega_\sigma} \left[\left(\frac{\partial v}{\partial \sigma} \right)^2 + (\nabla_x v)^2 \right] dx d\sigma, \quad \forall v \in V_\sigma.$$

□

REMARK 3.3. *From Proposition 3.1 one infers that the seminorm defined on $H_{s_0}^1(D_\sigma)$ by*

$$(3.15) \quad v \rightarrow \int_{D_\sigma} \left[\left(\frac{\partial v}{\partial \sigma} \right)^2 \sin \theta + \left(\frac{\partial v}{\partial \theta} \right)^2 \sin \theta + \frac{1}{\sin \theta} \left(\frac{\partial v}{\partial \phi} \right)^2 \right] d\theta d\phi$$

is equivalent to the usual norm on $H_{s_0}^1(D_\sigma)$.

THEOREM 3.2. *There exists a unique solution $\overline{\psi_s}$ to the problem (3.1)-(3.2).*

PROOF. By Proposition 3.1, operator A_2 is invertible; consequently, the problem (3.3) is equivalent to the following one:

$$(3.16) \quad \overline{\psi_s} + A_2^{-1} B_2 \psi_s = -\frac{1}{4\pi} A_2^{-1} (B_2(1))$$

Observe $A_2^{-1} B_2$ is continuous and compact and maps $L_s^2(D_\sigma)$ onto itself. By Fredholm theory, proving the existence and uniqueness of solutions to (3.16) is tantamount to proving the kernel of $A_2 + B_2$ reduces to $\{0\}$.

Let $u \in H_{s_0}^1(D_\sigma)$ be chosen such that $A_2 u + B_2 u = 0$. Then $u \in V_\sigma$ and we have for any $\hat{v} \in V_\sigma$:

$$(3.17) \quad \int_{\Omega_\sigma} \left(\frac{\alpha_1}{r^2} \frac{\partial u}{\partial \sigma} \frac{\partial \hat{v}}{\partial \sigma} + \alpha_2 \nabla_x u \cdot \nabla_x \hat{v} \right) dx d\sigma - \int_{\Omega_\sigma} \hat{a} u \cdot \nabla_x \hat{v} dx d\sigma = 0$$

where \hat{a} is the same as in Lemma 3.1.

Next, we proceed as in [7]. For any $\epsilon > 0$, let $v = \frac{u^+}{u^+ + \epsilon}$. Then:

$$\nabla_{x,\sigma} v = \epsilon \frac{\nabla_{x,\sigma} u^+}{(u^+ + \epsilon)^2}$$

One obtains:

$$\begin{aligned} & \int_{\Omega_\sigma} \left[\frac{\alpha_1}{r^2} \frac{1}{(u^+ + \epsilon)^2} \left(\frac{\partial u^+}{\partial \sigma} \right)^2 + \alpha_2 \frac{(\nabla_x u^+)^2}{(u^+ + \epsilon)^2} \right] dx d\sigma = \\ & \int_{\Omega_\sigma} \hat{a} u^+ \frac{\nabla_x u^+}{(u^+ + \epsilon)^2} dx d\sigma \leq \int_{\Omega_\sigma} |\hat{a}| \left| \frac{\nabla_x u^+}{u^+ + \epsilon} \right| dx d\sigma \\ (3.18) \quad & \leq \frac{\alpha_2}{2} \int_{\Omega_\sigma} \left| \frac{\nabla_x u^+}{u^+ + \epsilon} \right|^2 dx d\sigma + c \end{aligned}$$

Therefore:

$$(3.19) \quad \left\| \frac{\nabla_x u^+}{u^+ + \epsilon} \right\|_{L^2(\Omega_\sigma)} \leq c$$

where c is a constant which is independent of ϵ . Observe that

$$\nabla_{x,\sigma} \log \left(1 + \frac{u^+}{\epsilon} \right) = \frac{\nabla_{x,\sigma} u^+}{u^+ + \epsilon}$$

and that $\log \left(1 + \frac{u^+}{\epsilon} \right) = 0$ whenever $\sigma = 0$ and $\sigma = 1$. Invoking Poincaré's

inequality one gets $\left\| \log \left(1 + \frac{u^+}{\epsilon} \right) \right\|_{L^2(\Omega_\sigma)} \leq c$. The latest, in turn, gives $u^+ = 0$,

therefore $u \leq 0$. Reasoning on u^- instead on u^+ and proceeding likewise leads to $u \geq 0$, which ultimately gives $u = 0$. We have thus obtained the existence and uniqueness of $\overline{\psi}_s \in L^2_s(D_\sigma)$, solution to equation (3.16).

Next, let $\psi_s = \frac{1}{4\pi} + \overline{\psi}_s$. Then ψ_s solves equation (3.17) (with ψ_s instead of u).

As $\psi_s = \frac{1}{4\pi}$ for $\sigma = 0$ or $\sigma = 1$, one has $\psi_s^- \in V_\sigma$. Let now a test function be given by $v = \frac{\psi_s^-}{\psi_s^- + \epsilon}$. Proceeding as above, one obtains $\psi_s^- = 0$, therefore $\frac{1}{4\pi} + \overline{\psi}_s \geq 0$.

Now, take any $\varphi = \varphi(\sigma) \in H_0^1(]0, 1[)$ in the weak formulation given in equation

$$(3.3); \text{ it gives } \alpha_2 \int_{D_\sigma} \frac{\partial \overline{\psi}_s}{\partial \sigma} \varphi'(\sigma) \sin \theta d\theta d\phi d\sigma = 0$$

Denote $\tilde{\psi}_s := \int_{D_\sigma} \overline{\psi}_s \sin \theta d\theta d\phi$. Then $\tilde{\psi}_s''(\sigma) = 0$. The latest result, together with $\tilde{\psi}_s(0) = \tilde{\psi}_s(1) = 0$, gives $\tilde{\psi}_s = 0$, ending the proof. \square

REMARK 3.4. Notice that $\psi_s = \overline{\psi}_s + \frac{1}{4\pi}$ is the unique solution to the following problem: find $\psi_s \in V_\sigma + \frac{1}{4\pi}$ such that, for all $v \in V_\sigma$,

$$\int_{\Omega_\sigma} \left(\frac{\alpha_1}{r^2} \frac{\partial \psi_s}{\partial \sigma} \frac{\partial v}{\partial \sigma} + \alpha_2 \nabla_x \psi_s \cdot \nabla_x v \right) dx d\sigma - \int_{\Omega_\sigma} \frac{\hat{a} \psi_s}{r} \cdot \nabla_x v dx d\sigma = 0$$

The above is actually the weak formulation of the problem:

$$\begin{aligned} -\frac{\alpha_1}{r^2} \frac{\partial^2 \psi_s}{\partial \sigma^2} - \alpha_2 A \psi_s + \nabla_x \left(\frac{1}{r} \hat{a} \psi_s \right) &= 0, \quad \text{on } \Omega_\sigma \\ -\alpha_2 \frac{\partial \psi_s}{\partial \nu} + \frac{\hat{a} \cdot \nu}{r} &= 0, \quad \text{on } \partial \Omega_\sigma \\ \psi_s|_{\sigma=0} &= \psi_s|_{\sigma=1} = \frac{1}{4\pi} \end{aligned}$$

4. Final comments

There is growing interest in using phase-space kinetical theories for modeling the thermo-rheological behavior of complex fluids, all the more that, for polymer mixtures and chemically reacting liquids, reptation based approaches seem to be less suitable. In [3] Bird et al exposed at length the physical assumptions and many underpinnings of their polymer dynamics theory.

Crucial to basically any mean field theory is the configurational (probability) density function: it incorporates all inter- and intra-molecular interactions of relevance to a given molecular system. It is thus quite natural to have one's attention focused on ways to solve it. To the best of our knowledge, the question of existence and uniqueness of solutions to this PDE, within the framework of the general phase space theory, has not been answered. In Section 2 we proved that, under physically meaningful initial boundary conditions, the evolutionary PDE has unique solutions.

For large enough times, one is interested in stationary probability density equation solutions. In Section 3 we made use of the Krein-Rutman's Theorem to prove the existence and uniqueness of solutions to the steady-state probability density equation of Bird et al [3] kinetic theory for polymeric systems.

The matter of time depending solutions convergence, for $t \rightarrow +\infty$, towards the stationary ones will be addressed in a subsequent paper.

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