

Glass Transition Seen through Asymptotic Expansions

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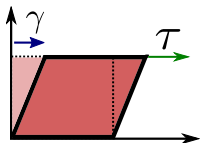
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Joint work with M. Renardy (VirginiaTech)

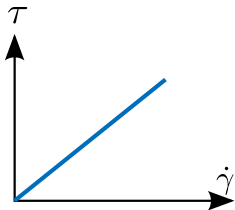
Outline

- 1 Glassy materials
 - Rheological properties
 - Hébraud -Lequeux Model
- 2 Hébraud -Lequeux and the Glass Transition
 - Physical input
 - Direct computations
 - Asymptotic expansions approach
- 3 A multidimensional extension of Hébraud -Lequeux
 - Presentation of the model
 - Formal results

Simple shear

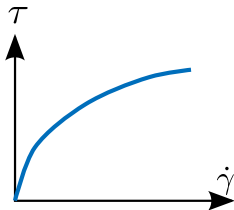


- τ : stress
- γ : shear
- $\dot{\gamma}$: shear rate



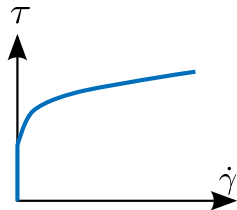
Newton

$$\tau = \eta \dot{\gamma}$$



Power law

$$\tau = A \dot{\gamma}^n$$



Herschell-Bulkley

$$\tau = \tau_0 + A \dot{\gamma}^n$$

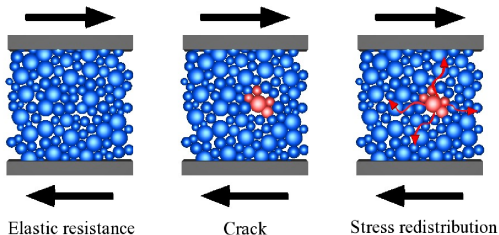
Solid or fluid?



Pitch drop experiment currently at University of Queensland.

Zoom to the mesoscopic scale

- Several type of response to a same external forcing



- Glassy transition

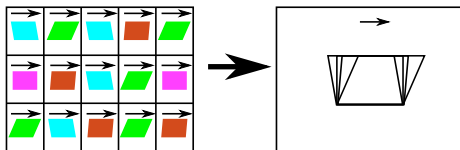
$$A\dot{\gamma}^n \quad \Phi_c \quad \tau_0 + B\dot{\gamma}^p$$

—————|—————→

Principles of the model

Generic glassy material.

- Replace spatial heterogeneities of local stresses \rightarrow global statistics p :



- Write the evolution equation of p directly
- Recover the macroscopic stress by averaging :

$$\tau = \int_{\sigma \in \mathbf{R}} \sigma p(t, \sigma) d\sigma$$

Hébraud -Lequeux equation

Elasticity

$$\partial_t p = -G_0 \dot{\gamma}(t) \partial_\sigma p - \frac{1}{T_0} H(|\sigma| - \sigma_c) p + \bar{\Gamma}(p(t)) \delta_0(\sigma) + D(p(t)) \partial_\sigma^2 p$$

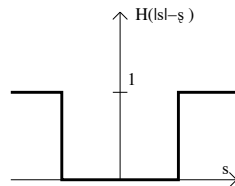
- G_0 : shear modulus
- $\dot{\gamma}$: shear rate

Hébraud -Lequeux equation

Relaxation

$$\partial_t p = -G_0 \dot{\gamma}(t) \partial_\sigma p - \frac{1}{T_0} H(|\sigma| - \sigma_c) p + \bar{\Gamma}(p(t)) \delta_0(\sigma) + D(p(t)) \partial_\sigma^2 p$$

- T_0 : relaxation time
- H : Heaviside step function



Hébraud -Lequeux equation

Relaxation

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- $\bar{\Gamma}(p(t)) = \frac{1}{T_0} \int_{|\sigma| > \sigma_c} p(t, \sigma) d\sigma$: **fluidity**
- δ_0 Dirac measure at 0

Hébraud -Lequeux equation

Plasticity

$$\partial_t p = -G_0 \dot{\gamma}(t) \partial_\sigma p - \frac{1}{T_0} H(|\sigma| - \sigma_c) p + \bar{\Gamma}(p(t)) \delta_0(\sigma) + D(p(t)) \partial_\sigma^2 p$$

- $D(p(t)) = \alpha \bar{\Gamma}(p(t)) = \frac{\alpha}{T_0} \int_{|\sigma| > \sigma_c} p(t, \sigma) d\sigma$
- α : Transition parameter

Initial question

Stationary dimensionless Hébraud -Lequeux equation

$$\begin{cases} -\alpha \bar{\Gamma}(p) \partial_{\sigma}^2 p + \dot{\gamma} \partial_{\sigma} p + h(\sigma) p = \bar{\Gamma}(p) \delta_0(\sigma) \\ p \geq 0, \int_{\mathbf{R}} p(\sigma) d\sigma = 1 \end{cases}$$

Does this model accounts for a glass transition?

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Does this model accounts for a glass transition?

[HÉBRAUD, LEQUEUX, 1998] : Yes, without formal proof

Results of [HL, 98]

If $\alpha > 1/2$, Newtonian behaviour,

$$\tau \approx \eta \dot{\gamma} \quad \eta \approx (\alpha - 1/2)^{-2}$$

If $\alpha = 1/2$, power law behaviour,

$$\tau \approx A \dot{\gamma}^{1/5}$$

If $\alpha < 1/2$, threshold behaviour,

$$\tau \approx \tau_0 \quad \tau_0 \approx (1/2 - \alpha)^{1/2}$$

$$\begin{array}{c} A\dot{\gamma}^n \\ \Phi_c \\ \tau_0 + B\dot{\gamma}^p \end{array}$$

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$$A \dot{\gamma}^n \quad \Phi_c \quad \tau_0 + B \dot{\gamma}^p$$

Goal : Prove mathematically this result.

Direct approach

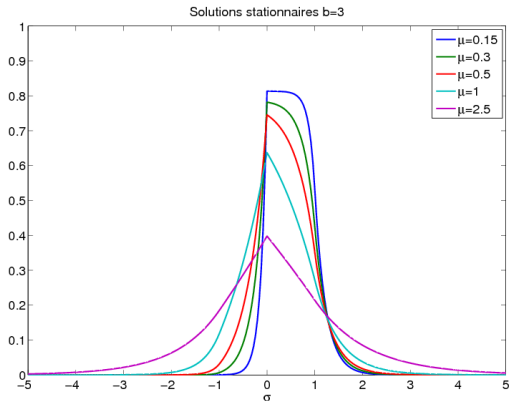


Figure: Examples of solution to the HL model

Direct approach

- Self consistency : $f_\alpha(\alpha\Gamma, \dot{\gamma}) = 0$

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 f_\alpha(\alpha\Gamma, \dot{\gamma}) = & \frac{1}{\alpha} \left[\frac{2\alpha\Gamma^2}{\dot{\gamma}^2} \left(\text{ch} \left(\frac{\dot{\gamma}}{\alpha\Gamma} \right) - 1 \right) + \alpha\Gamma \text{ch} \left(\frac{\dot{\gamma}}{\alpha\Gamma} \right) \right. \\
 & + \left(\frac{3\alpha\Gamma^2}{\dot{\gamma}} + \alpha\Gamma\dot{\gamma} \right) \text{sh} \left(\frac{\dot{\gamma}}{\alpha\Gamma} \right) + \sqrt{\dot{\gamma}^2 + 4\alpha\Gamma} \left(\frac{\alpha\Gamma^2}{\dot{\gamma}^2} \left(\text{ch} \left(\frac{\dot{\gamma}}{\alpha\Gamma} \right) - 1 \right) \right. \\
 & \left. \left. + \frac{\alpha\Gamma}{\dot{\gamma}} \text{sh} \left(\frac{\dot{\gamma}}{\alpha\Gamma} \right) + \alpha\Gamma \text{ch} \left(\frac{\dot{\gamma}}{\alpha\Gamma} \right) \right) \right] \\
 & - \sqrt{\dot{\gamma}^2 + 4\alpha\Gamma} \text{ch} \left(\frac{\dot{\gamma}}{\alpha\Gamma} \right) - \left(\frac{2\alpha\Gamma}{\dot{\gamma}} + \dot{\gamma} \right) \text{sh} \left(\frac{\dot{\gamma}}{\alpha\Gamma} \right)
 \end{aligned}$$

Direct approach

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 \end{aligned}$$

- Singularity removal : $X = \alpha\Gamma, Y = \dot{\gamma}/(\alpha\Gamma)$

Stress

Assuming $\Gamma = \phi_\alpha(\dot{\gamma}) \sim \phi_{\text{app}}(\dot{\gamma})$, how to prove the theorem?

$$\begin{aligned} \tau(\alpha\Gamma, \dot{\gamma}) &= \dot{\gamma} + \frac{\alpha\Gamma}{2\alpha\dot{\gamma}} - \frac{(\alpha\Gamma)^3}{\alpha\dot{\gamma}^3} \\ &\quad + \frac{(\alpha\Gamma)^2}{\dot{\gamma}^3\Delta(\alpha\Gamma, \dot{\gamma})} \left(\frac{\dot{\gamma}^2}{\alpha\Gamma} - 2 \left(\text{ch} \left(\frac{\dot{\gamma}}{\alpha\Gamma} \right) - 1 \right) \right) \\ &\quad + \frac{(\alpha\Gamma)^3}{\dot{\gamma}^4\Delta(\alpha\Gamma, \dot{\gamma})} \left(\dot{\gamma} \left(\left(\frac{\dot{\gamma}}{\alpha\Gamma} \right)^2 + \frac{4}{\alpha\Gamma} \right)^{1/2} + 2\text{sh} \left(\frac{\dot{\gamma}}{\alpha\Gamma} \right) \right) \end{aligned}$$

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Theorem

Glass transition is as announced by HÉBRAUD and LEQUEUX.

Link to the penalization

$$\begin{cases} -\alpha \bar{\Gamma}(p) \partial_{\sigma}^2 p + \dot{\gamma} \partial_{\sigma} p + h(\sigma) p = \bar{\Gamma}(p) \delta_0(\sigma) \\ p \geq 0, \int_{\mathbf{R}} p(\sigma) d\sigma = 1 \end{cases}$$

What is the behaviour of this system when $\dot{\gamma} \rightarrow 0^+$?

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- From previous proof : $\Gamma \sim c\dot{\gamma}$ when $\alpha < 1/2$.
- Replace Γ by its equivalent :

$$-\alpha c \partial_{\sigma}^2 p + \partial_{\sigma} p + \frac{1}{\dot{\gamma}} h(\sigma) p = c \delta_0(\sigma)$$

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$$-\eta \Delta u + V \cdot \nabla u + \frac{1}{\varepsilon} \mathbf{1}_{\omega} u + \nabla \pi = f \quad \text{div } u = 0$$

Boundary layers

By analogy with the penalization : **boundary layers**.

Example, for $\sigma > 1$:

$$p(\sigma) \approx \sum_k \dot{\gamma}^{k/2} \bar{R}^k(\sigma) + \dot{\gamma}^{k/2} R^k \left(\frac{\sigma - 1}{\dot{\gamma}^{1/2}} \right).$$

Goal :

- 1 find the expansion of p **without *a priori* assumptions**
- 2 justification of the expansion in an appropriate space

Rewriting

Note $q = p_{[-1,1]}$ and $r = p_{[-1,1]^c}$.

$$\left\{ \begin{array}{ll} -\alpha\Gamma\partial_\sigma^2 q + \dot{\gamma}\partial_\sigma q = \Gamma\delta_0 & \text{in }]-1, 1[, \\ -\mu\Gamma\partial_\sigma^2 r + \dot{\gamma}\partial_\sigma r + r = 0 & \text{in } [-1, 1]^c, \\ r(\pm 1) = q(\pm 1), \\ \partial_\sigma r(\pm 1) = \partial_\sigma q(\pm 1), \\ \int_{|\sigma|>1} r(\sigma)d\sigma + \int_{-1}^1 q(\sigma)d\sigma = 1. \end{array} \right.$$

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Ansätze for q and r

We use ansätze for q and r but of **unknown scale** and boundary layer size.

$$q(\sigma) = \sum_{k=0}^{+\infty} (\dot{\gamma}^{1/s})^k \bar{Q}^k(\sigma),$$

$$r(\sigma) = \sum_{k=0}^{+\infty} (\dot{\gamma}^{1/s})^k \bar{R}^k(\sigma) + (\dot{\gamma}^{1/s})^k R^k \left(\text{sign}(\sigma), \frac{|\sigma| - 1}{\dot{\gamma}^{l/s}} \right).$$

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Ansaetze for Γ

From $\Gamma = \int_{|\sigma|>1} r(\sigma)d\sigma$ we also have

$$\Gamma = \sum_{k=0}^{+\infty} \tilde{c}_k y^{k/s}$$

with

$$\tilde{c}_k = \begin{cases} \bar{c}_k & \text{if } 0 \leq k \leq l-1, \\ \bar{c}_k + c_{k-l} & \text{if } k \geq l, \end{cases}$$

$$\bar{c}_k = \int_{|\sigma|>1} \bar{R}^k(\sigma) d\sigma,$$

$$c_k = \int_0^{+\infty} [R^k(-1, z) + R^k(1, z)] dz.$$

Scales and sizes

Goal : find the expansion of p **without *a priori* assumptions**

Theorem (J. O., M. RENARDY, 2011)

$\alpha > 1/2$: $s = 1$, *all R^k vanish*, $\Gamma(\dot{\gamma}) \rightarrow \Gamma(0) > 0$

$\alpha < 1/2$: $s = 2$, $l = 1$, *all \bar{R}^k vanish*, $\Gamma(\dot{\gamma}) \sim c\dot{\gamma}$

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$\alpha < 1/2$: $s = 2$, $l = 1$, **all \bar{R}^k vanish**, $\Gamma(\dot{\gamma}) \sim c\dot{\gamma}$

$\alpha = 1/2$: $s = 5$, $l = 2$, **all \bar{R}^k vanish**, $\Gamma(\dot{\gamma}) \sim c\dot{\gamma}^{4/5}$

Proof

- First relate the shape of the expansion to the first non zero coefficient \tilde{c}_k .
 - $\tilde{c}_0 \neq 0$: no boundary layer terms
 - $\tilde{c}_0 = 0$: no non boundary layer terms. First non zero term necessarily $\tilde{c}_{2l} = c_l$.
- Next relate the fundamental problem to the range of α that gives a solution.
- Finally find the next non trivial profile and deduce the minimal s and the corresponding l .

Example: the case $\tilde{c}_0 = 0$ (I)

Assume $2l \geq s$.

- $2l \geq s \implies 2l = s$.
- Fundamental problem

$$\left\{ \begin{array}{l} -\alpha c_l \partial_\sigma^2 \bar{Q}^0 + \partial_\sigma \bar{Q}^0 = c_l \delta_0, \\ \bar{Q}^0(\pm 1) = 0, \\ \int_{-1}^1 \bar{Q}^0(\sigma) d\sigma = 1, \\ c_l \neq 0. \end{array} \right.$$

- $c_l \neq 0$ satisfies $\alpha = \alpha c_l \tanh(1/(2\alpha c_l))$. Solvable iff $\mu < 1/2$.
- Next non trivial interior problem for \bar{Q}^l : $l = 1$ and $s = 2$.

Example: The case $\tilde{c}_0 = 0$ (II)

Assume $2l + 1 \leq s$.

- $2l \leq s - 1$.
- Fundamental problem

$$\left\{ \begin{array}{l} -\alpha c_l \partial_\sigma^2 \bar{Q}^0 = c_l \delta_0, \\ \bar{Q}^0(\pm 1) = 0, \\ \int_{-1}^1 \bar{Q}^0(\sigma) d\sigma = 1, \\ c_l \neq 0. \end{array} \right.$$

- Only fixes $\alpha = 1/2$.

Example: The case $\tilde{c}_0 = 0$ (II)

- Non trivial following interior problem on \overline{Q}^{s-2l} .
Incompatibility with $c_l \neq 0$ if $l \leq s - 2l$ so $s \leq 3l - 1$ and $l \geq 2$.
- c_l still not defined!
- Next problem is for \overline{Q}^{2s-4l} .
Incompatibility with $c_l \neq 0$ except if $l = 2s - 4l$ that is $2s = 5l$.
- $c_l = 1/(3\sqrt{2})^{2/5}$.
- Minimize the number of profile to compute by taking $l = 2$ and $s = 5$.

Convergence Theorem

Theorem (J. O., M. RENARDY (2010))

For all $\alpha > 0$ the described ansätze converge (that is the series converge on small intervals $[0, \varepsilon(\alpha)]$) in **weighted Sobolev spaces**.

Corollary

The macroscopic stress $\tau(\dot{\gamma}) = \int_{\mathbf{R}} \sigma p^{\dot{\gamma}}(\sigma) d\sigma$ has the following expansion:

$$\alpha > 1/2: \tau(\dot{\gamma}) = \eta_0 \dot{\gamma} + \eta_1 \dot{\gamma}^2 + \eta_2 \dot{\gamma}^3 + \dots$$

$$\alpha < 1/2: \tau(\dot{\gamma}) = \tau_0 + \tau_1 \sqrt{\dot{\gamma}} + \tau_2 \dot{\gamma} + \dots$$

$$\alpha = 1/2: \tau(\dot{\gamma}) = A_0 \dot{\gamma}^{1/5} + A_1 \dot{\gamma}^{2/5} + A_2 \dot{\gamma}^{3/5} + \dots$$

Proof

- Rewrite as a two parameter model in $a = \dot{\gamma}/\Gamma$ and $b = \sqrt{\Gamma}$ (plus one for the exponential decay).
- Use analytic perturbation “à la Kato” + analytic local inversion theorem.

Multidimensional flows

Some rheological properties **cannot be accessed** in simple shear flows.

Example : normal differences.

Extension from simple shear models to general flow models : **not systematic**.

Example : Maxwell 1d \rightarrow Upper/under Convected Maxwell.

Typical rheological flows

- Shear flows:

$$\nabla u = \dot{\gamma} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

- 3d elongational flow

$$\nabla u = \dot{\gamma} \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

- 2d axisymmetric elongational flow

$$\nabla u = \dot{\gamma} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Frame indifference

Principle of frame indifference

The constitutive law of a material must be the same in all frames.

- If a block of material at point x has stress tensor Σ then in the frame $x^* = x_0(t) + Q(t)x$ it must have the stress:

$$\Sigma^* = Q\Sigma Q^{-1}.$$

- Consequence: a model based on $p(t, x, \Sigma)$ must be invariant by the change $p^*(t, x^*, \Sigma^*)$

A possible extension

- Works only for **incompressible** flows
- Σ : generic point of the space of symmetric tensors (**not traceless**)

$$\begin{aligned} \partial_t p(t, x, \Sigma) + u \cdot \nabla_x p - g_a(\Sigma, \nabla u) : \nabla_\Sigma p = \\ - 2\lambda D(\nabla u) : \nabla_\Sigma p(t, x, \Sigma) \\ - \frac{\mathbf{1}_{|\Sigma|>1}(\Sigma)}{We} p(t, x, \Sigma) + \frac{1}{We} \Gamma(p)(t, x) \rho(\Sigma) \\ + \frac{\alpha}{We} \Gamma(p)(t, x) \Delta_\Sigma p(t, x, \Sigma) \end{aligned}$$

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Glass transition in this model?

Theorem

- 1 *Same formal asymptotic expansion as in the 1d case.*
- 2 *There exists $\alpha_c(\rho)$ so that*
 - if $\alpha > \alpha_c$, “Newtonian” or “threshold”*
 - if $\alpha = \alpha_c$, “power-law” or “threshold”*
 - if $\alpha < \alpha_c$, only “threshold”*

Some of the difficulties

- If one wants $\rho = \delta_0$: non variationnal elliptic theory.
- Unable to compute any of the profiles.
- Needs some properties on the characteristics of $\Sigma \mapsto g_a(\nabla u, \Sigma) - 2\lambda D(\nabla u)$.
- Careful study of the symmetry of the profile equations.
- ...