Introduction

Onsager Equation
General Goals
Examples

Onsager equation for general corpora

Kinetics

Physical space connections

Embedding in Fluid

Outlook

The zero temperature limit of interacting corpora

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IMA, July 21, 2008

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Thanks: N. Masmoudi, A. Zlatos.

Support: NSF

Complex Fluid Models

- Landau Equilibrium models: order parameter (Director = Oseen, Zöcher, Frank, Ericksen, Leslie. Tensor = de Gennes.)
- Onsager Equilibrium models: (pdf of state), free energy derived from physics
- Passive Kinetic models: Doi, FENE and variants (pdf of state) effects of shear on dilute suspensions of rigid or extensible corpora = linear Fokker-Planck
- Tensorial models: (conformation tensors): closure of certain kinetic models, e.g. Oldroyd B
- Active Kinetic Models: (pdf) Onsager-Smoluchowski: Nonlinear Fokker-Planck, stochastic models

Applications

- Nanoscale self-assembly
- Microfluidics
- Biomaterials
- Gels and Foams
- Soft Lattices, Jamming
- Pattern recognition

Major Problems

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2. Dissipation of Energy: Complex Fluids “Onsager” conjecture

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4. Modeling of interactions in the correct moduli space

- Configuration space: M = compact, separable, metrizable space. $m \in M$ = corpus.

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- Free Energy

$$\mathcal{E}[f] = \int_M f \log f d\mu - \frac{1}{2}\int_M (\mathcal{K}f)\, f d\mu$$

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- Minima of Free Energy: Onsager Equation

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6. Dynamics

Example: Rods, Maier-Saupe potential

$M = \mathbb{S}^{n-1}, \quad d\mu = \text{area}.$

$$\mathcal{K}f(p) = b \int_{\mathbb{S}^{n-1}} \left((p \cdot q)^2 - \frac{1}{n} \right) f(q) d\mu$$

b = intensity, inverse temperature.

Dimension Reduction, Maier-Saupe

$n \times n$ symmetric, traceless matrix S:

$$S \mapsto Z(S)$$

$$Z(S) = \int_{\mathbb{S}^{n-1}} e^{b(S^{ij} m_i m_j)} d\mu.$$

$$f_S(m) = (Z(S))^{-1} e^{b(S^{ij} m_i m_j)}$$

$$\sigma(S)_{ij} = \int_{\mathbb{S}^{n-1}} \left(m_i m_j - \frac{\delta_{ij}}{n} \right) f_S(m) d\mu.$$

Theorem

Onsager's equation with Maier-Saupe potential is equivalent to

$$\sigma(S) = S.$$

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Prolate:

$$\lim_{b\to\infty} [\phi] = \phi(m), \quad m \in \mathbb{S}^2.$$

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$$\widetilde{f}(p_1, \dots p_N) = f_1(p_1) f(p_2) \dots f_N(p_N) \quad \text{product measure}$$

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with $e(p) = (\cos p, \sin p)$ if $p \in [0, 2\pi]$.

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with

$$\begin{cases} [\phi](a) = \int_0^{2\pi} \phi(\theta) g(\theta) d\theta \\ g(\theta) = Z^{-1} e^{-b(\sin(\theta) - a)^2} \\ Z = \int_0^{2\pi} e^{-b(\sin(\theta) - a)^2} d\theta \end{cases}$$

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As $b \to \infty$ this tends to $\delta((p_1 - p_2)\text{mod}\pi)$.

Consider

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$$\lim_{\tau\to 0} \lambda(a,\tau) = 2\sqrt{\pi}\frac{1}{\sqrt{1-a^2}}, \quad 0 < a < 1.$$

Increasing.

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In fact, phase transition at positive τ

$$\partial_a \lambda((a(\tau),\tau) = 0$$

and limit $\lim_{\tau\to 0} a(\tau) = 1$, and consequently

$$\lim_{b\to\infty} f(p_1 - p_2) = \delta\left(\left(p_1 - p_2 - \frac{\pi}{2}\right) \mathrm{mod}\pi\right)$$

More degrees of freedom

$$M = [0, L] \times [0, L] \times [0, \pi], \; d\mu = \frac{1}{\pi L^2} dx_1 dx_2 d\theta.$$

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$$a = \int_M (x_1 x_2 \sin\theta) g(x_1, x_2, \theta) d\mu$$

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$a \to 0$, as $b \to \infty$.

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Connection to the example of freely articulated $2n$ corpora, jamming, perhaps...

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$$\mathcal{E}[f] = \int_M f \log f d\mu + \frac{b}{2}\int_M \int_M u(p,q) f(p) d\mu(p) f(q) d\mu(q).$$

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The function g is normalized $\int g d\mu = 1$, strictly positive and Lipschitz continuous.

The ur-corpus

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(C-Zlatos) *Let ν be a weak limit of a sequence $f_n d\mu$ of minima of the free energy $\mathcal{E}$ corresponding to $b_n \to \infty$. Then there exists $m \in M$ such that ν is concentrated on the level set $\Sigma(m) = \{p \mid u(m, p) = 0\}$.*

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$$\lim_{b\to\infty}\frac{1}{b}\left\{\min_{f>0,\ \int_M f d\mu=1}\mathcal{E}[f]\right\}=0$$

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$\exists\ p_n,\ \int_{Q(p_n,\epsilon_n)} f_n(q)d\mu(q)\ge 1-2\epsilon_n$. Pass to subsequence $p_n\to p$.

Principle: if a μ measure-preserving transformation T exists such that locally around $p = p_0$, $u(Tp, Tq) \le cu(p, q)$ with $c < 1$, then p_0 cannot be an ur-corpus.

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If a local u-preserving transformation around $p = p_0$ has the property that $\mu(T(B)) \geq C\mu(B)$ for small balls around p_0, with $C > 1$, then p_0 cannot be an ur-corpus.

Example: Rhombi centered at the origin. The ur-rhombus is the square.

Kinetics

M compact connected Riemannian manifold with metric g.

The zero temperature limit of interacting corpora

Peter Constantin

Introduction

Onsager Equation
General Goals
Examples

Onsager equation for general corpora

Kinetics

Physical space connections

Embedding in Fluid

Outlook

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Gradient system, steady solutions = Onsager equation.

$$\partial_t f = \Delta_g f - \mathrm{div}_g (f \nabla_g (\mathcal{K} f))$$

Embedding in Physical Space

$f : \mathbb{R}^n \times M \times [0, \infty) \to (0, \infty)$:

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Standing Waves, Traveling Waves.

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Macro-Micro Effect: from first principles, in principle...

Active: Navier-Stokes

$$\partial_t v + v \cdot \nabla v + \nabla p = \nu \Delta v + \nabla \cdot \sigma$$
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added stress tensor.

Micro-Macro Effect

$$\sigma_j^i(x) = -\int_M \left(\mathrm{div}_g c_j^i + c_j^i\cdot\nabla_g\mathcal{K}f(x,m)\right) f(x,m)d\mu(m) \quad *$$

Theorem

*3DNS + Fokker-Planck eqns with *. Then*

$$E(t) = \frac{1}{2}\int |v|^2 dx + \\ + \int \left\{ f \log f - \frac{1}{2}(\mathcal{K}f)f \right\} dx d\mu.$$

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If the smooth solution is time independent, then $v = 0$ *and* f *solves the Onsager equation*

$$f = Z^{-1} e^{\mathcal{K}[f]}.$$

NFP + 3D time-dependent Stokes

$$\partial_t f + v\cdot\nabla_x f + \mathrm{div}_g(Wf) = \mathrm{div}_g(f\nabla_g(\log f - \mathcal{K}f)),$$
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Theorem

Let v_0 divergence-free, in $W^{2,r}(\mathbb{T}^3)$, $r > 3$, f_0 positive, $\int_M f_0(x,m)d\mu = 1$, $f_0 \in L^\infty(dx;\mathcal{C}(M)) \cap \nabla_x f_0 \in L^r(dx; H^{-s}(M))$, $s \le \frac{d}{2}+1$.

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$$\|v\|_{L^p[(0,T);W^{2,r}(dx)]}<\infty,$$
$$\|\nabla_x f\|_{L^\infty[(0,T);L^r(dx;H^{-s}(M))]}<\infty$$

for any $p>\frac{2r}{r-3}$, $T>0$.

NFP + 2D time dependent Navier-Stokes

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Outlook

1. n-gons, Hausdorff-Gromov distance

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3. kinetics w/o Riemannian structure