Coagulating Brownian Particles, Gelation and Smoluchowski Equation

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Outline

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  - x_i and x_j coagulate when $x_i - x_j = \varepsilon(r_i + r_j)$ (or a smoother variant with a potential). The new particle of mass $m = m_i + m_j$ is at x_i with probability m_i/m.

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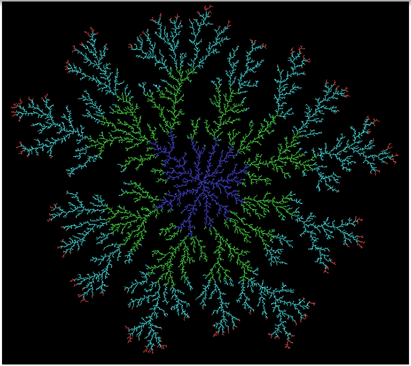
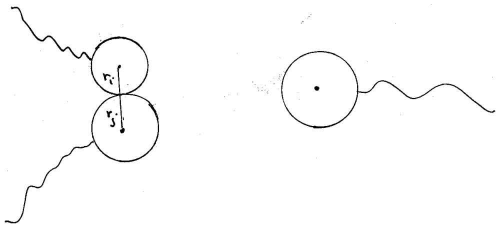
  - x_i fragments into two particles of masses m and $m_i - m$ with rate $\gamma(m, m_i - m)$. The new particles are at x_i and y.





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- Relationship between mass and radius: $r_i = m_i^\chi$.
- The central object to study is the cluster density of a given size; Empirical measures

$$g_n^\varepsilon(dx,t) = K_\varepsilon^{-1} \sum_i \delta_{x_i(t)}(dx) 1\!\!1(m_i(t) = n),$$

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Theorem (FR and Hammond when $\chi = 0$ and FR when $\chi < (d-2)^{-1}$, 2007)

$g_n^\varepsilon(dx, t)$ converges to $f_n(x, t)dx$ where f_n is a solution to the Smoluchowski's equation.

Smoluchowski's equation (solution is unique as we will see later)

$$\frac{\partial f_n}{\partial t}(x, t) = d(n)\Delta_x f_n(x, t) + Q_n^{+,c}(\mathbf{f}) - Q_n^{-,c}(\mathbf{f}) + Q_n^{+,f}(\mathbf{f}) - Q_n^{-,f}(\mathbf{f}),$$

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- $\alpha(m, n) = 2\pi(d(m) + d(n))$ when $d = 2$.

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- (Conjecture) Instantaneous Gelation occurs when $\chi > (d-2)^{-1}$. Smoluchowski is no longer relevant.

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We verify the conjecture for a simpler model. Ignore the location of particles.

Marcus-Lushnikov (ML) Process

- (Configuration) $L_n \in \mathbb{Z}^+$ denotes the number of particles of size n. We assume that the total mass $\sum_n nL_n = N$ is fixed.

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- (Dynamics)
  - When $n \neq m$, $(L_n, L_m, L_{m+n}) \to (L_n - 1, L_m - 1, L_{m+n} + 1)$ with rate $N^{-1}\alpha(m,n)L_mL_n$
  - $(L_n, L_{2n}) \to (L_n - 2, L_{2n} + 1)$ with rate $N^{-1}\alpha(n,n)L_n(L_n - 1)$

Theorem (FR 2012)

- Assume $\alpha(m,n) \geq m^q + n^q$ with $q > 1$. Then for every $\delta \in (0,1)$, δ fraction of particles are of size $\frac{\log N}{\log \log N}$ at a random time τ that in average is of size $const.|\log N|^{-\theta}$.

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  Assume $\alpha(m,n) \geq m^q n + n^q m$ with $q > 1$. Then complete gelation occurs at a random time τ' that in average is of size $const.(\frac{\log N}{\log\log N})^{1-q}$.

- Remark: Jeon (2000) proved complete gelation under $\alpha(m,n) \geq m^q n + n^q m$ with no bound on τ'.

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- ***Uniqueness:*** If f and g are two solutions, then

$$\frac{d}{dt}\int \sum_{n=1}^{\infty} n|f_n(x,t) - g_n(x,t)|dx$$
$$= c_0 \int \left[\sum_{n=1}^{\infty} n|f_n - g_n|\right]\left[\sum_{m=1}^{\infty} m^2(f_m + g_m)\right] dx.$$

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- ***Moral:*** We have uniqueness for solutions satisfying

$$\|\sum_{m=1}^{\infty} m^2 f_m\|_{L^\infty} < \infty$$

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- Gelation:

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  and $\int \infty f_\infty(x,t)dx > 0$ for $t > T_{gel}$.
- (FR and Hammond, 2007) No Gelation if

$$\int_0^T\int\sum_{n,m} nm(n+m)(d(n)+d(m))f_n(x,t)f_m(x,t)dxdt < \infty$$

How do we get various bounds on the solutions?

Theorem (FR and Hammond 2007)

L^1 ***bounds***: Under appropriate assumptions on the initial data,

$$\sup_t \|\sum_n n^a f_n(\cdot, t)\|_{L^1} < \infty$$

$$\int_0^\infty \int \sum_{n,m} nm(n^{a-1} + m^{a-1})(d(n) + d(m)) f_n(x,t) f_m dxdt < \infty,$$

provided

$$\lim_{n+m \to \infty} \frac{\alpha(n,m)}{(n+m)(d(n)+d(m))} = 0.$$

Theorem (FR and Hammond 2007)

L^∞ ***bounds:*** Under appropriate assumptions on the initial data,

$$\sup_t \| \sum_n n d(n)^{d/2} f_n(\cdot, t) \|_{L^\infty} < \infty$$

provided that $d(\cdot)$ is nonincreasing.

Using the previous results we obtain

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for all $a > 0$, provided that $d(\cdot)$ is nonincreasing and $d(n) \geq n^{-b}$ for large n.

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for all $a > 0$, provided that the total positive variation of $\log d(\cdot)$ is finite and $d(n) \geq n^{-b}$ for large n. In particular, if $d(\cdot)$ is uniformly positive and bounded.

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Comment on L^∞ bound when $d(\cdot)$ is nonincreasing:

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  is increasing in D.
- $$d(n)^{d/2} P_{d(n)}(x,t) = (4\pi)^{-d/2} \exp\left(-\frac{|x|^2}{4d(n)t}\right)$$
  is nonincreasing in n.

Comment on L^∞ bound when the increasing part of $d(\cdot)$ is controlled:

- Set $\phi(1) = 1$ and

$$\phi(n) = \prod_{m=1}^{n-1} \min\left\{1, \frac{d(m)}{d(m+1)}\right\},$$

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  Then $\phi(\cdot)$ and $d(\cdot)\phi(\cdot)$ are nonincreasing
- Differentiate

$$G(t) = \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} \sum_{\mathbf{n}} \Lambda^{\mathbf{n}} K(\mathbf{x}) \prod_{r=1}^{k} \gamma_k(n_r) f_{n_r}(x_r, t) dx_r.$$

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- $\Lambda^{\mathbf{n}} K(\mathbf{x})$ is

$$\int \left(\frac{|x_1 - z_1|^2}{d(n_1)} + \cdots + \frac{|x_k - z_k|^2}{d(n_k)} \right)^{1-\frac{kd}{2}} K(\mathbf{z}) \prod_{r=1}^{k} d(n_r)^{-\frac{d}{2}} dz_r.$$