Modeling and analysis of micro-magnetism of nano-particles and nano-wires

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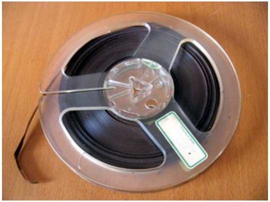
Joint works with P-A. Hervieux, G. Manfredi (IPCMS) and with R. Côte, C. Courtès, G. Ferrière, Y. Privat (IRMA) at Strasbourg (France).

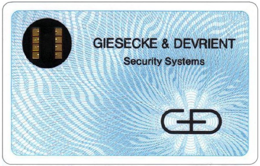
Introduction to micro-magnetism

Definition

The *micro-magnetism* aims at studying the magnetic phenomenon at micro or nano-metric scale where arises specific behaviors due to quantum effects (electron-exchange interaction).



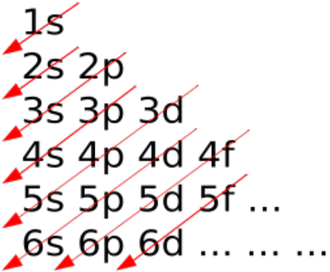
Magnetic tape 1/4-inch for audio recording (1950')



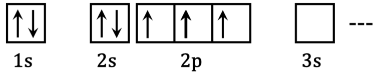
First chip card manufactured by Giesecke & Devrient in 1979.

Solid-state drive (SSD) Serial ATA storage unit.

Klechkowski-Hund rules for the filling of electronic orbits:



The Klechkowski rule gives the order of filling the electronic layers.



The Hund rule states the maximization of the spin inside a layer.

Definition

The *exchange interaction* is a quantum mechanical effect that only occurs when two electrons partially exchange position.

- Symmetric or anti-symmetric interaction.
- Creates ferro or anti-ferro magnetism.

The Brown model consists in the minimization of

$$\mathcal{E}(M) := A\int_\Omega |\nabla M|^2 + K\int_\Omega G(M,x) - \int_\Omega H_a \cdot M\,dx - \frac{1}{2}\int_\Omega H_d(M)\cdot M\,dx,$$

under the constraint $\forall x \in \Omega,\ M(x) \in \mathbb{S}^2$. We have:

- A the interaction constant ($A > 0$ for ferro-magnetism).
- K the anisotropy constant and $G : \mathbb{S}^2 \times \Omega \to \mathbb{R}$ the anisotropy profile.
- H_a the external magnetic field.
- H_d the self-induced magnetic field (demagnetizing field).

The demagnetizing field is solution to

$$\begin{cases} \operatorname{div}\big(H_d + M\big) = 0, \\ \operatorname{curl}\ H_d = 0, \\ H_d(x) \longrightarrow 0. \quad \text{as } |x| \to +\infty. \end{cases}$$

Some pictures from F. Alouges book:

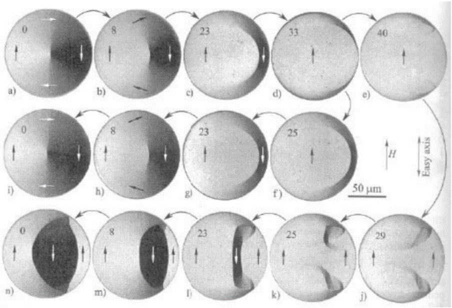


FIG. 1.1 – Historique de l'évolution d'un vortex à l'intérieur d'une particule

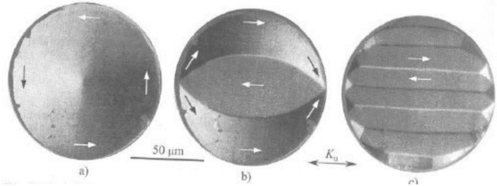


FIG. 1.4 – Trois configurations en domaines dans une même particule circulaire.

The Landau Lifschitz Gilbert equation:

$$\frac{dM}{dt} = -M \wedge H_{eff} - \alpha M \wedge (M \wedge H_{eff}),$$

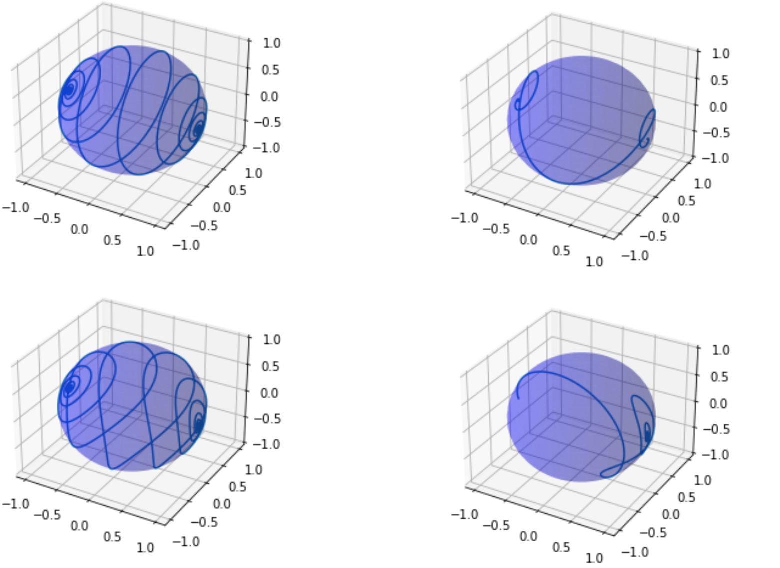
with H_{eff} the effective magnetic field and $\alpha \ll 1$ the damping coefficient.The effective field is computed using the Brown Energy. It involves :

- The external magnetic field H_a.
- The demagnetizing self-induced field H_d.
- The exchange interaction $-\Delta M$.
- The anisotropy potential $G'(M, x)$.

The first term in the equation (Landau-Lifschitz term) is derived using the Schrödinger equation and the Maxwell equations.

The second term (Gilbert term) is phenomenological. Theoretical works from physicists suggests a relativistic effect (Dirac equations).

Simulations of the LLG on a single spin in a magnetic field (low or strong damping, with or without anisotropy):



About Anisotropy :

Theorem (Alouges, Beauchard, 2009)

Study the Brown energy without anisotropy on a small domain $\varepsilon\Omega$.

(i) *After a rescale, the energy Γ-converges towards a situation where the magnetisation is constant.*

(ii) *Without rescale, we obtain an ODE that keep trace of the geometry of the domain.*

When the domain is small : only one Weiss domain remains.

Presentation of the nano-particles model

Dynamique d'aimantation ultra-rapide de nano-particules magnétique,
PhD thesis by Guillaume Klughertz (IPCMS, Strasbourg)

Model :

- Nanometric spherical magnetic particles
- Magnetic spin immobile in the particle frame
- Particles immersed in a very viscous fluid (low Reynolds)
- Fluid assumed immobile in comparison to the particles movement
- Particles cannot intersect each-other (collisions)
- Optional thermal effects (white noise effects)

The equations of the dynamics

- **Magnetic field generated by a magnetic dipole $\boldsymbol{m}$**:

$$B(r) = \frac{\mu_0}{4\pi}\left(\frac{3(m\cdot r)\,r}{|r|^5} - \frac{m}{|r|^3}\right).$$

- **Force exerted by dipole $\boldsymbol{m_1}$ on $\boldsymbol{m_2}$ separated by vector $\boldsymbol{r}$:**

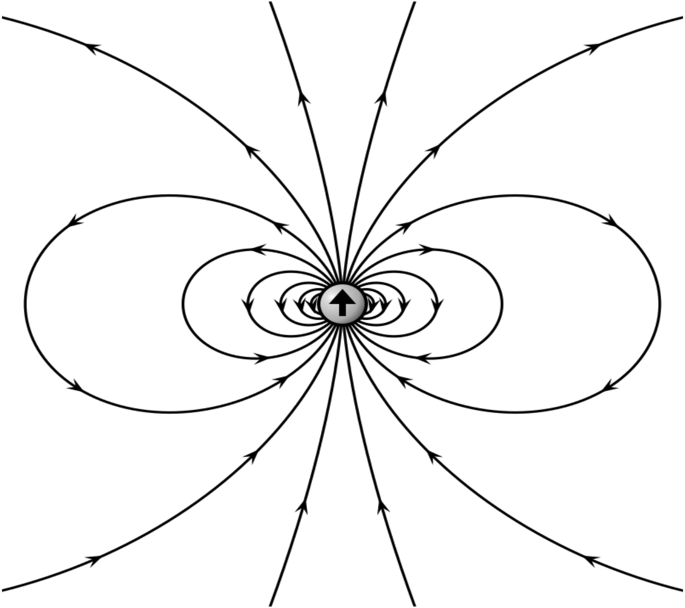
$$F_{dip}(r) = \nabla(m_2 \cdot B_1) = \frac{3\mu_0}{4\pi|r|^5}\left((m_1\cdot r)m_2 + (m_2\cdot r)m_1 + (m_1\cdot m_2)r - \frac{5(m_1\cdot r)(m_2\cdot r)r}{|r|^2}\right)$$

- **Repulsive force that models collisions of particles:**

$$F_{rep}(r) := C\left(\frac{R}{|r|}\right)^{\alpha}\frac{r}{|r|}.$$

- **Viscosity coefficients:**

$$\zeta_{tr} = 6\pi\eta R, \qquad \textbf{and} \qquad \zeta_r = 8\pi\eta R^3.$$



Magnetic field generated by a Magnetic dipole (source Wikipedia).

The equations of the dynamics

- **Dynamics in translation, the second Newton law gives:**

$$m\frac{dv_i}{dt} = F_i - \zeta_{tr} v_i,$$

where F_i the sum of all conservative forces acting on dipole m_i.

- **Dynamics in rotation:**

$$I\frac{d\omega_i}{dt} = T_i - \zeta_r \omega_i,$$

where $I = mR^2/10$ the moment of inertia of the sphere and $T_i = m_i \times B_i$ the magnetic couple.

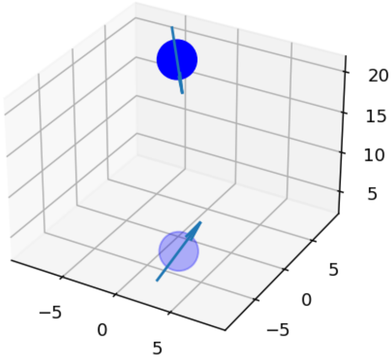
- **Dynamics of the spins, change of frame equation gives:**

$$\frac{d}{dt} m_{i|\mathcal{R}} = \frac{d}{dt} m_{i|\mathcal{R}'} + \omega_i \times m_i.$$

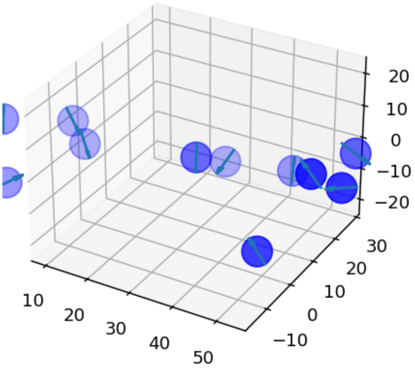
Time-scale separation hypothesis : $\frac{d}{dt} m_{i|\mathcal{R}'} = 0$.

Numerical simulations

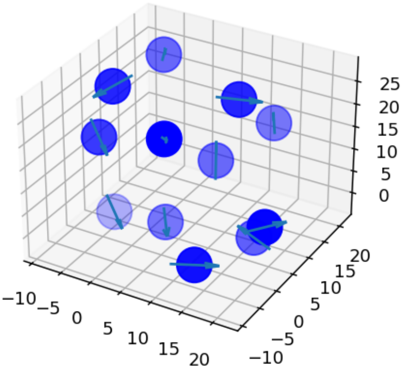
Dynamics of the 2 particles system :



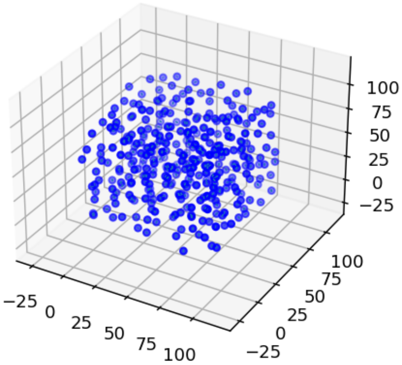
Dynamics of the 12 particles system (Aligned structure) :



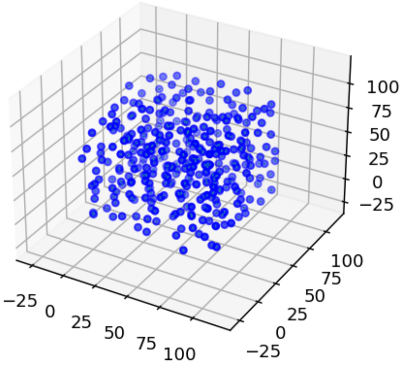
Dynamics of the 12 particles system (Ring structure) :



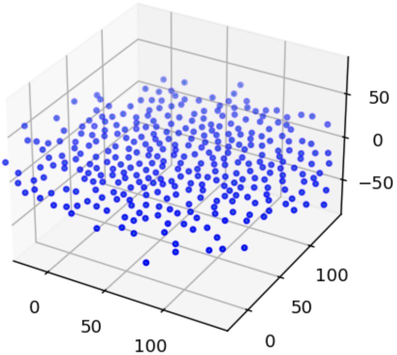
Dynamics of the 343 particles system (Complex structure) :

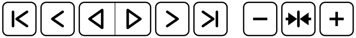


Dynamics of the 343 particles system with magnetic field :

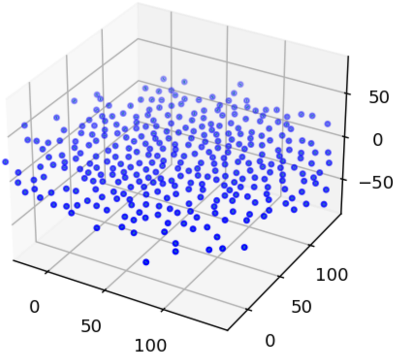


Dynamics of the 324 particles system with planar constraint ($z = 0$): :

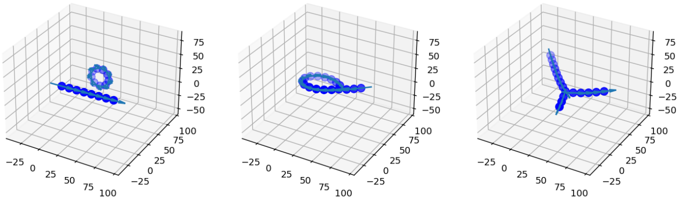




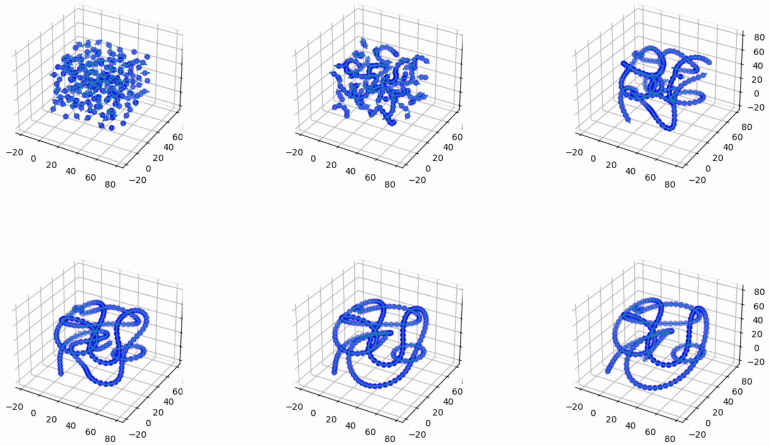
Dynamics of the 324 particles system with planar constraint and magnetic field :



Simple structures when N is small:

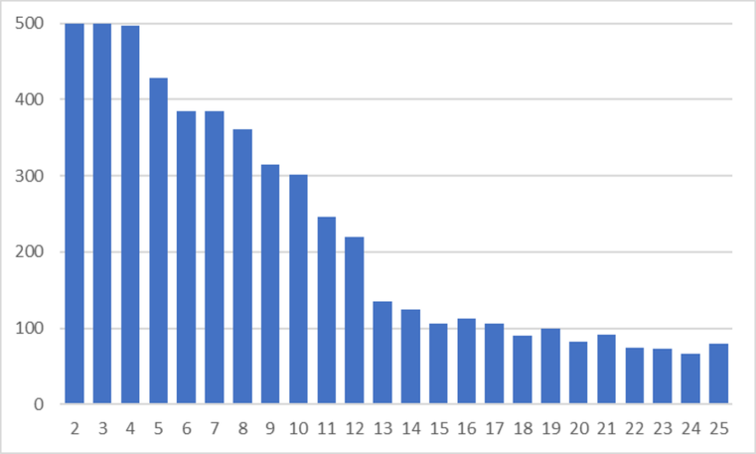


Complex structures when N is large:

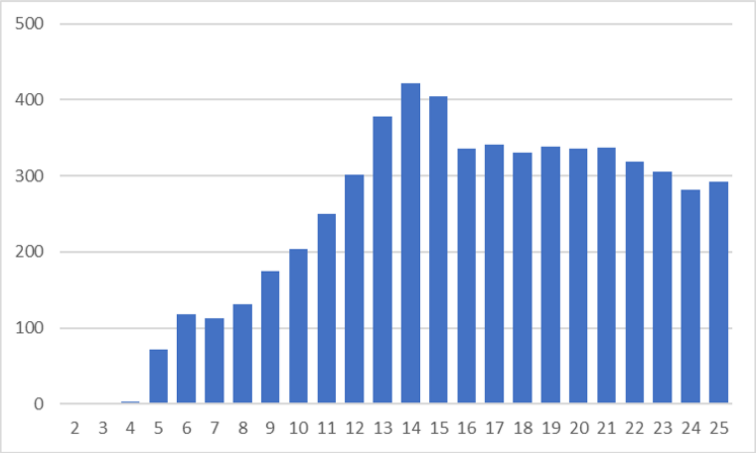


Evolution of 216 nano-particles at times 0, 1, 10, 30, 60, and 100 μ-seconds.

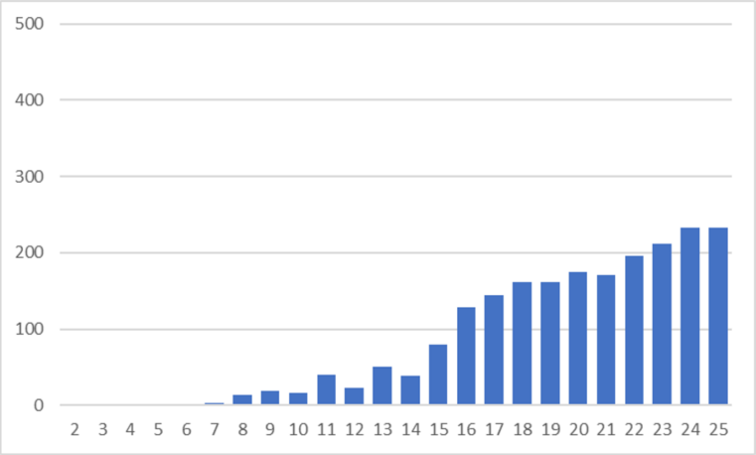
To study these structures : statistics (500 init. with $N = 2, 3, \ldots$)



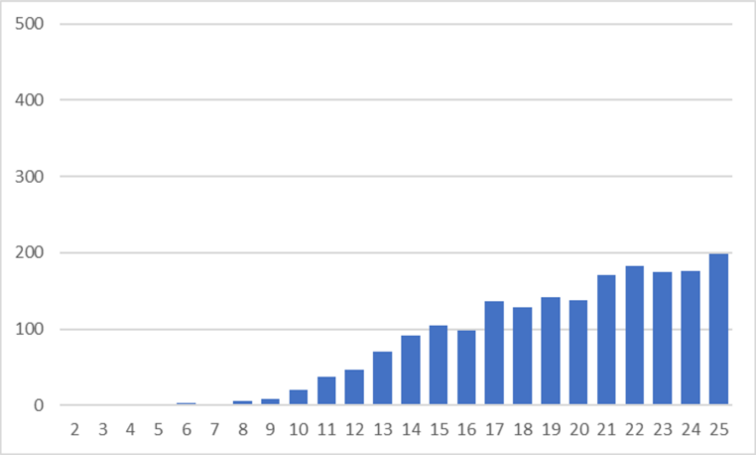
Probability to have one connected component that is an **aligned structure**.



Probability to have one connected component that is a **ring** structure.



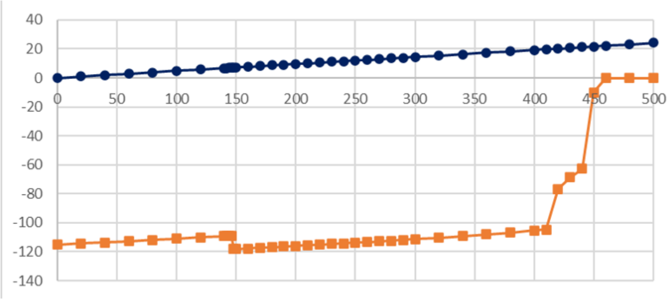
Probability to have one connected component that is **neither aligned nor ring**.



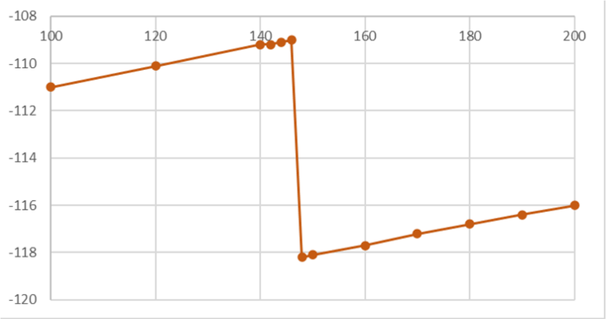
Probability to have **more than one connected component**.

Stability of structures in presence of temperature

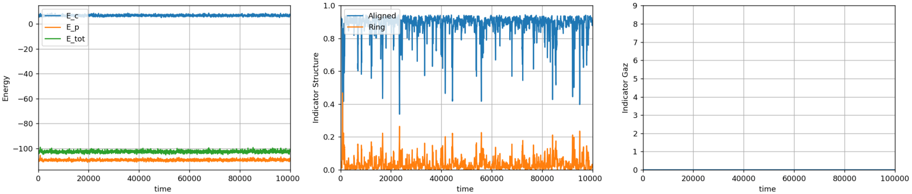
We add temperature and compute the mean potential and kinetic energy when the thermodynamical regime is reached:



Mean kinetic and potential energy with respect to the temperature (Blue : kinetic, orange : potential)

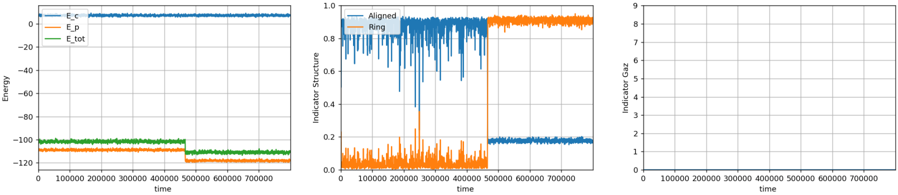


Zoom around the temperature 150 (first phase transition)



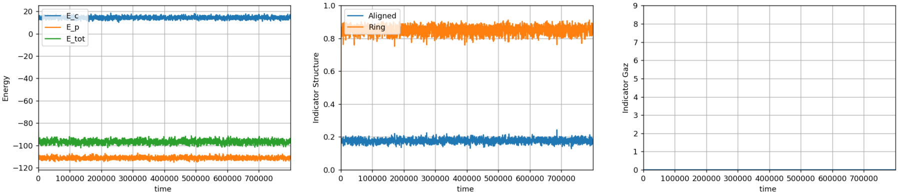
Evolution in time of the system at temperature $T = 140K$

- **Initial datum:** 9 particles with aligned structure
- **Left:** Kinetic and potential Energy
- **Middle:** Indicators of structure (aligned or ring)
- **Right:** Number of isolated particles



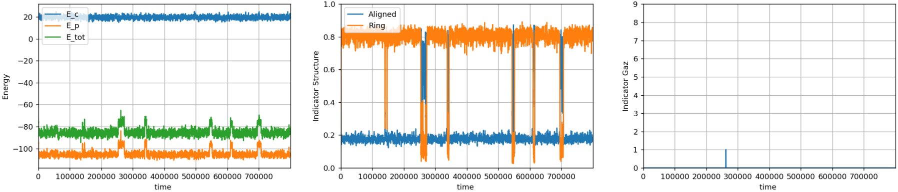
Evolution of the system at temperature $T = 150K$

- **Initial datum:** 9 particles with aligned structure
- **Left:** Kinetic and potential Energy
- **Middle:** Indicators of structure (aligned or ring)
- **Right:** Number of isolated particles



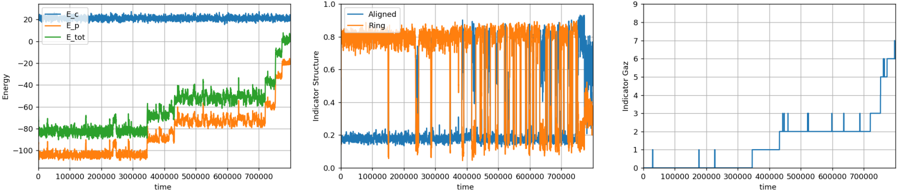
Evolution of the system at temperature $T = 300K$

- **Initial datum:** 9 particles with aligned structure
- **Left:** Kinetic and potential Energy
- **Middle:** Indicators of structure (aligned or ring)
- **Right:** Number of isolated particles



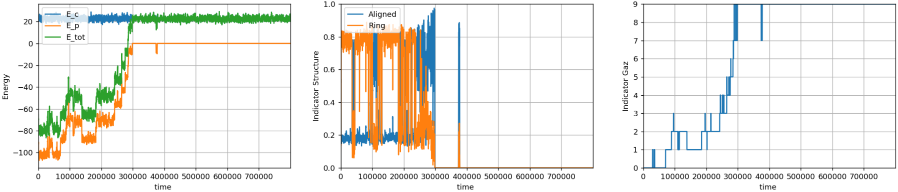
Evolution of the system at temperature $T = 410K$

- **Initial datum:** 9 particles with aligned structure
- **Left:** Kinetic and potential Energy
- **Middle:** Indicators of structure (aligned or ring)
- **Right:** Number of isolated particles



Evolution of the system at temperature $T = 440K$

- **Initial datum:** 9 particles with aligned structure
- **Left:** Kinetic and potential Energy
- **Middle:** Indicators of structure (aligned or ring)
- **Right:** Number of isolated particles



Evolution of the system at temperature $T = 470K$

- **Initial datum:** 9 particles with aligned structure
- **Left:** Kinetic and potential Energy
- **Middle:** Indicators of structure (aligned or ring)
- **Right:** Number of isolated particles

The described phenomenon is the following:

- An “aligned phase” until $T = 147K$.
- Brutal switch to a “ring phase” until $T = 410K$.
- Alternate switch between “aligned” and “ring”.
- Evaporation phenomenon.
- “Gaz phase” from $T = 510K$.

AND : we can see a modification of the structure of nano-particles in the variations of the potential energy.

What about theory ?

Theorem (R. Côte, C. Courtès, G. Ferrière, L.G-C., Y. Privat)

(i) *The system of N magnetic nano-particles admits a stationary state.*

(ii) *A unique stationary state where positions and spins are aligned.*

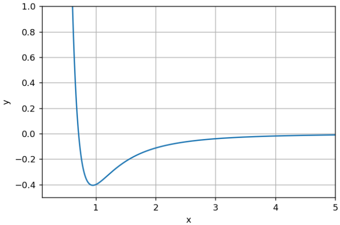
(iii) *Study of the properties of this stationnary states (details after).*

If the positions and spins are initially aligned, the dynamic becomes 1D. It is the gradient flow for $x_1, \ldots, x_N \in \mathbb{R}$ of:

$$\mathcal{J}_0(X) := \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} L\big(|x_i - x_j|\big), \qquad \text{with} \qquad L(s) := \frac{A}{|s|^\alpha} - \frac{B}{|s|^\beta}.$$

- Invariance by permutation: we can asssume $x_{k+1} > x_k$.
- Invariance by translation: we work with $h_k := x_{k+1} - x_k > 0$:

$$\mathcal{J}(H) := \sum_{i=1}^{N} \sum_{j=1}^{i-1} L\Big(\sum_{\ell=j}^{i-1} h_\ell\Big).$$



Lemma

The function $L(s) := \dfrac{A}{|s|^\alpha} - \dfrac{B}{|s|^\beta}$ *is decreasing, then increasing towards* 0 *as infinity and it admits as global minimizer:*

$$\overline{s} = \left(\frac{\alpha A}{\beta B}\right)^{\frac{1}{\alpha-\beta}}.$$

Corollary (upper bound on the distances)

The minimizers of $\mathcal{J}(H) := \sum_{i=1}^{N}\sum_{j=1}^{i-1} L\Big(\sum_{\ell=j}^{i-1} h_\ell\Big)$ *are such that* $h_\ell < \overline{s}$ *for all* ℓ.

Proof. Compute the sign of the derivative of $\mathcal{J}$ with respect to h_ℓ. □

Lemma (lower bound on the distances)

The minimizers of $\mathcal{J}$ *are such that* $h_\ell > \overline{c}$ *for all* ℓ*, where*

$$\overline{c} := \left(\frac{\alpha A}{\beta B\,\zeta(\beta)}\right)^{\frac{1}{\alpha-\beta}},$$

where ζ *is the Riemann zeta function,*

This gives existence of a minimizer by compactness arguments.

Proof.
Let $X \in \mathbb{R}^N$ a minimizer of $\mathcal{J}_0$ and i_0 be such that $|x_{i_0} - x_{i_0+1}| = \min_j |x_j - x_{j+1}|$.
We now define $\widetilde{X}$ by

$$\widetilde{x}_i = x_i, \quad \text{if } i \leq i_0, \qquad \text{and} \qquad \widetilde{x}_i = x_i + \delta, \quad \text{otherwise},$$

where $\delta > 0$. Since X is a minimizer, then

$$\mathcal{J}_0(X) - \mathcal{J}_0(\widetilde{X}) = \sum_{i=1}^{i_0} \sum_{j=i_0+1}^{N} \Big(L\big(|x_i - x_j|\big) - L\big(|\widetilde{x}_i - \widetilde{x}_j|\big) \Big) \leq 0.$$

Dividing by δ and letting $\delta \to 0$ (isolate the case $j = i_0 + 1$):

$$\sum_{i=1}^{i_0-1} L'\big(|x_i - x_{i_0}|\big) + \sum_{i=1}^{i_0} \sum_{j=i_0+2}^{N} L'\big(|x_i - x_j|\big) \geq -L'\big(|x_{i_0} - x_{i_0+1}|\big).$$

With the explicit formula for L' (removing terms in $\alpha + 1$ in the left-hand side):

$$\sum_{i=1}^{i_0-1} \frac{\beta B}{|x_i - x_{i_0+1}|^{\beta+1}} + \sum_{i=1}^{i_0} \sum_{j=i_0+2}^{N} \frac{\beta B}{|x_i - x_j|^{\beta+1}} \geq \frac{\alpha A}{|x_{i_0} - x_{i_0+1}|^{\alpha+1}} - \frac{\beta B}{|x_{i_0} - x_{i_0+1}|^{\beta+1}}.$$

If we denote the smallest distance $\delta_0 := |x_{i_0} - x_{i_0+1}|$:

$$\frac{\beta B}{\delta_0^{\beta+1}} \left(\sum_{i=1}^{i_0-1} \frac{1}{|i - (i_0+1)|^{\beta+1}} + \sum_{i=1}^{i_0} \sum_{j=i_0+2}^{N} \frac{1}{|i-j|^{\beta+1}} \right) \geq \frac{\alpha A}{\delta_0^{\alpha+1}} - \frac{\beta B}{\delta_0^{\beta+1}}.$$

If we denote the smallest distance $\delta_0 := |x_{i_0} - x_{i_0+1}|$:

$$\frac{\beta B}{\delta_0^{\beta+1}}\left(\sum_{i=1}^{i_0-1} \frac{1}{|i-(i_0+1)|^{\beta+1}} + \sum_{i=1}^{i_0} \sum_{j=i_0+2}^{N} \frac{1}{|i-j|^{\beta+1}}\right) \geq \frac{\alpha A}{\delta_0^{\alpha+1}} - \frac{\beta B}{\delta_0^{\beta+1}}.$$

Standard manipulations on the double sums:

$$\sum_{i=1}^{i_0} \sum_{j=i_0+2}^{N} \frac{1}{|i-j|^{\beta+1}} = \sum_{i=1}^{i_0} \sum_{k=i_0+2-i}^{N-i} \frac{1}{k^{\beta+1}} = \sum_{k=2}^{N-1} \sum_{i=\max(1,i_0+2-k)}^{\min(i_0,N-k)} \frac{1}{k^{\beta+1}}$$

Moreover, we can easily prove that

$$\min(i_0, N-k) - \max(1, i_0+2-k) + 1 \leq k-1.$$

Thus,

$$\sum_{i=1}^{i_0-1} \frac{1}{|i-i_0+1|^{\beta+1}} + \sum_{i=1}^{i_0} \sum_{j=i_0+2}^{N} \frac{1}{|i-j|^{\beta+1}} \leq \sum_{k=2}^{i_0} \frac{1}{k^{\beta+1}} + \sum_{k=2}^{N} \frac{k-1}{k^{\beta+1}} \leq \sum_{k=2}^{+\infty} \frac{1}{k^{\beta}}$$

Plugging this back into the main estimate:

$$\frac{\beta B}{\delta_0^{\beta+1}}(\zeta(\beta)-1) \geq \frac{\alpha A}{\delta_0^{\alpha+1}} - \frac{\beta B}{\delta_0^{\beta+1}}, \qquad \Longrightarrow \qquad \delta_0 \geq \left(\frac{\alpha A}{\beta B \zeta(\beta)}\right)^{\frac{1}{\alpha-\beta}}.$$

□

In the asymptotic $\alpha \to +\infty$ we recover a hard sphere model: $\bar{s}, \bar{c} \longrightarrow 1$.

On the contrary : what is the asymptotic $N \to +\infty$? with fixed parameters A, B, α, β ?

Lemma (Equation satisfied by the minimizer)

The equation solved by H^* is, for all $k = 1, \dots, N$,
$$\sum_{i=1}^{k} \sum_{j=k+1}^{N} L'\left(\sum_{\ell=i}^{j-1} h_\ell^* \right) = 0.$$

Difficulty: the limit distance is different in the center or at the extremities.

In the center, we expect the distances to converge towards some $\bar{h} > 0$. Formally:

$$\sum_{i=-\infty}^{0} \sum_{j=1}^{\infty} L'\left((j-i)\bar{h} \right) = 0. \qquad \text{This give:} \quad \bar{h} := \left(\frac{\alpha A \, \zeta(\alpha)}{\beta B \, \zeta(\beta)} \right)^{\frac{1}{\alpha - \beta}}.$$

On the opposite, at the extremities:

$$\sum_{j=1}^{\infty} L'\left(j\widehat{h} \right) = 0. \qquad \text{This give:} \quad \widehat{h} := \left(\frac{\alpha A \, \zeta(\alpha + 1)}{\beta B \, \zeta(\beta + 1)} \right)^{\frac{1}{\alpha - \beta}}.$$

Lemma

For all $k = 1, \dots, N$, we have:
$$\bar{h} + \frac{C}{N^{\beta - 1}} \leq h_k^* \leq \widehat{h} + \frac{C}{N^{\beta}}.$$

$\to$ remark that $\bar{c} < \bar{h} < \widehat{h} < \bar{s}$.

Proposition (Property of the Hessian matrix [going toward uniqueness !])

Let $H \in [\overline{c}, \overline{s}]^{N-1}$. Assume $\alpha > \beta > 1$ and α "large enough". The Hessian $\mathrm{Hess}\,\mathcal{J}(H)$ *of J at H satisfies:*

- *The diagonal terms are positive :*

$$\partial^2_{h_\mu, h_\mu} \mathcal{J}(H) \geq \frac{\beta B}{\overline{s}^{\beta+2}}(\alpha - \beta) - \frac{\beta B(\beta+1)}{\overline{c}^{\beta+2}}(\zeta(\beta+1) - 1) =: \Lambda_d > 0$$

- *The non-diagonal terms are non positive and decrease away of the diagonal:*

$$0 \geq \partial^2_{h_\mu, h_\nu} \mathcal{J}(H) \geq -C \frac{\beta B(\beta+1)}{\overline{c}^{\beta+2}} |\mu - \nu|^{-\beta} =: -\frac{\Lambda_{nd}}{|\mu - \nu|^\beta}.$$

- *The Hessian is a uniformly diagonally dominant matrix : for all μ,*

$$\sum_{\nu \neq \mu} |\partial^2_{h_\mu, h_\nu} \mathcal{J}(H)| = -\sum_{\nu \neq \mu} \partial^2_{h_\mu, h_\nu} \mathcal{J}(H) \leq \frac{\beta B(\beta+1)}{\overline{c}^{\beta+2}}(\zeta(\beta) - 1),$$

which leads in particular to

$$|\partial^2_{h_\mu, h_\mu} \mathcal{J}(H)| - \sum_{\nu \neq \mu} |\partial^2_{h_\mu, h_\nu} \mathcal{J}(H)| \geq \frac{\beta B}{\overline{s}^{\beta+2}}(\alpha - \beta) - \frac{\beta B(\beta+1)}{\overline{c}^{\beta+2}}\Big(\zeta(\beta+1) + \zeta(\beta)\Big) =: \Lambda_1 > 0.$$

Lemma (Uniqueness result !)

$\mathcal{J}$ is strictly convex in $[\overline{c}, \overline{s}]^{N-1}$. Furthermore, $\mathcal{J}$ admits a unique critical point which is its minimizer on $]\overline{c}, \overline{s}[^{N-1}$.

Proof.

- From previous lemma and the Gershgorin circle theorem, it is standard to show that the lowest eigenvalue of Hess $cJ(H)$ is larger than $\Lambda_1 > 0$ (for every H in the set $[\overline{c}, \overline{s}]^{N-1}$).
- Thus $\mathcal{J}$ is strictly convex on $[\overline{c}, \overline{s}]^{N-1}$.
- Then it admits at most one critical point.
- We already know that there are no critical points for $\mathcal{J}$ outside $]\overline{c}, \overline{s}[^{N-1}$.
- This proves uniqueness.

□

→ This conclude the proof of the theorem !

Nevertheless: Can we use the information on the Hessian matrix to improve the study of the asymptotic $N \to +\infty$??? **YES !**

Theorem (Convergence theorem)

Let $N \in \mathbb{N}$ large enough and $1 \le k \le N$. Recall that $\overline{h} := \left(\dfrac{\alpha A\,\zeta(\alpha)}{\beta B\,\zeta(\beta)}\right)^{\frac{1}{\alpha-\beta}}$.

Then there holds: $\quad |\overline{h} - h_k^*| \lesssim \left(\dfrac{1}{k^{\beta-1}} + \dfrac{1}{(N-k)^{\beta-1}} + \dfrac{1}{N^{\beta-1}}\right).$

Related work : Gardner and Radin, The infinite-volume ground state of the Lennard-Jones potential. *Journal of statistical physics* (1979).

Proposition (Quantitative Gerschgorin circles)

Let $\gamma > 1$ and $\delta = 2(1+2^\gamma)\zeta(\gamma)$. Then for $c, d > 0$ such that $r_+ := \dfrac{c}{d}\,\dfrac{\delta + \sqrt{\delta^2 + 4\zeta(2\gamma)}}{2} < 1$.
Let $A \in \mathcal{M}_n(\mathbb{C})$ such that A is strictly diagonally dominant and

$$|A_{ij}| \le \frac{c}{|i-j|^\gamma} \quad \text{for } i \neq j, \quad \text{and} \quad |a_{ii}| \ge d.$$

Then A is invertible and there exist $\kappa = \kappa(\gamma, \frac{c}{d})$ (bounded as $\frac{c}{d} \to 0$) such that

$$|(A^{-1})_{ij}| \le \kappa \frac{c}{d^2|i-j|^\gamma} \quad \text{for } i \neq j, \qquad \text{and} \qquad (A^{-1})_{ii} \le \kappa d^{-1} + \kappa \frac{c}{d}, \quad \text{for all } i.$$

Proof of the theorem. Let H^* realize the min of $\mathcal{J}$ and $\overline{H} = (\overline{h}, \dots, \overline{h})$. The equation on $\overline{h}$ gives:

$$\begin{aligned}
\partial_{h_k} \mathcal{J}(\overline{H}) &= \sum_{i=1}^{k} \sum_{j=k+1}^{N} L'((j-i)\overline{h}) = \sum_{i=1-k}^{0} \sum_{j=1}^{N-k} L'((j-i)\overline{h}) \\
&= \mathbf{0} - \sum_{i=-\infty}^{-k} \sum_{j=1}^{\infty} L'((j-i)\overline{h}) - \sum_{i=1-k}^{0} \sum_{j=N-k+1}^{\infty} L'((j-i)\overline{h}) \\
&= - \sum_{i=-\infty}^{-k} \sum_{\ell=1-i}^{\infty} L'(\ell\overline{h}) - \sum_{i=1-k}^{0} \sum_{\ell=N-k+1-i}^{\infty} L'(\ell\overline{h}) \\
&= - \sum_{\ell=1+k}^{\infty} \sum_{i=1-\ell}^{-k} L'(\ell\overline{h}) - \sum_{\ell=N-k+1}^{\infty} \sum_{i=\max(1-k, N-k+1-\ell)}^{0} L'(\ell\overline{h}) \\
&= - \sum_{\ell=1+k}^{\infty} (\ell-k) L'(\ell\overline{h}) - \sum_{\ell=N-k+1}^{\infty} (k - \max(0, N-\ell)) L'(\ell\overline{h}) \\
&= - \sum_{\ell=1+k}^{\infty} (\ell-k) L'(\ell\overline{h}) - \sum_{\ell=N-k+1}^{N} (\ell+k-N) L'(\ell\overline{h}) - \sum_{\ell=N+1}^{\infty} k L'(\ell\overline{h}).
\end{aligned}$$

Since $\ell \geq 2$ in each of those terms, we know that all the $L'(\ell\overline{h})$ are positive, which leads to $\partial_{h_k} J(\overline{H}) \leq 0$.

On the other hand, we also know that $L'(x) \leq \frac{\beta B}{x^{\beta+1}}$, which implies:

$$
\begin{aligned}
|\partial_{h_k} \mathcal{J}(\overline{H})| &= \left| \sum_{\ell=1+k}^{\infty} (\ell - k) L'(\ell \overline{h}) + \sum_{\ell=N-k+1}^{N} (\ell + k - N) L'(\ell \overline{h}) + \sum_{\ell=N+1}^{\infty} k L'(\ell \overline{h}) \right| \\
&\leq \sum_{\ell=1+k}^{\infty} (\ell - k) \frac{\beta B}{(\ell \overline{h})^{\beta+1}} + \sum_{\ell=N-k+1}^{N} (\ell + k - N) \frac{\beta B}{(\ell \overline{h})^{\beta+1}} + \sum_{\ell=N+1}^{\infty} k \frac{\beta B}{(\ell \overline{h})^{\beta+1}} \\
&\leq \frac{\beta B}{\overline{h}^{\beta+1}} \left(\sum_{\ell=1+k}^{\infty} (\ell - k) \ell^{-(\beta+1)} + \sum_{\ell=N-k+1}^{\infty} (\ell + k - N) \ell^{-(\beta+1)} + \sum_{\ell=N+1}^{\infty} (\ell - N) \ell^{-(\beta+1)} \right) \\
&\leq \frac{\beta B}{\overline{h}^{\beta+1}} \Big(\xi(k) + \xi(N-k) + \xi(N) \Big),
\end{aligned}
$$

where $\xi(n) = \sum_{\ell=n+1}^{\infty} (\ell - n) \ell^{-(\beta+1)}$. Moreover, we know that $\xi(n) \leq \frac{C_\beta}{n^{\beta-1}}$ for some C_β depending only on $\beta > 1$. Thus,

$$
|\partial_{h_k} \mathcal{J}(\overline{H})| \leq C_\beta \frac{\beta B}{\overline{h}^{\beta-1}} \left(\frac{1}{k^{\beta-1}} + \frac{1}{(N-k)^{\beta+1}} + \frac{1}{N^{\beta-1}} \right).
$$

We also have: $\nabla \mathcal{J}(\overline{H}) = \nabla \mathcal{J}(\overline{H}) - \nabla \mathcal{J}(H^*) = \int_0^1 \text{Hess}\, \mathcal{J}(\overline{H} + t(H^* - \overline{H}))dt\, (\overline{H} - H^*)$.

For all $t \in (0,1)$, there holds $\overline{H} + t(H^* - \overline{H}) \in [\overline{c}, \overline{s}]^{N-1}$, therefore Hess $\mathcal{J}(\overline{H} + t(H^* - \overline{H}))$ satisfies the hypothesis of the Refined Gerschorin Circles lemma. The inversion of the Hessian matrix leads to:

$$\overline{H} - H^* = \left(\int_0^1 \text{Hess}\, \mathcal{J}(\overline{H} + t(H^* - \overline{H}))dt \right)^{-1} \nabla J(\overline{H}).$$

Thus,

$$|\overline{h} - h_k^*| \leq \sum_{\ell=1}^{N-1} \left| \left(\left(\int_0^1 \text{Hess}\, \mathcal{J}(\overline{H} + t(h^* - \overline{h}))dt \right)^{-1} \right)_{k\ell} \right| \left| \partial_{h_\ell} J(\overline{H}) \right|$$
$$\leq \kappa \frac{1 + \Lambda_{nd}}{\Lambda_d} \left| \partial_{h_k} \mathcal{J}(\overline{H}) \right| + \sum_{\ell \neq k} \kappa \frac{\Lambda_{nd}}{\Lambda_d^2 |\ell - k|^{\beta+1}} \left| \partial_{h_\ell} J(\overline{H}) \right|.$$

Using now the previous estimate on $\nabla_{h_k} J(\overline{H})$ gives:

$$|\overline{h} - h_k^*| \leq \kappa C_\beta \frac{1 + \Lambda_{nd}}{\Lambda_d} \frac{\beta B}{\overline{h}^{\beta-1}} \left(\frac{1}{k^{\beta-1}} + \frac{1}{(N-k)^{\beta-1}} + \frac{1}{N^{\beta-1}} \right)$$
$$+ \kappa C_\beta \frac{\Lambda_{nd}}{\Lambda_d^2} \frac{\beta B}{\overline{h}^{\beta+1}} \sum_{\ell \neq k} \frac{1}{|\ell - k|^{\beta-1}} \left(\frac{1}{\ell^{\beta-1}} + \frac{1}{(N-\ell)^{\beta-1}} + \frac{1}{N^{\beta-1}} \right).$$

How to estimate the second term in the estimate above ?

Lemma

$$\sum_{k\in[\![1,n]\!]\setminus\{i,j\}} \frac{1}{|i-k|^\gamma}\frac{1}{|k-j|^\gamma} \leq 2\frac{(1+2^\gamma)\zeta(\gamma)}{|i-j|^\gamma}.$$

It suffices to consider the case $i<j$. Then

$$\sum_{k=1}^{i-1}\frac{1}{(i-k)^\gamma}\frac{1}{(j-k)^\gamma} = \sum_{h=1}^{i-1}\frac{1}{h^\gamma}\frac{1}{(j-i+h)^\gamma} \leq \frac{1}{(j-i)^\gamma}\sum_{h=1}^{+\infty}\frac{1}{h^\gamma} \leq \frac{\zeta(\gamma)}{(j-i)^\gamma}.$$

Similarly,

$$\sum_{k=j+1}^{n}\frac{1}{(k-i)^\gamma}\frac{1}{(k-j)^\gamma} = \sum_{h=1}^{n-j}\frac{1}{(j-i+h)^\gamma}\frac{1}{h^\gamma} \leq \frac{1}{(j-i)^\gamma}\sum_{h=1}^{+\infty}\frac{1}{h^\gamma} \leq \frac{\zeta(\gamma)}{(j-i)^\gamma}.$$

Finally, splitting the middle sum around $(j-i)/2$, there hold

$$\begin{aligned}\sum_{k=i+1}^{j-1}\frac{1}{(k-i)^\gamma}\frac{1}{(j-k)^\gamma} &\leq 2\sum_{k=i+1}^{\lceil\frac{j-i}{2}\rceil}\frac{1}{(k-i)^\gamma}\frac{1}{(j-k)^\gamma}\\ &\leq 2\sum_{k=i+1}^{\lceil\frac{j-i}{2}\rceil}\frac{1}{(k-i)^\gamma}\frac{2^\gamma}{(j-i)^\gamma} \leq \frac{2^{\gamma+1}\zeta(\gamma)}{(j-i)^\gamma}.\end{aligned}$$

Summing up the three bounds concludes the proof. □

What about the One Ring ?

The ring structure of radius $r > 0$, noted $\mathfrak{R}_r \in (\mathbb{R}^3 \times \mathbb{S}^2)^n$ is characterized by:

$$x_j = r \begin{pmatrix} \cos\left(\frac{2j\pi}{n}\right) \\ \sin\left(\frac{2j\pi}{n}\right) \\ 0 \end{pmatrix} \qquad \text{and} \qquad m_j = \begin{pmatrix} -\sin\left(\frac{2j\pi}{n}\right) \\ \cos\left(\frac{2j\pi}{n}\right) \\ 0 \end{pmatrix}.$$

Theorem (R. Côte, C. Courtès, G. Ferrière, L.G-C., Y. Privat)

(i) *Existence and Uniqueness of a critical point with a "ring" structure.*

(ii) *An explicit formula for the radius of the ring.*

Lemma

The gradient of the energy at the ring $\mathfrak{R}_r$ is given by:

$$\nabla_{x_i} U(\mathfrak{R}_r) = \nabla_{x_i} U^d(\mathfrak{R}_r) + \nabla_{x_i} U^s(\mathfrak{R}_r) \qquad \text{and} \qquad \nabla_{m_i} U(\mathfrak{R}_r) = \nabla_{m_i} U^d(\mathfrak{R}_r),$$

where

$$\nabla_{x_i} U^d(\mathfrak{R}_r) = \frac{3}{16\, r^4} \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} \frac{1}{\left|\sin\left(\frac{j\pi}{n}\right)\right|^3} \left(\cos^2\left(\frac{j\pi}{n}\right) + 2 \right) \frac{x_i}{|x_i|},$$

$$\nabla_{x_i} U^s(\mathfrak{R}_r) = -\frac{2}{r^{\alpha+1}} \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} \frac{1}{\left|2\sin\left(\frac{j\pi}{n}\right)\right|^{\alpha}} \frac{x_i}{|x_i|}$$

$$\nabla_{m_i} U^d(\mathfrak{R}_r) = \frac{1}{4r^3} \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} \left(\frac{1}{\left|\sin\left(\frac{j\pi}{n}\right)\right|} - \frac{2}{\left|\sin\left(\frac{j\pi}{n}\right)\right|^3} \right) \frac{m_i}{|m_i|}.$$

The conclusions on the theorem then follows from direct study of the function

$$r \longmapsto \frac{A}{r^{\alpha+1}} - \frac{B}{r^4},$$

with A and B given by the lemma.

"Proof" of the lemma. To start, we compute:

$$\nabla_{x_0} U^d = \sum_{j=1}^{n-1} \frac{-3}{|r_{0j}|^5} \left[(m_0 \cdot r_{0j}) m_j + (m_j \cdot r_{0j}) m_0 + (m_0 \cdot m_j) r_{0j} - 5 \frac{(m_0 \cdot r_{0j})(m_j \cdot r_{0j})}{|r_{0j}|^2} r_{0j} \right].$$

$$\nabla_{x_0} U^s = - \sum_{j=1}^{n-1} \left(\frac{1}{|r_{0j}|} \right)^{\alpha+1} \frac{r_{0j}}{|r_{0j}|}, \qquad \text{and} \qquad \nabla_{m_j} U^d = \sum_{j=1}^{n-1} \left[\frac{m_j}{|r_{0j}|^3} - 3 \frac{(m_j \cdot r_{0j}) r_{0j}}{|r_{0j}|^5} \right].$$

Since we have a ring structure, the scalar products write

$$|r_{0j}| = r\sqrt{2 - 2\cos\left(\frac{2j\pi}{n}\right)} = 2r\left|\sin\left(\frac{j\pi}{n}\right)\right|, \qquad m_0 \cdot r_{0j} = -r \sin\left(\frac{2j\pi}{n}\right),$$

$$m_j \cdot r_{0j} = -r \sin\left(\frac{2j\pi}{n}\right), \qquad m_0 \cdot m_j = \cos\left(\frac{2j\pi}{n}\right).$$

The lemma is given by tedious but straightforward computation (involving classical trigonometry formulas for simplifications).

$\rightarrow$ **The main important point is to gather the terms associated to the indices j and $n - j$ to obtain cancellations due to the symmetry of the structure.** □

The magnetic nano-wire

A 1D model of ferro-magnetic nano-wire

We consider here a simple and rich model introduced in works by Carbou for notched ferro-magnetic nano-wires:

- G. Carbou. Notch-Induced Domain Wall Pining in Ferromagnetic Nanowires (2020).
- G. Carbou and D. Sanchez. Stabilization of walls in notched magnetic nanowires (2018).

The magnetization behavior is obtained thanks to a Γ-convergence reasoning: a cylindrical material $\mathcal{D}_\eta$ is considered by

$$\mathcal{D}_\eta = \{(x, y, z) \in \mathbb{R}^3,\ y^2 + z^2 \leq \eta^2 \rho(x)^2\},$$

whose circular section, parametrized by a function ρ, has radius $\eta\rho(x)$ with $\eta > 0$.

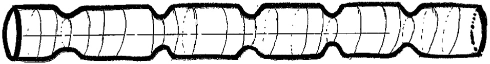
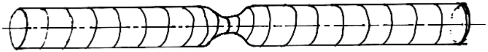


Figure: An example of domain $\mathcal{D}_\eta$.

A 1D model is then derived by making η tend towards 0. The 1D model involves the cross section area s defined by $s(x) = \pi\rho(x)^2$.

In this work we focus on the 1 notch case for the infinite nano-wire.



We work on the class of localized and symmetric notches ($s_0 > 0$):

$$\mathcal{S}_a(\Omega) = \big\{ s \in BV(\mathbb{R}; [s_0; 1]) \ : \ s \equiv 1 \text{ outside } [-a, a], \quad s \text{ is even and non-decreasing on } \mathbb{R}_+. \big\}.$$

The asymptotic $1D$ Landau-Lifshitz-Gilbert model for magnetization in notched nanowires reads:

$$\begin{cases} \partial_t \boldsymbol{m} = -\boldsymbol{m} \times \mathcal{H}(\boldsymbol{m}) - \alpha \boldsymbol{m} \times (\boldsymbol{m} \times \mathcal{H}(\boldsymbol{m})) \\ \mathcal{H}(\boldsymbol{m}) = \frac{\ell^2}{s(x)} \partial_x (s \partial_x \boldsymbol{m}) - \frac{1}{2}(m_2 \mathbf{e_2} + m_3 \mathbf{e_3}), \end{cases}$$

It has been proved in Carbou's works that every steady solution reads

$$\boldsymbol{m}(x) = R_\varphi \begin{pmatrix} \sin\theta(x) \\ \cos\theta(x) \\ 0 \end{pmatrix}, \quad \text{with} \quad R_\varphi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & \sin\varphi & \cos\varphi \end{pmatrix},$$

where $\varphi \in \mathbb{R}$ is the rotation angle, and θ solves the non-linear Sturm-Liouville equation:

$$s(x)\theta''(x) + s'(x)\theta'(x) + s(x)\cos\theta(x)\sin\theta(x) = 0, \qquad \forall\, x \in \mathbb{R}.$$

$$\theta''(x) + \frac{s'(x)}{s(x)}\theta'(x) + \frac{\sin 2\theta(x)}{2} = 0, \qquad \forall x \in \mathbb{R}.$$

Theorem (Carbou)

This Strum-Liouville Equation admits a non-trivial solution θ_0 in $W := \left\{\vartheta \in \dot{H}^1(\mathbb{R}) \ : \ \cos(\vartheta) \in L^2\right\}$. This solution is odd, increasing, with limits $\pm\frac{\pi}{2}$ at $\pm\infty$.

→ *Idea:* Proceed by analogy with the simple pendulum and solve a shooting problem.

Theorem (Carbou)

*For θ a solution to this Strum-Liouville Equation, the associated steady magnetization **m** is asymptotically stable (up to rotations around the x-axis) whenever $\theta \in W$, provided that $s \not\equiv 1$.*

→ *Idea:* The solutions are the critical points of the following energy

$$E_s(\theta) := \frac{1}{2}\int_{\mathbb{R}} \theta'(x)^2 s(x)\,dx + \frac{1}{2}\int_{\mathbb{R}} \cos^2\left(\theta(x)\right) s(x)\,dx.$$

Stability is then given by the computation of the second derivative at a critical point.

Theorem (R. Côte, C. Courtès, G. Ferrière, L.G-C., Y. Privat)

There exists a **unique** *non-trivial solution in W (up to symmetry or additive constant) if $s \not\equiv 1$.*

Deny the existence of 2 solutions by constructing a $3rd$, using the mountain-pass theorem (contradiction with the previous result).

Thank-you for your attention !