# Limite thermodynamique pour des systèmes coulombiens quantiques désordonnés.

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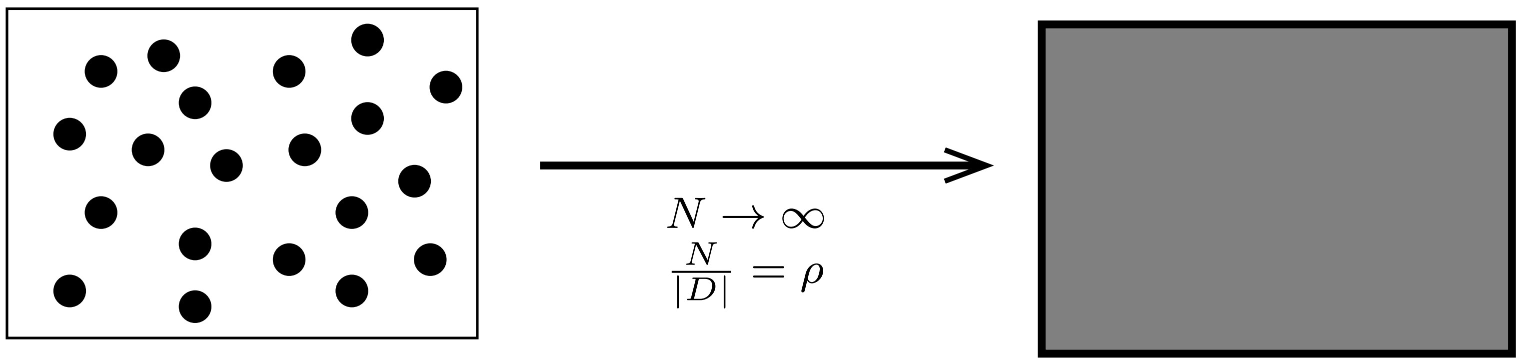
ANR NONAP

# Thermodynamic limit problem

Problem: determine macroscopic behaviour of microscopic systems. $\mathcal{F}(D)$ energy in domain $D$.




Fisher-Ruelle, 1966 :

- Notion of stability of matter: $\dfrac{\mathcal{F}(D)}{|D|} \geq -C.$
- Notion of thermodynamic limit: $\lim\limits_{|D|\to\infty} \dfrac{\mathcal{F}(D)}{|D|} = f.$

# Thermodynamic limit problem

Notion of stability of matter: $\dfrac{\mathcal{F}(D)}{|D|} \geq -C.$

- Dyson-Lenard, 1967.
- Lieb-Thirring, 1975.
- Reviews: Lieb, 1976, 1990, and Lieb-Seiringer, 2010.

Notion of thermodynamic limit: $\lim_{|D|\to\infty} \dfrac{\mathcal{F}(D)}{|D|} = f.$

- Short-range interaction: Ruelle, 1963, Fisher, 1964.
- Coulomb interactions: Lieb-Lebowitz, 1972.
- Crystals: Fefferman, 1985.
- Conlon-Lieb-Yau, 1989.
- Graf-Schenker, 1995.
- Hainzl-Lewin-Solovej, 2009.

# Stochastic setting

Our work:

generalize proof of Hainzl-Lewin-Solovej (periodic setting) to a stochastic setting.

Nuclei = classical static particles,
electrons = quantum particles,
interaction = Coulomb.

Stochastic setting:

- No interaction case (Germinet, Hislop, Kirsch, Klopp, ...)
- Interacting case : Veniaminov, 2011.

# Outline of the talk

- Stochastic lattices and ergodic theorem
- Statement of the problem
- Main results
  - Stability of matter
  - Thermodynamic limit
  - Asymptotic neutrality
- Example: i.i.d case
- Ideas of proof
  - Upper bound
  - Convergence of the expectation value of the energy
  - Liminf for the energy: Graf-Schenker inequality

# Stochastic lattices

## Stationary ergodic setting

$(\Omega, \mathcal{F}, \mathbb{P})$ probability space. $(\tau_k)_{k \in \mathbb{Z}^3}$ action of $\mathbb{Z}^3$ on $\Omega$ such that:

$\tau$ is a morphism: $\quad \tau_{k+j} = \tau_k \circ \tau_j,$

$\tau$ preserves $\mathbb{P}$: $\quad \forall A \in \mathcal{F}, \quad \mathbb{P}(\tau_k A) = \mathbb{P}(A),$

$\tau$ is ergodic: $\quad \left(\forall k \in \mathbb{Z}^3, \quad \tau_k A = A\right) \Rightarrow \mathbb{P}(A) = 0$ or $1.$

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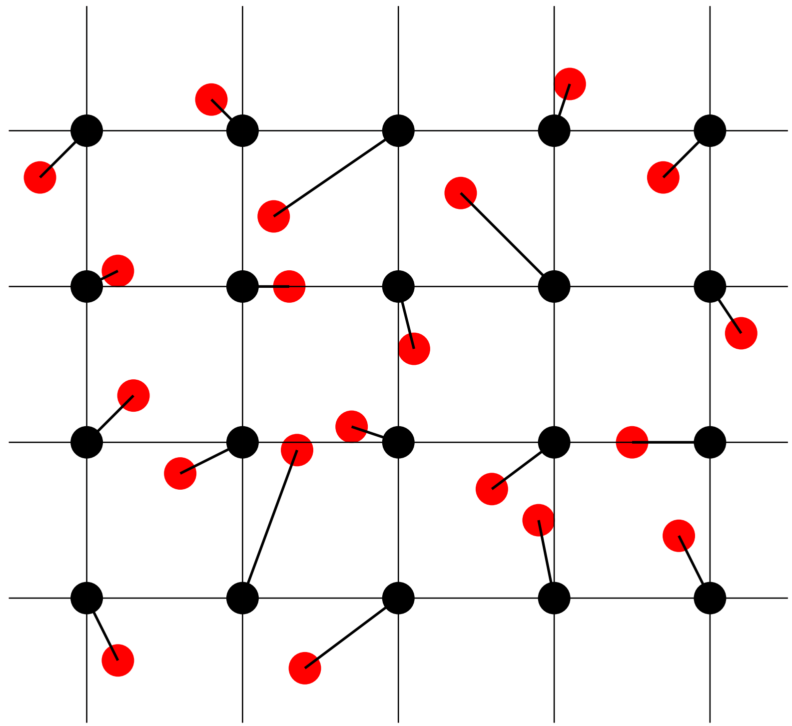
The discrete lattice $\mathcal{K} = \mathcal{K}(\omega)$ is said to be stationary if

$$\forall k \in \mathbb{Z}^3, \quad \mathcal{K}(\tau_k \omega) = \mathcal{K}(\omega) - k.$$

Example: i.i.d case $\mathcal{K}(\omega) = \left\{ i + Y_i(\omega), i \in \mathbb{Z}^3 \right\}$, $Y_i$ i.i.d.

# Stochastic lattices

Example: i.i.d case: $\mathcal{K}(\omega) = \left\{ i + Y_i(\omega), i \in \mathbb{Z}^3 \right\}$,
where $Y_i$ is an i.i.d sequence.



Typically, the law of $Y_i$ is $d\nu(x) = \dfrac{1}{(2\pi\sigma)^{3/2}} e^{-\frac{|x|^2}{2\sigma}}$.

# Ergodic theorem

Theorem (Tempel'man, 1972): Let $X \in L^p(\Omega)$, $1 \leq p < \infty$.
Consider a sequence of sets $D_n \subset \mathbb{R}^3$ such that $|D_n| \to \infty$ and which is regular in the sense of Fisher. Then we have

$$\frac{1}{|D_n|} \sum_{k \in \mathbb{Z}^3 \cap D_n} X(\tau_k \omega) \underset{n \to \infty}{\longrightarrow} \mathbb{E}(X) \quad \text{in} \quad L^p(\Omega).$$

If moreover $D_n \subset B_{c|D_n|^{1/3}}$ for some $c > 0$ and all $n$, then

$$\frac{1}{|D_n|} \sum_{k \in \mathbb{Z}^3 \cap D_n} X(\tau_k \omega) \underset{n \to \infty}{\longrightarrow} \mathbb{E}(X) \quad \text{almost surely.}$$

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Fisher regularity: $\forall t \in [0, t_0]$, $\left| \left\{ x \in \mathbb{R}^3 \ : \ \mathrm{d}(x, \partial D_n) \leq t \, |D_n|^{1/3} \right\} \right| \leq |D_n| \, \eta(t)$ for some $t_0 > 0$ and some function $\eta$ with $\lim_{t \to 0} \eta(t) = 0$.

# Statement of the problem

$$H(\omega, D, N) = \sum_{n=1}^{N} (-\Delta)_{x_n} - \sum_{n=1}^{N} \sum_{R \in \mathcal{K}(\omega) \cap D} \frac{1}{|x_n - R|}$$

$$+ \frac{1}{2} \sum_{1 \leq n \neq m \leq N} \frac{1}{|x_n - x_m|} + \frac{1}{2} \sum_{\substack{R \in \mathcal{K}(\omega) \cap D \\ R' \in \mathcal{K}(\omega) \cap D \\ R \neq R'}} \frac{1}{|R - R'|}.$$

$$\mathcal{F}_0(\omega, D, N) = \inf \sigma\Big(H(\omega, D, N)\Big) = \inf_{\substack{\Psi \in \bigwedge_1^N H_0^1(D) \\ \int_{D^N} |\Psi|^2 = 1}} \langle \Psi \,,\, H(\omega, D, N) \Psi \rangle.$$

$$\boxed{\mathcal{F}_0(\omega, D) := \inf_{N \geq 0} \mathcal{F}_0(\omega, D, N).}$$

# Statement of the problem

- Stability of matter:

$$\mathcal{F}_0(\omega, D) \geq -C|D|,$$

$C > 0$ independent of $D$ and $\omega$.

- Thermodynamic limit:

$$\frac{\mathcal{F}_0(\omega, D)}{|D|} \underset{|D|\to\infty}{\longrightarrow} f.$$

Need of geometric assumptions:

- On the set $\mathcal{K}(\omega)$: nuclei should not be too close.
- On the regularity of the set $D$. Typically, $|\partial D| \ll |D|$.

# Statement of the problem

Positive temperature $T > 0$, chemical potential $\mu \in \mathbb{R}$

$$\boxed{\mathcal{F}_{T,\mu}(\omega, D) = -T \log \left( \sum_{N \geq 0} \mathrm{Tr}_{\bigwedge_1^N L^2(\mathbb{R}^3)} e^{-\big(H(\omega,D,N) - \mu N\big)/T} \right)}$$

Fermionic Fock space

$$\mathscr{F} := \mathbb{C} \oplus \bigoplus_{N \geq 1} \bigwedge_1^N L^2(D).$$

Hamiltonian

$$\mathbb{H}(\omega, D) := 0 \oplus \bigoplus_{N \geq 1} H(\omega, D, N) \quad \text{and} \quad \mathcal{N} := 0 \oplus \bigoplus_{N \geq 1} N.$$

# Main results

Stability of matter: There exists a universal constant $C > 0$ such that

$$\mathcal{F}_{T,\mu}(\omega, D) \geq -C\big(1 + T^{5/2} + \mu_+^{5/2}\big)|D|,$$

almost surely. In particular, $\mathcal{F}_0(\omega, D) \geq -C|D|$.

This result does not use stationarity.

Main tools:

- Lieb-Yau inequality (lower bound on the interaction).
- Lieb-Thirring inequality (lower bound on the kinetic energy).

# Main results

Thermodynamic limit: If $\mathcal{K}$ is stationary and satisfies

$$X_1 := \sum_{R \in \mathcal{K} \cap W} \frac{1}{\delta(R)} \in L^2(\Omega), \quad \delta(x) = \inf \{|x - R|, R \in \mathcal{K} \cap D \setminus \{x\}\}$$

then there exists a function $f(T,\mu)$ such that for any regular sequence $D_n$ satisfying

$$|D_n| \underset{n\to\infty}{\longrightarrow} \infty, \quad \frac{\mathrm{diam}(D_n)}{|D_n|^{1/3}} \leq C,$$

$$\frac{\mathcal{F}_{T,\mu}(\omega, D_n)}{|D_n|} \underset{n\to\infty}{\longrightarrow} f(T,\mu) \quad \text{in } L^1(\Omega).$$

# Regular sets

We say that the domain $D$ is regular if

- it is regular in the sense of Fisher:
  $\exists a > 0$, such that

$$\forall t \in [0, 1/a), \quad \left| \left\{ x \in \mathbb{R}^3 \mid \mathsf{d}(x, \partial D) \leq |D|^{1/3} t \right\} \right| \leq |D| \, a \, t,$$

- it satisfies the $\varepsilon$-cone condition:
  $\exists \varepsilon > 0$, such that for any $x \in D$, there is a unit vector $v_x \in \mathbb{R}^3$ such that

$$\{ y \in \mathbb{R}^3 \mid (x - y) \cdot v_x > (1 - \varepsilon^2) |x - y|, \ |x - y| < \varepsilon \} \subseteq D.$$

- The set $\mathbb{R}^3 \setminus D$ satisfies the $\varepsilon$-cone condition.

# About almost sure convergence

Almost sure thermodynamic limit should hold:

$$\frac{\mathcal{F}_{T,\mu}(\omega, D_n)}{|D_n|} \underset{n\to\infty}{\longrightarrow} f(T,\mu) \quad \text{almost surely.}$$

A natural hypothesis for that would be

$$D_n \subseteq B_{c|D_n|^{1/3}}.$$

(cf Birkhoff's almost sure convergence theorem).

We can prove, under this assumption,

$$\liminf_{n\to\infty} \frac{\mathcal{F}_{T,\mu}(\omega, D_n)}{|D_n|} = f(T,\mu) \quad \text{almost surely.}$$

# Main results

Asymptotic neutrality: if $\mathcal{K}$ is stationary and $X_1 \in L^1(\Omega)$, then, letting

$$N_{T,\mu}(\omega, D_n) := \frac{\sum_{N\geq 0} N \ \mathrm{Tr}_{\bigwedge_1^N L^2(\mathbb{R}^3)} e^{-\left(H(\omega,D_n,N)-\mu N\right)/T}}{\sum_{N\geq 0} \mathrm{Tr}_{\bigwedge_1^N L^2(\mathbb{R}^3)} e^{-\left(H(\omega,D_n,N)-\mu N\right)/T}},$$

$$\lim_{n\to\infty} \frac{N_{T,\mu}(\cdot, D_n)}{|D_n|} = \underbrace{\mathbb{E}\left(\#\mathcal{K}\cap W\right)}_{:=Z_{\mathrm{av}}} \text{ in } L^2(\Omega)$$

Moreover, we have $\boxed{f(T,\mu) = f(T,0) - \mu\, Z_{\mathrm{av}},}$ and $T \mapsto f(T,0)$ is concave.

# Example: i.i.d case

$\mathcal{K}(\omega) = \left\{ i + Y_i(\omega), i \in \mathbb{Z}^3 \right\}$. $Y_i$ i.i.d sequence. $\nu$ law of $Y_i$

$$X_0(\omega) = \#\left(\mathcal{K}(\omega) \cap W\right) = \#\left\{ j \in \mathbb{Z}^3 \ : \ j + Y_j(\omega) \in W \right\}$$

- $X_0 \in L^1(\Omega)$, and $\mathbb{E}(X_0) = 1$.
- $\|X_0\|_{L^p(\Omega)} \leq \sum_{j \in \mathbb{Z}^3} \nu(W + j)^{1/p}$.
- If supp$(\nu)$ is not compact, then $X_0 \notin L^\infty(\Omega)$.
- If $\sum_{j \neq 0} \|\nu\|_{L^\infty(W + B_\eta - j)}^{1/p} < \infty$, $\eta > 0$ and $1 \leq p < 3$, then $X_1 \in L^p(\Omega)$.

In particular, if $\nu(x) = \dfrac{1}{(2\pi\sigma)^{-3/2}} e^{-|x|^2/(2\sigma)}$, the above results apply.

# Ideas of proof

- Step 1: $\sup_{n\in\mathbb{N}} \frac{\mathbb{E}\left(\left|\mathcal{F}_{T,\mu}(D_n)\right|\right)}{|D_n|} < \infty$. Uses $X_1 \in L^1(\Omega)$.
- Step 2: $\lim_{n\to\infty} \frac{\mathbb{E}\left(\mathcal{F}_{T,\mu}(D_n)\right)}{|D_n|} = f(T,\mu)$. Periodic case.
- Step 3: $\lim_{n\to\infty} \mathbb{E}\left[\frac{\mathcal{F}_{T,\mu}(\omega, D_n)}{|D_n|} - f(T,\mu)\right]_- = 0$.
  Graf-Schenker inequality.
- Step 4: 2 & 3 imply $\lim_{n\to\infty} \mathbb{E}\left|\frac{\mathcal{F}_{T,\mu}(\omega, D_n)}{|D_n|} - f(T,\mu)\right| = 0$.

# Upper bound: $\sup_{n\in\mathbb{N}} \frac{\mathbb{E}\left(\left|\mathcal{F}_{T,\mu}(D_n)\right|\right)}{|D_n|} < \infty.$

- $\mathcal{F}(D,\omega) \geq -C|D|,$ almost surely.
- Construction of an adpated trial function.

$$\delta(x,\omega) = \inf\Big\{|x-R|, R \in \mathcal{K} \cap D \setminus \{x\}\Big\},$$

For each nucleus $R$, a radially symmetric electron in $B_{\delta(R)/2}(R)$.

  - Kinetic energy: $\propto \sum_{R\in\mathcal{K}\cap D} \frac{1}{\delta(R)^2}$.
  - Inner electrostatic interactions: non-positive.
  - Boundary electrostatic interactions: dipoles $\propto \sum_{R\in\mathcal{K}\cap D} \sum_{R'\in\mathcal{K}\cap(\partial D)_\varepsilon\setminus\{R\}} \frac{1}{|R-R'|\,(1+|R-R'|^2)}$

# **Limit in average:** $\lim \frac{\mathbb{E}\Big(\mathcal{F}_{T,\mu}(D_n)\Big)}{|D_n|} = f(T,\mu).$

- Periodicity: $\mathbb{E}(\mathcal{F}_{T,\mu}(D+k)) = \mathbb{E}(\mathcal{F}_{T,\mu}(D)).$
- Continuity:
  $\forall D' \subset D, \quad \mathbb{E}\Big(\mathcal{F}_{T,\mu}(D)\Big) \leq \mathbb{E}\Big(\mathcal{F}_{T,\mu}(D')\Big) + C|D \setminus D'|.$
- Sub-average property:

$$\mathcal{F}_{T,\mu}(\omega, D) \geq \left(1 - \frac{C}{\ell}\right) \int_G \frac{\mathcal{F}_{T,\mu}(\omega, D \cap g\ell\triangle)}{|\ell\triangle|}\, dg \\ - \frac{C}{\ell}\Big(\#(\mathcal{K}(\omega) \cap D) + |D|\Big).$$

$\triangle$ is a simplex, $G = \mathbb{R}^3 \rtimes SO(3)$, $dg$ Haar measure.

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Hainzl-Lewin-Solovej: $\mathbb{E}\left(\mathcal{F}_{T,\mu}(D_n)\right)$ has a thermodynamic limit.

# Graf-Schenker inequality

Graf, Schenker, 1995: let $\triangle$ be a simplex, $z_i \in \mathbb{R}$, $x_i \in \mathbb{R}^3$, $\ell > 0$. Then

$$\sum_{1\le i<j\le N} \frac{z_i z_j}{|x_i - x_j|} \ge \int_G \frac{dg}{|\ell\triangle|} \sum_{1\le i<j\le N} \frac{z_i z_j \mathbb{1}_{g\ell\triangle}(x_i)\mathbb{1}_{g\ell\triangle}(x_j)}{|x_i - x_j|} - \frac{C}{\ell}\sum_{i=1}^N z_i^2.$$

Localization in Fock space (Dereziński-Gérard, 1999, Ammari, 2004):

$$H(\omega, D, N) \ge \frac{1 - C/\ell}{|\ell\triangle|}\int_G dg H_{g\theta^\ell}(\omega, D, N) + \frac{C}{2\ell}\sum_{i=1}^N(-\Delta_{x_i}) - \frac{C}{\ell}\#(\mathcal{K}\cap D).$$

$H_\chi(\omega, D, N) = \chi H(\omega, D, N)\chi$,
$\theta^\ell$ localization function around $\ell\triangle$.

**Lower bound:** $\lim \mathbb{E}\left[\frac{\mathcal{F}_{T,\mu}(\omega,D_n)}{|D_n|} - f(T,\mu)\right]_- = 0.$

Graf-Schenker inequality:

$$\frac{\mathcal{F}_{T,\mu}(\omega,D)}{|D|} \geq \frac{1}{|D|}\left(1-\frac{C}{\ell}\right)\int_G \frac{\mathcal{F}_{T,\mu}(\omega, D\cap g\ell\triangle)}{|\ell\triangle|}\,dg - \frac{C}{\ell}\underbrace{\left(\frac{\#(\mathcal{K}(\omega)\cap D)}{|D|}+1\right)}_{\text{bounded in } L^1(\Omega)}.$$

$$\frac{1}{|D|}\int_G \frac{\mathcal{F}_{T,\mu}\big(\omega, D\cap (g\ell\triangle)\big)}{|\ell\triangle|}\,dg$$

$$= \frac{1}{|D|}\sum_{j\in\mathbb{Z}^3}\int_W dy \int_{SO(3)} dR\,\frac{\mathcal{F}_{T,\mu}\big(\omega, D\cap(R\ell\triangle+y+j)\big)}{|\ell\triangle|}.$$

## **Lower bound:** $\lim \mathbb{E}\left[\frac{\mathcal{F}_{T,\mu}(\omega,D_n)}{|D_n|} - f(T,\mu)\right]_- = 0.$

Graf-Schenker inequality:

$$\frac{\mathcal{F}_{T,\mu}(\omega,D)}{|D|} \geq \frac{1}{|D|}\left(1-\frac{C}{\ell}\right)\int_G \frac{\mathcal{F}_{T,\mu}(\omega, D\cap g\ell\triangle)}{|\ell\triangle|}\,dg - \frac{C}{\ell}\underbrace{\left(\frac{\#(\mathcal{K}(\omega)\cap D)}{|D|}+1\right)}_{\text{bounded in } L^1(\Omega)}.$$

$$\frac{1}{|D|}\int_G \frac{\mathcal{F}_{T,\mu}\big(\omega, D\cap(g\ell\triangle)\big)}{|\ell\triangle|}\,dg = \frac{1}{|D|}\int_W dy\int_{SO(3)} dR\,\underbrace{\sum_{j\in\mathbb{Z}^3}\frac{\mathcal{F}_{T,\mu}\big(\tau_j\omega, D\cap(R\ell\triangle+y)\big)}{|\ell\triangle|}}_{\text{ergodic sum}}.$$

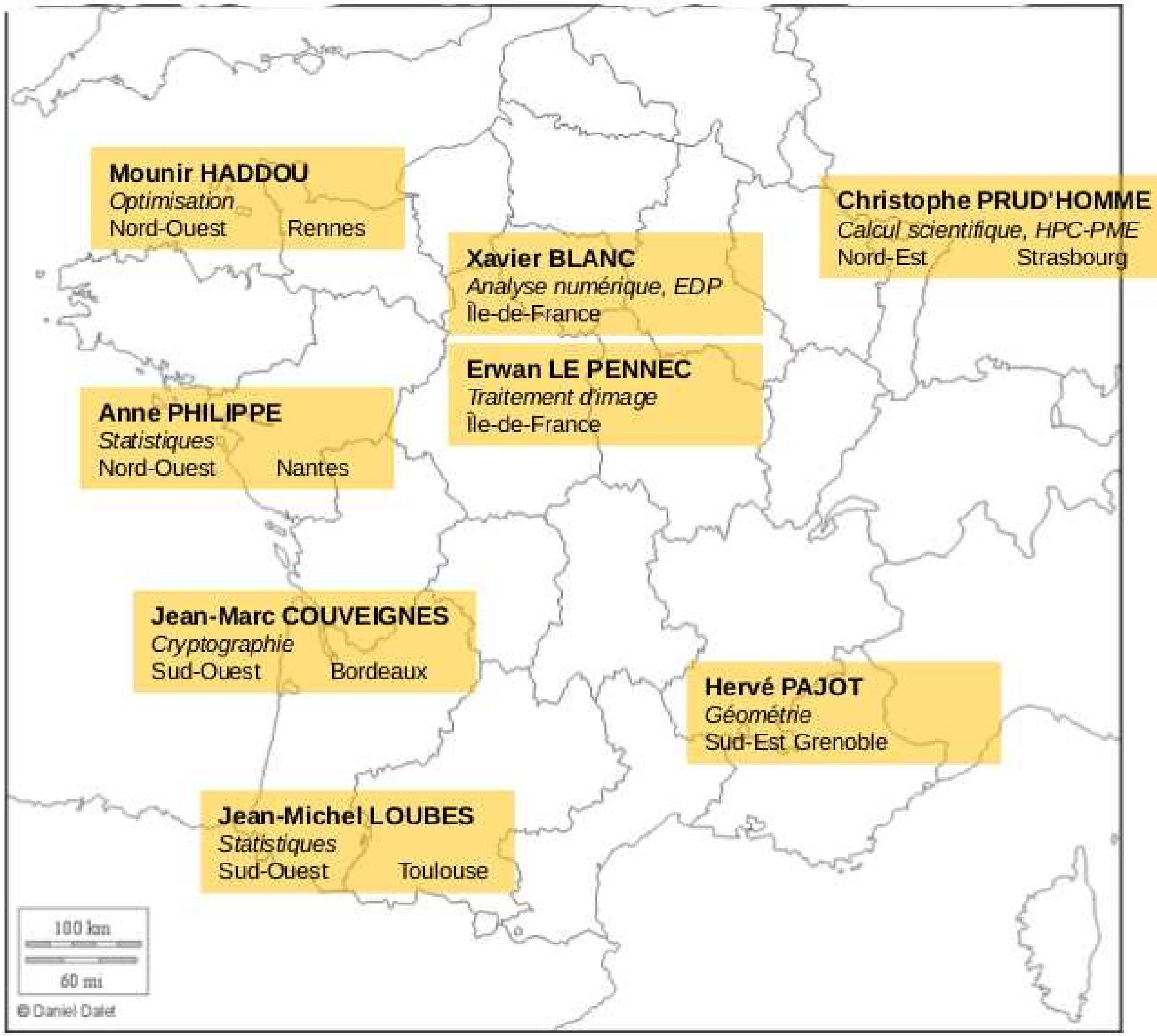
AMIES :
Agence pour les Mathématiques en Interaction avec l'Entreprise et la Société.

- Un Labex créé en 2011.
- Objectif : promouvoir et fluidifier les transferts mathématiques-entreprise/société, notamment les PME.
- Partenaires : CNRS (porteur), INRIA, UJF.
- Actions :
  - Formation
  - Stimulation de la recherche
  - Communication

# Programmes d'AMIES

- Stimulation de la recherche :
  - Connecter entreprises et chercheurs/étudiants via un réseau de facilitateurs
  - Organisation et soutien de manifestations impliquant étudiants-labos-entreprises
  - Soutien à projets exploratoires (PEPS) : candidature en ligne sur le site, au fil de l'eau
- Vitrine :
  - Communiquer sur les interactions Math. Entreprise : site de l'agence, newsletter, groupes de discussion sur les réseaux sociaux
  - Cartographier l'expertise des laboratoires : base de données en construction

# Facilitateurs



# Exemple

Collaboration de P. Helluy (IRMA) avec Axessim (PME) pour la simulation numérique d'un générateur de rayon X.

- simuler les flux d'électrons entre la cathode et l'anode lors d'une radiographie médicale par un générateur de rayons X
- coupler une méthode d'éléments finis/méthode Particle-In-Cell (PIC)
- Projet PEPS (1 stage + fonctionnement) et maintenant 1 thèse CIFRE