Nonlinear models for moiré materials

David Gontier
joint work with Solal Perrin-Roussel and Eric Cancès

CERMICS, Ecole Nationale des Ponts et Chaussées

February 6 2026

Nice, Dynamical and Quantum Systems... and Eric's Séré birthday.
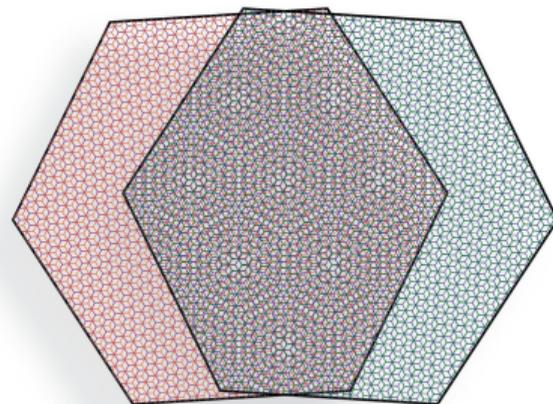
Moiré materials

Moiré = comes from the French "moiré" (which comes from English "mohair", which is a textile from Angora goats) = *watered silk* = one piece of silk folded and compressed.

Used nowadays for decorative textile and ribbons.

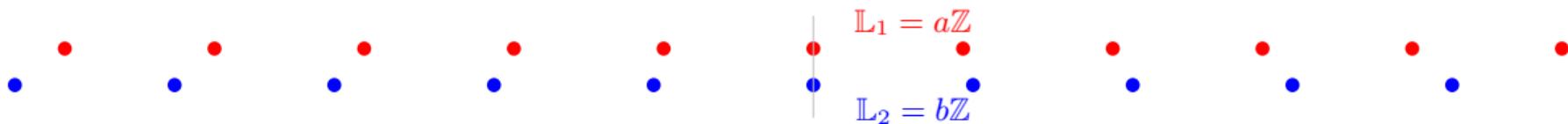Écharpe en moiré de Grand'Croix de l'Ordre de Léopold, Belgique.

Twisted Bilayer Graphene.

Two scales are involved: the microscopic scale (graphene), and the moiré scale.
In this presentation, we focus on the microscopic scale.

Bilayer materials

We consider a charge distribution of the form

$$\mu(x) = \mu_1(x) + \mu_2(x), \qquad \begin{cases} \mu_1 & \text{is } \mathbb{L}_1\text{-periodic,} \\ \mu_2 & \text{is } \mathbb{L}_2\text{-periodic.} \end{cases}$$

$$\mathbb{L}_1 = a\mathbb{Z}$$

$$\mathbb{L}_2 = b\mathbb{Z}$$

Remark: One should not fix an **offset** between the two lattices...

It is more physical to consider the family of charge distributions, parametrized by the **configuration** $\omega = (\omega_1, \omega_2)$.

$$\mu(\omega, x) = \mu_1(x - \omega_1) + \mu_2(x - \omega_2), \qquad \begin{cases} \mu_1 & \text{is } \mathbb{L}_1\text{-periodic,} \\ \mu_2 & \text{is } \mathbb{L}_2\text{-periodic,} \end{cases} \qquad \omega = (\omega_1, \omega_2) \in \mathbb{T}_1 \times \mathbb{T}_2.$$

Remark: We have $\mu(\omega_1, \omega_2; x) = \mu(\omega_1 - x, \omega_2 - x; 0)$.

Stationary functions

Definition

We say that a function $f(\omega, x) : \Omega \times \mathbb{R}^d \to \mathbb{R}$ is **stationary** (for the action α) iff it is of the form

$$f(\omega, x) = F(\alpha_x \omega), \quad \text{for a function } F : \Omega \to \mathbb{R},$$

where $x \mapsto \alpha_x$ is a measure preserving group action on $\Omega := \mathbb{T}_1 \times \mathbb{T}_2$.

Example 1: periodic functions

If $\Omega = \mathbb{T} := \mathbb{R}^d / \mathbb{L}$ and $\alpha_x(\omega) := \omega - x$ (modulo $\mathbb{L}$), a function $f(\omega, x) : \mathbb{T} \times \mathbb{R}^d \to \mathbb{R}$ is stationary iff $x \mapsto f(\omega - x, 0)$ is $\mathbb{L}$ periodic.
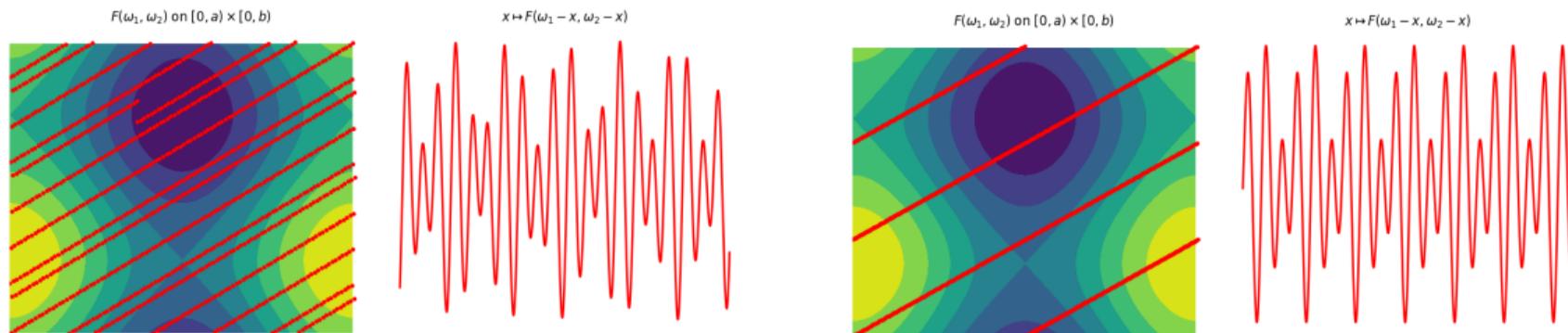
It is a nice way to describe periodic functions in $\mathbb{R}^d$.

Example 2: Bi-layered case

The previous charge distributions is stationary in the case $\Omega = \mathbb{T}_1 \times \mathbb{T}_2$ with the action

$$\alpha_x(\omega) := (\omega_1 - x, \omega_2 - x).$$

Sationary functions for bi-layered materials: $f(x) = F(\omega_1 - x, \omega_2 - x)$ with $F : \mathbb{T}_1 \times \mathbb{T}_2 \to \mathbb{R}$ periodic.

$F(\omega_1, \omega_2)$ on $[0, a) \times [0, b)$ $x \mapsto F(\omega_1 - x, \omega_2 - x)$

(a) Case $a = 1, b = \sqrt{2} = 1.414....$

$F(\omega_1, \omega_2)$ on $[0, a) \times [0, b)$ $x \mapsto F(\omega_1 - x, \omega_2 - x)$

(b) Case $a = 1, b = 1.5$.

We are wrapping a line on a torus $\mathbb{T}_1 \times \mathbb{T}_2$.

Incommensurate case: the line fills the whole torus.
All **configurations** are «similar», up to translations $\implies$ **ergodic case**.

Commensurate case: the line loops, and does not fill the torus
The *relative position* between the two lattices plays an important role!

It looks *nicer* to work with the smooth function F... but we added (several) dimensions...

Stationary operators

Consider a **stationary potential** $V(\omega, x)$. Our goal is study operators of the form

$$\boxed{H_\omega = -\Delta + V_\omega,} \qquad \text{acting on } L^2(\mathbb{R}^d),$$

Remark: we have $U_y H_\omega U_y^* = H_{\alpha_y(\omega)}$, where $[U_y f](x) := f(x - y)$ is the **translation operator**.

Step 1: we augment the space. We *superpose* all configurations:

$$\boxed{\widetilde{H} := \int_\Omega^\oplus H_\omega \, d\omega,} \qquad \text{acting on } L^2(\Omega \times \mathbb{R}^d), \qquad (\widetilde{g} = \widetilde{H} f \text{ means } g_\omega = H_\omega f_\omega)$$

In practice, we are interested in a *single* configuration $\omega_0 \in \Omega$, but it makes sense to study the whole family directly.

Fact: The set of (bounded) operators of the form $\widetilde{A} = \int_\Omega^\oplus A_\omega \, d\omega$ with $U_y A_\omega U_y^* = A_{\alpha_y(\omega)}$ forms a C^*-algebra.

This C^*-algebra is the **crossed product** $L^\infty(\Omega) \rtimes_\alpha \mathbb{R}^d$, which has been studied by Bellissard (1992), Schulz-Baldes, Simon, Avron, ...

Let's recover some results with slightly different tools.

Decomposition of stationary operators

Introduce the **generalized translation operator** $[T_y F](\omega, x) := F(\tau_y \omega, x - y)$, acting on $L^2(\Omega \times \mathbb{R}^d)$.

> **Lemma**
>
> *The operator $\widetilde{H}$ commutes with all operators T_y. As a consequence, we have*
>
> $$\boxed{\mathcal{F} \widetilde{H} \mathcal{F}^* = \int_{\mathbb{R}^d}^{\oplus} H_k \mathrm{d}k,} \quad \text{for a family } \{H_k\}_{k \in \mathbb{R}^d} \text{ acting on } L^2(\Omega),$$
>
> *where $\mathcal{F} : L^2(\Omega \times \mathbb{R}_x^d) \to L^2(\Omega \times \mathbb{R}_k^d)$ is the* stationary Fourier transform, *defined by*
>
> $$(\mathcal{F}f)(\omega, k) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} f(\alpha_{-x}\omega, x) \mathrm{e}^{-\mathrm{i}kx} \mathrm{d}x.$$

Example 1: periodic operators. With $\alpha_x \omega = \omega - x, \omega \in \Omega := \mathbb{R}^d / \mathbb{L}$, we find

$$H_k := (-\mathrm{i}\nabla_\omega + k)^2 + V(\omega) \quad \text{acting on } L^2(\Omega),$$

Remark: We recover the usual formula of H_j, but with a Fourier transform (instead of a Bloch transform).
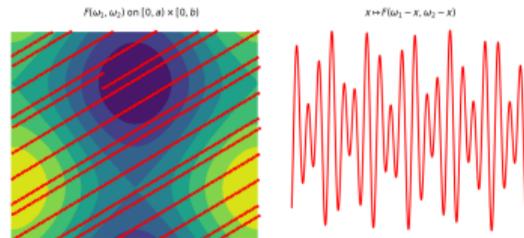
Decomposition of bilayered Hamiltonians

Example 2: bilayered operators. With $\alpha_x \omega = (\omega_1 - x, \omega_2 - x)$, $\omega \in \Omega := \mathbb{T}_1 \times \mathbb{T}_2$, we find

$$H_k := (-i\nabla_{\omega_1} - i\nabla_{\omega_2} + k)^2 + V(\omega_1, \omega_2) \quad \text{acting on } L^2(\mathbb{T}_1 \times \mathbb{T}_2),$$

Remarks:

$F(\omega_1, \omega_2)$ on $[0, a] \times [0, b]$ $x \mapsto F(\omega_1 - x, \omega_2 - x)$

- No coercivity: the derivative is along one direction only...
- Ω is $2d$–dimensional.

In the Fourier basis of $\mathbb{T}_1 \times \mathbb{T}_2$, parametrized by $K = (K_1, K_2) \in \mathbb{L}_1^* \times \mathbb{L}_2^*$, we have

$$[H_k]_{K,K'} := (K_1 + K_2 + k)^2 \delta_{K=K'} + \widehat{V}[K_1 - K_1', K_2 - K_2'].$$

For all K'', we have $[H_k]_{K+K'', K'+K''} = \left[H_{k+K_1''+K_2''}\right]_{K,K'}$.

Consider $G := \{K_1 + K_2, \quad K_1 \in \mathbb{L}_1^*, \ K_2 \in \mathbb{L}_2^*\} \subset \mathbb{R}^d$. Then H_k is unitary equivalent to H_{k+g} for all $g \in G$.

Commensurate case: G is discrete.

Incommensurate case: G is **dense**...

Definition. The two lattices $\mathbb{L}_1$ and $\mathbb{L}_2$ are **incommensurate** if $\mathbb{L}_1^* \cap \mathbb{L}_2^* = \{0\}$.

Some spectral surprises

> **Lemma**
>
> *In the incommensurate case, the spectrum of H_k is independent of $k \in \mathbb{R}^d$.*
> *In the incommensurate case, the spectrum of H_ω is independent of $\omega \in \Omega$ ([Pastur-Figotin 1992]).*

Example 3: convolution operator. Consider the operator

$$J : f \mapsto j * f = \int_{\mathbb{R}^d} j(\cdot - y) f(y) \mathrm{d}y, \quad \text{and its augmented version} \quad \widetilde{J} := \int_\Omega^\oplus J \mathrm{d}\omega.$$

Then $\widetilde{J}$ is a stationary operator, and we find (in the bi-layered case),

$$J_k := \sum_{K=(K_1,K_2) \in \mathbb{L}_1^* \times \mathbb{L}_2^*} \widehat{j}(k + K_1 + K_2) |e_K\rangle \langle e_K|.$$

In the incommensurate case,

- The spectrum is pure point essential, equal Im $\widehat{j}$, independent of $k \in \mathbb{R}^d$,
- The *nature* of the spectrum may depend on k.
- The operator J_k is never compact.

Still, efficient numerical methods exists to study these operators.
[Cancès, Cazeaux, Luskin 2017], [Zhou, Chen, Zhou 2019], [Etter, Massat, Luskin, Ortner 2020], [Wang, Chen, Zhou, Zhou, Massat 2025], ...

Density of a stationary operator

We consider a stationary operator

$$A = \int_\Omega^\oplus A_\omega \, \mathrm{d}\omega, \quad \text{and} \quad \mathcal{F} A \mathcal{F}^* = \int_{\mathbb{R}^d}^\oplus A_k \, \mathrm{d}k.$$

Assume that A_ω is locally trace class, with density ρ_ω.

Then, the function $\rho(\omega, x) = \rho_\omega(x)$ is stationary.

Lemma (A cute result)

In the incommensurate case, we have

$$\rho(\omega, 0) = \int_{\mathbb{R}^d} A_k \, \mathrm{d}k \qquad \text{as bounded operators on } L^2(\mathbb{R}^d).$$

In particular, $\rho(\omega, 0) = \int_{\mathbb{R}^d} A_k |e_0\rangle \mathrm{d}k$, as functions on Ω.

Idea of the proof

The operator $B := \int_{\mathbb{R}^d} A_k$ satisfies

$$[B]_{K+K'', K'+K''} = \int_{\mathbb{R}^d} \left[A_{k+K_1''+K_2''} \right]_{K,K'} \mathrm{d}k = [B]_{K,K'}.$$

So B is a convolution operator in Fourier space, hence a multiplication operator. $\quad\square$

Trace per unit volume

Since $\rho(\omega, x)$ is stationary, the quantity $\fint_\Omega \rho_\omega(x)\mathrm{d}\omega$ is independent of x (the action α_x is measure preserving...).
In particular, for any $\chi \in L^2(\mathbb{R}^d)$ with $\|\chi\|_2 = 1$, we have

$$\fint_\Omega \mathrm{Tr}(\chi A_\omega \chi) = \fint_\Omega \int_{\mathbb{R}^d} \rho_\omega(x)|\chi|^2(x)\mathrm{d}x\mathrm{d}\omega = \fint_\Omega \left(\lim_{R \to \infty} \frac{1}{|B_R|} \int_{B_R} \rho_\omega(x)\mathrm{d}x \right) \mathrm{d}\omega.$$

Incommensurate case: **Birkhoff theorem** states that the last parenthesis is independent of $\omega \in \Omega$.
(one configuration represents all of them.)

Commensurate case: The generalized density differs from the *usual* density (it is averaged over all configurations...)

Trace per unit volume

$$\underline{\mathrm{Tr}}(\widetilde{A}) := \fint_\Omega \rho(\omega, x)\mathrm{d}\omega = \fint_\Omega \underbrace{\left(\lim_{R \to \infty} \frac{1}{|B_R|}\mathrm{Tr}(\mathbb{1}_{B_R} A_\omega \mathbb{1}_{B_R}) \right)}_{\text{independent of } \omega \text{ in the incommensurate case, by Birkhoff}} \mathrm{d}\omega = \int_{\mathbb{R}^d} \langle e_0, A_k e_0 \rangle \, \mathrm{d}k.$$

Example:

$$\underline{\mathrm{Tr}}\left(-\widetilde{\Delta}\widetilde{\gamma}\right) = \int_{\mathbb{R}^d} \langle e_0, (-\mathrm{i}\partial_{\omega_1} - \mathrm{i}\partial_{\omega_2} + k)^2 \gamma_k e_0 \rangle \, \mathrm{d}k = \int_{\mathbb{R}^d} |k|^2 \langle e_0, \gamma_k e_0 \rangle \, \mathrm{d}k.$$

Thermodynamic limits

Thermodynamic limits $\implies$ one can **export** some tools from the finite world to the stationary one.

Example: Lieb-Thirring inequalities
For $0 \leq \gamma \leq 1$ on $L^2(\mathbb{R}^d)$, we have

$$C_{\mathrm{TL}} \int_{\mathbb{R}^d} \rho^{\frac{d+2}{d}}(x) \mathrm{d}x \leq \mathrm{Tr}(-\Delta \gamma).$$

For any stationary **ergodic** operator $0 \leq \widetilde{\gamma} \leq 1$ on $L^2(\Omega \times \mathbb{R}^d)$, we have *see also [Cancès, Lahbabi, Lewin 2012]*.

$$C_{\mathrm{LT}} \fint_{\Omega} \rho^{\frac{d+2}{d}}(\omega) \mathrm{d}\omega \leq \underline{\mathrm{Tr}}\left(-\widetilde{\Delta}\widetilde{\gamma}\right) = \int_{\mathbb{R}^d} |k|^2 \langle e_0, \gamma_k e_0 \rangle \, \mathrm{d}k.$$

Non linear models

Thomas–Fermi models

Consider a stationary charge density $\mu(\omega, x)$, and its finite version $\mu_R(x) := \mu(\omega, x) \mathbb{1}(x \in B_R)$

Thomas Fermi model

$$I_R := \inf\left\{ C_{\text{TF}} \int_{\mathbb{R}^3} \rho^{5/3}(x)\mathrm{d}x + \frac{1}{2}D(\rho - \mu_R), \quad \rho \in L^{5/3}(\mathbb{R}^3, \mathbb{R}^+),\ \rho > 0 \right\},$$

with the Hartree interaction

$$\forall f : \mathbb{R}^3 \to \mathbb{R}, \qquad D(f) := \iint_{\mathbb{R}^d \times \mathbb{R}^d} \frac{f(x)f(y)}{|x-y|}\mathrm{d}x\mathrm{d}y = 4\pi \int_{\mathbb{R}^d} \frac{|\widehat{f}|^2(k)}{|k|^2}\mathrm{d}k.$$

Theorem (Blanc, Le Bris, Lions 2007)

*In the **incommensurate case**, the energy per unit volume $\frac{1}{R^3}I_R$ converges to some limit I_*, given by the stationary limiting problem*

$$I_* := \inf\left\{ C_{\text{TF}} \fint_{\Omega} \rho^{5/3}(\omega)\mathrm{d}\omega + \frac{1}{2}\widetilde{D}(\rho - \mu_R), \quad \rho \in L^{5/3}(\Omega),\ \rho > 0 \right\},$$

with the stationary Hartree interaction

$$\forall F : \Omega \to \mathbb{R}, \quad \widetilde{D}(F) := 4\pi \sum_{K=(K_1, K_2) \in \mathbb{L}_1^* \times \mathbb{L}_2^*} \frac{|c_K(F)|^2}{|K_1 + K_2|^2}.$$

Idea of the proof (from *[Blanc, Le Bris, Lions 2007]*)

WARNING:
- Given a function $F(\omega)$, one can create a *finite* function $f_\omega(x) = F(\alpha_x \omega) \mathbb{1}(x \in B_R)$
- But the reverse operations is not so clear : how to **create** a stationary function $F(\omega)$ from $f_\omega(x)$?

  The construction of test functions *to compare the energies only works in one direction...*

Main idea: study the Euler–Lagrange equations

Let ρ_R be the (unique) optimal finite density for I_R, then the function $u_R := c\rho_R^{3/2}$ satisfies

$$-\Delta u_R + u_R^{3/2} = \mu_R.$$

Lemma (Brezis 1984)

For every $1 < p < \infty$ and every $f \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$, there exists a unique $u \in L^p_{\mathrm{loc}}(\mathbb{R}^d)$ satisfying

$$-\Delta u + u^p = f.$$

In addition, if u_R is the solution for $f_R := f\mathbb{1}_{B_R}$, then $u_R \to u$ in $L^1_{\mathrm{loc}}(\mathbb{R}^d)$ and almost everywhere.

Final argument
- The corresponding solution $\rho = cu^{2/3}$ solves the stationary Euler-Lagrange equations
- It is a critical point of the convex stationary Thomas–Fermi problem
- Hence it is the unique minimizer.

Hartree models

Consider the reduced Hartree-Fock (rHF) energy

$$\inf\left\{\underline{\mathrm{Tr}}\,(-\widetilde{\Delta}\widetilde{\gamma}) + \frac{1}{2}\widetilde{D}_\kappa(\rho - \mu), \qquad 0 \le \widetilde{\gamma} \le 1, \qquad \widetilde{\gamma} \quad \text{stationary}\right\},$$

with the Yukawa potential

$$\forall F \in C^\infty(\Omega), \quad \widetilde{D}_\kappa(F) := 4\pi \sum_{K=(K_1,K_2)\in\mathbb{L}_1^*\times\mathbb{L}_2^*} \frac{|c_K(F)|^2}{|K_1 + K_2|^2 + \kappa^2}.$$

Lemma (Cancès, Gontier, Perrin-Roussel 2026)

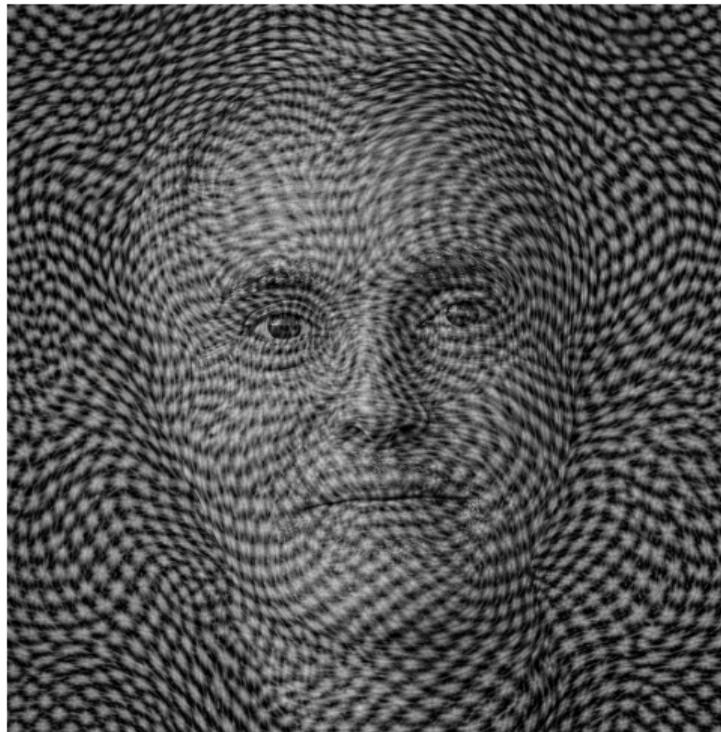*The stationary rHF minimisation problem is well-posed.*

Probably also true for Coulomb ($\kappa = 0$).

Open questions

- Thermodynamic limit?
- Continuity with respect to the rotation of the two layers?
  ([Avron, Simon 1983] True in the linear setting, for the averaged energy $\underline{\mathrm{Tr}}\,(f(\widetilde{H}_\theta))$.)

Thank you for your attention, and...
Joyeux anniversaire Eric !

Moire pattern of Selenium (Se) + Rhenium (Re).