

Linear elliptic homogenization with non-periodic highly oscillating potentials

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Purpose : To address an homogenization problem for stationary Schrödinger equation with highly oscillating potential :

$$\begin{cases} -\Delta u^\varepsilon + \frac{1}{\varepsilon} V(\cdot/\varepsilon) u^\varepsilon = f & \text{on } \Omega \\ u_\varepsilon = 0 & \text{on } \partial\Omega. \end{cases} \quad (1)$$

Where :

- $\Omega \subset \mathbb{R}^d$ is a bounded domain ($d \geq 1$).
- $f \in L^2(\Omega)$.
- $\varepsilon > 0$ is a small scale parameter.
- $V \in L^\infty(\mathbb{R}^d)$ is a non-periodic potential that models a perturbed periodic geometry.
- $\lim_{\varepsilon \rightarrow 0} V(\cdot/\varepsilon) = 0$ in $L^\infty(\mathbb{R}^d) - \star$. ← necessary assumption due to the exploding term $\frac{1}{\varepsilon} V(\cdot/\varepsilon)$

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Main questions :

Can we identify the limit of u^ε when the scale parameter $\varepsilon \rightarrow 0$ and study the convergence for several topologies ($L^2(\Omega)$, $H^1(\Omega)$, ...) ?

→ $\exists u^*$ s.t. $u^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} u^*$?

→ $\exists V^*$ s.t. $-\Delta u^* + V^* u^* = f$?

The periodic case

The periodic problem, when $V = V_{per}$ and $\langle V_{per} \rangle = \int_Q V_{per} = 0$, is well known ¹ :

→ If u^ε converges, a formal approach shows that its limit u^* is a solution to the *homogenized* equation :

$$\begin{cases} -\Delta u^* + \langle w_{per} V_{per} \rangle u^* = f & \text{on } \Omega \\ u^* = 0 & \text{on } \partial\Omega. \end{cases} \quad (2)$$

and w_{per} is a periodic *corrector* solution to corrector equation :

$$\Delta w_{per} = V_{per} \quad \text{on } \mathbb{R}^d \quad (3)$$

→ When $\varepsilon \rightarrow 0$, we expect

$$u^\varepsilon \sim u^* + \varepsilon u^* w_{per}(\cdot/\varepsilon).$$

¹[Bensoussan, Lions, Papanicolaou '1978]

Results in the periodic case :

1. Existence of a corrector ?

$\langle V_{per} \rangle = 0 \Rightarrow \exists w_{per}$ periodic solution to $\Delta w_{per} = V_{per}$.

Remark : $\Delta w_{per} = V_{per} \xrightarrow{\text{Green formula}} \langle w_{per} V_{per} \rangle = - \langle |\nabla w_{per}|^2 \rangle$.

2. Well-posedness of $-\Delta u^\varepsilon + \frac{1}{\varepsilon} V(\cdot/\varepsilon)u^\varepsilon = f$?

Let μ_1 and λ_1^ε be respectively the first eigenvalue of $-\Delta$ and the first eigenvalue of $-\Delta + \frac{1}{\varepsilon} V(\cdot/\varepsilon)$ with homogeneous Dirichlet b.c. on Ω .

Then :

$$\lambda_1^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} \mu_1 - \langle |\nabla w_{per}|^2 \rangle.$$

Consequence: $\mu_1 - \langle |\nabla w_{per}|^2 \rangle > 0$ and ε small \Rightarrow Existence and uniqueness of u^ε in $H_0^1(\Omega)$.

Results in the periodic case :

3. Assume $\mu_1 - \langle |\nabla w_{per}|^2 \rangle > 0$, then $\lim_{\varepsilon \rightarrow 0} u^\varepsilon = u^*$ **strongly** in $L^2(\Omega)$, **weakly** in $H^1(\Omega)$.
4. Define $R^\varepsilon = u^\varepsilon - u^* - \varepsilon u^* w_{per}(\cdot/\varepsilon)$, then $\lim_{\varepsilon \rightarrow 0} R^\varepsilon = 0$ **strongly** in $H^1(\Omega)$.

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Essential properties of w_{per} for the proofs :

- **Strict sublinearity at infinity** : $\varepsilon w_{per}(\cdot/\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} 0$ in $L^\infty(\Omega)$.
- **Average of $|\nabla w_{per}|^2$** : $|\nabla w_{per}(\cdot/\varepsilon)|^2 \xrightarrow{\varepsilon \rightarrow 0} \langle |\nabla w_{per}|^2 \rangle$ in $L^\infty(\mathbb{R}^d) - \star$

The perturbed problem

- Our purpose is to extend these results to the setting of a perturbed periodic problem when

$$V = g_{per} + \sum_{k \in \mathbb{Z}^d} \varphi(\cdot - k - Z_k),$$

where

- g_{per} is a regular periodic function,
- $\varphi \in \mathcal{D}(\mathbb{R}^d)$,
- $Z := (Z_k)_{k \in \mathbb{Z}^d} \in (l^\infty(\mathbb{Z}^d))^d$

→ V is a perturbation of $V_{per} = g_{per} + \sum_{k \in \mathbb{Z}^d} \varphi(\cdot - k)$.

→ Setting inspired by a work related to minimization of the energy of an infinite non-periodic system of particles ^a.

^a[Blanc, Lions, Le Bris, 2003]

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→ Follows up on some previous works^a addressing perturbed elliptic homogenization problems for **local defects**.

→ Here Z_k does not necessarily vanish at infinity → **non-local defects**.

^a[Blanc, Le Bris, Lions, 2012, 2018] & [Blanc, Josien, Le Bris, 2020]

Examples of Z_k ($d = 2$)

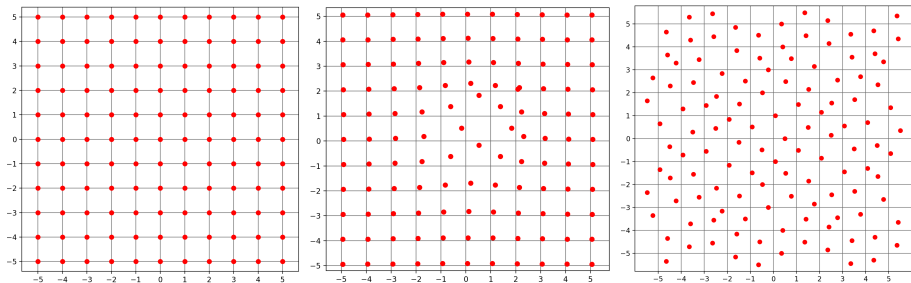


Figure: Illustration of $X_k = k + Z_k$ for several examples of sequence Z_k .

Left. Reference periodic case : $Z_k = 0$.

Center. Local perturbation : $\lim_{|k| \rightarrow \infty} Z_k = 0$.

Right. Non-local perturbations.

Corrector equation

Aim : To prove the **existence** of a solution w to the corrector equation :

$$\Delta w = V, \quad (4)$$

such that :

$$\lim_{\varepsilon \rightarrow 0} \varepsilon w(\cdot/\varepsilon) = 0 \text{ on } L^\infty(\Omega), \quad (5)$$

$$\text{weak } \lim_{\varepsilon \rightarrow 0} |\nabla w(\cdot/\varepsilon)|^2 \text{ exists on } \Omega. \quad (6)$$

Remark : $\text{weak } \lim_{\varepsilon \rightarrow 0} \nabla w(\cdot/\varepsilon) = 0 \Rightarrow (5)$

\implies Properties of weak convergence satisfied by ∇w are sufficient.

Questions :

- Can we use the structure of V to prove the existence of a corrector ?
- Which distribution of Z_k in the space ensures (5) and (6) ?

Corrector equation : Existence ?

Main difficulties :

- We have to establish some bounds satisfied by ∇w , at least on $\Omega/\varepsilon = \{x/\varepsilon, x \in \Omega\}$.
- V is *non-periodic* : the corrector equation cannot be reduced to an equation posed on a fixed bounded domain.
→ Prevents to use classical techniques (Lax-Milgram Lemma).

Corrector equation : Existence ?

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Idea ($d \geq 2$) : V has a particular structure.

$$V = [\text{periodic potential } V_{per}] + [\text{perturbation } \tilde{V} := \sum_{k \in \mathbb{Z}^d} \varphi(\cdot - k - Z_k) - \varphi(\cdot - k)].$$

→ We want to find $w = w_{per} + \tilde{w}$ where $\Delta w_{per} = V_{per}$ and $\nabla \tilde{w}$ is expected to formally read as

$$\nabla \tilde{w} = \sum_{k \in \mathbb{Z}^d} \nabla G * (\varphi(\cdot - k - Z_k) - \varphi(\cdot - k)).$$

→ $G(x) = C(d) \frac{1}{|x|^{d-2}}$ ($d \geq 3$) is the Green function associated with Δ (ie. $\Delta G = \delta$).

Corrector equation : Existence ?

Well definition of $\nabla \tilde{w} = \sum_{k \in \mathbb{Z}^d} \nabla G * (\varphi(\cdot - k) - \varphi(\cdot - k - Z_k))$?

Remark : $\nabla G(x - k) \underset{k \rightarrow \infty}{\sim} \frac{C(d)}{|x - k|^{d-1}}$

→ obtaining a series that normally converges requires to increase by more than one the exponent in the rate of decay ($\frac{1}{|k|^d}$ is the critical decay in ambient dimension d).

Approach : Taylor expansion of $\varphi(x - k - Z_k)$ with respect to Z_k :

$$\begin{aligned} \varphi(x - k - Z_k) - \varphi(x - k) &= -Z_k \cdot \nabla \varphi(x - k) \\ &+ \int_0^1 (1-t) Z_k^T D^2 \varphi(x - k - tZ_k) Z_k dt \end{aligned}$$

⇒ Two different contributions in the series : $\nabla \tilde{w} = \nabla \tilde{w}_1 + \nabla \tilde{w}_2$?

Corrector equation : Existence ?

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$$\varphi(x - k - Z_k) - \varphi(x - k) = -Z_k \cdot \nabla \varphi(x - k) \quad \leftarrow \begin{array}{l} \text{1}^{\text{st}}\text{-order derivatives of } \varphi, \\ \text{linear w.r. to } Z \end{array}$$

$$\begin{array}{l} \text{2}^{\text{nd}}\text{-order derivatives,} \\ \text{non-linear w.r. to } Z \end{array} \quad \rightarrow \quad + \int_0^1 (1-t) Z_k^T D^2 \varphi(x - k - tZ_k) Z_k dt$$

⇒ Two different contributions in the series : $\nabla \tilde{w} = \nabla \tilde{w}_1 + \nabla \tilde{w}_2$?

Corrector equation : Existence ?

1) Convergence of $\nabla \tilde{w}_1 = \sum_{k \in \mathbb{Z}^d} \nabla G * (-Z_k \cdot \nabla \varphi(x - k))$
 $= \sum_{k \in \mathbb{Z}^d} \nabla^2 G * (-Z_k \varphi(x - k)) ?$

- $\nabla^2 G(x - k) \sim \frac{1}{|x - k|^d} \rightarrow$ Critical rate of convergence !

Two parameters may ensure the convergence of the sum in L_{loc}^∞ :

1. Properties of φ . Ex : $\int_{\mathbb{R}^d} \varphi = 0 \Rightarrow |\nabla^2 G * \varphi(x)| \leq \frac{1}{|x|^{d+1}}$
2. Properties of Z_k . Ex : Z_k rapidly decreases at infinity.

→ Very specific assumptions... What if $\int_{\mathbb{R}^d} \varphi \neq 0$ and $\lim_{|k| \rightarrow \infty} Z_k \neq 0$?

Corrector equation : Existence ?

→ Convergence of $\sum_{k \in \mathbb{Z}^d} \nabla^2 G * (Z_k \varphi(\cdot - k))$?

- $\nabla^2 G(x - k) \sim \frac{1}{|x - k|^d} \rightarrow$ Critical rate of convergence !

In general : Convergence of the sum only in a weak sense, in $BMO(\mathbb{R}^d)$

→ Related to the continuity of $T : f \mapsto \nabla^2 G * f$ from $L^\infty(\mathbb{R}^d)$ to $BMO(\mathbb{R}^d)$
(theory of Calderón-Zygmund operators)

BMO ? "Bounded Mean Oscillations" :

$$BMO(\mathbb{R}^d) = \left\{ f \in L^1_{loc}(\mathbb{R}^d) \mid \sup_{R>0, x_0 \in \mathbb{R}^d} \int_{B_R(x_0)} \left| f - \int_{B_R(x_0)} f(y) dy \right| < +\infty \right\}.$$

ex : $x \mapsto \log(|x|) \in BMO(\mathbb{R}^d) \Rightarrow BMO(\mathbb{R}^d) \not\subset L^\infty(\mathbb{R}^d)$

Corrector equation : Existence ?

2) Convergence of $\nabla \tilde{w}_2 = \sum_{k \in \mathbb{Z}^d} \nabla G * \left(\int_0^1 (1-t) Z_k^T D^2 \varphi(x - k - tZ_k) Z_k dt \right) ?$

2^{nd} -order derivatives of $\varphi \rightarrow D^3 G(x)$ decays like $\frac{1}{|x|^{d+1}}$

\Rightarrow yields an absolutely converging contribution and $\nabla \tilde{w}_2 \in L^\infty(\mathbb{R}^d)^d$.

Conclusions : We have the existence of \tilde{w}_1 and \tilde{w}_2 such that :

- $\nabla \tilde{w}_1 \in BMO(\mathbb{R}^d)^d \not\subset L^\infty(\mathbb{R}^d)^d$, ← generates some technicalities to establish the homogenization results
- $\nabla \tilde{w}_2 \in L^\infty(\mathbb{R}^d)^d$.

Corrector equation : Existence ?

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- $\nabla \tilde{w}_1 \in BMO(\mathbb{R}^d)^d \not\subset L^\infty(\mathbb{R}^d)^d$, ← generates some technicalities to establish the homogenization results
- $\nabla \tilde{w}_2 \in L^\infty(\mathbb{R}^d)^d$.
- Which bounds satisfied by the corrector on Ω/ε ?

Properties of *BMO* show the existence of $C_{\varepsilon, \Omega} \in \mathbb{R}^d$ s.t., $\forall p \in [1, +\infty[$:

$$\nabla W_{\varepsilon, \Omega}(\cdot/\varepsilon) = \nabla w_{per}(\cdot/\varepsilon) + \nabla \tilde{w}_1(\cdot/\varepsilon) - C_{\varepsilon, \Omega} + \nabla \tilde{w}_2(\cdot/\varepsilon) \text{ is bounded in } (L^p(\Omega))^d$$

$\rightarrow \varepsilon$ -dependent sequence of correctors

Corrector equation : Properties of weak-convergence ?

If the existence of $W_{\varepsilon, \Omega}$ is established, can we obtain the weak convergence of $\nabla W_{\varepsilon, \Omega}(\cdot/\varepsilon)$ and $|\nabla W_{\varepsilon, \Omega}(\cdot/\varepsilon)|^2$?

→ requires a specific distribution of Z_k .

Assumptions :

1) Convergence of $\nabla W_{\varepsilon, \Omega}(\cdot/\varepsilon)$?

→ Assumption regarding the average of Z :

$$\bullet \exists \langle Z \rangle \in \mathbb{R}^d, \forall R > 0, \forall x_0 \in \mathbb{R}^d, \lim_{\varepsilon \rightarrow 0} \frac{\varepsilon^d}{|B_R|} \sum_{k \in \frac{B_R(x_0)}{\varepsilon}} Z_k = \langle Z \rangle. \quad (\text{A1})$$

Corrector equation : Properties of weak-convergence ?

Assumptions :

2) Convergence of $|\nabla \tilde{w}_1(\cdot/\varepsilon)|^2 = \left| \sum_{k \in \mathbb{Z}^d} \nabla^2 G * (-Z_k \varphi(x-k)) \right|^2$

→ Assumptions regarding the auto-correlations of Z :

• $\left\{ \begin{array}{l} \forall i, j, \forall l \in \mathbb{Z}^d, \exists C_{l,i,j} \in \mathbb{R}^d, \lim_{\varepsilon \rightarrow 0} \frac{\varepsilon^d}{|B_R|} \sum_{k \in \frac{B_R(x_0)}{\varepsilon}} (Z_k - \langle Z \rangle)_i (Z_{k+l} - \langle Z \rangle)_j = C_{l,i,j}. \\ \text{+ Logarithmic convergence rates.} \end{array} \right.$ (A2.a)

• $x \mapsto \sum_{|l| \leq L} C_{l,i,j} (\partial_i \partial_j G * \varphi)(x-l)$ converges in $L^1_{loc}(\mathbb{R}^d)$ when $L \rightarrow +\infty$. (A2.b)

Corrector equation : Properties of weak-convergence ?

Assumptions :

$$3) \text{ Convergence of } |\nabla \tilde{w}_2(\cdot/\varepsilon)|^2 = \left| \sum_{k \in \mathbb{Z}^d} \nabla G * \left(\int_0^1 (1-t) Z_k^T D^2 \varphi(x - k - tZ_k) Z_k dt \right) \right|^2$$

→ Assumption regarding the 2nd-order correlations of Z :

- $\forall F \in \mathcal{C}^0(\mathbb{R}^d \times \mathbb{R}^d), \forall l \in \mathbb{Z}^d, \exists C_{F,l} \in \mathbb{R},$

$$\lim_{\varepsilon \rightarrow 0} \frac{\varepsilon^d}{|B_R|} \sum_{k \in \frac{B_R(x_0)}{\varepsilon}} F(Z_k, Z_{k+l}) = C_{F,l}. \quad (\text{A3})$$

Example of non-periodic admissible sequences

- Local perturbations : $\lim_{|k| \rightarrow \infty} Z_k = 0$

1. Some sequences such that Z_k "slowly" converges to 0 when $|k| \rightarrow \infty$.
(Typically $Z_k = O(\ln(|k|)^{-\alpha})$ for $\alpha > \frac{1}{2}$);

- Non-local perturbations : $\lim_{|k| \rightarrow \infty} Z_k \neq 0$

2. Some deterministic approximations of random variables

→ Deterministic sequences Z that share the properties of i.i.d sequences of random variables (used to simulate random processes).

→ Example for $d = 1$: $Z_k = k\theta^p \bmod 1$, for $p \geq 2$ and almost all irrational number $\theta \in \mathbb{R}$ (Approximation of uniform distribution on $[0, 1]$).

3. Many other non-periodic sequences.

Example for $d = 2$: $Z_{(k_1, k_2)} := (\cos(\sqrt{2}k_1), \sin(\sqrt{2}k_2))$

Existence result for the corrector equation

Theorem 1 : Existence of the corrector

Assume (A1) to (A3). Then, for every $R > 0$ and every $\varepsilon > 0$, there exists $W_{\varepsilon,R} \in L^1_{loc}(\mathbb{R}^d)$ solution to

$$\Delta W_{\varepsilon,R} = V \quad \text{on } B_{R/\varepsilon},$$

such that

- $\varepsilon W_{\varepsilon,R}(\cdot/\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} 0$ strongly in $L^\infty(B_R)$,
- $\exists \mathcal{M} \in \mathbb{R}, \quad |\nabla W_{\varepsilon,R}|^2(\cdot/\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} \mathcal{M}$ weakly in $L^p(B_R), \forall p \in [1, +\infty[$.
- **Remark** : $W_{\varepsilon,R} = w_{per} + \tilde{w}_1 - x \cdot \int_{B_R} \nabla \tilde{w}_1(y/\varepsilon) dy + \tilde{w}_2,$
→ Contrary to the periodic case, the corrector depends on ε and R .

Well-posedness of $-\Delta u^\varepsilon + \frac{1}{\varepsilon} V(\cdot/\varepsilon) u^\varepsilon = f$

- Assume (A1) to (A3).
- Denote $W_{\varepsilon, \Omega} := W_{\varepsilon, R}$ where $R = \text{Diam}(\Omega)$ and $\mathcal{M} = \text{weaklim}_{\varepsilon \rightarrow 0} |\nabla W_{\varepsilon, \Omega}(\cdot/\varepsilon)|^2$.

Idea : The first eigenvalue of $-\Delta + \frac{1}{\varepsilon} V(\cdot/\varepsilon)$ converges to the first eigenvalue of $-\Delta - \mathcal{M}$.

Proposition

Denote by λ_1^ε the first eigenvalue of $-\Delta + \frac{1}{\varepsilon} V(\cdot/\varepsilon)$ on Ω with homogeneous Dirichlet b.c. Then,

$$|\lambda_1^\varepsilon - \mu_1 + \mathcal{M}| \xrightarrow{\varepsilon \rightarrow 0} 0.$$

Proof : Asymptotic expansion of λ_1^ε using the properties of the corrector

Consequence : We obtain a sufficient condition for the well-posedness

$\mu_1 - \mathcal{M} > 0 + \varepsilon$ small $\Rightarrow -\Delta u^\varepsilon + \frac{1}{\varepsilon} V(\cdot/\varepsilon) u^\varepsilon = f$ is well-posed in $H_0^1(\Omega)$.

Application to homogenization

Homogenization of $-\Delta u^\varepsilon + \frac{1}{\varepsilon} V(\cdot/\varepsilon)u^\varepsilon = f$ when $\varepsilon \rightarrow 0$?

Theorem 2 : Homogenization result

- Assume (A1) to (A3).
- Denote $W_{\varepsilon,\Omega} := W_{\varepsilon,R}$ where $R = \text{Diam}(\Omega)$ and $\mathcal{M} = \text{weaklim}_{\varepsilon \rightarrow 0} |\nabla W_{\varepsilon,\Omega}(\cdot/\varepsilon)|^2$.
- Assume $\mu_1 - \mathcal{M} > 0$, where μ_1 is the first eigenvalue of $-\Delta$ with homogeneous Dirichlet boundary condition on Ω .

Then the sequence u^ε is well defined in $H_0^1(\Omega)$ for ε small and converges, **strongly** in $L^2(\Omega)$ and **weakly** in $H^1(\Omega)$, to u^* solution to

$$\begin{cases} -\Delta u^* - \mathcal{M}u^* = f & \text{on } \Omega, \\ u^* = 0 & \text{on } \partial\Omega. \end{cases} \quad (7)$$

In addition, the sequence of remainders $R^\varepsilon := u^\varepsilon - u^* - \varepsilon u^* W_{\varepsilon,\Omega}(\cdot/\varepsilon)$ converges to 0 **strongly** in $H^1(\Omega)$.

- Generalization of Theorem 2 : homogenization when $\mu_l - \mathcal{M} \neq 0$
 $\forall l \in \mathbb{N}^*$, where μ_l is the l^{th} eigenvalue of $-\Delta$.

Main idea : Convergence of all the eigenvalues of $-\Delta + \frac{1}{\varepsilon}V(\cdot/\varepsilon)$ to the eigenvalues of $-\Delta - \mathcal{M}$.

- Extension for more general potentials. 2 complementary approaches :

1) Extension by density in $L^\infty(\mathbb{R}^d)$:

$$V = \sum_{k \in \mathbb{Z}^d} g(\cdot - k - Z_k) \text{ where } |g(x)| \leq \frac{1}{|x|^{d+\alpha}} \text{ for } \alpha > 0.$$

2) Extension by algebraic operations :

$$V = \sum_{k_1, \dots, k_n \in \mathbb{Z}^d} \varphi_1(\cdot - k_1 - Z_{k_1}) \varphi_2(\cdot - k_2 - Z_{k_2}) \dots \varphi_n(\cdot - k_n - Z_{k_n})$$

→ Assumptions up to the $2n$ -order correlations of Z are required.

Thank you for your attention !