CONSTRUCTION OF COARSE APPROXIMATIONS FOR A SCHRÖDINGER PROBLEM WITH HIGHLY OSCILLATORY COEFFICIENTS

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An Inverse Multiscale Schrödinger Problem

Objectives

We define a **methodology to contruct coarse approximations** of highly oscillating PDEs when coefficients are *not* known but only measurements of *a few* solutions are available. This methodology is **inspired by homogenization theory** but overcome many of its limitations (e.g. periodicity assumptions) and is more **versatile** (e.g. valid outside the homogenization regime).

Assume we are able to measure solutions $u_\varepsilon(f)$ to the multiscale Schrödinger equation (1) for a few selected RHS $f_1, ..., f_P$.

$$\mathcal{L}_\varepsilon u_\varepsilon \coloneqq \left(-\Delta + \varepsilon^{-1} V(\varepsilon^{-1}\cdot)\right) u_\varepsilon = f \text{ in } \Omega. \tag{1}$$

How can we define an *effective constant potential* $\overline{V}$ such that solutions u_ε to (1) for new RHS are *well* approximated by the solutions $\overline{u}$ to the coarse Schrödinger problem

$$\overline{\mathcal{L}}\overline{u} \coloneqq \left(-\Delta + \overline{V}\right) \overline{u} = f \text{ in } \Omega. \tag{2}$$

Can we *improve these approximations*, e.g. by building a first order term ?

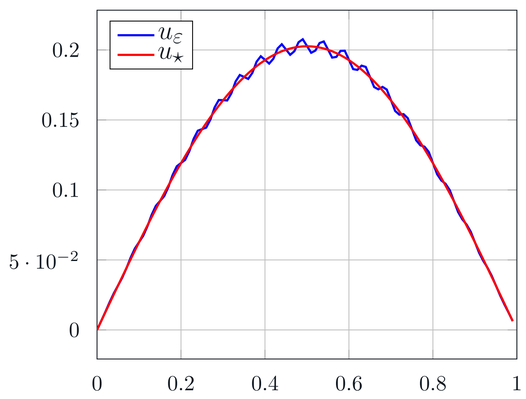

Fig 1. : Schrödinger Solutions

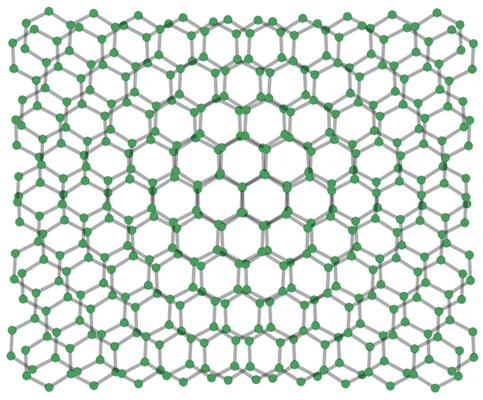

Fig 2. : Moiré Materials

Homogenization theory assess the existence of an homogenized coefficient $V_\star$ and a corrector w to obtain satisfactory L^2 and H^1 approximations. But ...

	Homogenization	Our Methodology
Pros	○ **Analytical expressions** available (in periodic regime) $\begin{cases} \Delta w = V, \text{ in } Q=(0,1)^d, \\ V_\star = -\|\nabla w\|^2_{L^2(Q)}, \\ u_\varepsilon \approx_{L^2} u_\star, \\ u_\varepsilon \approx_{H^1} u_\star(1+\varepsilon w(\varepsilon^{-1}\cdot)). \end{cases}$	○ Inverse Problem **(IP) adapted** (only require few measurement $u_\varepsilon(f)$) ○ **wide range of applications** (w.r.t ε) ○ **versatility** (valid in non-periodic context)
Limitations	○ based on **strong hypothesis** (e.g. periodicity), ○ **limited range of validity** (vanishing ε), ○ not IP adapted (require to know V)	○ No analytical expression

Tab 1. : Homogenization vs Our Methodology

An Optimization Formulation

Strategy For Best Effective Coefficient

We examine the worst case scenario and try to minimize it upon $\overline{V}$.

$$\inf_{\overline{V}\in\mathbb{R}} \max_{\substack{f \in \text{Span}(f_i)_{1\le i\le P}, \\ \|f\|_{L^2(\Omega)}=1.}} \left(\|u_\varepsilon(f) - \overline{u}(f)\|_{L^2(\Omega)}\right) \tag{3}$$

The arginf $\overline{V}$ gives a satisfaying macroscopic description of the system : **the related solutions $\overline{u}$ are good L^2 approximation of u_ε.**

Numerical Aspects :

- **Iterative Algorithm** : starting from $(\overline{V}^n, f^n)$, we solve the $\max$ at fixed $\overline{V}^n$, hence finding the argmax f^{n+1}, then we solve the $\inf$ with fixed f^{n+1}, hence finding $\overline{V}^{n+1}$.
- **Quadratic formulation in $\overline{V}$** : we apply the 0^{th}-operator $(-\Delta)^{-1}(-\Delta+\overline{V})$ to $u_\varepsilon(f) - \overline{u}(f)$ to recover a quadratic formulation in $\overline{V}$.
- **Computational Cost** : Each step require only solving a $P \times P$ eigenvalue problem. We need $N_{\text{iter}} \approx 10$ iterations.

Strategy For Corrector

Inspired by the relation $\nabla u_\varepsilon \approx_{L^2} \nabla u_\star + u_\star(\nabla w)(\varepsilon^{-1}\cdot))$ (stemming from homogenization theory), we define a first order corrected term C by considering

$$\inf_{C\in(L^2(\Omega))^2} \sum_{p=1}^{P} \|\nabla u_\varepsilon(f_p) - \nabla\overline{u}(f_p) - \overline{u}(f_p)C\|_{L^2(\Omega)} \tag{4}$$

The arginf $\overline{C}$ can be used to *correct* the previous coarse solutions $\overline{u}$, hence **obtaining good H^1 approximations**.

Numerical Aspects :

- **Piecewise constant functions** : in practice, u_ε and $\overline{u}$ are $\mathbb{P}^1$ elements, and C is searched among piecewise constant functions. The problem can be reduced to many optimization problems of small size
- **Computational Cost** : On each N_K triangles of the mesh, we perform a local integral to define the value of $\overline{C}$.

Numerical Results

Experiments have been performed in 2D ($\Omega = [0,1]^2$) using the potential

$$V(x,y) = \pi^2\sqrt{8}\left(\sin(2\pi x) + \sin(2\pi y)\right).$$

For loadings, we consider the eigenmodes of $(-\Delta)$-operator, denoted $(f_p)_{p\ge1}$.

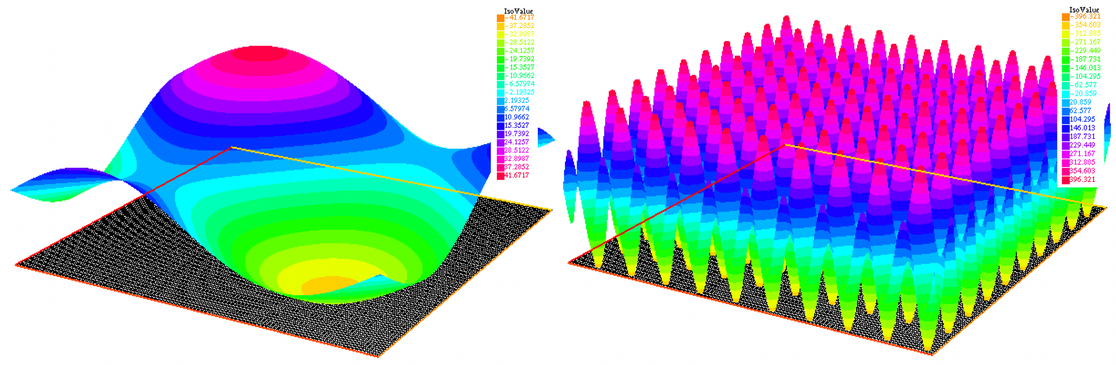

Fig 3 : Kernel Potential V and Oscillating Potential $V_\varepsilon = \varepsilon^{-1}V\left(\varepsilon^{-1}\cdot\right)$ (for $\varepsilon = 0.1$).

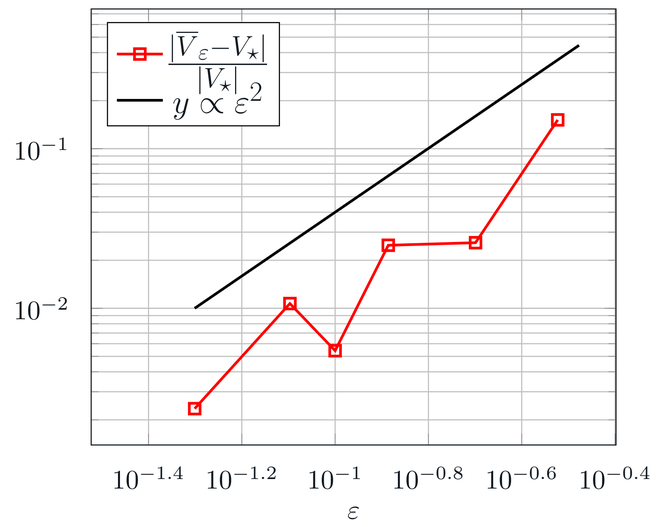

Fig 4 : Error between homogenized potential $V_\star$ and effective potential $\overline{V}_\varepsilon$ (computed with $P=1$) as a function of ε.

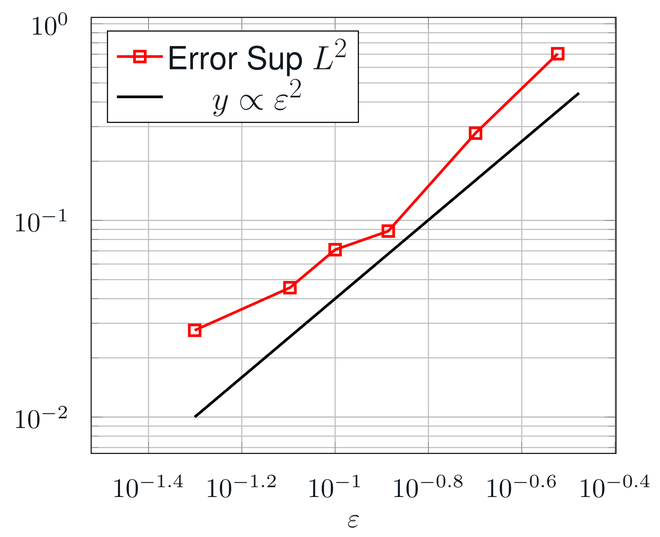

Fig 5 : L^2 maximal error $\sup_{f\in\text{Span}_{1\le p\le 10}(f_p)} \left(\frac{\|u_\varepsilon(f)-\overline{u}(f)\|_{L^2(\Omega)}}{\|u_\varepsilon(f)\|_{L^2(\Omega)}}\right)$ ($\overline{V}$ computed with $P=3$) as a function of ε.

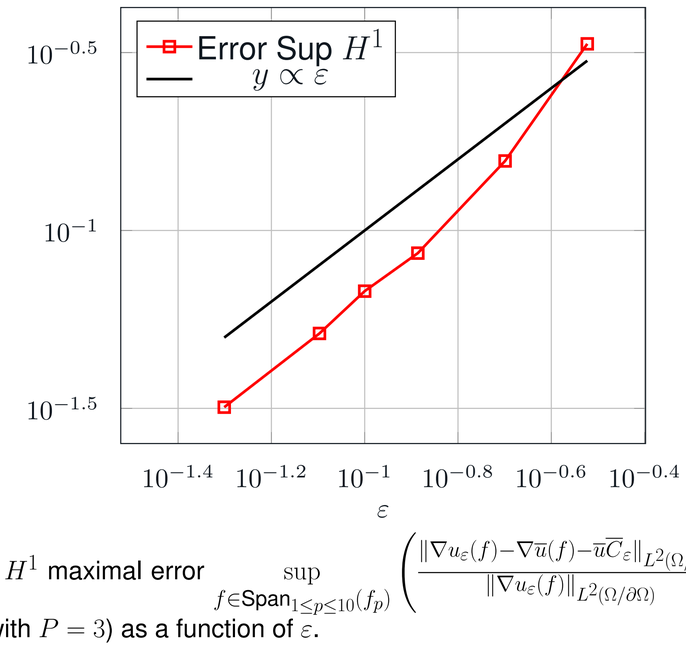

Fig 6 : H^1 maximal error $\sup_{f\in\text{Span}_{1\le p\le 10}(f_p)} \left(\frac{\|\nabla u_\varepsilon(f)-\nabla\overline{u}(f)-\overline{u}\overline{C}_\varepsilon\|_{L^2(\Omega/\partial\Omega)}}{\|\nabla u_\varepsilon(f)\|_{L^2(\Omega/\partial\Omega)}}\right)$ ($\overline{V}$ computed with $P=3$) as a function of ε.

References

[1] A. Bensoussan, J.-L. Lions, and G. Papanicolaou. *Asymptotic analysis for periodic structures*. Vol. 374. American Mathematical Soc., 2011.

[2] C. Le Bris, F. Legoll, and S. Lemaire. "On the best constant matrix approximating an oscillatory matrix-valued coefficient in divergence-form operators". In: *ESAIM: Control, Optimisation and Calculus of Variations* 24.4 (2018), pp. 1345–1380.

[3] C. Le Bris, F. Legoll, and K. Li. "Approximation grossière d'un problème elliptique à coefficients hautement oscillants". In: *Comptes Rendus Mathematique* 351.7-8 (2013), pp. 265–270.