Homogenization and Numerical Approximation of Elliptic Problems

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Based on joint work with Rafael Orive Santander, December 2006

- Introduction & Motivation
- 2 The 1 d case
- 3 The multi-dimensional case
- 4 The continuous Bloch wave decomposition
- 6 The Discrete Bloch wave decomposition
- O Numerical experiments
- Conclusion
- Open problems
- Related issues

- 1 Introduction & Motivation
- 2 The 1 d case
- 3 The multi-dimensional case
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- 5 The Discrete Bloch wave decomposition
- O Numerical experiments
- Conclusion
- 📵 Open problems
- Related issues

- Introduction & Motivation
- 2 The 1 d case
- The multi-dimensional case
- 4 The continuous Bloch wave decomposition
- 5 The Discrete Bloch wave decomposition
- 6 Numerical experiments
- Conclusion
- Open problems
- Related issues

- Introduction & Motivation
- 2 The 1 d case
- 3 The multi-dimensional case
- 4 The continuous Bloch wave decomposition
- 5 The Discrete Bloch wave decomposition
- 6 Numerical experiments
- Conclusion
- Open problems
- Related issues

- Introduction & Motivation
- 2 The 1 d case
- 3 The multi-dimensional case
- 4 The continuous Bloch wave decomposition
- 5 The Discrete Bloch wave decomposition
- 6 Numerical experiments
- 7 Conclusion
- **8** Open problems
- Related issues

- Introduction & Motivation
- 2 The 1 d case
- 3 The multi-dimensional case
- 4 The continuous Bloch wave decomposition
- 5 The Discrete Bloch wave decomposition
- 6 Numerical experiments
- 7 Conclusion
- 8 Open problems
- 9 Related issues

- Introduction & Motivation
- 2 The 1 d case
- 3 The multi-dimensional case
- 4 The continuous Bloch wave decomposition
- 5 The Discrete Bloch wave decomposition
- 6 Numerical experiments
- 7 Conclusion
- 8 Open problems
- 9 Related issues

- Introduction & Motivation
- 2 The 1 d case
- 3 The multi-dimensional case
- 4 The continuous Bloch wave decomposition
- 5 The Discrete Bloch wave decomposition
- 6 Numerical experiments
- 7 Conclusion
- 8 Open problems
 - 9 Related issues

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- 3 The multi-dimensional case
- 4 The continuous Bloch wave decomposition
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- Conclusion
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- Multiscale analysis: Two scales are involved: ε for the size of the microstructure and h for that of the numerical mesh;
- As usual, three different regimes: $h << \varepsilon$, $h \sim \varepsilon$, $\varepsilon << h$;
- Slow convergence of standard approximations (finite elements, finite differences): h << ε.
- Resonances may occur when $\varepsilon \sim h!$
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- Analyze the limit behavior as the characteristic size of the medium and the mesh-size tend to zero.

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B. Engquist, Th. Hou [1989,1993], M.Avellaneda, Th. Hou, G. Papanicolaou [1991], Babuška, Osborn [2000]. In other words:

- According to classical homogenization theory: u^{ε} converges to the homogenized solution u^* as $\varepsilon \to 0$;
- This is not necessarily the case for the numerical solution u^ε_h as both h, ε → 0.
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Problem formulation:

We consider the periodic elliptic equation associated to the following rapidly oscillating coefficients:

$$A^{\varepsilon} = -\frac{\partial}{\partial x_k} \left(a_{k\ell}^{\varepsilon}(x) \frac{\partial}{\partial x_\ell} \right),$$

with $a_{k\ell}^{\varepsilon}(x) = a_{k\ell}(x/\varepsilon)$, and $a_{k\ell}$ satisfying

$$\begin{cases} a_{kl} \in L^{\infty}_{\#}(Y) \text{ are } Y\text{-periodic, where } Y =]0,1[^{N}, \\ \exists \alpha > 0 \text{ s.t. } \sum_{k,\ell=1}^{N} a_{kl}(y)\eta_{k}\bar{\eta}_{l} \ge \alpha |\eta|^{2}, \quad \forall \eta \in \mathbb{C}^{N}, \\ a_{kl} = a_{lk} \quad \forall l, k = 1, ..., N. \end{cases}$$

Homogenization: u^* limit of the solutions of $A^{\varepsilon}u^{\varepsilon} = f$, satisfies

$$A^*u^* = -\frac{\partial}{\partial x_k} \left(a^*_{k\ell} \frac{\partial u^*}{\partial x_\ell} \right) = f.$$

Discretization: Let $h = (h_1, \ldots, h_d)$ with

$$h_i = rac{1}{n_i}$$
 with $n_i \in \mathbb{N}$.

The following is a natural numerical approximation scheme by finite-differences:

$$\sum_{i,j=1}^{d} -\nabla_i^{-h} \left[a_{ij}^{\varepsilon}(x(i,j)) \nabla_j^{+h} u_h^{\varepsilon}(x) \right] = f(x), \quad x \in \Gamma_h,$$

where Γ_h is the numerical mesh and

$$x(i,j) = x + \frac{1}{2}h_ie_i + (1 - \delta_{ij})\frac{1}{2}h_je_j.$$

0		0			
		i, j +	1		
	×	+	×		
o	+	o	+	0	
		i, j		i+1, j	• pts. of Γ_h where u is approximated
		+	×		+ pts. where $a_{\ell\ell}$ is evaluated
		o		o	${\pmb{x}}_{}$ pts. where $a_{k\ell},k\neq\ell$ is evaluated

Classical Numerical Analysis ensures

$$||u_h^{\varepsilon}-u^*||\leq crac{h}{arepsilon}+c'arepsilon.$$

Note that, in particular, no convergence is guaranteed for $h\simarepsilon$.

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In Avellaneda, Hou, Papanicolaou [1991] for the 1 - d problem with Dirichlet conditions the following was proved:

Theorem

If f is continuous and bounded in (0,1), then

$$\lim_{\varepsilon,h\to 0}||u_h^{\varepsilon}-u^*||_{\infty}\to 0,$$

for sequences h, ε such that $h/\varepsilon = r$ with r irrational.

- Analyze the behavior when ε/h =rational;
- Reprove the same result as in the Theorem above using diophantine approximation.
- Do it using explicit Bloch wave representations of solutions.

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and $h \rightarrow 0?????????$.

In this case the numerical mesh, despite of the fact that $h \rightarrow 0$, only samples a finite number of values in each periodicity cell of the coefficient a(x). Thus, it is impossible that the numerical schemes recovers the continuous homogenized limit u^* . One rather expects a discrete homogenized limit $u^*_{a/p}$ such that

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Main 1 - d result

Theorem

Assume that a = a(x) is Lipschitz, 1-periodic and $\alpha \le a(x) \le \beta$. Let $\{u_h^{\varepsilon}(x_i)\}_{i=0}^n$ the approximation of u^{ε} with $h/\varepsilon = q/p$. Then,

$$||u_h^{\varepsilon} - u_{q/p}^{*}||_{\infty} \leq c hp$$

Moreover, $u_{q/p}^*$ is a discrete Fourier approximation with mesh-size h of the solution of

$$\begin{cases} -a_p^* \frac{\partial^2 v}{\partial x^2}(x) = f(x), & 0 < x < 1, \\ v(0) = v(1) = 0, \end{cases}$$

with $a_p^* = \left(\frac{1}{p} \sum_{j=1}^p \frac{1}{a((j+1/2)/p)}\right)^{-1}.$

Recall that the continuous homogenized solution u^* is a solution of the same Dirichlet problem but with a continuous effective coefficient a^* defined as

$$a^* = \left(\int_0^1 (1/a(x))dx\right)^{-1}.$$

Furthermore,

$$||u_{q/p}^* - u^*||_{\infty} \le c' \frac{1}{p}.$$

In conclusion,

$$||u_h^{\varepsilon} - u^*||_{\infty} \leq c hp + c'/p$$

where c and c' depend on α , β , $||a'||_{\infty}$ and $||f||_{\infty}$.

Note that, this estimate, together with diophantine approximation results, allows recover convergence for h/ε irrational.

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The main multi-dimensional result

Theorem

Assume that $d \ge 2$ and $\{a_{ij}\} \in C^1$ and consider the elliptic problem with periodicity boundary conditions. Let $\varepsilon = 1/s$ and h

 $h_i/\varepsilon = q_i/p_i$, with H.C.F. $(p_i, q_i) = 1$, $i = 1, \dots, d$.

Furthermore, assume that

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ho}{p}, \quad ext{with } \left|rac{
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where c_a depends only on the lower and upper bounds of the coefficients. Then,

$$\left| u_h^{\varepsilon} - u_{q/p}^* \right|_h \leq c \left| ph \right| ||f||_{\infty},$$

for all $h, \varepsilon > 0$ as above with c > 0 independent of h, ε, f .

 $u_{q/p}^*$ is the discrete Fourier approximation with mesh-size h of

$$-a_{ij}^{*,q/p}\frac{\partial^2 v}{\partial x_i\partial x_j}=f \quad \text{ in } \quad Y, \quad v\in H^1_\#(Y), \qquad \int_Y vdx=0.$$

In general, this solution does not coincide with the homogenized solution:

$$u_{q/p}^* - u^*\Big|_h \leq c\,\delta\,||f||_\infty,$$

where $\delta > 0$ is given by

$$\delta = \max\left(\left| \frac{\rho}{\rho} \right|, 1 - \frac{\sigma_m}{\sigma_M}, \frac{\sigma_M}{\sigma_m} - 1 \right)$$

with $\sigma_M = \max(\sigma_i)$ and $\sigma_m = \min(\sigma_i)$, where $\sigma = q/\rho$.

Continuous Bloch wave decomposition

Following the presentation by C. Conca & M. Vanninathan:

Spectral problem family with parameter $\eta \in Y' = [-1/2, 1/2[^d:$

 $A\psi(\cdot;\eta) = \lambda(\eta)\psi(\cdot;\eta)$ in \mathbb{R}^d ,

 $\psi(\cdot;\eta)$ is (η, Y) -periodic, i.e., $\psi(y + 2\pi m; \eta) = e^{2\pi i m \cdot \eta} \psi(y;\eta)$. $\psi(y;\eta) = e^{iy \cdot \eta} \phi(y;\eta)$, ϕ being Y-periodic in the variable y.

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$$\begin{cases} 0 \leq \lambda_1(\eta) \leq \cdots \leq \lambda_n(\eta) \leq \cdots \to \infty, \\ \lambda_m(\eta) \text{ is a Lipschitz function of } \eta \in Y', \forall m \geq 1. \end{cases}$$

$$\lambda_2(\eta) \geq \lambda_2^{(N)} > 0, \quad \forall \eta \in Y',$$

where $\lambda_2^{(N)} > 0$ is the second eigenvalue of A in the cell Y with Neumann boundary conditions.

The eigenfunctions $\psi_m(\cdot; \eta)$ and $\phi_m(\cdot; \eta)$, form orthonormal bases in the subspaces of $L^2_{loc}(\mathbb{R}^d)$ of (η, Y) -periodic and Y-periodic functions, respectively.

$$\lambda_m^{\varepsilon}(\xi) = \varepsilon^{-2}\lambda_m(\varepsilon\xi), \qquad \phi_m^{\varepsilon}(x;\xi) = \phi_m(\frac{x}{\varepsilon};\varepsilon\xi).$$

Given f, the mth Bloch coefficient of f at the ε scale:

$$\widehat{f}_m^{\varepsilon}(k) = \int\limits_Y f(x)e^{-ik\cdot x}\overline{\phi_m^{\varepsilon}}(x;k)dx \quad \forall m \ge 1, \ k \in \Lambda_{\varepsilon},$$

$$\Lambda_{\varepsilon} = \{k = (k_1, \ldots, k_d) \in \mathbb{Z}^d : [-1/2\varepsilon] + 1 \le k_i \le [1/2\varepsilon]\}.$$

$$\begin{split} f(x) &= \sum_{k \in \Lambda_{\varepsilon}} \sum_{m \ge 1} \widehat{f}_m^{\varepsilon}(k) e^{ik \cdot x} \phi_m^{\varepsilon}(x;k). \\ &\int_{Y} |f(x)|^2 dx = \sum_{k \in \Lambda_{\varepsilon}} \sum_{m \ge 1} |\widehat{f}_m^{\varepsilon}(k)|^2. \\ &\lambda_m^{\varepsilon}(k) \widehat{u}_m^{\varepsilon}(k) = \widehat{f}_m^{\varepsilon}(k), \quad \forall \ m \ge 1, \ k \in \Lambda_{\varepsilon}. \end{split}$$

$$u^{\varepsilon}(x) = \sum_{k \in \Lambda_{\varepsilon}} \sum_{m=1}^{\infty} \frac{\widehat{f}_{m}^{\varepsilon}(k)}{\lambda_{m}(\varepsilon k)/\varepsilon^{-2}} e^{ik \cdot x} \phi_{m}^{\varepsilon}(x;k).$$
$$u^{\varepsilon}(x) \sim \varepsilon^{2} \sum_{k \in \Lambda_{\varepsilon}} \frac{\widehat{f}_{1}^{\varepsilon}(k)}{\lambda_{1}(\varepsilon k)} e^{ik \cdot x} \phi_{1}^{\varepsilon}(x;k).$$

$$\begin{split} c_1|\eta|^2 &\leq \lambda_1(\eta) \leq c_2|\eta|^2, \quad \forall \eta \in Y', \\ \lambda_1(0) &= \partial_k \lambda_1(0) = 0, k = 1, \dots, N, \\ \partial_{k\ell}^2 \lambda_1(0) &= 2a_{k\ell}^*, k, \ell = 1, \dots, N, \end{split}$$

where $a_{k\ell}^*$ are the homogenized coefficients.

$$\eta \in B_{\delta} \to \phi_{1}(y;\eta) \in L^{\infty} \cap L^{2}_{\#}(Y) \text{ is analytic,}$$

$$\phi_{1}(y;0) = (2\pi)^{-\frac{d}{2}}.$$

$$\widehat{f}_{1}^{\varepsilon}(k) \sim \widehat{f}_{k}$$

$$\widehat{u}_{1}^{\varepsilon}(k) \sim \widehat{u}_{k}^{*} \quad \text{as } \varepsilon \to 0,$$

$$u^{\varepsilon}(x) \sim \sum_{k \in \Lambda_{\varepsilon}} \frac{\widehat{f}_{1}^{\varepsilon}(k)}{\lambda_{1}(\varepsilon k)/\varepsilon^{-2}} e^{ik \cdot x} \phi_{1}^{\varepsilon}(x;k) \sim \sum_{k \in \mathbb{Z}^{d}} \frac{\widehat{f}^{k}}{a_{ij}^{*}k_{i}k_{j}} e^{ik \cdot x}$$

which is the solution of the homogenized problem in its Fourier representation.

- In 1 d one can use the explicit representation formula for discrete solutions. But, of course, this is impossible for multi-dimensional problems.
- In 1 d the homogenized coefficient a* can be computed explicitly as above. But in several space dimensions, the homogenized coefficients depend on test functions x_k that are defined by solving elliptic problems on the unit cell.
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Explicit 1 - d computations.

$$\begin{cases} -a_i^{\varepsilon}u_{i+1}^{\varepsilon} + (a_i^{\varepsilon} + a_{i-1}^{\varepsilon})u_i^{\varepsilon} - a_{i-1}^{\varepsilon}u_{i-1}^{\varepsilon} = h^2f_i, & 1 \le i \le n-1, \\ u_0^{\varepsilon} = b, & u_n^{\varepsilon} = c. \end{cases}$$

Therefore,

$$u_{i}^{\varepsilon} = b + U_{0}^{\varepsilon,h} \sum_{j=1}^{i} \frac{h}{a_{j}^{\varepsilon}} - \sum_{j=1}^{i} \frac{h}{a_{j}^{\varepsilon}} \sum_{k=1}^{j} hf_{k} \quad 1 \le i \le n-1,$$

with $U_{0}^{\varepsilon,h} = a_{h}^{\varepsilon,*}(c-b) + a_{h}^{\varepsilon,*} \sum_{j=1}^{n-1} \left(\frac{1}{a_{j}^{\varepsilon}} \sum_{k=1}^{j} h^{2}f_{k}\right),$
and $a_{h}^{\varepsilon,*} = \left(\sum_{j=0}^{n-1} \frac{h}{a_{j}^{\varepsilon}}\right)^{-1}.$

Using that $a_{p+i}^{\varepsilon} = a_i^{\varepsilon}$, $\frac{a_h^{\varepsilon,*}}{a_h} \to \frac{a_p^*}{p}$ (with explicit estimates).

DISCRETE BLOCH WAVE METHOD: 1 - d

Since
$$h/\varepsilon = q/p$$
, $a^{\varepsilon}(x + ph) = a^{\varepsilon}(x)$, $x \in \Gamma_h$
 $\Gamma_h^p = \{x = zh : 0 \le z < p, z \in \mathbb{Z}\}$
 $f(x,k) = hp^{\frac{1}{2}} \sum_{z \in \Gamma_{hp}} f(x+z)e^{-i2\pi k \cdot (x+z)}$, $k \in \Lambda_{q\varepsilon}$,
 $\Lambda_{q\varepsilon} = \left\{k \in \mathbb{Z}^d$, such that $\left[\frac{-1}{2q\varepsilon}\right] + 1 \le k \le \left[\frac{1}{2q\varepsilon}\right]\right\}$.

The discrete Bloch waves are defined by the family of eigenvalue problems:

$$\begin{aligned} -\nabla^{-h} \left[a^{\varepsilon} \left(x \right) \nabla^{+h} (e^{i2\pi x \cdot \xi} \phi_{h}^{\varepsilon} (x, \xi)) \right] &= \lambda(\xi) e^{ix \cdot \xi} \phi_{h}^{\varepsilon} (x, \xi), \quad x \in \Gamma_{h}^{p}, \\ \phi_{h}^{\varepsilon} (x, \xi) \text{ is } ph \text{-periodic in } x, \text{ i.e., } \quad \phi_{h}^{\varepsilon} (x + ph, \xi) &= \phi_{h}^{\varepsilon} (x, \xi). \end{aligned}$$

There exist a sequence $\lambda_1(\xi), ..., \lambda_p(\xi) \ge 0$ and their eigenfunctions $\{\phi_{h,m}^{\varepsilon}(x,\xi)\}_{m=1}^{p}$.

$$\lambda_m(\xi) \ge rac{c}{arepsilon^2 q^2} > 0, \quad m \ge 2$$

 $\xi \in B_{\delta} \mapsto (\lambda_1(\xi), \phi_1(\cdot, \xi)) \in \mathbb{R} \times \mathbb{C}^p$ is analytic.

$$\phi_1(y,0) = p^{-1/2}$$
$$\lambda_1(0) = \partial \lambda_1(0) = 0, \partial^2 \lambda_1(0) = \left(\frac{1}{p} \sum_{i=1}^p \frac{1}{a((i+0.5)/p))}\right)^{-1}.$$

1 10

This method allows obtaining sharp estimates on both $||u_h^\varepsilon - u_{q/p}^*||$ and $||u^* - u_{q/p}^*||$. Indeed,

- All solutions involved can be represented in a similar form by means of Bloch wave expansions;
- The contribution of Bloch components *m* ≥ 2 is uniformly negligible;
- The dependence of the first Bloch component, both in what concerns the eigenvalue and eigenfunction, can be estimated very precisely in terms of the various parameters.

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Numerical experiments

One dimension. Errors of the solutions with q = 5, p = 19.

h	ε	$\ u^arepsilon-u_h^arepsilon\ _h$	$\ u^arepsilon-u_h^arepsilon\ _\infty$	$\ u^*-u_h^arepsilon\ _h$	$\ u^*-u_h^arepsilon\ _\infty$	$\ u_{q/p}^* - u_h^{arepsilon}\ _h$
<u>2π</u> 38	$\frac{1}{10}$	0.038	0.0217	0.078	0.069	0.0778
$\frac{2\pi}{380}$	$\frac{1}{100}$	0.0039	0.0027	0.0086	0.0085	0.0079
$\frac{2\pi}{1900}$	<u>1</u> 500	0.0033	0.0018	0.0036	0.0022	0.0016
$\frac{2\pi}{19000}$	1 5000	0.0033	0.0018	0.0033	0.0018	$1.5 \cdot 10^{-4}$
$\frac{2\pi}{190000}$	1 50000	0.0033	0.0018	0.0033	0.0018	1.58 · 10 ⁻⁵

One dimension. Errors of the solutions with different values of q, p.

h	ε	q	р	$\ u^arepsilon-u_h^arepsilon\ _h$	$\ u^*-u_h^arepsilon\ _h$	$\ u_{q/p}^*-u_h^arepsilon\ _h$	$\left a^{*}-a_{p}^{*} ight $
$\frac{2\pi}{19000}$	1 5000	5	19	0.0033	0.0033	$1.5 \cdot 10^{-4}$	$2.08 \cdot 10^{-4}$
$\frac{2\pi}{19100}$	1 5100	51	191	$5.37 \cdot 10^{-5}$	$1.61 \cdot 10^{-4}$	$1.57 \cdot 10^{-4}$	$2.06 \cdot 10^{-6}$
$\frac{2\pi}{19100}$	$\frac{1}{5110}$	511	1910	$3.72 \cdot 10^{-5}$	$1.56 \cdot 10^{-4}$	$1.55 \cdot 10^{-4}$	$2.06 \cdot 10^{-8}$

Numerical homogenized coefficients with different values of p and q.

q1, q2, p1, p2	1, 1, 71, 71	72,71,71,70	72,72,71,71	31, 103, 70, 72	1031,121,70,72
$a_{11}^{*,q/p}$	1.3728	1.3727	1.3727	1,3684	1.3656
$a_{22}^{*,q/p}$	1.3728	1.3727	1.3727	1.3679	1.3672
$a_{12}^{*,q/p}$	0.5010	0.5009	0.5010	0.4939	0.4896


Top: approximation by finite differences of the continuous Bloch waves.

Bottom: Discrete Bloch waves with $(q_1; q_2) = (30, 120)$

- Discrete Bloch waves allow getting a complete representation formula for the numerical approximations when h/ε is rational.
- This allows deriving the discrete homogenized solution with convergence rates.
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Related topics and works:

The pathologies on the numerical approximation of homogenization problems arise, as we have shown, due to the interaction of the two scales involved in the problem: ε for the characteristic size of the medium and h for the numerical mesh-size.

Here we have considered an elliptic homogenization problem. Thus, we have worked on a low frequency regime in which the wave-length does not enter.

Similar phenomena arise and have been analyzed in other contexts:

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Numerical approximation and control of high frequency waves.



Enrique Zuazua

Due to high frequency numerical spurious oscillations $(\sqrt{\lambda} \sim 1/h)$ controls of a numerical approximation of the wave equation diverge. Convergence is restablished when the high frequency components are filtered out.



E. Z. Propagation, observation, and control of waves approximated by finite difference methods. SIAM Review, 47 (2) (2005), 197-243.

Similar phenomena arise in the context of the homogenization of the continuous wave equation

$$y_{tt}-(a(x/\varepsilon)y_x)_x=0.$$

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Numerical approximation of NLS.

Similar issues arise when dealing with numerical approximation schemes for nonlinear dispersive equations. High frequency components $(|\xi| \sim 1/h)$ may distroy the dispersive properties of the numerical schemes. The so-called Strichartz estimates then fail to be uniform as $h \rightarrow 0....$

L. IGNAT, E. Z., Dispersive Properties of Numerical Schemes for Nonlinear Schrödinger Equations, Proceedings of FoCM'2005.

- Inverse Problems, optimal design,
- Transparent boundary conditions, PML,...

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Motivation 1 - d N - d Bloch-c Bloch-d Experiments C

Continuous Homogenization

The limit of the solutions solves an elliptic equation related to the following constant coefficient homogenized operator A^* :

$$A^* = -a^*_{ij} \frac{\partial^2}{\partial x_i \partial x_j}.$$
 (1)

The homogenized coefficients a_{ij}^* are defined as follows

$$2a_{ij}^{*} = \frac{1}{|Y|} \int_{Y} \left(2a_{ij} - \frac{\partial a_{j\ell}}{\partial y_{\ell}} \chi^{i} - \frac{\partial a_{i\ell}}{\partial y_{\ell}} \chi^{j} \right) dy, \qquad (2)$$

where, for any $k = 1, \ldots, d$, χ^k is the unique solution of the cell problem

$$\begin{cases} A\chi^k = \frac{\partial a_{k\ell}}{\partial y_\ell} & \text{in } Y, \\ \chi^k \in H^1_{\#}(Y), \quad m(\chi^k) = 0. \end{cases}$$

The classical theory of homogenization provides the following result (see [BLP]:

Theorem

Then, if f belongs to $L^2_{\#}(Y)$ with m(f) = 0, the sequence of solutions u^{ε} converges weakly in $H^1(Y)$, as $\varepsilon \to 0$, to the so-called homogenized solution u^* characterized by

$$\begin{cases} A^*u^* = f & \text{in } Y, \\ u^* \in H^1_{\#}(Y), & m(u^*) = 0. \end{cases}$$

Furthermore, we have

$$\left|u^{\varepsilon}-u^{*}\right|_{0}\leq c\varepsilon\left|f\right|_{0}.$$

Diophantine approximation

Given r irrational there exist rational numbers (p_n, q_n) s. t.

$$\left| r - \frac{q_n}{p_n} \right| \le \frac{1}{\sqrt{5}p_n^2} \to 0 \quad \text{when } n \to \infty.$$

Then $\{a_n\} \subset \mathbb{N}$ for $a_n \to \infty$. Then,

$$arepsilon = 1/(a_nq_n), \ h = 2\pi/(a_np_n)$$

 $\sup_{x\in\Gamma_h} |u_h^{arepsilon}(x) - u^*(x)| \le c\left(rac{1}{a_n} + rac{1}{p_n}
ight)$