Optimizing the diffusion for overdamped Langevin dynamics

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Joint work with: T. Lelièvre, G. Pavliotis, G. Robin, G. Stoltz

S26: Modeling, analysis and simulation of molecular systems

Molecular dynamics

System: **average total energy** of the system is **fixed** (NVT)

Canonical ensemble: system samples the **Boltzmann–Gibbs measure** μ

$$\mathrm{d}\mu = Z_\mu^{-1} \mathrm{e}^{-\beta H(q,p)} \mathrm{d}q \, \mathrm{d}p, \qquad H(q,p) = V(q) + \frac{1}{2} p^\mathsf{T} M^{-1} p.$$

Langevin dynamics: configurational space $\mathcal{E} = \mathbb{T}^d \times \mathbb{R}^d$

$$\begin{cases} \mathrm{d}q_t = M^{-1} p_t \, \mathrm{d}t, \\ \mathrm{d}p_t = -\nabla V(q_t) \, \mathrm{d}t - \gamma M^{-1} p_t \, \mathrm{d}t + \sqrt{2\beta^{-1}\gamma} \, \mathrm{d}W_t, \end{cases}$$

Compute averages of observables $f \in L^1(\mu)$, rely on ergodic averages:

$$\boxed{\int_{\mathcal{E}} f \, \mathrm{d}\mu = \lim_{t \to +\infty} \frac{1}{t} \int_0^t f(q_s, p_s) \, \mathrm{d}s}$$

Diffusion dependent Overdamped Langevin dynamics - I

Sampling the marginal in position is the problem !

$$\mathrm{d}\mu = \underbrace{Z_\pi^{-1}\mathrm{e}^{-\beta V(q)}\mathrm{d}q}_{=:\mathrm{d}\pi}\, Z_\kappa^{-1}\mathrm{e}^{-\frac{\beta}{2}p^\mathsf{T} M^{-1}p}\mathrm{d}p$$

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Idea: only consider the position variable using the **overdamped limit**

$$\mathrm{d}q_t = -\nabla V(q_t)\,\mathrm{d}t + \sqrt{2\beta^{-1}}\,\mathrm{d}W_t$$

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Generalization: Position dependent pos. def. sym. matrix $\mathcal{D}$[1]

$$\boxed{\mathrm{d}q_t = \left(-\mathcal{D}(q_t)\nabla V(q_t) + \beta^{-1}\,\mathrm{div}\,\mathcal{D}(q_t)\right)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathcal{D}(q_t)^{1/2}\mathrm{d}W_t}$$

$\mathcal{D} \equiv$ inverse of position-dependent mass tensor

[1] Jardat/Bernard/Turq/Kneller (1999)

Diffusion dependent Overdamped Langevin dynamics - II

From physics to statistics $\rightarrow$ *we can choose* $\mathcal{D}$ *!*

- **Estimate** $\mathbb{E}_\pi[f] = \int_{\mathbb{T}^d} f(q)\pi(q)\mathrm{d}q$

with

$$\hat{I}_N := \frac{1}{N}\sum_{i=1}^{N} f(q^i), \qquad q^i \sim \pi$$

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- **Difficulty**: explore **anisotropic** potentials with **multiple minima**

- Find **optimal diffusion coefficient** $\mathcal{D}$ to accelerate convergence

Quantify convergence rate

- Related to the **spectral gap** of the dynamics' generator $\mathcal{L}_\mathcal{D}$:

$$\mathcal{L}_\mathcal{D}\varphi = \left(-\mathcal{D}\nabla V + \beta^{-1}\operatorname{div}\mathcal{D}\right)\cdot\nabla\varphi + \beta^{-1}\mathcal{D} : \nabla^2\varphi$$

Then the law π_t of the process q_t satisfies[2]

$$\boxed{\left\|\frac{\pi_t}{\pi} - 1\right\|_{L^2(\pi)} \leqslant \mathrm{e}^{-\Lambda(\mathcal{D})\beta^{-1}t}\left\|\frac{\pi_0}{\pi} - 1\right\|_{L^2(\pi)}}$$

$\Lambda(\mathcal{D})$: spectral gap of $-\beta\mathcal{L}_\mathcal{D} \geqslant 0$

[2] Lelièvre/Nier/Pavliotis (2013)

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- **Examples**: Approach mainly used in Bayesian Inference[3]: $\mathcal{D} \equiv (\nabla^2 V)^{-1}$

Other works[4] suggest $\mathcal{D} \propto \mathrm{e}^{\beta V}\mathrm{I}_d$

[2] Lelièvre/Nier/Pavliotis (2013)

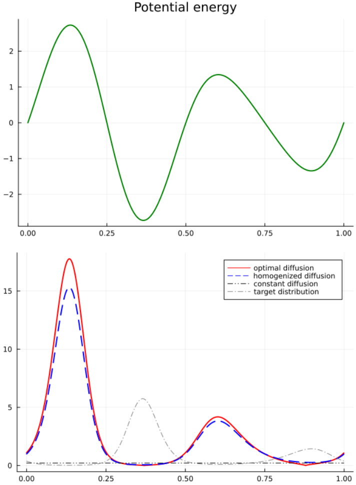
[3] Girolami/Calderhead (2011)

[4] Roberts/Stramer (2002), Lelièvre/Pavliotis/Robin/Santet/Stoltz (In prep.)

Which diffusion coefficient? Metastability case

- Example with $V(q) = \sin(4\pi q)(2 + \sin(2\pi q))$

$\mathcal{D}_{\mathrm{opt}}, \mathcal{D}_{\mathrm{exp}} = \mathrm{e}^{\beta V}, \mathcal{D}_{\mathrm{cst}} = a \in \mathbb{R}$ (all three normalized in $L^2(\pi)$)



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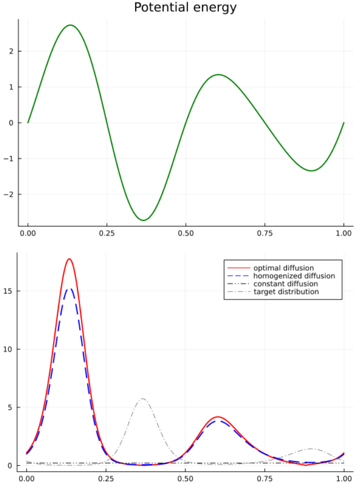

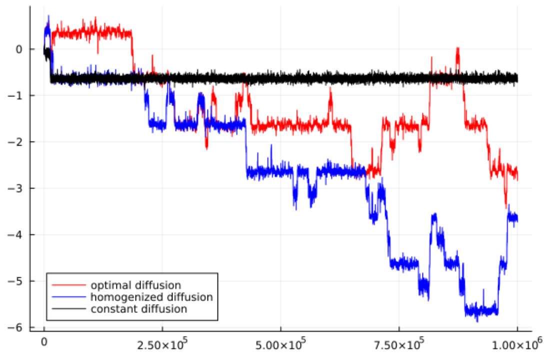

Typical trajectory (same noise)

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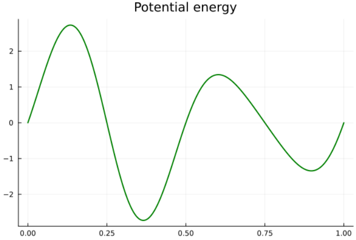

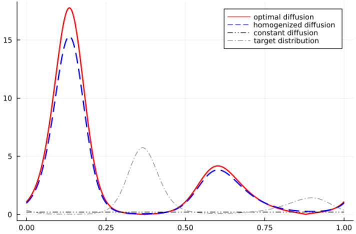

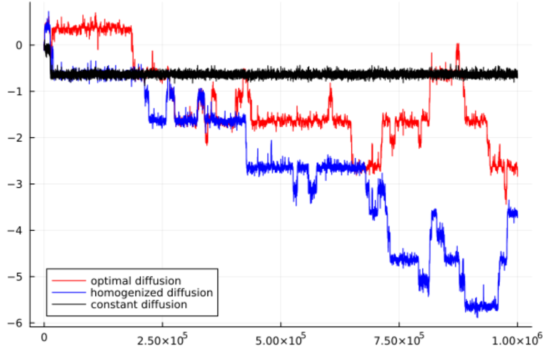

Typical trajectory (same noise)

- 'Optimal' $\mathcal{D}$ helps to **cross energy barriers** (if $V \uparrow$, then $\mathcal{D} \uparrow$)

Formulation of the optimization problem

- Using $\mathcal{L}_{\mathcal{D}} = -\beta^{-1}\nabla^{\star}\mathcal{D}\nabla$ on $L^2(\pi)$, the spectral gap of $-\beta\mathcal{L}_{\mathcal{D}}$ is

$$\boxed{\Lambda(\mathcal{D}) = \min_{u\in H^1(\mathbb{T}^d)\setminus\{0\}} \left\{ \frac{\int_{\mathbb{T}^d} \nabla u^{\mathsf{T}}\mathcal{D}\nabla u \,\mathrm{d}\pi}{\int_{\mathbb{T}^d} u^2 \,\mathrm{d}\pi} \;\middle|\; \int_{\mathbb{T}^d} u \,\mathrm{d}\pi = 0 \right\}}$$

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- L^p **constraints** on $\mathcal{D}$:

$$\boxed{\mathfrak{D}_p^{a,b} = \left\{ \mathcal{D} \in L^\infty_\pi(\mathbb{T}^d, \mathcal{M}_{a,b}) \,\middle|\, \|\mathcal{D}\|_{L^p_\pi} \leqslant 1 \right\}}$$

endowed with the norm

$$\|\mathcal{D}\|_{L^p_\pi} = \left(\int_{\mathbb{T}^d} |\mathcal{D}(q)|_\mathrm{F}^p \,\mathrm{e}^{-\beta p V(q)} \,\mathrm{d}q \right)^{1/p}$$

$\mathcal{D} \in L^p_\pi\left(\mathbb{T}^d, \mathcal{M}_{a,b}\right)$ for $1 \leqslant p \leqslant +\infty,\ a, b \geqslant 0$ if

$\mathrm{e}^{-\beta V(q)}\mathcal{D}(q) \in \mathcal{M}_{a,b} = \left\{ M \in \mathcal{S}_d^+ \,\middle|\, \forall \xi \in \mathbb{R}^d, a\,|\xi|^2 \leqslant \xi^\mathsf{T} M \xi \leqslant b^{-1}\,|\xi|^2 \right\}$ a.e.

Theoretical analysis of the optimization problem

- $V \in \mathcal{C}^\infty(\mathbb{T}^d)$
- $\mathcal{D} \mapsto \Lambda(\mathcal{D})$ concave
- $\mathfrak{D}_p^{a,b}$ weakly closed for the L^p_π norm

V and π bounded on $\mathbb{T}^d \Rightarrow \pi$ satisfies a Poincaré inequality

Theorem [Existence of a maximizer]

For any $p \in [1, +\infty]$, there exists

$$\boxed{\mathcal{D}_p^\star = \underset{\mathcal{D} \in \mathfrak{D}_p^{a,b}}{\arg\max}\, \Lambda(\mathcal{D})}$$

The maximizer is such that

- $\|\mathcal{D}\|_{L^p_\pi} = 1$;
- For any open set $\Omega \subset \mathbb{T}^d$, there exists $q \in \Omega$ such that $\mathcal{D}_p^\star(q) \neq 0$

Maximizer characterization

Euler–Lagrange equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\Lambda\left(\mathcal{L}_{\mathcal{D}_p^\star+t\delta\mathcal{D}}\right)\Big|_{t=0} + \gamma\,\frac{\mathrm{d}}{\mathrm{d}t}\left\|\mathcal{D}_p^\star + t\delta\mathcal{D}\right\|_{L^p_\pi}^p\Big|_{t=0} = 0$$

leads to ($s_p \geqslant 0$)

$$\boxed{\mathcal{D}_p^\star(q) \propto \left(\sum_{i=1}^{N_2} \nabla u^i_{\mathcal{D}_p^\star}(q) \otimes \nabla u^i_{\mathcal{D}_p^\star}(q)\right)^{s_p}}$$

with $\left(u^i_{\mathcal{D}_p^\star}\right)_{1\leqslant i\leqslant N_2}$ eigenvectors associated to $\Lambda(\mathcal{D}_p^\star)$

Numerical approximation of the optimization problem

- Piecewise constant approximation for $\mathcal{D}$ on $\mathbb{T}^d$

- $\mathbb{P}_1$ Finite Elements approximation to compute $(\Lambda(\mathcal{D}), u_{\mathcal{D}})$:

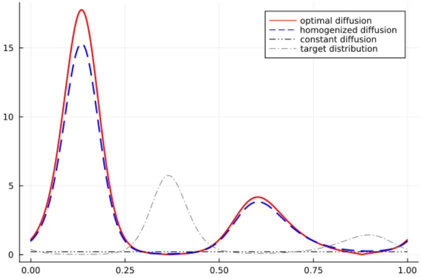
$$\boxed{A(\mathcal{D})u_{\mathcal{D}} = \Lambda(\mathcal{D})Bu_{\mathcal{D}}}$$

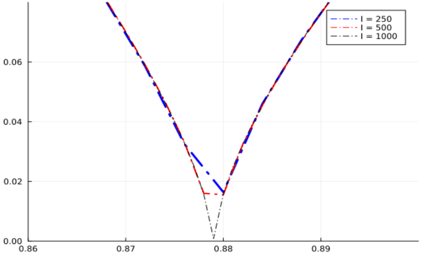
with

$$A_{i,j}(\mathcal{D}) = \int \nabla\varphi_j^{\mathsf{T}}\mathcal{D}\nabla\varphi_i \, \mathrm{d}\pi, \qquad B_{i,j} = \int \varphi_j\varphi_i \, \mathrm{d}\pi$$

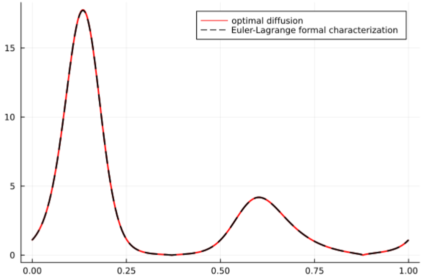
- Generalized eigenvalue problem: A sym., B pos. def. sym.

Numerical results - 1

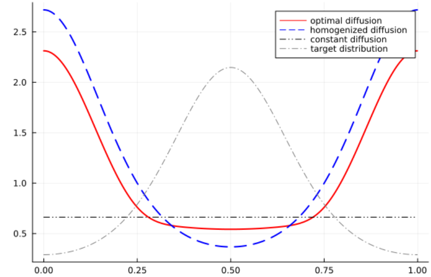


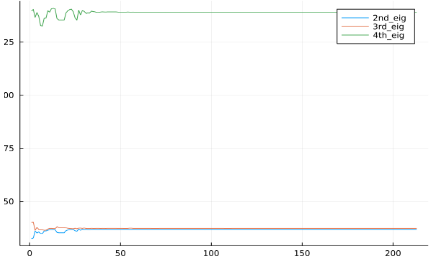


$$\boxed{V(q) = \sin(4\pi q)(2 + \sin(2\pi q))}$$

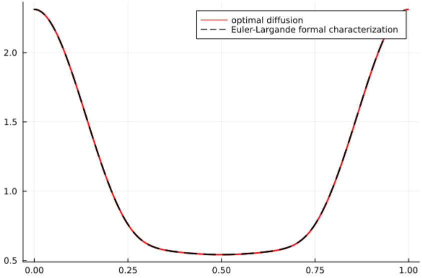


Non-degenerate eigenvalue





$$\boxed{V(q) = \cos(2\pi q)}$$



Degenerate eigenvalue

Optimal diffusion in the homogenized limit

- Previous procedure only helpful in low dimensions
- Need to solve a high-dimensional generalized eigenvalue problem

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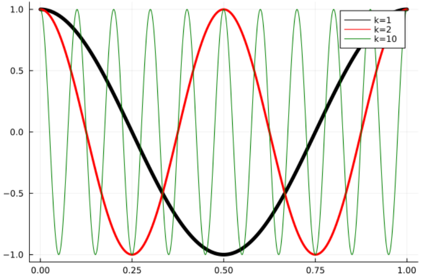
Idea: use **homogenization theory** to obtain a good approximation



$$\begin{tikzcd} \mathcal{D} \arrow[r, "\text{Homogenization}", "k\to+\infty"'] \arrow[d, "\text{Optimization}"'] & \mathcal{D}_{\text{Hom}} \arrow[d, "\text{Optimization}"] \\ \mathcal{D}^\star \arrow[r, "\text{Homogenization}", "k\to+\infty"'] & \mathcal{D}^\star_{\text{Hom}} \end{tikzcd}$$

Optimization of the homogenized limit

Goal: compute

$$\boxed{\Lambda^\star_{\mathrm{Hom}} = \Lambda(\mathcal{D}^\star_{\mathrm{Hom}})}$$

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Theorem [Analytic expression]

- Linear constraint: For a fixed $M \in \mathcal{S}_d^{++}$, under the constraint, $\int_{\mathbb{T}^d} \mathcal{D}\,\mathrm{d}\pi = M$,

$$\boxed{\mathcal{D}^\star_{\mathrm{Hom}}(q) = M/\pi(q)}$$

is a maximizer.

- L^p_π constraint, $d=1$: Under the constraint $\|\mathcal{D}\|_{L^p_\pi} \leqslant 1$,

$$\boxed{\mathcal{D}^\star_{\mathrm{Hom}}(q) = \mathrm{e}^{\beta V(q)}}$$

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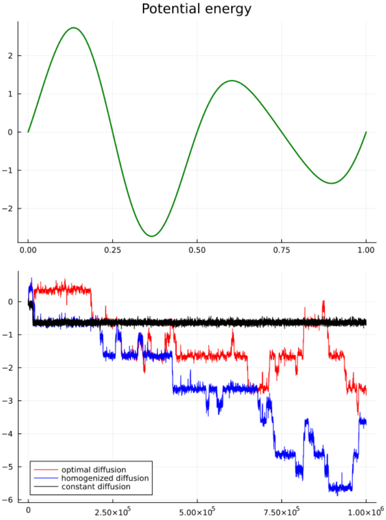
Numerical results - Application to sampling experiments - 1



Typical trajectories

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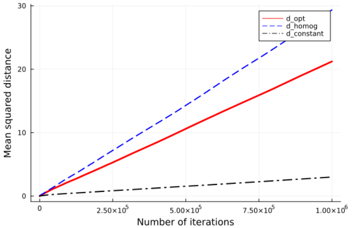
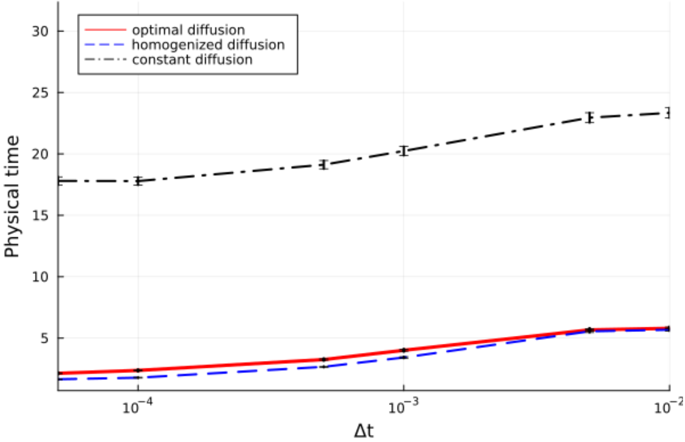


Mean square distance (averaged)

Numerical results - Application to sampling experiments - 2

Diffusion coefficient	Constant	Homogenized	Optimal
Spectral gap	2.16	10.57	11.23



Transition times between the two wells, $N_{\mathrm{transitions}} = 10^5$

Conclusion

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- In high-dimension, use free energy F and coordinate reaction ξ:

$$\mathcal{D}(q) \propto \mathrm{e}^{\beta F(\xi(q))}$$

- Good approximation with homogenization procedure: $\mathcal{D}^{\star}_{\mathrm{Hom}} = \mathrm{e}^{\beta V}$

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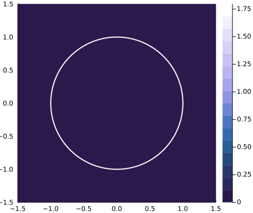
Thank you !

Which diffusion coefficient? Anisotropic case

- Anisotropic diffusion coefficient $\mathcal{D}_{\mathsf{Tan}}(q) = \varepsilon \mathrm{I}_2 + \tilde{q}\tilde{q}^{\mathsf{T}}/\|q\|^2,\ \tilde{q} = (-y\ x)^{\mathsf{T}}$
- Isotropic diffusion coefficient $\mathcal{D}_{\mathsf{One}} \equiv (1+\varepsilon)\mathrm{I}_2, \quad \varepsilon = 0.1$



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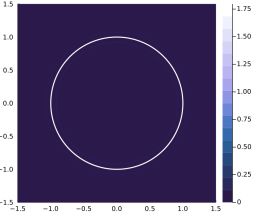
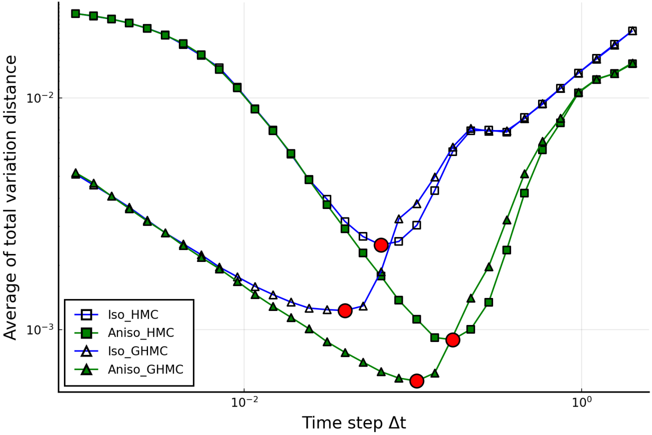
Computing: after fixed number of iterations, distance to the invariant measure of the angle distribution (uniform on $[0, 2\pi]$)





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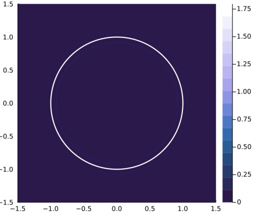

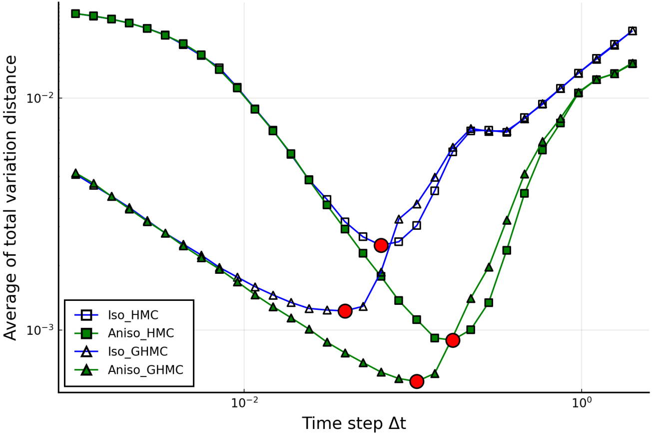

$\Rightarrow$ Compromise: small/large time steps (exploration vs rejection)

Periodic homogenization procedure

- Decrease the period: $(\mathbb{Z}/k)^d$-periodic functions $V_{\#,k}(q) = V(kq)$ and $\mathcal{D}_{\#,k}(q) = \mathcal{D}(kq)$
- Write the spectral gap problem:

$$\Lambda_{\#,k}(\mathcal{D}) = \min_{u \in H^1(\mathbb{T}^d)\setminus\{0\}} \left\{ \frac{\int_{\mathbb{T}^d} \nabla u^\mathsf{T} \mathcal{D}_{\#,k} \nabla u \, \mathrm{e}^{-\beta V_{\#,k}}}{\int_{\mathbb{T}^d} u^2 \, \mathrm{e}^{-\beta V_{\#,k}}} \,\middle|\, \int_{\mathbb{T}^d} u \, \mathrm{e}^{-\beta V_{\#,k}} = 0 \right\}$$

[5] See for instance Allaire, *Shape Optimization by the Homogenization Method* (2002)

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• Decrease the period: $(\mathbb{Z}/k)^d$-periodic functions $V_{\#,k}(q) = V(kq)$ and $\mathcal{D}_{\#,k}(q) = \mathcal{D}(kq)$

• Write the spectral gap problem:

$$\Lambda_{\#,k}(\mathcal{D}) = \min_{u \in H^1(\mathbb{T}^d)\setminus\{0\}} \left\{ \frac{\int_{\mathbb{T}^d} \nabla u^\mathsf{T} \mathcal{D}_{\#,k} \nabla u \, \mathrm{e}^{-\beta V_{\#,k}}}{\int_{\mathbb{T}^d} u^2 \, \mathrm{e}^{-\beta V_{\#,k}}} \,\middle|\, \int_{\mathbb{T}^d} u \, \mathrm{e}^{-\beta V_{\#,k}} = 0 \right\}$$

• Use **H-convergence**:[5] $\exists \overline{\mathcal{D}} \in \mathfrak{D}_p^{a,b}$, $\Lambda_{\#,k}(\mathcal{D}) \xrightarrow[k\to+\infty]{} \Lambda_{\mathrm{Hom}}(\mathcal{D})$ with

$$\boxed{\Lambda_{\mathrm{Hom}}(\mathcal{D}) := \min_{u \in H^1(\mathbb{T}^d)\setminus\{0\}} \left\{ \frac{\int_{\mathbb{T}^d} \nabla u^\mathsf{T} \overline{\mathcal{D}} \nabla u}{\int_{\mathbb{T}^d} u^2} \,\middle|\, \int_{\mathbb{T}^d} u = 0 \right\}}$$

• $\overline{\mathcal{D}}$ can be expressed using $\mathcal{D}$ and corrector functions appearing in the H-convergence procedure

[5] See for instance Allaire, *Shape Optimization by the Homogenization Method* (2002)

H-convergence

Definition [H-convergence]

A sequence $(\mathcal{A}^k)_{k\geqslant 1} \subset L^\infty(\mathbb{T}^d, \mathcal{M}_{a,b})$ H-converges to $\overline{\mathcal{A}} \in L^\infty(\mathbb{T}^d, \mathcal{M}_{a,b})$ if, for any $f \in H^{-1}(\mathbb{T}^d)$ such that $\langle f, \mathbf{1} \rangle_{H^{-1},H^1} = 0$, the sequence $(u^k)_{k\geqslant 1} \subset H^1(\mathbb{T}^d)$ of solutions to

$$\begin{cases} -\operatorname{div}\left(\mathcal{A}^k \nabla u^k\right) = f \quad \text{on } \mathbb{T}^d, \\ \displaystyle\int_{\mathbb{T}^d} u^k(q)\mathrm{d}q = 0 \end{cases}$$

satisfies in the limit $k \to +\infty$,

$$\begin{cases} u^k \rightharpoonup u & \text{weakly in } H^1(\mathbb{T}^d), \\ \mathcal{A}^k \nabla u^k \rightharpoonup \overline{\mathcal{A}} \nabla u & \text{weakly in } L^2(\mathbb{T}^d)^d, \end{cases}$$

where $u \in H^1(\mathbb{T}^d)$ is the solution of the homogenized problem

$$\begin{cases} -\operatorname{div}\left(\overline{\mathcal{A}} \nabla u\right) = f \quad \text{on } \mathbb{T}^d, \\ \displaystyle\int_{\mathbb{T}^d} u(q)\mathrm{d}q = 0 \end{cases}$$

Definition [Correctors]

If $\mathcal{A} = \mathcal{D} \exp(-\beta V)$, $(w_i)_{1 \leqslant i \leqslant d} \subset H^1(\mathbb{T}^d)$ is the family of unique solutions to the problem

$$\begin{cases} -\operatorname{div}(\mathcal{A}(e_i + \nabla w_i)) = 0, \\ \displaystyle\int_{\mathbb{T}^d} w = 0 \end{cases}$$

Then for any $\xi \in \mathbb{R}^d$,

$$\xi^{\mathsf{T}} \overline{D} \xi = \xi^{\mathsf{T}} \left(\int_{\mathbb{T}^d} \mathcal{D}(q) \mathrm{d}\pi \right) \xi - \int_{\mathbb{T}^d} \nabla w_\xi^{\mathsf{T}} \mathcal{D} \nabla w_\xi \mathrm{d}\pi.$$

Homogenization of the optimal diffusion

Goal: optimize for a given $k \geqslant 1$, then let $k \to +\infty$

- Recall the oscillating potential $V_{\#,k}(q) = V(kq)$. Let $\mathfrak{D}^{a,b}_{\#,k,p} \equiv \mathfrak{D}^{a,b}_{p}$ but defined with $V_{\#,k}$ instead of V.
- Let

$$\Lambda^k(\mathcal{D}) = \min_{u \in H^1(\mathbb{T}^d)\setminus\{0\}} \left\{ \frac{\int_{\mathbb{T}^d} \nabla u^\mathsf{T} \mathcal{D} \nabla u \, \mathrm{e}^{-\beta V_{\#,k}}}{\int_{\mathbb{T}^d} u^2 \, \mathrm{e}^{-\beta V_{\#,k}}} \,\middle|\, \int_{\mathbb{T}^d} u \, \mathrm{e}^{-\beta V_{\#,k}} = 0 \right\}$$

and

$$\boxed{\Lambda^{k,\star} = \max_{\mathcal{D} \in \mathfrak{D}^{a,b}_{\#,k,p}} \Lambda^k(\mathcal{D})}$$

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and

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Lemma

There exists a maximizer $\mathcal{D}^{k,\star} \in \mathfrak{D}^{a,b}_p$ such that, denoting by $\mathcal{D}^{k,\star}_{\#,k}(q) = \mathcal{D}^{k,\star}(kq)$,

$$\Lambda^k(\mathcal{D}^{k,\star}_{\#,k}) = \Lambda^{k,\star}$$

Commutation between Homogenization and Optimization

$$
\begin{tikzcd}
\Lambda(\mathcal{D}) \arrow[r, "\text{Hom.}", "k\to+\infty"'] \arrow[d, "\text{Opt.}"'] & \Lambda_{\mathrm{Hom}}(\mathcal{D}) \arrow[d, "\text{Opt.}"] \\
\Lambda^{k,\star} \arrow[r, "\text{Hom.}", "k\to+\infty"'] & \Lambda^{\star}_{\mathrm{Hom}}
\end{tikzcd}
$$

Theorem

The sequence $(\Lambda^{k,\star})_{k\geqslant 1}$ converges to $\Lambda^{\star}_{\mathrm{Hom}} := \Lambda(\mathcal{D}^{\star}_{\mathrm{Hom}})$.

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\end{tikzcd}$$

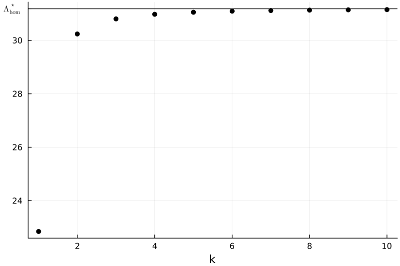
Theorem

The sequence $(\Lambda^{k,\star})_{k\geqslant 1}$ converges to $\Lambda^{\star}_{\mathrm{Hom}} := \Lambda(\mathcal{D}^{\star}_{\mathrm{Hom}})$.

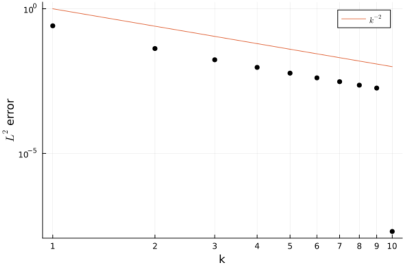
- This implies that a good proxy $(d = 1)$ is $\mathcal{D}^{\star}_{\mathrm{Hom}} = \mathrm{e}^{\beta V}$
- In this case, $\overline{\mathcal{D}} = \left(\int_{\mathbb{T}} \mathrm{e}^{-\beta V}\right)^{-1} := Z^{-1}$, and

$$\boxed{\Lambda^{\star}_{\mathrm{Hom}} = 4\pi^2 Z^{-1}}$$

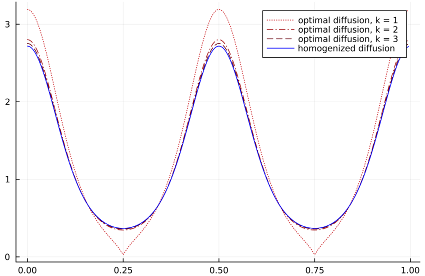
Numerical results - 3



$(\Lambda^{k,\star})_{k\geqslant 1}$ converges to $\Lambda^\star_{\mathrm{Hom}}$



$$\boxed{V(q) = \cos(4\pi q)}$$



$(\mathcal{D}^{k,\star})_{k\geqslant 1}$ and $\mathcal{D}^\star_{\mathrm{Hom}}$ (rescaled with $1/k$ unit cell)