OPTIMAL PARTITIONS FOR EIGENVALUES*

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Abstract. We introduce a new numerical method to approximate partitions of a domain minimizing the sum of Dirichlet-Laplacian eigenvalues of any order. First we prove the equivalence of the original problem and a relaxed formulation based on measures. Using this result, we build a numerical algorithm to approximate optimal configurations. We describe numerical experiments aimed at studying the asymptotic behavior of optimal partitions with large numbers of cells.

Keywords: γ-convergence, shape analysis

1. Introduction and motivation. This paper deals with the optimal partition problem for Dirichlet-Laplacian eigenvalues. Precisely, given a bounded open set $D \subset \mathbb{R}^2$, we are looking for a family of subsets $\{\Omega_i\}_{i=1}^n$ such that

$$\Omega_1 \cup \cdots \cup \Omega_n \subseteq D,\ \Omega_i \cap \Omega_j = \emptyset \text{ for } i \neq j$$

and which minimizes

$$\mathcal{J}_n(\Omega_1, \ldots, \Omega_n) = \sum_{i=1}^n \lambda_k(\Omega_i) \tag{1.1}$$

among all possible such partitions. Above, $\lambda_k(\Omega)$ denotes the k-th eigenvalue of the Dirichlet-laplacian on Ω, counted with multiplicity.

Existence of optimal partitions for problem (1.1) in the class of quasi-open sets was proved in [7]. For $k = 1$ regularity and qualitative studies of the optimal partitions were obtained by Conti, Terracini, and Verzini in [12] and Caffarelli, and Lin in [9]. Caffarelli and Lin obtained regularity results for the optimal partition and estimates for the asymptotic behavior of (1.1) when $n \to +\infty$. In particular, they conjectured that for the optimal partition $\{\Omega_i^*\}_{i=1}^n$

$$\sum_{i=1}^n \lambda_1(\Omega_i^*) \simeq n^2 \lambda_1(H), \tag{1.2}$$

where H is the regular hexagon of area 1 in $\mathbb{R}^2$. Roughly speaking this estimate says that, far from ∂D, a tiling by regular hexagons of area $\frac{|D|}{n}$ is asymptotically close to the optimal partition.

A close problem, still for $k = 1$, was considered by Bonnaillie-Noël, Helffer and Vial in [4], where the cost functional is replaced by

$$\mathcal{L}_n(\Omega_1, \ldots, \Omega_n) = \max_{i=1\ldots n} \lambda_1(\Omega_i). \tag{1.3}$$

We notice that for fixed n, problems (1.1) and (1.3) may have different solutions (see [7] for remarks in relation with Payne conjecture). Nevertheless, Van den Berg conjectured the following asymptotic behavior :

$$\lim_{n \to +\infty} \frac{\mathcal{L}_n(\Omega_1^*, \ldots, \Omega_n^*)}{n} = \lambda_1(H) \tag{1.4}$$

It is quite easy to notice that, at least for smooth sets D, the asymptotic estimate (1.2) implies (1.4). The main feature of the case $k = 1$ is that the cost function (1.1) is of energy type. Namely, it can be written as:

$$\min_{u_1,\ldots,u_n} \left\{ \sum_{i=1}^n \int_D |\nabla u_l|^2 : u_i \in H_0^1(D),\ \int_D u_i^2 = 1,\ u_i u_j = 0 \text{ for } 1 \leq i < j \leq n \right\}.$$

*Support for the first author was provided in part by the National Science Foundation grant DMS-0605320. The numerical experiments were performed using the National Science Foundation TeraGrid resources [14] provided by NCSA at the University of Illinois at Urbana-Champaign and TACC at the University of Texas under the Resource Allocation TG-DMS060011N.

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This kind of energy formulation was used by Chang [11] (see also [10]) to carry out a numerical study of optimal partitions of the disk. As expected, for m large enough, a regular hexagon tiling was observed.

The main purpose of this paper is to propose a numerical scheme for the approximation of the optimal partitions of problem (1.1) for any k. Our method relies on the approximation of "true domains" by positive Borel measures, the relaxation process introduced by Dal Maso and Mosco (see [13] and also Buttazzo and Timofte [8]). Based on a density argument, we replace the unknown m-upple of domains $(\Omega_1, \ldots, \Omega_n)$ by an n-upple of functions $(\varphi_1, \ldots, \varphi_n)$ such that

$$\varphi_l : D \longmapsto [0,1], \sum_{i=1}^{n} \varphi_i(x) = 1, \text{ a.e. } x \in D$$

For each index i, the k-th eigenvalue associated to φ_i is defined by the k-th eigenvalue of

$$\begin{cases} -\Delta u + C(1-\varphi_i)u & = \lambda_k(\varphi_i)u \text{ in } D, \\ u \in H_0^1(D). \end{cases}$$

We notice that if φ_i equals the characteristic function 1_{Ω_i} of a smooth set Ω_i and $C \to +\infty$, then $\lambda_k(\varphi_l) \to \lambda_k(\Omega_l)$.

In this paper we propose a rigorous proof of the equivalence between problem (1.1) and our relaxed formulation when $C \to +\infty$ providing a complete justification of our numerical approach. Based on this method, we performed numerical simulations for $k = 1, 2, 3$ and large values of n. As expected, and up to boundary effects, in our numerical experiments, we obtain partitions that are very close to a tiling by regular hexagons in the case $k = 1$. Provided that the conjecture (1.2) is true, it can be easily proved that the asymptotic optimal partition for $k = 2$ is made of unions of pairs of regular hexagons (of measure $\frac{|D|}{2n}$). Again our numerical computations illustrate this fact.

Surprisingly as a consequence of our theoretical analysis, for every $k \in \mathbb{N}$ we prove the existence of an optimal partition with a mild regularity property, precisely : it is not consisting of quasi-open but open sets. Usually, the gain of regularity from quasi-open to open is a quite difficult task working only for energy functionals (see [5]).

2. Analysis of the optimal partition problem. Let $d \geq 2$ and $D \subseteq \mathbb{R}^d$ be a bounded open connected set. For every open (or quasi-open) subset $A \subseteq D$ we denote by $\lambda_k(A)$ the k-th Dirichlet eigenvalue of the Laplace operator (multiplicities are counted)

$$\begin{cases} -\Delta u & = \lambda_k(A)u \text{ in } A \\ u & = 0 \text{ on } \partial A. \end{cases}$$

The previous equation has to be understood in a weak sense:

$$u \in H_0^1(A), \ \forall \varphi \in H_0^1(A) \int_A \nabla u \cdot \nabla \varphi dx = \lambda_k(A) \int_A u\varphi dx,$$

the eigenvalues being given by the Courant Fischer formula

$$\lambda_k(A) = \min_{S \in \mathcal{S}_k} \max_{u \in S} \frac{\int_A |\nabla u|^2 dx}{\int_A u^2 dx},$$

where $\mathcal{S}_k$ denotes the family of subspaces of dimension k of $H_0^1(A)$. Let

$$O_n = \{(\Omega_1, .., \Omega_n) : \Omega_i \text{ open}, \Omega_i \subseteq D, \Omega_i \cap \Omega_j = \emptyset, \ i \neq j\}.$$

Given $k, n \in \mathbb{N}$, the optimal partition problem reads

$$\inf_{(\Omega_1,..,\Omega_n) \in O_n} \sum_{i=1}^{n} \lambda_k(\Omega_i) := O(k,n). \tag{2.1}$$

In order to justify the numerical computations, we first introduce a relaxed version of the problem. Let

$$Q_n = \{(A_1, .., A_n) : A_i \text{ quasi-open}, A_i \subseteq D, \text{cap}(A_i \cap A_j) = 0,\ i \neq j\},$$

where $\text{cap}(U)$ stands for the capacity of U, and consider the problem

$$\inf_{(A_1,..,A_n)\in Q_n} \sum_{i=1}^{k} \lambda_k(A_i) := Q(k, n). \tag{2.2}$$

For every $k \geq 1$, the existence of a solution of problem (2.2) was proved in [7].

We begin with a first result asserting that problem (2.2) is indeed a relaxed version of problem (2.1). We rely on the γ-convergence which is a suitable topology in the family of quasi-open sets for which the eigenvalues are continuous (see [6]).

THEOREM 2.1. *The set O_n is dense in Q_n for the γ-convergence. As a consequence, for every $k, n \in \mathbb{N}$ we have*

$$O(k, n) = Q(k, n).$$

Proof. Clearly, $O_n \subseteq Q_n$. In order to prove the density for the γ-convergence, we consider $(A_1, .., A_n) \in Q_n$. For every A_i, there exists a sequence of open sets U_i^j such that

$$A_i \subseteq U_i^j, \textit{a.e.}, \text{ and } \text{cap}(U_j^i \setminus A_i) \to 0 \text{ when } j \to \infty.$$

For each U_1^j there exists a smooth open subset V_1^j such that

$$\overline{V}_1^j \subseteq U_1^j,\ d_\gamma(U_1^j, V_1^j) \leq 1/j.$$

We set $\Omega_1^j = V_1^j$ and observe that $\Omega_1^j \xrightarrow{\gamma} A_1$, since

$$d_\gamma(A_1, \Omega_1^j) \leq d_\gamma(A_1, U_1^j) + d_\gamma(U_1^j, V_1^j).$$

For U_2^j there exists a smooth open subset V_2^j such that

$$\overline{V}_2^j \subseteq U_2^j,\ d_\gamma(U_2^j \setminus \overline{V}_1^j, V_2^j \setminus \overline{V}_1^j) \leq 1/j.$$

We set $\Omega_2^j = V_2^j \setminus \overline{V}_1^j$ and observe that $\Omega_2^j \xrightarrow{\gamma} A_2$. Indeed,

$$d_\gamma(A_2, \Omega_2^j) \leq d_\gamma(A_2, U_2^j \setminus \overline{V}_1^j) + d_\gamma(U_2^j \setminus \overline{V}_1^j, V_2^j \setminus \overline{V}_1^j).$$

The second term on the right hand is no greater than $1/j$, while for the first term we notice that

$$\text{cap}(A_2 \setminus (U_2^j \setminus \overline{V}_1^j)) = \text{cap}(A_2 \cap \overline{V}_1^j) \leq \text{cap}(A_2 \cap U_1^j) \leq \text{cap}(U_1^j \setminus A_1) \to 0,$$

and

$$\text{cap}((U_2^j \setminus \overline{V}_1^j) \setminus A_2) \leq \text{cap}(U_2^j \setminus A_2) \to 0.$$

Since in general $\text{cap}(A_n \Delta A) \to 0$ implies $A_n \xrightarrow{\gamma} A$, we get that $\Omega_2^j \xrightarrow{\gamma} A_2$.

We continue the same procedure taking $\Omega_3^j = V_3^j \setminus (\overline{V}_1^j \cup \overline{V}_2^j)$, where V_3^j is chosen such that

$$d_\gamma(V_j^3 \setminus (\overline{V}_1^j \cup \overline{V}_2^j), U_j^3 \setminus (\overline{V}_1^j \cup \overline{V}_2^j)) \leq 1/j,$$

and iterating the same construction, we obtain that $(\Omega_1^j, .., \Omega_n^j) \in O_n$ and

$$(\Omega_1^j, .., \Omega_n^j) \xrightarrow{\gamma^n} (A_1, .., A_n).$$

The second assertion of the theorem is an immediate consequence of the density result. □

Let M be a measurable subset of D. There exists a quasi-open set A such that

$$H_0^1(A) = \{u \in H_0^1(D) : \quad u = 0 \text{ a.e. on } D \setminus M\}.$$

This set is precisely the union of all finely open sets U such that

$$1_U \leq 1_M \ a.e.$$

This remark provides a natural way to extend the optimal partition problem to partitions of n measurable, pairwise disjoint sets. Let $\varphi : D \to [0,1]$ be a measurable function. For any $C > 0$, by $\lambda_k(\varphi, C)$, we denote the k-th eigenvalue (counting multiplicity) of $-\Delta u + C(1-\varphi)u$, *i.e.*

$$\begin{cases} -\Delta u + C(1-\varphi)u & = \lambda_k(\varphi, C)u \text{ in } D \\ u & \in H_0^1(D) \end{cases} \tag{2.3}$$

Again, we have

$$\lambda_k(\varphi, C) = \min_{S \in \mathcal{S}_k} \max_{u \in S} \frac{\int_D |\nabla u|^2 + C(1-\varphi)u^2 dx}{\int_D u^2 dx},$$

$\mathcal{S}_k$ being the family of subspaces of $H_0^1(D)$ of dimension k. We introduce the set

$$M = \{(\varphi_1, .., \varphi_n) | \varphi : D \to [0,1] \text{ measurable } \sum_{i=1}^n \varphi_i = 1 \ a.e. \ D\},$$

and the problem

$$\inf_{(\varphi_1, .., \varphi_n) \in M} \sum_{i=1}^n \lambda_k(\varphi_i, C) := M(C, k, n). \tag{2.4}$$

Proposition 2.2. *Problem* (2.4) *admits at least one solution* $(\varphi_1^C, .., \varphi_n^C)$.

Proof. The existence of a solution is a consequence of the weak * $L^\infty(D)$ sequential compactness of M and of the fact that if $\varphi_h \overset{w*-L^\infty(D)}{\longrightarrow} \varphi$ then $C(1-\varphi_h)dx \overset{\gamma}{\longrightarrow} C(1-\varphi)dx$. □

Theorem 2.3. *Let* $k = 1$. *The mapping*

$$\varphi \longrightarrow \lambda_1(\varphi, C)$$

is concave and every solution of problem (2.4) *is an extremal point of* M.

Proof. We give the details of the proof for $n = 2$. It is straightforward to generalize the following arguments for $n > 2$.

Let us first establish the concavity of

$$\varphi \longrightarrow \lambda_1(\varphi, C)$$

Let $\varphi_1, \varphi_2 \in L^\infty(D, [0,1])$ and $\theta \in (0,1)$. Then

$$\lambda_1(\theta\varphi_1 + (1-\theta)\varphi_2, C) = \frac{\int_D |\nabla u|^2 + C[1 - \theta\varphi_1 - (1-\theta)\varphi_2]u^2 dx}{\int_D u^2 dx}$$

where u is a non zero first eigenfunction associated to $\lambda_1(\theta\varphi_1 + (1-\theta)\varphi_2, C)$. Moreover, by definition of the Rayleigh quotient we have

$$\lambda_1(\theta\varphi_1 + (1-\theta)\varphi_2, C) = \theta \frac{\int_D |\nabla u|^2 + C(1-\varphi_1)u^2 dx}{\int_D u^2 dx} + (1-\theta) \frac{\int_D |\nabla u|^2 + C(1-\varphi_2)u^2 dx}{\int_D u^2 dx},$$

so that

$$\lambda_1(\theta\varphi_1 + (1-\theta)\varphi_2, C) \geq \theta\lambda_1(\varphi_1, C) + (1-\theta)\lambda_1(\varphi_2, C), \tag{2.5}$$

which proves the concavity of the functional.

Let us prove now that every solution of problem (2.4) is an extremal point of M. First we notice that if equality occurs in (2.5), then $\varphi_1 - \varphi_2$ must be a constant function. Indeed, if equality occurs, the eigenfunction u associated to $\lambda_1(\theta\varphi_1 + (1-\theta)\varphi_2, C)$ is also a first eigenfunction of $\lambda_1(\varphi_1, C)$ and $\lambda_1(\varphi_2, C)$. Subtracting the two equations of type (2.3) satisfied by u with $\varphi = \varphi_1$ and $\varphi = \varphi_2$ we get

$$\varphi_1(x) - \varphi_2(x) = \frac{\lambda_1(\varphi_2, C) - \lambda_1(\varphi_1, C)}{C} \text{ a.e. } x \in D$$

since $u \neq 0$ a.e. on D.

Assume now that $(\varphi_1, .., \varphi_n)$ is an optimal solution for problem (2.4) and not an extremal point. We may assume the existence of $\varepsilon > 0$, a measurable set A such that $0 < |A| < |D|$ and

$$A \subseteq \{\varepsilon < \varphi_1 < 1-\varepsilon\} \cap \{\varepsilon < \varphi_2 < 1-\varepsilon\}.$$

We have from the concavity property

$$\lambda_1(\varphi_1, C) \geq \frac{1}{2}\lambda_1(\varphi_1 + \varepsilon 1_A, C) + \frac{1}{2}\lambda_1(\varphi_1 - \varepsilon 1_A, C),$$

$$\lambda_1(\varphi_2, C) \geq \frac{1}{2}\lambda_1(\varphi_2 - \varepsilon 1_A, C) + \frac{1}{2}\lambda_1(\varphi_2 + \varepsilon 1_A, C). \tag{2.6}$$

or

$$\lambda_1(\varphi_1, C) + \lambda_1(\varphi_2, C) \geq \min\{\lambda_1(\varphi_1 + \varepsilon 1_A, C) + \lambda_1(\varphi_2 - \varepsilon 1_A, C), \lambda_1(\varphi_1 - \varepsilon 1_A, C) + \lambda_1(\varphi_2 + \varepsilon 1_A, C)\}.$$

Finally, we have

$$\lambda_1(\varphi_1, C) + \lambda_1(\varphi_2, C) = \lambda_1(\varphi_1 + \varepsilon 1_A, C) + \lambda_1(\varphi_2 - \varepsilon 1_A, C) = \lambda_1(\varphi_1 - \varepsilon 1_A, C) + \lambda_1(\varphi_2 + \varepsilon 1_A, C).$$

Since equality holds in all previous inequalities we should have that $\varphi_1 + \varepsilon 1_A - (\varphi_1 - \varepsilon 1_A) = 2\varepsilon 1_A$ is constant in D. This last assertion is only possible only $A = D$, in contradiction with the assumption $|A| < |D|$. □

THEOREM 2.4. *We have*

$$\lim_{C\to\infty} M(C, k, n) = O(k, n). \tag{2.7}$$

Moreover, if $(\varphi_1^C, .., \varphi_n^C)$ *is an optimal solution for problem* (2.4) *and* $\varphi_i^C \overset{w*L^\infty}{\longrightarrow} \varphi_i$ *then there exists an optimal solution* $(A_i)_{i=1,..,n}$ *for problem* (2.2) *such that* $A_i \subseteq \{\varphi_i = 1\}$ *a.e.*

Proof. There exists a constant K such that for every $C > 0$ and for every $i = 1, .., n$

$$\int_D C(1-\varphi_i^C) w_i^C dx \leq K \text{ and } \|w_i^C\| \leq K$$

where w_i^C is the solution of

$$\begin{cases} -\Delta w_i^C + C(1-\varphi_i^C) w_i^C & = 1 \text{ in } D \\ w_i^C & \in H_0^1(D) \end{cases}$$

Up to extracting a subsequence we have

$$w_i^C \overset{H_0^1(D)}{\rightharpoonup} w_i,$$

and we get

$$\int_D (1-\varphi_i) w_i dx = 0$$

hence

$$w_i = 0 \text{ a.e. on } \{\varphi_i < 1\}.$$

We define the quasi-open sets $A_i = \{w_i > 0\}$ and notice that $(A_i)_i$ satisfy

$$\sum_{i=1}^{n} \lambda_1(A_i) \leq \lim_{C\to\infty} M(C,k,n). \tag{2.8}$$

For the converse inequality, we fix a partition $(\Omega_1, .., \Omega_n)$ consisting of open, smooth and disjoint sets. We take

$$\varphi_i = 1_{\Omega_i}$$

and observe that

$$M(C,k,n) \leq \lim_{C\to\infty} \sum_{i=1}^{n} \lambda_1(C,\varphi_i) = \sum_{i=1}^{n} \lambda_1(\Omega_i).$$

Using Theorem 2.1, and taking the infimum in the right hand side, we get (2.7).

The second assertion of the theorem is a consequence of inequality (2.8).

□

THEOREM 2.5. *If $d = 2$, for every $k \geq 1$ there exists a solution of* (2.1) *consisting of open sets.*

Proof. Thanks to Theorem 2.1, we may take a minimizing sequence $(\Omega_1^h, .., \Omega_n^h)$ indexed by h consisting on polygonal disjoint sets. Assume that $\mathbb{R}^2 \setminus \Omega_1^h$ has more than $k(n-1)+1$ connected components. Since for every $i = 2, .., n$, the $k-th$ eigenvalue on Ω_i^h is given by at most k connected components, one can take the unused connected components of $\mathbb{R}^2 \setminus \Omega_1^h$ and add them to Ω_1^h in such a way that the cost functional decreases. The same procedure is repeated for every Ω_i^h, and finally we may assume that in the minimizing sequence every $\mathbb{R}^2 \setminus \Omega_i^h$ has at most $k(n-1)+1$ connected components.

Using Šverák's result (which is only valid in $\mathbb{R}^2$, see [17]) and the compactness of the Hausdorff complementary topology (see [6]), we can extract a subsequence (still denoted using the same index) such that

$$\Omega_i^h \xrightarrow{H^c} \Omega_i \text{ and } \lambda_k(\Omega_i^h) \to \lambda_k(\Omega_i).$$

Since the Ω_i are pairwise disjoint open sets, they form a solution of problem (2.1). □

3. Implementation and numerical results. The key to our numerical approach is the approximation Theorem 2.4. In order to obtain an approximation of the minimizers of (1.1), we fix C "large enough", and try to solve problem (2.4). In all the numerical experiments presented below, we assume that $\Omega = (0,1)\times(0,1)$, and use first order finite differences to represent the functions φ_l and their associated eigenvectors u_l. We decompose the domain D into a $N \times N$ grid with spacing $h = 1/(N-1)$. In order to simplify notations, we consider a renumbering operator $I : (0, N-1)\times(0, N-1) \mapsto 0, N^2-1$ such $I(i,j) = jN + i$. We refer to the components of a discrete field U as $U_{i,j}$ or $U_{I(i,j)}$ (which we abbreviate as U_I when there is no risk of confusion) depending on wether we want to insist on the spatial relation between the components or U or not. More precisely, to any $\varphi_l \in H_0^1(D)$, we associate a vector $\Phi_l \in \mathbb{R}^{N\times N}$ such that $[\Phi_l]_{i,j} = \varphi_l((i-1)h, (j-1)h)$, $1 \leq i,j \leq N$. By δ_x^2 and δ_y^2, we denote the classical finite difference operators, *i.e.* for any vector $U \in \mathbb{R}^{N\times N}$

$$\left[\delta_x^2 U\right]_{i,j} = \frac{U_{i-1,j} - 2U_{i,j} + U_{i+1,j}}{h^2},$$
$$\left[\delta_y^2 U\right]_{i,j} = \frac{U_{i,j-1} - 2U_{i,j} + U_{i,j+1}}{h^2}.$$

To each Φ_l, we associate the k-th Dirichlet eigenpair $(\lambda_{k,l}(\Phi_l), U_{k,l}(\Phi_l))$ (which we will denote by $(\lambda_{k,l}, U_{k,l})$ when there are no confusion possible) of the discrete operator $\mathrm{A}(\Phi_l)$ defined by

$$\mathrm{A}(\Phi)U := \left[-(\delta_x^2 + \delta_y^2) + C\mathrm{Id}\right] U - C\mathrm{M}(\Phi)U,$$

where $[\mathrm{M}(\Phi)]_{I,J} = \delta_{I,J}\,[\phi]_I$, for any $0 \le I \le N^2 - 1$, and Id denotes the identity matrix of dimension $N \times N$.

Accounting for the homogeneous Dirichlet boundary conditions, we have then

$$[\mathrm{A}(\Phi_l)U_{k,l}(\Phi_l)]_I = \lambda_{k,l}(\Phi_l)\,[U_{k,l}(\Phi_l)]_I\,, \tag{3.1}$$

for any I corresponding to an interior node $I = I(i,j), 1 \le i,j < N-1$, and $U_{k,l}(\Phi_l)$ otherwise, and our discrete problem is

$$\inf\left\{ J_n\left(\Phi_1,\ldots,\Phi_n\right) : \Phi_l \in \mathbb{R}^{N\times N},\, 0 \le [\Phi_l]_I \le 1,\, \sum_{l=1}^{n} [\Phi_l]_I = 1,\, 0 \le I < N^2,\, 1 \le l \le n \right\}, \tag{3.2}$$

where the discrete objective function J_n is defined by

$$J_n\left(\Phi_1,\ldots,\Phi_n\right) := \sum_{l=1}^{n} \lambda_{k,l}(\Phi_l).$$

The main difficulty in tailoring a numerical method for this problem is due the non-convexity of J_n, as stated in Theorem 2.3. As we are interested in the asymptotic behavior of the partitions function when n becomes large, the total number of degrees of freedom in the problem can become quite large (in the experiment presented in Figure 3.2, we have $N = 505$ and $n = 512$, leading to over 130,000,000 degrees of freedom), and to our knowledge, there are no global optimization algorithm capable of solving non-convex problems of this size. We note that the derivative of the objective function J_n with respect to the components of each of the Φ_l are easily obtained using a classical method in optimal design (see [3], for instance). We first differentiate (3.1) with respect to the I-th component of Φ_l (I corresponding to an interior node of the discrete domain):

$$A(\Phi_l)\frac{\partial U_{k,l}(\Phi_l)}{\partial[\Phi]_I} - C\frac{\partial \mathrm{M}(\Phi_l)}{\partial[\Phi]_I}U_{k,l}(\Phi_l) = \frac{\partial \lambda_{k,l}(\Phi_l)}{\partial[\Phi]_I}U_{k,l}(\Phi_l) + \lambda_{k,l}(\Phi_l)\frac{\partial U_{k,l}(\Phi_l)}{\partial[\Phi]_I}.$$

Taking the dot product with $U_{k,l}(\Phi_l)$ on both side gives

$$\begin{aligned} U_{k,l}^t(\Phi_l)A(\Phi_l)\frac{\partial U_{k,l}(\Phi_l)}{\partial[\Phi]_I} - CU_{k,l}^t(\Phi_l)\frac{\partial \mathrm{M}(\Phi_l)}{\partial[\Phi]_I}U_{k,l}(\Phi_l) \\ = \frac{\partial \lambda_{k,l}(\Phi_l)}{\partial[\Phi]_I}U_{k,l}^t(\Phi_l)U_{k,l}(\Phi_l) + \lambda_{k,l}(\Phi_l)U_{k,l}^t(\Phi_l)\frac{\partial U_{k,l}(\Phi_l)}{\partial[\Phi]_I}. \end{aligned}$$

Noticing now that the operator $A(\Phi)$ is self-adjoint, and using (3.1) we obtain

$$-CU_{k,l}^t(\Phi_l)\frac{\partial \mathrm{M}(\Phi_l)}{\partial[\Phi]_I}U_{k,l}(\Phi_l) = \frac{\partial \lambda_{k,l}(\Phi_l)}{\partial[\Phi]_I}U_{k,l}^t(\Phi_l)U_{k,l}(\Phi_l).$$

Last, we notice that $\left[U_{k,l}^t(\Phi_l)\frac{\partial \mathrm{M}(\Phi_l)}{\partial \Phi_I}U_{k,l}(\Phi_l)\right]_J = [U_{k,l}(\Phi_l)]_I^2\,\delta_{I,J}$, so that

$$\left[\frac{\partial \lambda_{k,l}(\Phi_l)}{\partial[\Phi]_I}\right]_J = -C\,\frac{[U_{k,l}(\Phi_l)]_I^2\,\delta_{I,J}}{U_{k,l}^t(\Phi_l)U_{k,l}(\Phi_l)},$$

and with the convention that the eigenvectors $U_{k,l}$ are normalized, we obtain the final expression for the sensitivity of $\lambda_{k,l}$ with respect to each component of each Φ field:

$$\left[\frac{\partial \lambda_{k,l}(\Phi_p)}{\partial[\Phi]_I}\right]_J = \begin{cases} -C\,[U_{k,l}(\Phi_l)]_I^2 & \text{if } l = p \text{ and } I = J, \\ 0 & \text{otherwise.} \end{cases}$$

3.1. Minimization algorithm. From Theorem (2.3), we know that the functional J_n is concave, (at least when $k = 1$) and expect therefore that it admits many local minima. Due to the overall size of the problem, global minimization approaches are not practical. Instead, our numerical method is based on a projected-gradient descent with adaptive step described in Algorithm 3.1, where $\Pi_{\mathbb{S}^{n-1}}$ denotes a projection operator over the $n-1$ dimensional unit simplex $\mathbb{S}^{n-1}$ defined by

$$\mathbb{S}^{n-1} = \left\{ X = (X_1, \ldots, X_n) \in [0,1]^n : \sum_{l=1}^{n} X_l = 1 \right\}.$$

Note that since each $\lambda_{k,l}$ depends only on Φ_l, the parallelization of (3.2) is very natural. In our implementa-

Algorithm 1 General form of the projected gradient algorithm

Require: α (step), α_{min}, α_{max}, ω, ε (tolerance), p_{max}

```
p = 1
repeat
    for l = 1 to n do
        Compute the eigenpair (λ_{k,l}, U_{k,l}) of A(Φ_l)
        Φ_l ← Φ_l − α∇_{Φ_l} λ_{k,l}
    end for
    Φ_l ← Π_{S^{n-1}} Φ_l, l = 1, ..., n.
    Compute J^n := J_n(Φ_1, ..., Φ_n)
    if J^p ≤ J^{p-1} then
        α ← min((1 + ω)α, α_max)
    else
        α ← max(α_min, (1 − ω)α)
    end if
    p ← p + 1
until p = p_max or sup_{i,j,l} |α Π_{S_n} (Φ_l)_I| ≤ ε
```

tion, we distributed each partition function Φ_l on its own processor. We relied on PETSc [2, 1] for the main parallel infrastructure and distributed linear algebra operations, and used m uncoupled eigenvalues solvers provided by SLEPc [15]. The most computationally intensive part of this algorithm is the evaluation of the eigenpair $(\lambda_{k,l}(\Phi_l), U_{k,l}(\Phi_l))$, which does not require any inter-processor communication. In Algorithm 3.1, the time spent in this step is virtually independent of the number of cells m. The I/O operations can also be distributed in a trivial way. The most communication intensive part of the algorithm is the projection step, which can be achieved using a fixed number of *all-to-one* operations on the partition functions Φ_l, so the overall implementation of perfectly scalable.

Of course, we cannot guaranty that such a method will lead to the global minimizer of a non-convex energy. In particular, the concavity of J_m implies that the global minimizers of (2.4) lie on the boundary of the admissible simplex, which by definition is not a regular set. Roughly speaking, this means that in the course of the minimization algorithm, the Φ_l evolve rapidly toward the closest vertex of $\mathbb{S}^n$ at which point they cannot move anymore, so that the outcome of the minimization algorithm depends strongly on the initial guess. Figure 3.1 illustrates this sensitivity. We used an orthogonal projection operator over the unit simplex devised in [16]. In order to simulate the effect of a large number of cells on a reasonably sized domain, we used periodic boundary conditions for the Φ and U fields, and 16 cells.[1] The domain size is the unit square discretized in 200×200 nodes, and the parameter C is 10,000. We solved the same problem several times, using randomly generated initial fields. The first row represents a composite map of the functions Φ_l obtained by plotting $\sum_l l\Phi_l$, the second represents the sum of associated eigenvalues.

[1] This choice is not innocent. It is of course impossible to construct a periodic paving of $\mathbb{R}^2$ by regular hexagons with periodicity cell the unit square. However, it is possible to do so using $4n^2$, $n \in \mathbb{N}$ slightly flattened regular hexagons. If conjecture 1.2 holds, it is reasonable to expect that such a paving realizes the global minimizer of J_m in this setting.

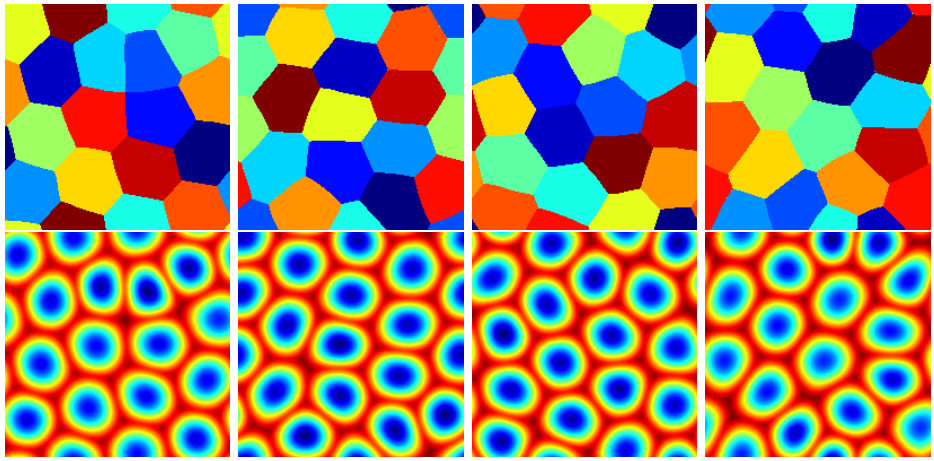

FIG. 3.1. *Dependence on the initial guess, using an orthogonal projection step. The initial values of the fields Φ are chosen randomly. The value of the objective function upon convergence is (left to right) 2,095.2, 2,108.5, 2,100.7, and 2,146.3*

In order to partially alleviate this effect, we then implemented the *simple* projection operator defined by

$$[\Pi_{\mathbb{S}^{n-1}}\Phi_l]_I = \frac{|[\Phi_l]_I|}{\sum_{i=1}^{n}|[\Phi_i]_I|}.$$

Note that this operator is not an orthogonal projection operator and instead tend to keep the Φ in the middle of the faces of the target simplex (see the comparison of the effect of both projection in Figure 3.2). The effect of such an operator is double edged: it tends to prevent the Φ's from becoming "stuck" at the vertices of the unit simplices, but at the same time makes the actual minimizers virtually unreachable.

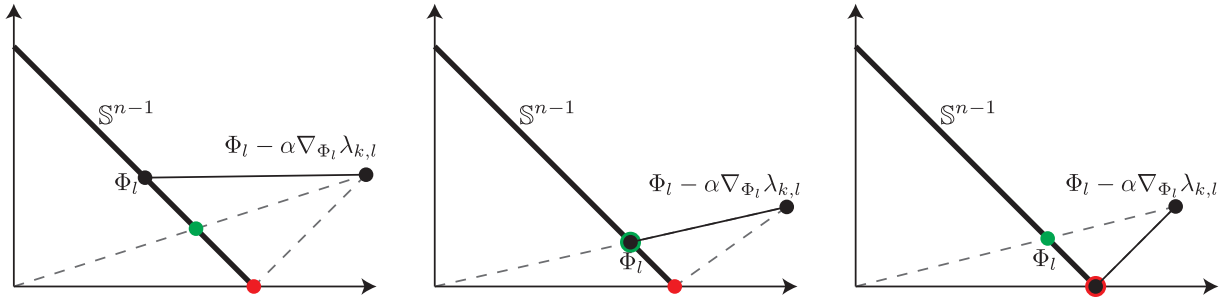

FIG. 3.2. *Behavior of the projection operators. The black dots represent Φ_l and $\Phi_l - \alpha\nabla_{\Phi_l}\lambda_{k,l}$ as labeled. The red ones are the orthogonal projection of $\Phi_l - \alpha\nabla_{\Phi_l}\lambda_{k,l}$, the green ones its* simple *projection. Simple projection has a lesser tendency to "send" the functions Φ_l towards the vertices of $\mathbb{S}^{n-1}$.*

We then combined both operators: in step 7 of Algorithm 3.1, we used the simple algorithm until we reach convergence, then restart the computation using the orthogonal projection step. Figure 3.3 displays the outcome of this approach. The parameters are that of Figure 3.1, and the initial guess for the Φ_l is the same as in the leftmost experiment of the aforementioned figure. Upon convergence, we still obtain a non-regular tiling, whose energy is lesser than that obtained using only orthogonal projection. As the size of the search space is very large, convergence to a local minimizer is very likely. Our final algorithm uses a implemented a multi-level approach akin to a continuation method to address that issue. We use the simple projection algorithm and upon convergence of Algorithm 3.1 project the solution onto a finer grid, and iterate this process. After several grid refinement, we switch to the orthogonal projection. Figure 3.4 displays the numerical results obtained using this approach for the problem solved in Figures 3.1 and 3.3. We tested this approach using several initial conditions. In each case, we obtained a regular paving by hexagons, as expected. All the experiments presented below were obtained using the multi-level algorithm.

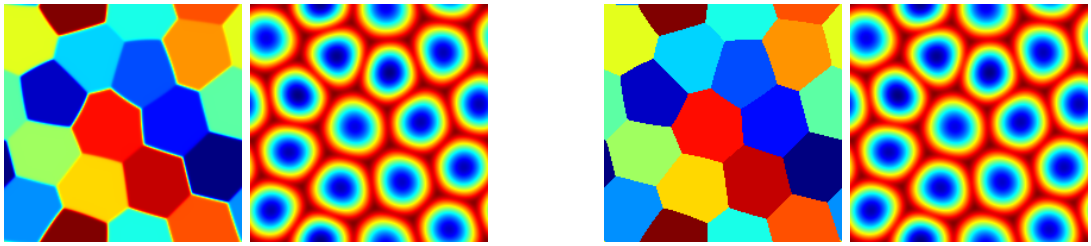

FIG. 3.3. *The problem from Figure 3.1(left) solved using a combination of simple and orthogonal projection. The leftmost figures represents the* Φ *and* U *fields upon convergence of the minimization algorithm using simple projection. Note how the functions* Φ *are not piecewise constant with values in* $\{0, 1\}$*. The rightmost figure corresponds to the final result obtained by using the orthogonal projection, starting from the configuration in th left. Compare the value of the objective function at 2,145.0 (left) and 2,073.8 (right) to that of the previous computations.*

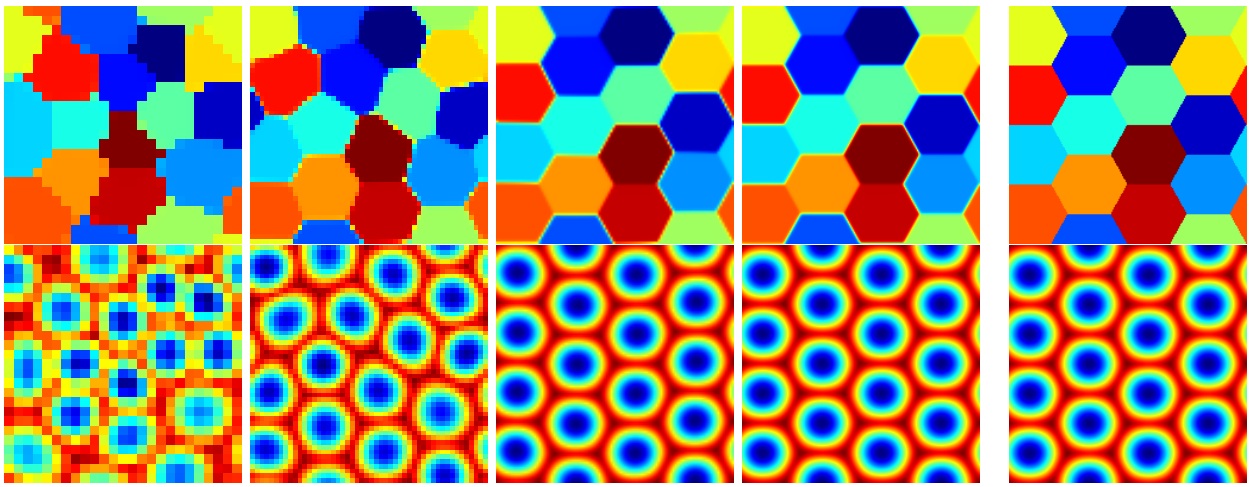

FIG. 3.4. *The same problem is solved again using the simple projection on increasingly refined grids (4 leftmost figures) then using the orthogonal projection on the final grid (right). The grid sizes are (from left to right)* 25×25, 50×50, 100×100, *and* 200×200. *The objective function upon convergence is (from left to right) 1,902.1, 2,033.8, 2,095.7, 2,124.6, and 2,048.8*

3.2. Numerical experiments. We were able to run a series of large computations on parallel supercomputers at the Texas Advanced Computing Center. In Figure 3.2, the domain is again the unit square. Periodicity boundary conditions are not used, as the number of cell ($n = 384$) is large enough that we expect that the effect of boundary conditions vanishes in the center of the domain. The computations were run on four layers of recursively refined grid of respective dimension (64×64), (127×127), (253×253), and (505×505). The parameter C is 10^5, the tolerance parameter $\epsilon = 10^6$, the bounds on the admissible steps are $\alpha_{min} = 1$, $\alpha_{max} = 10^4$. We used only the simple projection operator, and the final objective functions on each grid are $1.602\,10^6$, $1.248\,10^6$, $1.176\,10^6$, and $1.189\,10^6$. We observe that the solution corresponds to local patches of tiling by regular hexagons, as we would expect from a "good" local minimizer.

We obtained similar results while running the same computation of 512 processors, for 512 cells. The fields Φ and U are represented using the usual convention and the final energies are $2.342\,10^6$, $2.243\,10^6$, $2.024\,10^6$, and $2.051\,10^6$. Again, the local geometry away from the edges of the domain is that of a network of regular hexagons.

3.3. Extensions and conclusions. Our algorithm can easily be adapted to objective function involving higher order eigenvalues of linear combination of eigenvalues of different order. A classical numerical issue in this case comes from the potential non-differentiability of multiple eigenvalues with respect to changes of the function Φ. We did not try to address this problem, but obtained interesting results nevertheless. Figure (3.7) represent the Φ fields obtained with $n = 8$ for $k = 2$ and $k = 3$, respectively, using periodic boundary conditions. As explained in the introduction if (1.2) holds, the optimal partition for $k = 2$ is

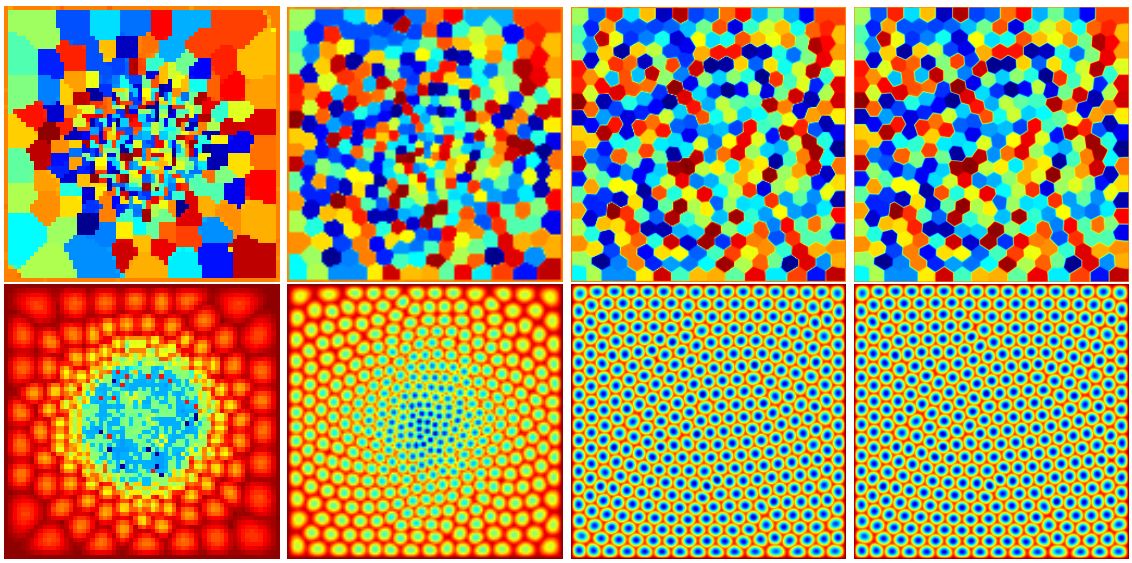

FIG. 3.5. *Optimization of the sum of the first eigenvalue of the Dirichlet Laplacian on 384 cells with* $C = 10^5$. *First row: cell shape on recursively refined grids* (64×64), (127×127), (253×253), *and* (505×505). *Second row: sum of the first eigenvalues on the same grids.*

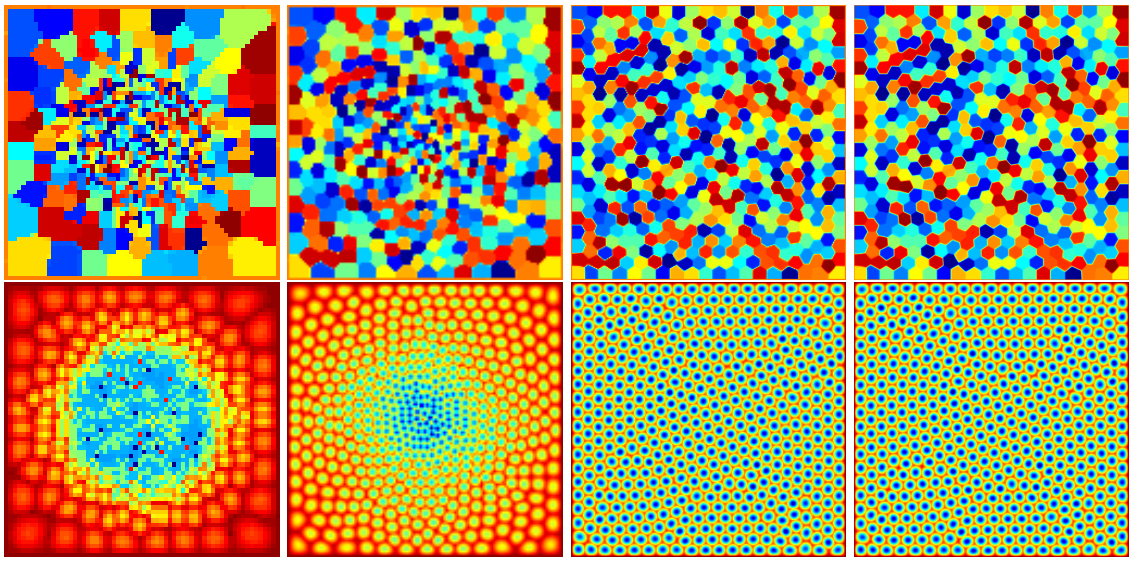

FIG. 3.6. *Optimization of the sum of the first eigenvalue of the Dirichlet Laplacian of 512 cells with* $C = 10^5$. *First row: cell shape on recursively refined grids* (64×64), (127×127), (253×253), *and* (505×505). *Second row: sum of the first eigenvalues on the same grids.*

obtained by a partition made of pairs of regular hexagons. Again, modulo the flattening necessary to achieve periodicity on a unit cell, this is the configuration that we observe. For $k = 3$ (Figure 3.7-right), we obtain a periodic tiling by non-regular hexagons, which can be proven to be a sub-optimal solution, as a tiling by regular hexagons would lead to a lower energy. Again, this is most certainly due to the fact that our objective function admits a great deal of local minima, which are difficult to avoid in optimization problems of this size. An additional difficulty when $k \geq 2$ is that the k-th eigenvalue of an optimal cell is expected to have multiplicity greater than 1 hence and may not be differentiable.

Noticing that the analysis and algorithm are not restricted to the two–dimensional case, we ported our program to the 3D case, but were unable to obtain any meaningful results. We believe that the convergence

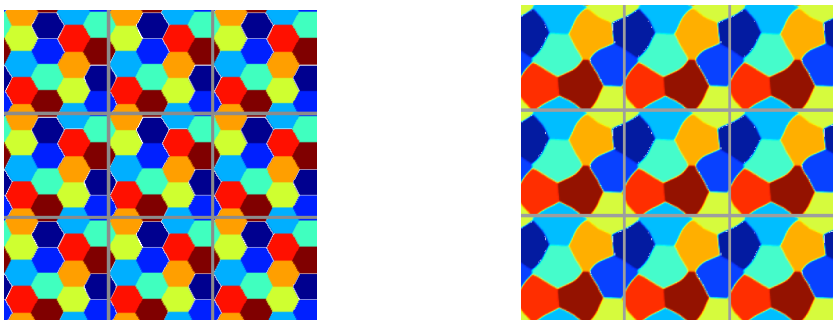

FIG. 3.7. *Optimal partitions of the sum of the second (left) and third (right) eigenvalues of the Dirichlet Laplacian for $n = 8$ cells. The periodicity is highlighted by repeating the unit cell 9 times on a two dimensional lattice.*

rate of our primitive algorithms is too slow to converge to a decent local minimizer in a reasonable time in 3D, when the dimension of the space of admissible fields Φ becomes very large, and the eigenvalue computation cannot be performed on a single processor in an acceptable time. Perhaps the current implementation needs to be improved by associating groups of processors to each function Φ (so as to improve the performance of the eigenvalue solver), and implement a more efficient minimization algorithm in order to reduce the number of necessary function evaluations in the minimization loop.

Acknowledgements. This work was initiated in an open-problems session during the Mini-Workshop "Shape Analysis for Eigenvalues" at the Mathematisches Forschungsinstitut Oberwolfach, organized by D. Bucur, G. Buttazzo, and A. Henrot. The authors would like to thank the MFO and the organizers of the mini-workshop for that.

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