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OPTIMAL PARTITIONS FOR EIGENVALUES*

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Abstract. We introduce a new numerical method for approximating 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.

Key words. γ-convergence, shape analysis

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1. Introduction and motivation.

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

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

and which minimizes

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

among all possible such partitions. Above, $\lambda_k(\Omega)$ denotes the kth 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 $\{\Omega_i^*\}_{i=1}^n$,

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

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.

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

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

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

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

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

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

This kind of energy formulation was used by Chang et al. [11] and Cybulski and Hołyst [13] (see also [10]) to carry out a numerical study of optimal partitions. 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 [14] and also Buttazzo and Timofte [8]). Based on a density argument, we replace the unknown n-tuple of domains $(\Omega_1, \dots, \Omega_n)$ by an n-tuple of functions $(\varphi_1, \dots, \varphi_n)$ such that

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

For each index i, the kth eigenvalue associated with φ_i is defined by the kth 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 $\lambda_k(\varphi_i) \to \lambda_k(\Omega_i)$.

In this paper we propose a rigorous proof of the equivalence between problem (1.1) and our relaxed formulation when $C \to +\infty$, provided a complete justification of our numerical approach. Based on this method, we perform 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; namely, it consists not of quasi-open but rather open sets. Usually, to gain regularity from quasi-open to open sets is quite a difficult task that works only for energy functionals (see [5]).

2. Analysis of the optimal partition problem. Let $d \geq 2$ and let $D \subseteq \mathbb{R}^d$ be a bounded open connected set. For every open (or quasi-open) subset $A \subseteq D$ we denote by $\lambda_k(A)$ the kth 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 as follows:

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

with the eigenvalues 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

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

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

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

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

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

where $cap(U)$ stands for the capacity of U, and consider the problem

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

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]). Roughly speaking, the topology of the γ-convergence is defined by the distance

$$d_\gamma(\Omega_1, \Omega_2) = \int_D |w_{\Omega_1} - w_{\Omega_2}| dx,$$

where w_Ω is the weak solution of the equation

$$\begin{cases} -\Delta w_\Omega = 1 & \text{in } \Omega, \\ w_\Omega \in H_0^1(\Omega). \end{cases}$$

Moreover, we recall (see [6, Chapter 4]) that if $(A_\varepsilon)_\varepsilon$ is a perturbation of a quasi-open set A such that

$$cap(A_\varepsilon \setminus A) + cap(A \setminus A_\varepsilon) \to 0$$

when $\varepsilon \to 0$, then $d_\gamma(A_\varepsilon, A) \to 0$ and thus $\lambda_k(A_\varepsilon) \to \lambda_k(A)$.

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*

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

A priori the infimum over partitions in quasi-open sets may lead to a lower infimum than partitions in open sets. It is well known that every quasi-open set is the intersection of a decreasing sequence of open sets. When approaching a partition of quasi-open sets by such open sets, it may be possible that the open sets overlap and do not realize a true partition. We prove below that these small regions of overlap are small in capacity so that they can be ignored asymptotically.

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

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

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

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

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

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

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

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

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

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

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

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

and

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

Since in general $cap(A_n \Delta A) \to 0$ 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

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

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

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

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

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

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

$$1_U \leq 1_M \text{ a.e.}$$

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 kth eigenvalue (counting multiplicity) of $-\Delta u + C(1-\varphi)u$, i.e.,

$$\left\{ \begin{array}{rl} -\Delta u + C(1-\varphi)u &= \lambda_k(\varphi, C)u \quad \text{in } D, \\ u &\in H_0^1(D). \end{array} \right. \tag{2.3}$$

Again, we have

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

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

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

and the problem

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

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

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 $C(1-\varphi_h)dx \xrightarrow{\gamma} C(1-\varphi)dx$. ∎

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 $n > 2$.

The concavity is a direct consequence of the definition of the functional $\varphi \longrightarrow \lambda_1(\varphi, C)$ as an infimum of affine functionals (the Rayleigh quotient is affine in φ), so that for every $\theta \in [0,1]$

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

Let us prove now the strict concavity of the functional, so that every solution of problem (2.4) is necessarily 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 with $\lambda_1(\theta\varphi_1 + (1-\theta)\varphi_2, C)$ 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

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

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

Assume now that $(\varphi_1, \dots, \varphi_n)$ 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

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

Finally, we have

$$\begin{aligned} \lambda_1(\varphi_1, C) + \lambda_1(\varphi_2, C) &= \lambda_1(\varphi_1 + \varepsilon 1_A, C) + \lambda_1(\varphi_2 - \varepsilon 1_A, C) \\ &= \lambda_1(\varphi_1 - \varepsilon 1_A, C) + \lambda_1(\varphi_2 + \varepsilon 1_A, C). \end{aligned}$$

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 possible only if $A = D$, in contradiction to 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 $(\varphi_1^C, \dots, \varphi_n^C)$ *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* $(A_i)_{i=1,\dots,n}$ *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 $i = 1, \dots, n$,

$$\int_D C(1 - \varphi_i^C) w_i^C \, dx \leq K \quad \text{and} \quad \|w_i^C\|_{H_0^1(D)} \leq K,$$

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

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

and we get

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

Hence,

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

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

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

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

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

and observe that

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

Using Theorem 2.1 and taking the infimum on 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 $k \ge 1$ there exists a solution of* (2.1) *consisting of open sets.*

Proof. Thanks to Theorem 2.1, we may take a minimizing sequence $(\Omega_1^h, \dots, \Omega_n^h)$ indexed by h consisted of polygonal disjoint sets. Assume that $\mathbb{R}^2 \setminus \Omega_1^h$ has more than $k(n-1)+1$ connected components. Since for every $i = 2, \dots, n$, the kth 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 valid only in $\mathbb{R}^2$; see [18]) and the compactness of the Hausdorff complementary topology (see [6]), we can extract a subsequence (still denoted using the same index) such that

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

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, Theorem 2.4. In order to obtain an approximation of the minimizers of (1.1), we fix C "large enough," and we try to solve problem (2.4). In all the numerical experiments presented below, we assume that

$\Omega = (0,1) \times (0,1)$, and we use first order finite differences to represent the functions φ_l and their associated eigenvectors u_l. We decompose the domain D into an $N \times N$ 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 that $I(i,j) = jN + i$. 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 whether we want to insist on the spatial relation between the components or U or not. More precisely, with any $\varphi_l \in H_0^1(D)$, we associate a vector $\Phi_l \in \mathbb{R}^{N \times N}$ such that $[\Phi_l]_{i,j} = \varphi_l((i-1)h, (j-1)h)$, $1 \le i, j \le N$. By δ_x^2 and δ_y^2, we denote the classical finite difference operators; i.e., for any vector $U \in \mathbb{R}^{N \times N}$,

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

With each Φ_l, we associate the kth 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 is no possible confusion) 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 then have

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

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 to the nonconvexity of J_n, as stated in Theorem 2.3. As we are interested in the asymptotic behavior of the partition 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 3.7, we have $N = 505$ and $n = 512$, leading to over 130,000,000 degrees of freedom), and to our knowledge, there is no global optimization algorithm capable of solving nonconvex 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 is easily obtained using a classical method in optimal design (see [3], for instance). We first differentiate (3.1) with respect to the Ith component of Φ_l (with 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 sides gives

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

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:

$$\left[\frac{\partial\lambda_{k,l}(\Phi_p)}{\partial[\Phi]_I}\right]_J = \begin{cases} -C\,[U_{k,l}(\Phi_l)]_I^2 & \text{if } l=p \text{ and } I=J,\\ 0 & \text{otherwise.}\end{cases} \tag{3.3}$$

3.1. Minimization algorithm. From Theorem 2.3, we know that the functional J_n is concave (at least when $k=1$) and we 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 1, where $\Pi_{\mathbb{S}^{n-1}}$ denotes a projection operator over the $(n-1)$-dimensional unit simplex $\mathbb{S}^{n-1}$ defined by

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

Note that since each $\lambda_{k,l}$ depends only on Φ_l, the parallelization of (3.2) is very natural. In our implementation, 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 we used m uncoupled eigenvalues solvers provided by SLEPc [16]. 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 interprocessor communication. In Algorithm 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 is perfectly scalable.

Of course, we cannot guarantee that such a method will lead to the global minimizer of a nonconvex 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 the outcome of the minimization algorithm

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 $(\lambda_{k,l}, U_{k,l})$ of $\mathrm{A}(\Phi_l)$
    $\Phi_l \leftarrow \Phi_l - \alpha \nabla_{\Phi_l} \lambda_{k,l}$
  end for
  $\Phi_l \leftarrow \Pi_{\mathbb{S}^{n-1}} \Phi_l$, $l = 1, \ldots, n$.
  Compute $J^n := J_n(\Phi_1, \ldots, \Phi_n)$
  if $J^p \leq J^{p-1}$ **then**
    $\alpha \leftarrow \min((1+\omega)\alpha, \alpha_{max})$
  else
    $\alpha \leftarrow \max(\alpha_{min}, (1-\omega)\alpha)$
  end if
  $p \leftarrow p + 1$
until $p = p_{max}$ or $\sup_{i,j,l} |\alpha \Pi_{S_n} (\Phi_l)_I| \leq \varepsilon$

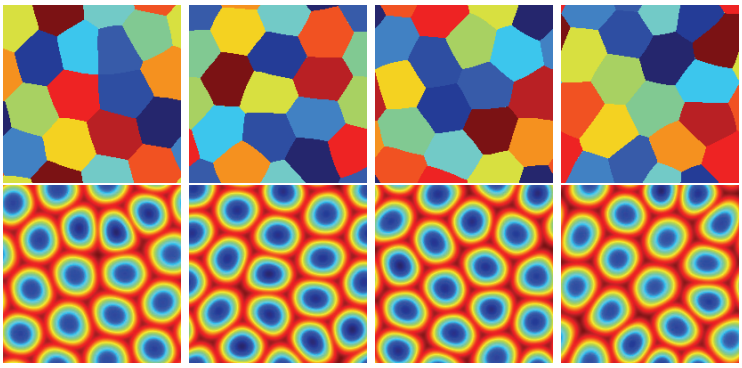

FIG. 3.1. *Dependence on the initial guess, using an orthogonal projection step. The initial values of the fields Φ are chosen randomly. The value of the objective function upon convergence is (left to right)* 2,095.2, 2,108.5, 2,100.7, *and* 2,146.3.

depends strongly on the initial guess. Figure 3.1 illustrates this sensitivity. We used an orthogonal projection operator over the unit simplex devised in [17]. 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.

In order to partially alleviate this effect, we then implemented the *simple* projec-

[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 equal to 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.

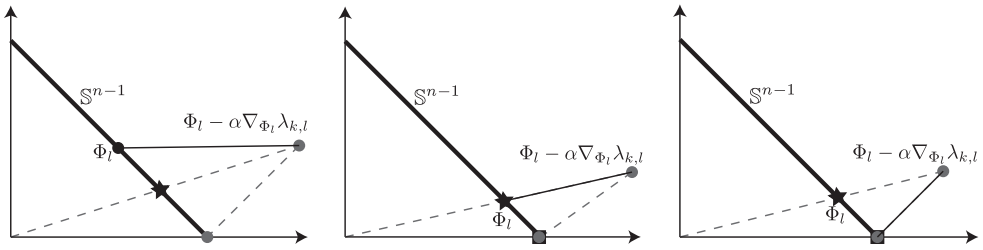

FIG. 3.2. *Behavior of the projection operators. The grey dots represent* Φ_l *and* $\Phi_l - \alpha\nabla_{\Phi_l}\lambda_{k,l}$ *as labeled. The black squares show the orthogonal projection of* $\Phi_l - \alpha\nabla_{\Phi_l}\lambda_{k,l}$*; the black stars its* simple *projection. The simple projection has a lesser tendency to "send" the functions* Φ_l *toward the vertices of* $\mathbb{S}^{n-1}$.

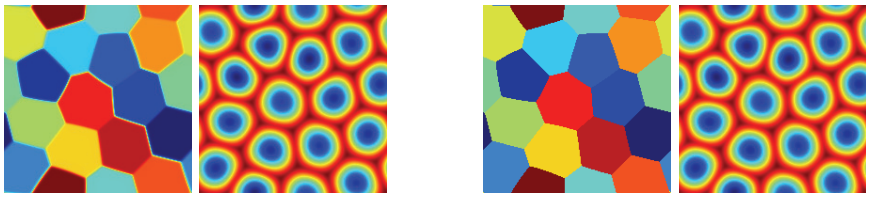

FIG. 3.3. *The problem from Figure* 3.1 *(left) solved using a combination of simple and orthogonal projection. The leftmost figure represents the* Φ *and* U *fields upon convergence of the minimization algorithm using simple projection. Note how the functions* Φ *are not piecewise constant with values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

tion 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 tends to keep the Φ in the middle of the faces of the target simplex (see the comparison of the effect of both projections 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.

We then combined both operators: in step 7 of Algorithm 1, we used the simple algorithm until we reached convergence and then restarted the computation using the orthogonal projection step. Figure 3.3 displays the outcome of this approach. The parameters are those 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 nonregular tiling, whose energy is less 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 multilevel approach akin to a continuation method to address that issue. We use the simple projection algorithm and upon convergence of Algorithm 1, we project the solution onto a finer grid and iterate this process. After several grid refinements, 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 multilevel algorithm.

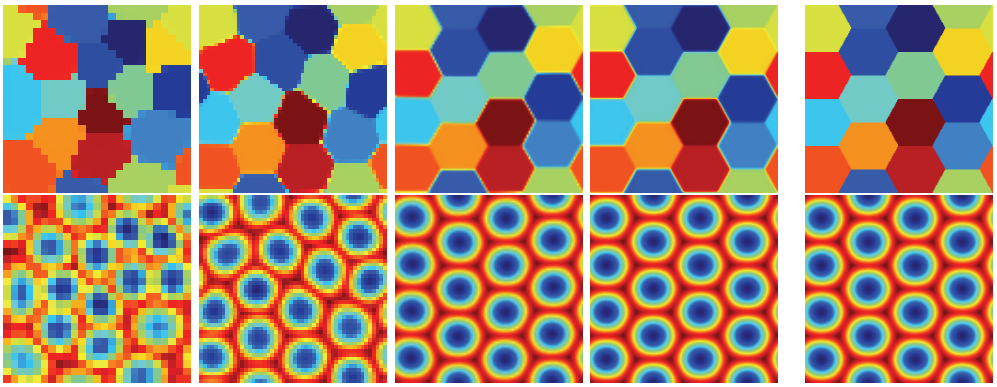

FIG. 3.4. *The same problem is solved again using the simple projection on increasingly refined grids (four leftmost figures) and then using the orthogonal projection on the final grid (right). The grid sizes are (from left to right)* 25×25, 50×50, 100×100, *and* 200×200. *The objective function upon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

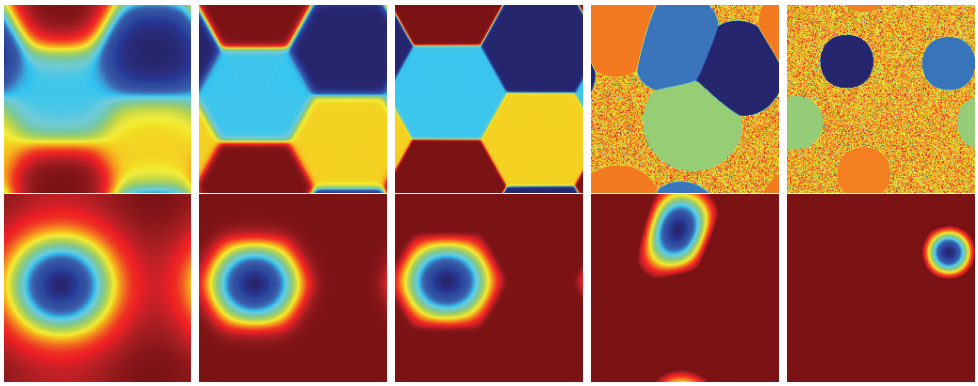

FIG. 3.5. *Optimization of the sum of the first eigenvalues of a periodic partition of size* 4 *on a grid of size* 200×200*: effect of the regularization parameter* C. *Composite view of the functions* φ *(top) and the first eigenfunctions* (u_1) *for* $C = 10^2, 10^3, 10^4, 10^5, 10^6$ *(left to right). For "smaller" values of* C, *support of the eigenfunctions* u_1 *does not appear to be included in that of their matching* ϕ *functions. For "larger" values of* C, *the problem becomes too stiff and the optimization algorithm does not converge in a reasonable time.*

3.2. Numerical experiments. We first explore the choice of the relaxation parameter C in the regularized problem. From the form of (2.3), we expect that given a φ, as C becomes "large" the associated eigenfunction u will approach 0 outside of the support of φ. Conversely, for "smaller" values of C, u will not necessarily be "close" to 0 outside of the support of φ, so then one may expect that C needs to be chosen "very large." The expression of the derivative of the eigenvalues for the discretized problem suggests a difficulty, if this is the case. From (3.3), one sees that if C is "too large," the problem becomes very stiff, and optimization become difficult. Figure 3.5 presents the phase function φ and the first eigenfunction u_1 for a simple problem with four cells and periodicity conditions. The parameter C was set to 10^2, 10^3, 10^4, and 10^6. The behavior is as expected. In what follows, we set C in such a way that the functions u and φ appear to share the same support (typically between 10^4 and 10^5 for the problem sizes and cell numbers we considered).

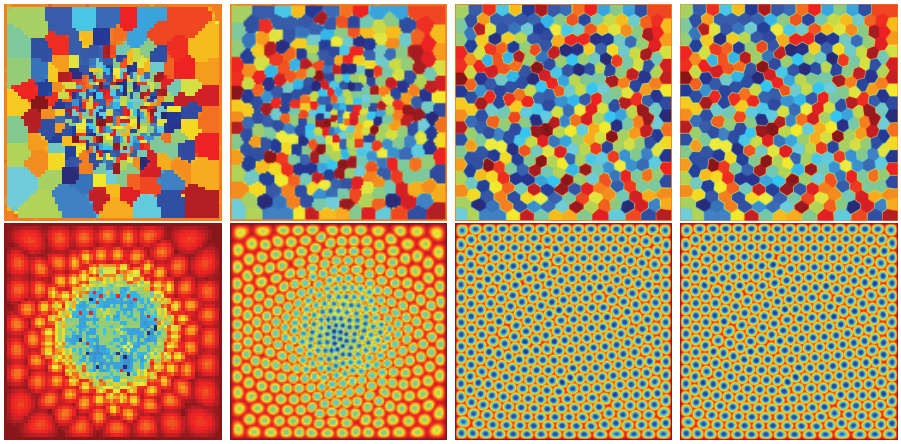

FIG. 3.6. *Optimization of the sum of the first eigenvalue of the Dirichlet–Laplacian on* 384 *cells with* $C = 10^5$. *First row: cell shape on recursively refined grids* (64×64), (127×127), (253×253), *and* (505×505). *Second row: sum of the first eigenvalues on the same grids.*

We were able to run a series of large computations on parallel supercomputers at the Texas Advanced Computing Center. In Figure 3.6, the domain is again the unit square. Periodicity boundary conditions are not used, as the number of cells ($n = 384$) is large enough that we expect that the effect of the boundary conditions vanishes in the center of the domain. The computations were run on four layers of recursively refined grids of respective dimensions (64×64), (127×127), (253×253), and (505×505). The parameter C is 10^5, the tolerance parameter $\epsilon = 10^6$, and 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 (see Figure 3.7). 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 functions involving higher order eigenvalues of linear combinations of eigenvalues of different order. A classical numerical issue in this case comes from the potential nondifferentiability of multiple eigenvalues with respect to changes of the function Φ. We did not try to address this problem, but we obtained interesting results nevertheless. Figure 3.8 represents 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 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 3.8(right)), we obtain a periodic tiling by nonregular hexagons, which can be proved to be a suboptimal 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

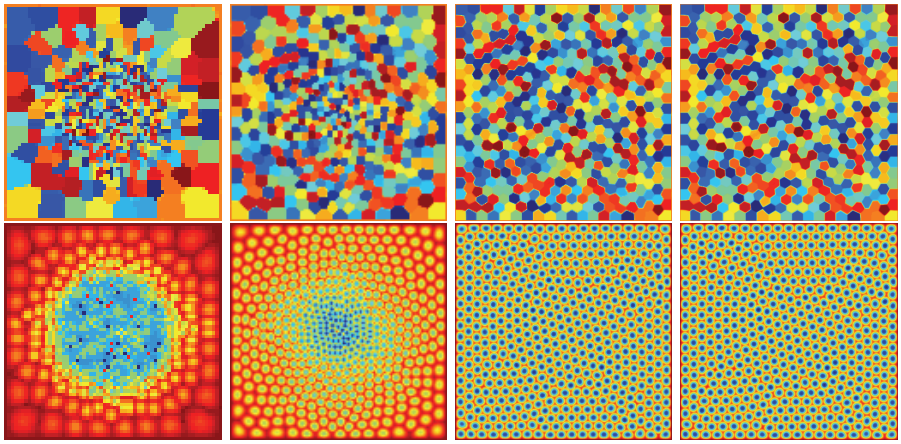

FIG. 3.7. *Optimization of the sum of the first eigenvalue of the Dirichlet–Laplacian of* 512 *cells with* $C = 10^5$. *First row: cell shape on recursively refined grids* (64×64), (127×127), (253×253), *and* (505×505). *Second row: sum of the first eigenvalues on the same grids.*

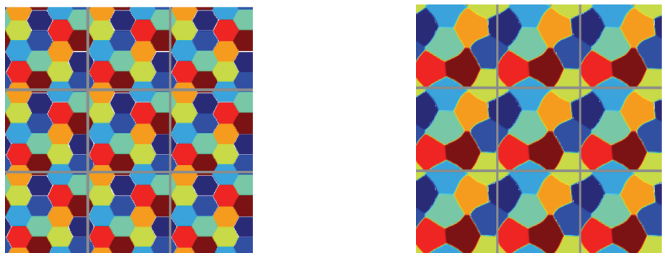

FIG. 3.8. *Optimal partitions of the sum of the second (left) and third (right) eigenvalues of the Dirichlet–Laplacian for* $n = 8$ *cells. The periodicity is highlighted by repeating the unit cell* 9 *times on a two-dimensional lattice.*

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 kth eigenvalue of an optimal cell is expected to have multiplicity greater than 1 and hence may not be differentiable.

Noticing that the analysis and algorithm are not restricted to the two-dimensional case, we ported our program to the three-dimensional case but were unable to obtain any meaningful results. We believe that the convergence rate of our primitive algorithms is too slow to converge to a decent local minimizer in a reasonable time in three dimensions, 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 with each function Φ (so as to improve the performance of the eigenvalue solver), and implementing a more efficient minimization algorithm in order to reduce the number of necessary function evaluations in the minimization loop.

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