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Small singular values of an extracted matrix of a Witten complex.

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ABSTRACT

It is shown how rather tricky induction processes, used for the accurate computation of exponentially small eigenvalues of Witten Laplacians, essentially amount to some Gaussian elimination after the proper rewriting.

RESUMEN

Se muestra cómo un proceso de inducción bastante truculento se usa para el cálculo preciso de los valores propios pequeños de los laplacianos de Witten utilizando esencialmente cantidades de eliminaciones gausianas después de una reescritura correcta.

Key words and phrases: *Induction process, Witten Laplacian, exponentially small eigenvalues, Gaussian elimination.*

Math. Subj. Class.: *81Q10, 15A18, 34L15, 58J10, 58J37.*

1 Introduction and motivations

The accurate computation of exponentially small eigenvalues of Witten Laplacians on 0-forms, or generators associated with reversible diffusion processes, relies on some rather tricky induction

process. In [2] [3], the induction scheme is modelled after the probabilistic picture of exit times. After [7] [8] [16] it appeared that this induction scheme could be extracted from its spectral analysis or probabilistic framework as a pure problem of finite dimensional linear algebra. The aim of this short text is to show that all these previous and rather involved inductions essentially amount, after a proper rewriting, to some Gaussian elimination.
We first recall that the Witten Laplacian writes

$$\Delta_{f,h}^{(0)} = d_{f,h}^{(0),*} d_{f,h}^{(0)} = -h^2\Delta + |\nabla f(x)|^2 - h\Delta f(x) \tag{1.1}$$

on functions and more generally on differential forms with arbitrary degree,

$$\Delta_{f,h} = \left(d_{f,h}^{*} + d_{f,h}\right)^2 \quad \text{with} \quad d_{f,h} = e^{-\frac{f}{h}}(hd)e^{\frac{f}{h}} \,. \tag{1.2}$$

Since it has a square structure, the eigenvalues of $\Delta_{f,h}^{(0)}$ (resp. $\Delta_{f,h}$) are the squares of the singular values of $d_{f,h}^{(0)}$ (resp. $(d_{f,h}^{*}+d_{f,h})$). Remember that in the study of Witten Laplacians d denotes the exterior differential on a Riemannian manifold, d^* the codifferential, $h > 0$ is a small parameter considered in the limit $h \to 0$ and f is a Morse function. In the case when the manifold is $\mathbb{R}^n$ with the Euclidean metric, recall that the Witten Laplacian on functions (1.1) in $L^2(\mathbb{R}^n, dx)$ is unitary equivalent to the following operator

$$-h(-2\nabla f(x).\nabla + h\Delta)$$

in $L^2(\mathbb{R}^n, e^{-2f/h}dx)$. This last operator fits better with the probabilistic presentation ([4] [17] [19]) and the simulated annealing framework ([14]).

The main purpose is the accurate computation of the smallest non zero eigenvalue of these operators among a finite collection of exponentially small eigenvalues, i.e. of order $e^{-\frac{C_k}{h}}$ as $h \to 0$. The inverse of this eigenvalue can be interpreted as the longest lifetime of metastable states. The issue is the suitable control of errors (which are in absolute values larger than the final result) at every step of the induction process. A usual Gramm-Schmidt type orthonormalisation process as it is used in the semiclassical multiple wells problem ([6] [9]) does not allow such a control.

As this was pointed out in [7] [16], working with singular values rather than with eigenvalues of the square operator allows to use the Fan inequalities ([5] [18]) in their simplest form. These multiplicative inequalities propagate the control of the small relative errors on the singular values through the induction process.

At the moment, this approach has been applied systematically only in the case of Witten Laplacian acting on functions. Some cases with higher order Witten Laplacians can be considered. The only condition is the construction of global quasimodes, which is not completely elucidated for the moment except in the case of 0-forms. Besides the simplification of previous proofs, this text aims at providing an abstract and general result to be referred to in the next future.

2 Result

Let $F^{(0)}$ and $F^{(1)}$ be two complex Hilbert spaces respectively of dimension $m_0 < +\infty$ and $m_1 < +\infty$. Let $\langle\,|\,\rangle$ denote the scalar product on $F^{(0)}$ or $F^{(1)}$ (without distinction), and let $\|\psi\|$ and $\|A\| = \sup_{\psi\neq 0}\frac{\|A\psi\|}{\|\psi\|}$ denote the norms of the vector ψ and of the linear application A associated with this scalar product. Let moreover h_0 and ε_0 be two positive numbers.
Consider a linear application $B(h)$ depending on $h \in (0,\, h_0]$:

$$B(h) : F^{(0)} \longrightarrow F^{(1)},$$

and set

$$A_0(h) = B^*(h)B(h) \geq 0\,.$$

Let

$$A_1(h) = B(h)B^*(h) \geq 0\,,$$

and note the intertwining relation:

$$B(h)A_0(h) = A_1(h)B(h)\,.$$

Definition 1. *For a number (resp. a linear operator) $g(h)$, the notation $g(h) = \mathcal{O}_\varepsilon(e^{-\frac{\alpha}{h}})$ means that, for all $\varepsilon \in (0, \varepsilon_0]$, there exists a constant $C_\varepsilon > 0$ such that:*

$$\forall h \in (0,\, h_0]\ , \quad |g(h)| \leq C_\varepsilon e^{-\frac{\alpha}{h}}\ (\textit{resp. } \|g(h)\| \leq C_\varepsilon e^{-\frac{\alpha}{h}})\,.$$

Assumption 2.1. *Assume that there exist two bases (of $F^{(0)}$ and $F^{(1)}$ respectively) depending on $(\varepsilon, h) \in (0, \varepsilon_0] \times (0,\, h_0]$ and a positive number α independent of $(\varepsilon\,, h) \in (0, \varepsilon_0] \times (0,\, h_0]$ such that:*

$$\begin{aligned}
\psi_k^{(0)} &= \psi_k^{(0)}(\varepsilon, h)\ (k \in \{1, \dots, m_0\})\,, \left\langle \psi_k^{(0)} \mid \psi_{k'}^{(0)} \right\rangle = \delta_{kk'} + \mathcal{O}_\varepsilon(e^{-\frac{\alpha}{h}}) \quad ,\\
\psi_j^{(1)} &= \psi_j^{(1)}(\varepsilon, h)\ (j \in \{1, \dots, m_1\})\,, \left\langle \psi_j^{(1)} \mid \psi_{j'}^{(1)} \right\rangle = \delta_{jj'} + \mathcal{O}_\varepsilon(e^{-\frac{\alpha}{h}}) \quad .
\end{aligned}$$

Assumption 2.2. *Assume furthermore that there exist an injective map $j : \{1, \dots, m_0\} \to \{1, \dots, m_1\}$, a decreasing sequence $(\alpha_k)_{k\in\{1,\dots,m_0\}}$ of real numbers, and a positive number d (independent of $(\varepsilon\,, h) \in (0, \varepsilon_0] \times (0,\, h_0]$) such that:*

$$\begin{aligned}
&\forall \varepsilon \in (0, \varepsilon_0],\ \exists C_\varepsilon > 1, \forall k \in \{1, \dots, m_0\}\,,\\
&\qquad \forall h \in (0, h_0], \quad C_\varepsilon^{-1} e^{-\frac{\alpha_k + d\varepsilon}{h}} \leq \left|\left\langle \psi_{j(k)}^{(1)} \mid B(h)\psi_k^{(0)} \right\rangle\right| \leq C_\varepsilon e^{-\frac{\alpha_k - d\varepsilon}{h}}\\
&\qquad \forall h \in (0, h_0], \forall j' \neq j(k), \quad \left|\left\langle \psi_{j'}^{(1)} \mid B(h)\psi_k^{(0)} \right\rangle\right| \leq C_\varepsilon e^{-\frac{\alpha_k + \alpha}{h}}\,.
\end{aligned}$$

Theorem 2.3. *There exist positive numbers $h_0' \leq h_0$ and $\varepsilon_0' \leq \varepsilon_0$ such that, under Assumptions 2.1 and 2.2, the eigenvalues $0 \leq \lambda_1(h) \leq \cdots \leq \lambda_{m_0}(h)$ of $A_0(h)$ satisfy:*

$$\begin{aligned}
&0 < \lambda_1(h) < \cdots < \lambda_{m_0}(h)\,,\\
&\forall k \in \{1, \dots, m_0\}\ , \quad \lambda_k(h) = \left|\left\langle \psi_{j(k)}^{(1)} \mid B(h)\psi_k^{(0)} \right\rangle\right|^2 (1 + \mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}}))\ ,
\end{aligned}$$

where $\eta > 0$ is a real number independent of $(\varepsilon,\, h) \in (0,\, \varepsilon_0'] \times (0,\, h_0']$.

Remark 2.4. *More generally, vanishing eigenvalues can be included. It suffices to allow the value $+\infty$ for the first values*

$$\alpha_1 = \cdots = \alpha_\ell = +\infty \quad \text{and} \quad \alpha_{m_0} < \cdots < \alpha_{\ell+1} \in \mathbb{R}\,,$$

for some given $\ell \in \{1, \ldots, m_0\}$. In this last case, the eigenvalues of $A_0(h)$ satisfy:

$$\lambda_1 = \cdots = \lambda_\ell = 0 \quad \text{and} \quad 0 < \lambda_{\ell+1} < \cdots < \lambda_{m_0}\,,$$

while the above estimates hold for the non-zero eigenvalues.

This theorem, or a modified form of this theorem according to Remark 2.4, can be applied to simplify the final proof done in [7] for the case of the Witten Laplacian acting on 0-forms on a Riemannian manifold without boundary or the one in [8] for some Dirichlet realization in the case with a boundary. This final part of the analysis in [7] [8] has been reconsidered in [16], without giving all the possible simplifications. The reader can also find in [16] various illustrations in practical cases of this approach .

Once the quasimodes satisfying Assumptions 2.1 and 2.2 are constructed, Theorem 2.3 can be applied as soon as we work with a self-adjoint operator with a square structure. The application to Witten Laplacians on 0-forms with alternative boundary conditions is in progress. Some examples of Witten Laplacians acting on p-forms for which quasimodes are constructed can be treated with this result and Theorem 2.3 may be useful for a future generalization.

While working with Witten Laplacians on 0-forms, the quasimodes $\psi_k^{(0)}$'s are constructed globally after truncating $e^{-\frac{f}{h}}$, while the $\psi_j^{(1)}$'s are introduced locally via a WKB approximation around saddle points of f, $U_{j(k)}^{(1)}$. Note that the discussion in [7] [16] about sending $U_{j(1)}^{(1)}$ to infinity when $\lambda_1 = 0$ is replaced by consedering $\alpha_1 = +\infty$ (according to Remark 2.4) with an arbitrary additionnal $\psi_{j(1)}^{(1)}$.

The application to some non self-adjoint Fokker-Planck operators with a distorted square strusture (see [1] [8] [11] [15]) seems more delicate (see Remark 3.6).

3 Proof

Let us begin by fixing the positive numbers ε_0' and η. We first choose ε_0' small enough such that:

$$\alpha' = \alpha - d\,\varepsilon_0' > 0 \quad \text{and} \quad \alpha'' = \underset{k>k'}{min}\,\{\alpha_{k'} - \alpha_k - 2d\,\varepsilon_0'\} > 0\,.$$

Then, we set:

$$\eta = min\,\{\alpha,\, \alpha'\,, \alpha''\} = min\,\{\alpha'\,, \alpha''\}\ .$$

To prove Theorem 2.3, it will be more convenient to work with matrices. Let us give a definition and an easy application which will be very useful.

Definition 2. *A square matrix $V(h)$ is said quasi-unitary if there exists an unitary matrix U such that:*

$$V(h) = U + \mathcal{O}_\varepsilon(e^{-\eta/h}).$$

Lemma 3.1. *The product of quasi-unitary matrices is a quasi-unitary matrix.*

Furthermore, to prove Theorem 2.3, we need a particular case of Fan inequalities that we recall here (we refer the reader to [18] for a proof).

Lemma 3.2. *Let B and C be respectively a compact and a bounded linear operator on a Hilbert space $\mathcal{H}$. The inequalities*

$$\begin{aligned} \mu_n(BC) &\leq \|C\|\, \mu_n(B) \\ \mu_n(CB) &\leq \|C\|\, \mu_n(B) \quad , \end{aligned}$$

where $\mu_n(B)$ is the n-th singular value of B, hold for all $n \leq \dim \mathcal{H}$.

We apply this lemma with $\mathcal{H} = \mathcal{H}_0 \overset{\perp}{\oplus} \mathcal{H}_1$, while identifying $B : \mathcal{H}_0 \to \mathcal{H}_1$ with $J_1 B \Pi_0 \in \mathcal{L}(\mathcal{H})$, where Π_0 is the orthogonal projection $\mathcal{H} \to \mathcal{H}_0$ and J_1 the embedding $\mathcal{H}_1 \to \mathcal{H}$.

Corollary 3.3. *Let $\mathcal{H}_0$, $\mathcal{H}_1$ be two Hilbert spaces. Let B be a compact linear operator from $\mathcal{H}_0$ to $\mathcal{H}_1$. Assume that $C \in \mathcal{L}(\mathcal{H}_1)$ and $D \in \mathcal{L}(\mathcal{H}_0)$ are two invertible operators with:*

$$\max\left\{\|C\|\,,\, \left\|C^{-1}\right\|\,,\, \|D\|\,,\, \left\|D^{-1}\right\|\right\} \leq 1 + \rho\,,$$

for some $\rho > -1$. Then the inequality

$$(1+\rho)^{-2}\mu_n(B) \leq \mu_n(CBD) \leq (1+\rho)^2 \mu_n(B)$$

holds for all $n \leq \min(\dim \mathcal{H}_0,\ \dim \mathcal{H}_1)$.

Remark 3.4. *We will apply this corollary in the particular case when C and D depend on $h \in (0,\, h_0']$ and are quasi-unitary:*

$$C(h) = U + \mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}}) \quad \text{and} \quad D(h) = V + \mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}})\,,$$

where U and V are unitary matrices and $\rho = \mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}})$. We obtain the equivalent relations:

$$\mu_n(CBD) = \mu_n(B)(1 + \mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}}))\ ,\ \mu_n(B) = \mu_n(CBD)(1 + \mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}}))\,. \tag{3.1}$$

From $A_0(h) = B^*(h)B(h)$, we deduce that the eigenvalues of $A_0(h)$ are the squares of the singular values of $B(h)$:

$$\forall k \in \{1, \ldots, m_0\}\ ,\ \lambda_k(h) = \mu^2_{m_0+1-k}(B(h)) \quad (\mu_1(B(h)) = \|B(h)\|)\,.$$

In order to apply Corollary 3.3, it will be easier to work with the singular values of $B(h)$ than with the eigenvalues of $A_0(h)$.

Choose now two arbitrary orthonormal bases $\mathcal{B}^{(0)}$ and $\mathcal{B}^{(1)}$ (of $F^{(0)}$ and $F^{(1)}$ respectively). We make the identifications:

$$B(h) = \underset{\mathcal{B}^{(0)},\, \mathcal{B}^{(1)}}{Mat}(B(h)), \quad B^*(h) = (\underset{\mathcal{B}^{(0)},\, \mathcal{B}^{(1)}}{Mat}(B(h)))^*.$$

Let be $B'(h) = \left(\left\langle \psi_j^{(1)} \mid B(h)\psi_k^{(0)} \right\rangle\right)_{j,k} = \left(b'_{j\,k}\right)_{j,\,k}$. For $i \in \{1, \ldots, m_l\}$ and $l \in \{0, 1\}$, we set

$$C_l = \mathrm{Mat}_{\mathcal{B}^{(l)}}\left(\psi_1^{(l)} \ldots \psi_{m_l}^{(l)}\right),$$

where $\psi_i^{(l)}$ is written as a column vector in $\mathcal{B}^{(l)}$. These change-of-coordinates matrices give $B'(h) = C_1^* B(h) C_0$.

Remark 3.5. *By Assumption 2.1, the matrices C_0 and C_1^* are quasi-unitary and Assumption 2.2 implies, for h'_0 small enough:*

$$\forall \quad 1 \le k' < k \le m_0\,, \quad b'_{j(k')\,k'} = b'_{j(k)\,k}.\mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}})\,, \tag{3.2}$$

$$\forall \quad 1 \le k \le m_0\,, \forall j \neq j(k)\,, \quad b'_{j\,k} = b'_{j(k)\,k}.\mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}})\,. \tag{3.3}$$

We now simplify $B'(h)$ by Gaussian elimination *in the following order*:

Step 0: By permuting the rows, that is by left-multiplying with permutation matrices which are unitary, put the coefficients $b'_{j(k)\,k}$ (for k in $\{1, \ldots, m_0\}$) on the k-th row and k-th column. The new matrix has the form:

$$B''(h) = \begin{pmatrix} b''_{1\,1} = b'_{j(1)\,1} & b'_{j(2)\,2}.\mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}}) & \ldots & b'_{j(m_0)\,m_0}.\mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}}) \\ \vdots & b''_{2\,2} = b'_{j(2)\,2} & & \vdots \\ b'_{j(1)\,1}.\mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}}) & \vdots & \ddots & \vdots \\ \vdots & b'_{j(2)\,2}.\mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}}) & & b''_{m_0\,m_0} = b'_{j(m_0)\,m_0} \\ \vdots & \vdots & & \vdots \end{pmatrix}.$$

Furthermore, the matrix $B''(h)$ satisfies the structure equations (3.2) and (3.3) with the injective map $j : \{1, \ldots, m_0\} \to \{1, \ldots, m_1\}$ replaced by the canonical injection $i : \{1, \ldots, m_0\} \to \{1, \ldots, m_1\}$, $i(k) = k$.

Step 1: For $j \in \{1, \ldots, m_1\} \setminus \{m_0\}$, replace the j-th row L_j by $L_j - \frac{b''_{j\,m_0}}{b''_{m_0\,m_0}} L_{m_0} = L_j - \mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}}).L_{m_0}$.

Step 2: Then, for $k \in \{1, \ldots, m_0 - 1\}$, replace the k-th column C_k by $C_k - \frac{b''_{m_0\,k}}{b''_{m_0\,m_0}} C_{m_0} = C_k - \mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}}).C_{m_0}$. Due to the previous operations, only the m_0-th row of the new matrix is changed by these operations.

Each operation of the two last steps preserves the structure of Assumption 2.2, or more precisely the structure of Remark 3.5 where we have replaced the injective map j by the canonical injection i. Moreover, these operations correspond to left multiplications or right multiplications by quasi-unitary matrices.
The new matrix only contains zeros on the m_0-th row and m_0-th column except for the (m_0, m_0)-coefficient which is $b'_{j(m_0)\,m_0} = \left\langle \psi^{(1)}_{j(m_0)} \mid B(h)\psi^{(0)}_{m_0} \right\rangle$.
When $m_0 \geq 2$, iterate the Gaussian elimination, Step 1 with the reference row $m_0 - \nu$ and Step 2 with the reference column $m_0 - \nu$, by taking successively $\nu = 1, \ldots, m_0 - 2$. At the end, we obtain a diagonal matrix $D(h) \in M_{m_0,m_1}(\mathbb{C})$ such that:

$$\forall k \in \{1, \ldots, m_0\}\,,\ (D(h))_{k,k} = \left\langle \psi^{(1)}_{j(k)} \mid B(h)\psi^{(0)}_k \right\rangle (1 + \mathcal{O}_\varepsilon(e^{-\eta/h})).$$

Moreover, by Lemma 3.1, there exist two quasi-unitary matrices $U(h) \in M_{m_0}(\mathbb{C})$ and $V(h) \in M_{m_1}(\mathbb{C})$ satisfying

$$D(h) = V(h)B'(h)U(h) = V(h)C_1^* B(h) C_0 U(h)\,.$$

Using again Lemma 3.1, $V'(h) = V(h)C_1^*$ and $U'(h) = C_0U(h)$ are quasi-unitary. From $D(h) = V'(h)B(h)U'(h)$, we conclude using Corollary 3.3 and (3.1).

Remark 3.6. ***a)*** *The square self-adjoint structure $A_0(h) = B^*(h)B(h)$ is essential here to be able to conclude.*
Even a small distortion, $A_0(h) = B^*(h)CB(h)$ with $C = Id + r$ with $r = \mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}})$, in dimension 2, destroys the above arguments, due to ill-conditioning problem.
In the decomposition

$$A_0(h) = B^*(h)B(h) + B^*(h)rB(h) = B^*(h)B(h) + B^*(h)\mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}})B(h)\,,$$

the remainder term $B^*(h)\mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}})B(h)$ cannot be put in general in the form $B^*(h)B(h)\mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}})$:

$$\begin{aligned} & B^*(h)rB(h) = B^*(h)B(h)\left(B(h)^{-1}rB(h)\right) \\ \textit{with}\quad & \left\|B(h)^{-1}rB(h)\right\| \leq \left\|B(h)^{-1}\right\| \|B(h)\| \|r\|\,. \end{aligned}$$

For example, take $\eta = 1$ and

$$B(h) = \begin{pmatrix} e^{-\frac{4}{h}} & 0 \\ 0 & e^{-\frac{2}{h}} \end{pmatrix} \quad \textit{and} \quad C(h) = \begin{pmatrix} 1 & e^{-\frac{1}{h}} \\ 0 & 1 \end{pmatrix}.$$

In this example the remainder factor equals

$$B(h)^{-1}rB(h) = \begin{pmatrix} 0 & e^{+\frac{1}{h}} \\ 0 & 0 \end{pmatrix}$$

with a norm of order $e^{\frac{1}{h}} = e^{\frac{2}{h}} \times e^{-\frac{\eta}{h}}$.
b) *A first attempt at the extension of this analysis to the non self-adjoint case related with Kramers-Fokker-Planck type operators, studied in [12] [13], led to the simple distortion* $A_0(h) = B^*(h)CB(h)$ *with* $C = Id + \mathcal{O}_\varepsilon(e^{-\frac{\eta}{h}})$. *The previous remark shows that it cannot work without including some additional information about the intimate link between these non self-adjoint operators coming from kinetic theory and Witten Laplacians ([1] [8] [11] [15]).*

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