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YVES COLIN DE VERDIÈRE

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We present a natural proof of a recent and surprising result of Gregory Berkolaiko interpreting the Courant nodal defect as a Morse index. This proof is inspired by a nice paper of Miroslav Fiedler published in 1975.

1. Introduction

The "nodal defect" of an eigenfunction of a Schrödinger operator is closely related to the difference between the upper bound on the number of nodal domains given by Courant's theorem and the number of nodal domains. Berkolaiko [2013] has proved a nice formula for the nodal defect of an eigenfunction of a Schrödinger operator on a finite graph in terms of the Morse index of the corresponding eigenvalue as a function of a magnetic deformation of the operator. His proof remains mysterious and rather indirect. In order to get a better understanding in view of possible generalizations, it is desirable to have a more direct approach. This is what we do here, with a proof inspired by [Fiedler 1975].

After reviewing our notations, we state the main result, as well as a reinterpretation in terms of Hessians of a determinant, and give an informal description of the proof in Section 3. The proof itself is implemented in Sections 4 and 5 with an alternative view provided in Appendix A. The continuous Schrödinger operator on a circle was considered in the preprint version of this paper [Colin de Verdière 2012]. The case of quantum graphs, i.e., graphs as 1-dimensional simplicial complexes, is worked out in [Berkolaiko and Weyand 2012].

2. Notation

Let G = (X, E) be a finite connected graph, where X is the set of vertices and E the set of unoriented edges. We denote by $\{x, y\}$ the edge linking the vertices x and y. We denote by \vec{E} the set of oriented edges and by [x, y] the edge from x to y; the set \vec{E} is a 2-fold cover of E. A 1-form α on G is a map $\vec{E} \to \mathbb{R}$ such that $\alpha([y, x]) = -\alpha([x, y])$ for all $\{x, y\} \in E$. We denote by $\Omega^1(G)$ the vector space of dimension #E of 1-forms on G. The operator $d : \mathbb{R}^X \to \Omega^1(G)$ is defined by df([x, y]) = f(y) - f(x). If Q is a nondegenerate, not necessarily positive, quadratic form on $\Omega^1(G)$, we denote by d^* the adjoint of d, where \mathbb{R}^X carries the canonical Euclidean structure and $\Omega^1(G)$ is equipped with the symmetric inner product \hat{Q} associated to Q. We have dim ker $d^* = \beta$, where $\beta = 1 + \#E - \#X$ is the dimension

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of the space of cycles of *G*. We will show later that, in our context, we have the Hodge decomposition $\Omega^1(G) = d\mathbb{R}^X \oplus \ker d^*$, where both spaces are \hat{Q} -orthogonal.

Following [Colin de Verdière 1998], we denote by \mathbb{O}_G the set of $X \times X$ real symmetric matrices H which satisfy $h_{x,y} < 0$ if $\{x, y\} \in E$ and $h_{x,y} = 0$ if $\{x, y\} \notin E$ and $x \neq y$. Note that the diagonal entries of H are arbitrary. An element H of \mathbb{O}_G is called a *Schrödinger operator* on the graph G. It will be useful to write the quadratic form associated to H as

$$q_1(f) = -\sum_{\{x,y\}\in E} h_{x,y}(f(x) - f(y))^2 + \sum_{x\in X} V_x f(x)^2,$$

with $V_x = h_{x,x} + \sum_{y \sim x} h_{x,y}$. A magnetic field on *G* is a map $B : \vec{E} \to U(1)$ defined by $B([x, y]) = e^{i\alpha_{x,y}}$, where $[x, y] \mapsto \alpha_{x,y}$ is a 1-form on *G*. We denote by $\mathfrak{B}_G = e^{i\Omega^1(G)}$ the manifold of magnetic fields on *G*. The magnetic Schrödinger operator H_B associated to $H \in \mathbb{O}_G$ and $B = e^{i\alpha}$ is defined by the quadratic form

$$q_B(f) = -\frac{1}{2} \sum_{[x,y] \in \vec{E}} h_{x,y} |f(x) - e^{i\alpha_{x,y}} f(y)|^2 + \sum_{x \in X} V_x |f(x)|^2$$

associated to a Hermitian form on \mathbb{C}^X . More explicitly, if $f \in \mathbb{C}^X$,

$$Hf(x) = h_{x,x}f(x) + \sum_{y \sim x} h_{x,y}e^{i\alpha_{x,y}}f(y).$$
 (1)

We fix H and we denote by

$$\lambda_1(B) \leq \lambda_2(B) \leq \cdots \leq \lambda_n(B) \leq \cdots \leq \lambda_{\#X}(B)$$

the eigenvalues of H_B . It will be important to notice that $\lambda_n(\bar{B}) = \lambda_n(B)$. Moreover, we have a gauge invariance: the operators H_B and $H_{B'}$ with $\alpha' = \alpha + df$ for some $f \in \mathbb{R}^X$ are unitarily equivalent. Hence they have the same eigenvalues. This implies that, if $\Omega^1(G) = d\mathbb{R}^X \oplus \ker d^*$ (this is not always the case because Q is not positive), it is enough to consider 1-forms in the subspace ker d^* of $\Omega^1(G)$ when studying the map $\Lambda_n : B \to \lambda_n(B)$. This holds in particular for investigations concerning the Hessian and the Morse index.

3. Statement of Berkolaiko's magnetic theorem

Before stating the main result, we recall:

Definition 1. The *Morse index* $j(q) \in \mathbb{N} \cup \{+\infty\}$ of a quadratic form q on a real vector space E is defined by $j(q) = \sup_F \dim F$, where F is a subspace of E such that $q|_{F\setminus 0}$ is less than 0. The *nullity* of q is the dimension of the kernel of q.

The *Morse index* of a smooth real-valued function f defined on a smooth manifold M at a *critical* point $x_0 \in M$ (i.e., a point satisfying $df(x_0) = 0$) is the Morse index of the Hessian of f, which is a canonically defined quadratic form on the tangent space $T_{x_0}M$. The critical point x_0 is called *nondegenerate* if the previous Hessian is nondegenerate. The *nullity* of the critical point x_0 of f is the nullity of the Hessian of f at the point x_0 .

The aim of this note is to prove the following nice results due to Berkolaiko [2008; 2013]:

Theorem 1. Let G = (X, E) be a finite connected graph and β the dimension of the space of cycles of G. We suppose that the n-th eigenvalue λ_n of $H \in \mathbb{O}_G$ is simple. We assume moreover that an associated nonzero eigenfunction ϕ_n satisfies $\phi_n(x) \neq 0$ for all $x \in X$. Then, the number ν of edges along which ϕ_n changes sign satisfies $n - 1 \leq \nu \leq n - 1 + \beta$.

Moreover $\Lambda_n : B \to \lambda_n(B)$ is smooth at $B \equiv 1$ which is a critical point of Λ_n and the nodal defect, $\delta_n = v - (n - 1)$, is the Morse index of Λ_n at that point. If M is the manifold of dimension β of magnetic fields on G modulo the gauge transforms, the function $[B] \to \Lambda_n(B)$ has [B = 1] as a nondegenerate critical point.

Remark 1. The previous results can be extended by replacing the critical point $B \equiv 1$ by $B_{x,y} = \pm 1$ for all edges $\{x, y\} \in E$. The number v is then the number of edges $\{x, y\} \in E$ satisfying $B_{x,y}\phi_n(x)\phi_n(y) < 0$ where ϕ_n is the corresponding eigenfunction.

Remark 2. The assumptions on *H* are satisfied for *H* in an open dense subset of \mathbb{O}_G .

The upper bound of ν in the first part of Theorem 1 is related to the Courant nodal theorem (see [Courant and Hilbert 1953, Section VI.6]) as follows: a nodal domain on a graph for the eigenfunction ϕ_n is a connected component of the subgraph G' of G obtained by removing the edges along which ϕ_n changes sign. Denoting by μ the number of nodal domains of ϕ_n , the Courant theorem for graphs (see [Colin de Verdière 1998, Theorem 2.4]) asserts that $\mu \leq n$; using the Euler formula for the graph G' and because $\mu = b_0(G')$, the number of connected components of the graph G', we get also a lower bound (see [Berkolaiko 2008]):

Corollary 1. Under the assumptions of Theorem 1, we have $n - \beta \le \mu \le n$.

Example 3.1 (bipartite graphs). Let G = (V, E) be a bipartite graph: $V = Y \cup Z$ and all edges have one vertex in Y and the other in Z. Let U be the involution on \mathbb{R}^V given by Uf(x) = -f(x) if $x \in Y$ and Uf(x) = f(x) if $x \in Z$ and let B be a magnetic field. Then $UH_BU = -H'_B$ with $H' \in O_G$, so that $\lambda_{|V|}(H_B) = -\lambda_1(H'_B)$. And hence it follows from the diamagnetic inequality that $B \to \lambda_{|V|}(H_B)$ has a maximum at $B \equiv 1$. And hence the Morse index of the Hessian of $B \to \lambda_{|V|}(H_B)$ at $B \equiv 1$ is the dimension of the manifold of magnetic fields, namely β . On the other hand the first eigenfunction ϕ_1 of H' is everywhere greater than 0 and the number of sign changes of $U\phi_1$ is |E|. So Berkolaiko's formula for $\lambda_{|V|}$ gives $(|V| - 1) + \beta = |E|$. This is the Euler formula.

Theorem 1 can be reinterpreted as follows:

Theorem 2. Under the assumptions as in Theorem 1, consider the functional $D_n : B \mapsto \det(H_B - \lambda_n(1))$. Then $B \equiv 1$ is a nondegenerate critical point of D_n whose Morse index is δ_n if n is odd and $\beta - \delta_n$ if n is even.

Proof. Under the assumptions of the theorem we have

$$\det(H_B - \lambda_n(1)) = (\lambda_n(B) - \lambda_n(1)) \det'(H_B - \lambda_n(1))$$

where det'(H_B) = F(B) is the product of the eigenvalues $\lambda_j - \lambda_n(1)$ for $j \neq n$. The following lemma is easy to check by direct computations of the second derivatives:

Lemma 1. Let F = fG where F, f, G are smooth real valued functions defined near a point x_0 on a smooth manifold. Let us assume that $f(x_0) = 0$ and $f'(x_0) = 0$; then the Hessian of F at the point x_0 is $G(x_0)$ times the Hessian of f at x_0 .

From the lemma, we get that the Hessian of D_n at $B \equiv 1$ is F(1) times the Hessian of Λ_n . We have $(-1)^{n-1}F(1) > 0$. The conclusion follows.

There is a formula for the characteristic polynomial of a magnetic Laplacian on graphs due to Robin Forman [1993] and reproved by Richard Kenyon [2012] and Yurii Burman [2012]. Using the gauge change $f \rightarrow f \phi_n$ as in [Colin de Verdière 1998] gives a Laplace type operator whose entries can be of any sign. Forman's formula extends to that case and it would be nice to relate Berkolaiko's formula to Forman's formula.

Important warning: Without loss of generality, we can and *will* assume in the rest of this note that $\lambda_n = \Lambda_n(1) = 0$. This implies that the Morse index of q_1 is n - 1.

In the course of the proof we will use a special choice of gauge in which we can compute the Hessian explicitly. More precisely, according to the classical perturbation formulae,

$$\ddot{\lambda} = (\phi, \ddot{H}\phi) + 2(\dot{H}\phi, \dot{\phi}),$$

where we assumed that λ is at a critical point: $\dot{\lambda} = 0$. The first term is easy to calculate explicitly; for perturbation in the direction of the 1-form ω it is

$$Q(\omega) = \frac{1}{2} \sum_{\vec{E}} a_{x,y} \omega([x, y])^2 \quad \text{with } a_{x,y} = -h_{x,y} \phi_n(x) \phi_n(y) = a_{y,x}.$$
 (2)

Considered as a quadratic form in ω , Q is already in the diagonal form. Its index is clearly the number of negative values among $\{-h_{x,y}\phi_n(x)\phi_n(y)\}$, or, in other words, the number ν of edges where ϕ_n changes sign!

We will present an explicit choice of gauge in which the second term vanishes. The condition for this is $\dot{H}\phi = 0$ which, after explicit calculation, can be interpreted as $\omega \in \ker d^*$, where d^* is the conjugate of d with respect to the inner product induced by (2).

Finally, we observe that the index of $Q(\omega)$ has been computed to be ν in the whole of $\Omega^1(G)$, whereas we should be restricting ourselves to our chosen gauge, $\omega \in \ker d^*$. We will show that this restriction reduces the index precisely by n - 1. Indeed, the splitting $\Omega^1(G) = d\mathbb{R}^X \oplus \ker d^*$ is orthogonal with respect to the form Q; therefore

$$\operatorname{ind}(Q) = \operatorname{ind}(Q|_{d\mathbb{R}^X}) + \operatorname{ind}(Q|_{\ker d^*}).$$

We establish that $\operatorname{ind}(Q|_{d\mathbb{R}^X}) = n - 1$ by relating the form Q on $d\mathbb{R}^X$ to the quadratic form q_1 around the point ϕ_n .

4. The quadratic form Q

Lemma 2. The set of forms $f \to (f(x) - f(y))^2$ where $\{x, y\} \in \mathcal{P}_2(X)$, the set of subsets with two elements of X, and $f \to f(x)^2$ with $x \in X$ is a basis of the set of quadratic forms on \mathbb{R}^X .

Definition 2. A quadratic form q on \mathbb{R}^X is said of Laplace type if for all $f \in \mathbb{R}^X$, $\hat{q}(1, f) \equiv 0$ where \hat{q} is the symmetric bilinear form associated to q.

Lemma 3. The set of forms $f \to (f(x) - f(y))^2$, $\{x, y\} \in \mathcal{P}_2(X)$ is a basis of the space of quadratic forms of Laplace type.

The form $\tilde{q}_1: f \to q_1(\phi_n f)$, where $\phi_n f$ is the pointwise product of ϕ_n and f, is of Laplace type because

$$\tilde{q}_1(1,g) = \langle H\phi_n | \phi_n g \rangle = \langle 0 | \phi_n g \rangle.$$

Hence $\widehat{\tilde{q}}_1(1, g) = 0$.

Moreover, $\tilde{q}_1(f) = Q(df)$. Indeed, because of Lemma 3, it is enough to compare the coefficients of the basis forms $f \to (f(x) - f(y))^2$. The form $f \to Q(df)$ is already expanded in this basis. To find the coefficient for the form $f \to \tilde{q}_1(f)$, we observe that (because we know it is of Laplace type) the coefficient in question is minus the coefficient in front of the term f(x)f(y), divided by two. This evaluates to $a_{x,y}$ (see (2)).

In fact, we will need to use $\hat{Q}(df, dg) = \langle H(\phi_n f) | \phi_n g \rangle$.

Lemma 4. The Morse index of $Q_{|d\mathbb{R}^X}$ is equal to n-1.

It is a general fact that the Morse index of the quadratic form $f \to Q(Af)$ is the same as the Morse index of the restriction of Q to the image of A. Hence, the Morse index of $Q_{|d\mathbb{R}^X}$ is the Morse index of \tilde{q}_1 on \mathbb{R}^X . Because $f \to \phi_n f$ is a linear isomorphism, this index is equal to the index of q_1 by the Sylvester theorem. Since $\lambda_n = 0$, the index of q_1 is n - 1 by elementary spectral theory.

Lemma 5. Let us denote by d^* the adjoint of d where \mathbb{R}^X is equipped with the canonical Euclidean structure and $\Omega^1(G)$ with the inner product associated to Q. The space $\Omega^1(G)$ splits as

$$\Omega^1(G) = d\mathbb{R}^X \oplus \ker d^*$$

(Hodge type splitting), and this decomposition is Q-orthogonal.

More explicitly d^* is given by

$$d^{\star}\omega(x) = \sum_{y \sim x} a_{x,y}\omega([y, x]).$$

If $\omega = df$ satisfies $d^*\omega = 0$, we have $d^*df = 0$. Hence $\hat{Q}(df, dg) = 0$ for all g and $\langle H(\phi_n f) | \phi_n g \rangle \rangle = 0$. Because λ_n is of multiplicity 1, this implies that f is constant and hence df = 0. So $d\mathbb{R}^X \cap \ker d^* = \{0\}$ and the conclusions follow.

At this point, we know that the nodal defect is the Morse index of the restriction of Q to the space ker d^* of dimension β . The first part of Theorem 1 follows.

5. The magnetic Hessian

We need one more fact to complete the proof: to identify the Hessian of Λ_n on $e^{i \ker d^*}$ at $B \equiv 1$ with the restriction of Q to ker d^* .

Let us denote by $S \subset \mathbb{C}^X$ the set of unit vectors f normalized so that $f(x_0)$ is real and $f(x_0) > 0$ where x_0 is chosen in X.

Lemma 6. The point $B \equiv 1$ is a critical point of Λ_n . If $\phi_n(B) \in S$ is the eigenfunction of H_B corresponding to the eigenvalue $\lambda_n(B)$, the differential of $B \to \phi_n(B)$ vanishes at $B \equiv 1$ on ker d^* .

The first property comes from the fact that $\Lambda_n(\bar{B}) = \Lambda_n(B)$. We can compute, for any variation $e^{it\alpha}$, t close to 0, of $B \equiv 1$, that $\dot{H}_B \phi_n + H \dot{\phi}_n = 0$. The condition $d^*\alpha = 0$ can be written as

$$\sum_{y \sim x} h_{x,y} \phi_n(y) \alpha_{x,y} = 0 \quad \text{for all } x \in X.$$

From (1), this is equivalent to $\dot{H}_B \phi_n = 0$. Hence $H(\dot{\phi}_n) = 0$ and $\dot{\phi}_n = c\phi_n$ since λ_n is simple. From the normalization $\|\phi_n(B)\| = 1$, we get $c \in i\mathbb{R}$ and, since $\dot{\phi}_n(x_0) \in \mathbb{R}$, the number *c* is real. We deduce that $\dot{\phi}_n = 0$.

Lemma 7. The function $F: S \times e^{i \ker d^*} \to \mathbb{R}$ defined by $F(f, e^{i\alpha}) = \langle H_{e^{i\alpha}} f | f \rangle$ admits $(\phi_n, 0)$ as a critical point and the Hessian of $(\Lambda_n)_{|e^{i \ker d^*}}$ at the point $B \equiv 1$ is the form Q.

The differential of *F* with respect to *f* vanishes because *f* is an eigenfunction of *H*. The differential with respect to ker d^* vanishes, because $F(f, e^{i\alpha}) = F(f, e^{-i\alpha})$. The Hessian of *F* at $(\phi_n, 0)$ is well defined. Because the differential at B = 1 of $B \to \phi_n(B)$ vanishes on $e^{i\ker d^*}$, the Hessians of $\Lambda_n : B \to F(\phi_n(B), B)$ and $M_n : B \to F(\phi_n(1), B)$ agree. A simple calculation of the Hessian of M_n gives the result:

$$\begin{split} M_n(e^{i\alpha}) &= -\frac{1}{2} \sum_{[x,y] \in \vec{E}} h_{x,y} |\phi_n(x) - e^{i\alpha_{x,y}} \phi_n(y)|^2 + \sum_{x \in X} V_x |\phi_n(x)|^2 \\ &= -\sum_{[x,y] \in E} h_{x,y} (\phi_n(x)^2 + \phi_n(y)^2 - 2\cos\alpha_{x,y} \phi_n(x) \phi_n(y)) + \sum_{x \in X} V_x |\phi_n(x)|^2. \end{split}$$

Computing the second derivative with respect to α at $\alpha = 0$ gives $\text{Hessian}(M_n) = Q(\alpha)$.

Appendix A: A pedestrian approach to the calculus of the Hessian of Λ_n in Section 5

We will derive a direct approach to the calculus of the second derivative of an eigenvalue which could be used directly in the proof of Lemma 7. Let $t \to A(t)$ be a C^2 curve defined near t = 0 in the space of Hermitian matrices on a finite-dimensional Hilbert space $(\mathcal{H}, \langle \cdot | \cdot \rangle)$. Let us assume that $\lambda(0)$ is an eigenvalue of A(0) of multiplicity one with a normalized eigenvector $\phi(0)$. Then, for t close to 0, A(t)has a simple eigenvalue $\lambda(t)$ of multiplicity one which is a C^2 function of t. We can choose an associated eigenfunction $\phi(t)$ which is C^2 with respect to t. The following assertions give the values of the first and second derivatives of $\lambda(t)$ at t = 0: **Proposition 1.** Under the previous assumptions, we have

$$\lambda'(0) = \langle A'(0)\phi(0) | \phi(0) \rangle.$$

If $\lambda'(0) = 0$, we have

$$\lambda''(0) = \langle A''(0)\phi(0)|\phi(0)\rangle + 2\langle \phi'(0)|A'(0)\phi(0)\rangle,$$

where $\phi'(0)$ is any solution of $(A(0) - \lambda(0))\phi'(0) = -A'(0)\phi(0)$. In particular, if $A'(0)\phi(0) = 0$,

$$\lambda''(0) = \langle A''(0)\phi(0)|\phi(0)\rangle.$$

Proof. We start with $(A(t) - \lambda(t))\phi(t) = 0$ where $\phi(t)$ is an eigenfunction of A(t) which depends in a C^2 way on t. Taking the first derivative, we get

$$(A'(t) - \lambda'(t))\phi(t) + (A(t) - \lambda(t))\phi'(t) = 0.$$
(3)

Putting t = 0 and taking the scalar product with $\phi(0)$, we get the formula for $\lambda'(0)$. Similarly, the *t*-derivative of (3) is

$$(A''(t) - \lambda''(t))\phi(t) + 2(A'(t) - \lambda'(t))\phi'(t) + (A(t) - \lambda(t))\phi''(t) = 0.$$
(4)

Putting t = 0, taking the scalar product with $\phi(0)$ and using $\lambda'(0) = 0$, we get the result.

We can apply this to $A(t) := H_{e^{it\alpha}}$ with $\alpha \in \ker d^*$ in order to get the Hessian of Λ_n in Section 5. The condition $A'(0)\phi(0) = 0$ is exactly $d^*\alpha = 0$!

Appendix B: The case where the eigenfunction vanishes at some vertex

In this appendix, we take $H \in \mathbb{O}_G$ and assume that $\lambda_n = 0$ is nondegenerate eigenvalue of H with a normalized eigenfunction ϕ . We have:

Proposition 2. Let us assume that, for all vertices x satisfying $\phi(x) = 0$, there exists a vertex $y \sim x$ so that $\phi(y) \neq 0$. Then, for any $\psi \in \mathbb{R}^X$ orthogonal to ϕ , there exists a smooth deformation $H_t \in \mathbb{O}_G$ of H so that $\dot{\phi} = \psi$.

It is enough to check that the space of $\dot{H}\phi$ is \mathbb{R}^X and to use the first variation formulae given in Appendix A.

Theorem 3. Let us assume that the function ϕ vanishes at the unique vertex x_0 . Then, the nullity of the Hessian of the "magnetic variation" of H is at least $|n_+ - n_-|$ where n_{\pm} is the number of vertices $x \sim x_0$ so that $\pm \phi(x) > 0$.

Proof. Choose a smooth variation H_t of H so that $\dot{\phi}(x_0) = 1$. Let ν be the number of sign changes of ϕ away from x_0 . Then, for t > 0 small enough, the number of sign changes of ϕ_t is $\nu + n_-$ while, for t < 0 small enough, it is $\nu + n_+$. We see from Theorem 1 that the magnetic Morse index is $\nu + n_- - (n-1)$ for t > 0 and $\nu + n_+ - (n-1)$. The discontinuity of the Morse index at t = 0 is $|n_+ - n_-|$. This gives the lower bound on the nullity.

Corollary 2. If $|n_+ - n_-| > \beta$, the eigenvalue 0 is degenerate.

Let us remark that this lower bound is not always sharp. In the following example, we have $n_+ = n_-$, $\beta = 2$ and the nullity of the Hessian is 2.

Example B.1. The graph G is made of 2 cycles of length 3 with a common vertex. The matrix of H is chosen as follows:

$$[H] = -\begin{pmatrix} 1 & 1 & 1 & 0 & 0\\ 1 & 1 & 2 & 0 & 0\\ 1 & 2 & 1 & 1 & 2\\ 0 & 0 & 1 & 1 & 1\\ 0 & 0 & 2 & 1 & 1 \end{pmatrix}.$$

Using the fact that the graph has a symmetry of order 2 exchanging the 2 cycles, one can split \mathbb{R}^X and the matrix *H* into the even and odd parts. This allows us to check that $\lambda_4 = 0$ is nondegenerate. In order to compute the magnetic Hessian, we check that it is possible to build a decomposition $\Omega^1(G) = d\mathbb{R}^X \oplus K$ which is *Q*-orthogonal and with $K \subset \ker d^*$. It is then easy to check that the magnetic Hessian evaluated on *K* vanishes.

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YVES COLIN DE VERDIÈRE: yves.colin-de-verdiere@ujf-grenoble.fr Unité Mixte de Recherche CNRS-UJF 5582, Institut Fourier, BP 74, 38402 Saint Martin d'Hères cedex, France http://www-fourier.ujf-grenoble.fr/~ycolver/



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László Lempert	Purdue University, USA lempert@math.purdue.edu	Gunther Uhlmann	University of Washington, USA gunther@math.washington.edu
Richard B. Melrose	Massachussets Institute of Technology, USA rbm@math.mit.edu	András Vasy	Stanford University, USA andras@math.stanford.edu
Frank Merle	Université de Cergy-Pontoise, France Da Frank.Merle@u-cergy.fr	n Virgil Voiculescu	University of California, Berkeley, USA dvv@math.berkeley.edu
William Minicozzi II	Johns Hopkins University, USA minicozz@math.jhu.edu	Steven Zelditch	Northwestern University, USA zelditch@math.northwestern.edu
Werner Müller	Universität Bonn, Germany mueller@math.uni-bonn.de		

PRODUCTION

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