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Magnetic interpretation of the nodal defect on graphs

Yves Colin de Verdière *†

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Abstract

In this note, 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. In the recent paper [2], Gregory Berkolaiko proves 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.

2 Notations

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

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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 non degenerate, 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 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 [3], we denote by \mathcal{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. 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 is a map $B : \vec{E} \to U(1)$ defined by $B([x,y]) = e^{i\alpha_{x,y}}$ where $[x,y] \to \alpha_{x,y}$ is a 1-form on G. We denote by $\mathcal{B}_G = e^{i\Omega^{1}(G)}$ the manifold of magnetic fields on G. The magnetic Schrödinger operator H_B associated to $H \in \mathcal{O}_{\mathcal{G}}$ 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 . We fix H and we denote by

$$\lambda_1(B) \le \lambda_2(B) \le \dots \le \lambda_n(B) \le \dots \le \lambda_{\#X}(B)$$

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 the

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 so that $q_{|F\setminus 0}$ is < 0.

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. 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 non degenerate if the previous Hessian is non degenerate.

The aim of this note is to prove the following nice results due to Berkolaiko [1, 2]:

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 $H \in \mathcal{O}_G$ is simple. We assume moreover that an associated non-zero 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, $\delta_n = \nu - (n-1)$ is the Morse index of Λ_n at that point. If M is the manifold of dimansion β of magnetic fields on G modulo the gauge transforms, the function $[B] \to \Lambda_n(B)$ has [1] as a non degenerate critical point.

Remark 1 The previous results can be extended by replacing $B \equiv 1$ by $B_{x,y} = \pm 1$ for all edges $\{x,y\} \in E$. The number ν 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 In fact, we will identify in a precise way the Hessian of Λ_n as a quadratic form on ker d^* , the tangent space to the manifold of magnetic fields modulo gauge transforms.

Remark 3 The assumptions on H are satisfied for H in an open dense subset of \mathcal{O}_G .

The upper bound of ν in the first part of Theorem 1 is related to Courant nodal Theorem (see [5] Section VI.6) as follows: a nodal domain on a graph for the eigenfunction ϕ_n is a connected component of the sub-graph 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 [3], Theorem 2.4) asserts that $\mu \leq n$; using 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 [1]):

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

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.

The scheme of proof will be to build a quadratic form Q on $\Omega^1(G)$ so that $\operatorname{ind}(Q) = \nu$, $\operatorname{ind}(Q_{|d\mathbb{R}^X}) = n-1$ and hence $\operatorname{ind}(Q_{|\ker d^*}) = \delta_n$. The form Q is defined by

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

The Morse index of Q is the number of edges so that $a_{x,y} < 0$. Since $h_{x,y} < 0$, this is precisely the number ν of sign changes of ϕ_n . It remains to identify δ_n with the Morse index of Λ_n restricted to $e^{i\ker d^*}$.

4 The quadratic form Q

Lemma 1 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 $\forall f \in \mathbb{R}^X$, $\hat{q}(1, f) \equiv 0$ where \hat{q} is the symmetric bi-linear form associated to q.

Lemma 2 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 point-wise product of ϕ_n and f, is of Laplace type because

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

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

Moreover, $\tilde{q}_1(f) = Q(df)$. Indeed, because of Lemma 2, 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 equation (1)).

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

Lemma 3 The Morse index of $Q_{|d\mathbb{R}^X}$ is equal to n-1.

Because the kernel of d is also the kernel of \tilde{q}_1 (the constant functions), the index of $Q_{|d\mathbb{R}^X}$ is the index of \tilde{q}_1 . This index is equal to the index of q_1 by Sylvester Theorem. Since $\lambda_n = 0$, the index of q_1 is n-1 by elementary spectral theory.

Lemma 4 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 $\langle H(\phi_n f)|\phi_n g\rangle = 0$. 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 the Theorem follows.

5 The Hessian of Λ_n and magnetic variations

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 5 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 $B \equiv 1$, $\dot{H}_B\phi_n + H\dot{\phi}_n = 0$. The condition $d^*\alpha = 0$ can be written as $\sum_{y \sim x} h_{x,y}\phi_n(y)\alpha_{x,y} = 0$ for all $x \in X$. This is exactly $i\dot{H}_B\phi_n$. 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 6 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:

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

$$-\sum_{[x,y]\in E} h_{x,y} \left(\phi_n(x)^2 + \phi_n(y)^2 - 2\cos\alpha_{x,y}\phi_n(x)\phi_n(y) \right) + \sum_{x\in X} V_x |\phi_n(x)|^2.$$

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

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 6. 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 $(\mathcal{H}, \langle .|.\rangle)$. 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 of t. Taking the first derivative, we get

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

Putting t = 0 and taking the scalar product with $\phi(0)$, we get the formula for $\lambda'(0)$. Similarly, the t-derivative of Equation (2) is

$$(A''(t) - \lambda''(t))\phi(t) + 2(A'(t) - \lambda'(t))\phi'(t) + (A(t) - \lambda(t))\phi''(t) = 0. (3)$$

Pouting 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: Hill's operators

In this Appendix, we will describe the case of a Schrödinger operator on the circle, also called the Hill's operator. This is the simplest continuous case, but it may be useful to do it with some details in order to try to extend the method to higher dimensional manifolds.

Eigenvalues and discriminant

The Hill's operator is

$$H = -\frac{d^2}{dx^2} + q(x)$$

where $q: \mathbb{R} \to \mathbb{R}$ is a smooth, 1-periodic, function. The spectral theory of Hill's operators has been well studied; in particular, the inverse spectral theory for this operator allows to solve non-linear evolution equations, like the Korteweg-de Vries one. A presentation of the properties of Hill's operators is given in [7].

The following facts are known:

Theorem 2 If we denote by λ_j^{\pm} , $j=1,\cdots$ the spectra of H acting on periodic (resp anti-periodic) functions of period 1, we have the inequalities

$$\lambda_1^+ < \lambda_1^- \le \lambda_2^- < \lambda_2^+ \le \lambda_3^+ < \cdots$$

and the spectrum of H on $L^2(\mathbb{R})$ is then union of intervals, called the bands,

$$[\lambda_1^+,\lambda_1^-] \cup [\lambda_2^-,\lambda_2^+] \cup [\lambda_3^+,\lambda_3^-] \cup \cdots .$$

These statements are linked to the properties of the discriminant $\Delta(\lambda)$: if $y_1(x,\lambda)$ and $y_2(x,\lambda)$ are the normalized solutions of $(H-\lambda)y=0$ whose Cauchy data are $y_1(0,\lambda)=1,\ y_1'(0,\lambda)=0,\ y_2(0,\lambda)=0,\ y_2'(0,\lambda)=1$, the discriminant Δ is the entire function given by $\Delta(\lambda):=y_1(1,\lambda)+y_2'(1,\lambda)$. The spectrum of H on $L^2(\mathbb{R})$ is the set of real λ 's so that $|\Delta(\lambda)| \leq 2$. The periodic (resp. anti-periodic) spectra are given by $\Delta(\lambda)=2$ (resp. $\Delta(\lambda)=-2$). The function $\Delta(\lambda)-2$ is a regularization of $\prod_{n=1}^{\infty}(\lambda-\lambda_n^+)$ in the spirit of [4]. It is proved in [7], Section II, that, if λ_n^+ is simple, $\Delta'(\lambda_n^+)\neq 0$ and the sign of this derivative is that of $(-1)^n$.

Magnetic fields

We will assume that λ_n^+ is equal to 0 and is a simple eigenvalue of H acting on 1-periodic functions. Up to gauge transform, every magnetic potential on the circle is a constant α . The bands are linked to the addition of a magnetic field as follows: the n-th band is the image of the circle $U = \{e^{i\alpha} | \alpha \in \mathbb{R}\}$ by the map Λ_n where $\Lambda_n(e^{i\alpha})$ is the n-th eigenvalue of H_α which is H acting on functions f so that $f(x+1) = e^{i\alpha} f(x)$. In particular, if n is even, λ_n^+ is a maximum of Λ_n while if n is odd, λ_n^+ is a minimum of Λ_n . This fits with Berkolaiko's formula because the (even!) number of zeros of the corresponding periodic eigenfunction ϕ_n is n = (n-1)+1 if n is even and n-1 = (n-1)+0 if n is odd (see [7] Theorem 2.14). In this appendix, we will use the general formula for the second derivative in order to reprove this result and to show that the critical points are non degenerate.

A direct computation of $d^2\Lambda_n/d\alpha^2(0)$ using the discriminant works as follows: the spectrum of H_{α} is given by $\Delta^{-1}(2\cos\alpha)$. Near $\lambda = \lambda_n^+$, we have $2 + \Delta'(\lambda_n^+)(\lambda_n(\alpha) - \lambda_n^+) \sim 2\cos\alpha$. This gives $\lambda_n(\alpha) \sim \lambda_n^+ - \alpha^2/\Delta'(\lambda_n^+)$, hence the Morse index of Λ_n at $\alpha = 0$ is 0 if n is odd and 1 is n is even.

A direct calculation of the Hessian

We will denote with a "dot" the derivatives w.r. to α and by a "prime" the derivatives w.r. to x. The operator H_{α} is unitarily equivalent to $K_{\alpha} = e^{-i\alpha x} H e^{i\alpha x}$ acting on 1-periodic functions. We have

$$K_{\alpha} = H - 2i\alpha \frac{d}{dx} + \alpha^2 .$$

The derivatives of K_{α} w.r. to α at $\alpha = 0$ are $\dot{K} = -2i\frac{d}{dx}$ and $\ddot{K} = 2$. Applying Proposition 1 and denoting by ϕ_n a corresponding normalized eigenfunction, we get

$$\ddot{\Lambda}_n(0) = 2 + 4i \int_0^1 \dot{\phi}_n(x) \phi'_n(x) dx$$
.

Moreover $H\dot{\phi}_n(x) = -\dot{K}\phi_n = 2i\phi'_n(x)$.

Let us denote by ψ the function $y_1(.,0)$. Then, using the method of "variation of parameters" (i.e. making the Ansatz $\dot{\phi}_n(x) = C_1(x)\psi(x) + C_2(x)\phi_n(x)$ with $C'_1(x)\psi(x) + C'_2(x)\phi_n(x) = 0$), we get

$$\dot{\phi}_n(x) = -ix\phi_n(x) + k\psi(x) + C\phi_n(x) , \qquad (4)$$

where the constant k is chosen so that $\dot{\phi}_n(x)$ is periodic and C is an arbitrary constant which can be fixed by a normalization of ϕ_n . We can always assume that $\phi_n(0) = \phi_n(1) = 0$ by shifting the origin of \mathbb{R} to some zero of ϕ_n . Using the wronskian, we see that $\dot{\phi}_n(1) = \dot{\phi}_n(0)$. We have to check the derivatives: $k\psi'(1) - i(\phi_n(1) + \phi'_n(1)) = k\psi'(0) - i\phi_n(0)$ or $k\psi'(1) = i\phi'_n(0)$. This gives, using Equation (4),

$$\dot{\phi}_n(x) = -ix\phi_n(x) + i\frac{\phi'_n(0)}{\psi'(1)}\psi(x) + C\phi_n(x) .$$

We get

$$\ddot{\Lambda}_n(0) = 2 + 4i \int_0^1 [-ix\phi_n(x) + k\psi(x) + C\phi_n(x)]\phi'_n(x)dx .$$

By integration by parts, we have $\int_0^1 2x\phi_n(x)\phi_n'(x)dx = -\int_0^1 \phi_n(x)^2 dx = -1$. Moreover, again by integration by parts, $\int_0^1 \psi(x)\phi_n'(x)dx = -\int_0^1 \psi'(x)\phi_n(x)dx$ and, since the Wronskian $\psi\phi_n' - \psi'\phi_n$ is constant and $\equiv \phi_n'(0)$, $\int_0^1 \psi(x)\phi_n'(x)dx = \frac{1}{2}\phi_n'(0)$. We get

$$\ddot{\Lambda}_n(0) = -2\phi'_n(0)^2/\psi'(1)$$
.

Moreover, it follows from Equation (2.13), page 16 in [7] and the fact that $\phi_n = \phi'_n(0)y_2$, that this is exactly $-2/\Delta'(\lambda_n^+)$.

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