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Hermitian matrices depending on three parameters: Coalescing eigenvalues[☆]

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ABSTRACT

We consider Hermitian matrix valued functions depending on three parameters that vary in a bounded surface of \mathbb{R}^3 . We study how to detect when such functions have coalescing eigenvalues inside this surface. Our criterion to locate these singularities is based on a construction suggested by Stone [20]. For *generic* coalescings, any such singularity is related to a particular accumulation of a certain phase, or lack thereof, as we cover the surface.

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Notation. With $\Omega \subset \mathbb{R}^3$ we indicate an open region of \mathbb{R}^3 diffeomorphic to the open unit ball. Points in Ω will use coordinates (x, y, z) and will be indicated by the symbol ξ . The metric is the Euclidean metric. With \mathbb{S}^2 we denote the unit sphere in \mathbb{R}^3 : $\mathbb{S}^2 = \{\xi \in \mathbb{R}^3 : \|\xi\|_2 = 1\}$. Closed pluri-rectangular regions of \mathbb{R}^3 will be denoted by R . With i we indicate the imaginary unit. We write $A \in C^k(\Omega, \mathbb{C}^{n \times n})$, $k \geq 1$, to indicate a smooth complex matrix-valued function defined on Ω . We write $A \in C^k_\tau(\mathbb{R}, \mathbb{C}^{n \times n})$ to indicate a smooth τ -periodic complex matrix-valued function, where $\tau > 0$ is the minimal period. Unless otherwise stated, the word *parameters* will always imply real valued.

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1. Introduction

To understand how eigenvalues, and eigenspaces, behave under perturbation is a classical problem, which finds wide applicability in dynamical systems studies, structural mechanics, numerical discretizations, and general stability studies. In essence, one has to study the behavior of eigenvalues of a matrix valued function depending (smoothly) on parameters. Clearly, the eigenvalues can always be chosen as continuous functions of the parameters, but further smoothness is generally precluded when there are multiple eigenvalues, with even more dramatic and pathological behaviors possible for the eigenspaces (e.g., see [12]), even in the friendlier cases of symmetric (in the real case) or Hermitian (complex case) functions. In a nutshell, as long as eigenvalues remain distinct, there are no obstacles to choosing them (and their corresponding eigenvectors) to vary smoothly in the parameters. However, severe lack of smoothness can be expected whenever there are multiple eigenvalues. Thus, the key problem one has to study is what happens when one or more eigenvalues of a matrix depending on parameters come together, that is, they *coalesce*.

By and large, most studies on this subject have been concerned with local perturbation results, and the book [15] gives an accessible and thorough introduction to this topic and its applications. In this work, however, we are interested in giving *global*, hence *topological*, localization results for values in parameter space where the eigenvalues coalesce, and our particular emphasis is on Hermitian matrices depending on three parameters. As we are reporting elsewhere, our theoretical results are adaptable to approximate numerically the location of the coalescing points; in particular, in [6] we present algorithmic details of a numerical realization of Theorem 4.13 of the present work.

Localization of coalescing points of eigenvalues of smooth symmetric and Hermitian matrix valued functions is a problem which has attracted the attention of the mathematics, physics and engineering communities for quite some time, with deep and varied ramifications ranging from random matrix theory and quantum mechanics to structural dynamics. Selected relevant references in the mathematical and quantum physics community include the pioneering works [1, 10, 18, 20] as well as the more recent studies [21–23, 25], whereas the references [8, 16, 19] offer an excellent starting point for studies in the structural dynamics communities.

In [7], we studied the problem of coalescing eigenvalues for symmetric (and real valued) functions depending on two parameters (and for the SVD as well). In that case, the original insight of the *non-crossing rule* of von Neumann and Wigner [24] was that having a pair of coalescing eigenvalues is a codimension-two phenomenon; that is one *should* need two parameters to observe coalescing eigenvalues. Moreover, these points *should* be isolated and at such coalescing points the surfaces describing the eigenvalues *should* come together as a double-cone, hence the name of conical intersections given to such exceptional points. In [7], a work which was preceded by the remarkable physical insight of [10], we gave rigorous and complete mathematical proofs that smoothly varying eigenvectors will change sign as one completes a loop around a *generic* coalescing point. We further showed what to expect in non-generic cases, and when there are multiple coalescing points inside the loop (for different or the same pairs of eigenvalues).

In this work, we are concerned with Hermitian matrix valued functions. A simple counting argument shows that in the Hermitian case a pair of coalescing eigenvalues is a real codimension-three phenomenon. Although this argument has appeared several times before, it is simple and insightful, so we report it here. “Consider a general Hermitian matrix, $A = A^* \in \mathbb{C}^{2 \times 2} = \begin{bmatrix} a & b+ic \\ b-ic & d \end{bmatrix}$. In general, there are 4 real degrees of freedom: a , b , c and d . Now, take a unitary decomposition of A : $A = U \Lambda U^*$, $U^* U = I$, with Λ being the matrix of (real) eigenvalues. If the two eigenvalues are equal, then A has to be a real multiple of the identity and this gives us three conditions to be satisfied: $a - d = 0$, $b = 0$, $c = 0$, hence a coalescing pair of eigenvalues is a codimension-three phenomenon”. Now, if we think of the solution set of the system $a - d = 0$, $b = 0$, $c = 0$, as the intersection of three surfaces in \mathbb{R}^3 , we see that – in general – we expect these surfaces to intersect, and to do so at isolated points.

As a consequence of the above considerations, for a Hermitian matrix valued function A , the natural setting to expect coalescing eigenvalues at isolated points is when A depends on three parameters; if A depended on fewer than three parameters, then we should not expect coalescing eigenvalues, while if A depended on four parameters (or more), then we should expect that coalescing eigenvalues are

not isolated (e.g., should occur along curves when A depends on four parameters, along surfaces when A depends on five parameters, and so forth).

We will thus focus on the study of $A \in C^k(\Omega, \mathbb{C}^{n \times n})$, $k \geq 1$, and Hermitian: $A = A^*$. In the present context, it is the work of Stone [20] which serves as a starting point of our study. The work of Stone does not seem to be as well known as it deserves to be, but in our opinion Stone had a truly remarkable insight. He considered what happens to the eigenvectors as they are moved smoothly along non-overlapping loops which cover a football-like surface, from the South to the North pole. He observed that if a certain phase factor¹ associated to an eigenvector completes a loop around the origin, then there is a coalescing point of the corresponding eigenvalues inside the surface. Our goal is to provide a rigorous and complete mathematical explanation of this phenomenon, and moreover to go the other way around; that is, to show that if a pair of eigenvalues coalesce inside the surface in a *generic* way (which we will characterize), then there is accumulation of phase. To justify our arguments, we will need some powerful geometrical results (e.g., [9]) that were not available at the time of the work of Stone. Furthermore, we will also generalize to the case of multiple coalescings.

To make some progress in our plan, we first need to recall some important results for Hermitian matrices which smoothly depend on one parameter. We do this next.

1.1. 1-d Compendium

It is a well known fact (e.g., see [12]) that eigenvalues of a smoothly varying matrix valued function are not smooth, in general, and of course neither are the eigenvectors (if they even exist!). Even in the case of a Hermitian function $A \in C^k(\mathbb{R}, \mathbb{C}^{n \times n})$, $k \geq 1$, the eigenvalues and eigenvectors may lose some smoothness at coalescing points (see [12,5]). At the same time, it is also well understood that any one-parameter smooth Hermitian matrix with simple eigenvalues is diagonalizable through a smooth unitary matrix: *unitary eigendecomposition*. [This is effectively Schur's theorem specialized to the Hermitian case; for this reason, below we will often refer to this unitary eigendecomposition just as a Schur's decomposition.]

More precisely, given $A \in C^k(\mathbb{R}, \mathbb{C}^{n \times n})$, $k \geq 1$, Hermitian and with distinct eigenvalues $\lambda_1(t) < \dots < \lambda_n(t)$ for all $t \in \mathbb{R}$, there exist unitary $U \in C^k(\mathbb{R}, \mathbb{C}^{n \times n})$ and diagonal $\Lambda \in C^k(\mathbb{R}, \mathbb{R}^{n \times n})$, $\Lambda(t) = \text{diag}(\lambda_1(t), \dots, \lambda_n(t))$, such that:

$$U^*(t)A(t)U(t) = \Lambda(t), \quad \forall t \in \mathbb{R}. \quad (1.1)$$

We remark that if A further depends smoothly (say, with degree of smoothness k) on other parameters varying in a compact region S , and the eigenvalues remain distinct as these extra parameters vary in S , then also the factors U and Λ will depend smoothly on these parameters. [This fact is a consequence of smooth dependence of solutions of differential equations on parameters; see (1.2) below.]

The factorization (1.1) is far from being unique, since $U(t)$ is determined up to a smooth *phase matrix*, that is up to a right diagonal factor $D(t) = \text{diag}(e^{i\alpha_1(t)}, \dots, e^{i\alpha_n(t)})$, where each α_j is an arbitrary C^k real-valued function. In other words, each eigenvector is determined only up to a smooth phase factor. The last statement, and the one about smooth dependence on the parameters, are easy to justify if we consider (as [5]) the differential equations satisfied by U and Λ . Since these differential equations models are important in what follows, let us summarize the above considerations in the form of a Theorem.

Theorem 1.1 [5]. *Let $A \in C^k(\mathbb{R}, \mathbb{C}^{n \times n})$, $k \geq 1$, be Hermitian and with distinct eigenvalues $\lambda_1(t) < \lambda_2(t) < \dots < \lambda_n(t)$, for all t . If, for all t , $A(t) = U(t)\Lambda(t)U^*(t)$ is a C^k unitary eigendecomposition of $A(t)$, with $\Lambda(t) = \text{diag}(\lambda_1(t), \dots, \lambda_n(t))$, and $U(t) = [u_1(t), \dots, u_n(t)]$, where $u_j(t)$ is the j th column of $U(t)$, then U and Λ satisfy the differential equations*

¹ This came to be known as the *Berry phase*, although the work of Stone predates that of Berry and Berry [1] refers to the work of Stone; in fairness, other authors as well had effectively introduced the same phase factor (see the recent review [2]). The equivalence of the choices of Stone and Berry will be further reviewed in the present work.

$$\begin{aligned}
 \dot{U} &= UH(A, U), \\
 H^* &= -H, \quad H_{hj} = u_h^* \dot{A} u_j / (\lambda_j - \lambda_h), \quad h < j \\
 \dot{\lambda}_j &= u_j^* \dot{A} u_j
 \end{aligned} \tag{1.2}$$

with $H_{jj} = u_j^* \dot{A} u_j$. Conversely, if $A(0) = U(0)\Lambda(0)U(0)^*$ is a given Schur decomposition at $t = 0$, then (1.2) define U , unitary, and Λ , diagonal with the ordered eigenvalues, giving a C^k Schur decomposition of A for all t , for any choice of $H_{jj} = i\phi_j$ where ϕ_j is any C^k (real valued) function.

In practice, to define U and Λ as solutions of (1.2), we need to resolve the lack of uniqueness in the choice of H_{jj} . We will resolve this non-uniqueness by imposing the following requirement:

$$H_{jj} = u_j^*(t)\dot{u}_j(t) = 0, \quad \forall t \in \mathbb{R}. \tag{1.3}$$

This way of resolving the non-uniqueness was suggested in [5], but it turns out to be equivalent to the ones proposed in [3,20], as shown in Theorem 2.6 below. For this reason, following the analogous definition in [3], we will call any decomposition satisfying (1.3) a *minimum variation decomposition*, or “MVD” for short.

2. Preliminary results

2.1. Berry phase

Let us consider condition (1.3) relatively to periodic matrix functions. In this case, (1.3) leads to the well known *Berry phase*.

Let $A \in C^k(\Omega, \mathbb{C}^{n \times n})$ be Hermitian. Let $\Gamma \subset \Omega$ be a smooth simple closed curve, parametrized as $\gamma \in C_1^k(\mathbb{R}, \Omega)$, and consider $A \circ \gamma = A_\gamma \in C_1^k(\mathbb{R}, \mathbb{C}^{n \times n})$. Assume that $A_\gamma(t)$ has distinct eigenvalues for all t , and let $U_\gamma^*(t)A_\gamma(t)U_\gamma(t) = \Lambda_\gamma(t)$ be the MVD of A_γ , for given $U_\gamma(0)$. Even though A_γ is 1-periodic, the smooth minimum variation eigenvectors will not, in general, be 1-periodic. That is, if we look at any MVD eigenvector u_j , for $t \in [0, 1]$, $j = 1, \dots, n$, we will have $u_j(1) = u_j(0)e^{i\alpha_j}$; in other words, each eigenvector of the MVD accrues a phase α_j after 1 period:

$$u_j(1) = u_j(0)e^{i\alpha_j} \rightarrow e^{i\alpha_j} = u_j(0)^* u_j(1). \tag{2.1}$$

From (2.1), we must appreciate that α_j is multi-valued, that is, in (2.1) α_j must be understood as being defined modulo 2π . This is an obvious consequence of the fact that the logarithm of a complex number is multi-valued. In (2.1) we can consider the principal branch of the logarithm, so that we will have $\alpha_j \in (-\pi, \pi]$; we call this the *principal phase*. This is effectively the choice of phase adopted by Berry in [1], and by virtue of Lemma 2.1 below, we call the value $e^{i\alpha_j}$ the *geometric phase factor*, and call the principal phase α_j the *Berry phase* associated to λ_j .

At the same time, from [4], it is known that a smooth 1-periodic eigendecomposition for A_γ does exist. That is, there is a $Q_\gamma \in C_1^k(\mathbb{R}, \mathbb{C}^{n \times n})$ unitary and such that $Q_\gamma^*(t)A_\gamma(t)Q_\gamma(t) = \Lambda_\gamma(t)$ for all t . Using this Q_γ , we now derive a useful explicit formula for the principal phase (see also [1, pp. 46–47]).

Lemma 2.1. *Let U_γ be the MVD unitary factor of a Hermitian function $A_\gamma \in C_1^1(\mathbb{R}, \mathbb{C}^{n \times n})$ with distinct eigenvalues along Γ , and let Q_γ be any smooth unitary 1-periodic factor of A , with $Q_\gamma(0) = U_\gamma(0)$. Partition Q_γ columnwise: $Q_\gamma(t) = [q_1(t), \dots, q_n(t)]$, $\forall t$. Then, for the principal phase α_j , we have:*

$$\alpha_j = i \int_0^1 q_j^*(t) \dot{q}_j(t) dt \pmod{2\pi}, \quad \forall j = 1, \dots, n. \tag{2.2}$$

Finally, the result is independent of the specific smooth 1-periodic function Q_γ considered.

Proof. Consider the smooth eigenvectors u_j and q_j relative to the eigenvalue λ_j . Since the eigenvalues are distinct, we have $u_j(t) = e^{i\eta_j(t)} q_j(t)$ for all t , where $\eta_j(\cdot)$ is a real-valued C^1 function with $\eta_j(0) = 0 \pmod{2\pi}$. Differentiating both sides in the relation $u_j(t) = e^{i\eta_j(t)} q_j(t)$, we get:

$$\dot{u}_j(t) = i\dot{\eta}_j(t)e^{i\eta_j(t)}q_j(t) + e^{i\eta_j(t)}\dot{q}_j(t).$$

Left-multiplication by $u_j^*(t)$ yields:

$$u_j^*(t)\dot{u}_j(t) = i\dot{\eta}_j(t) + q_j^*(t)\dot{q}_j(t).$$

By hypothesis $u_j^*(t)\dot{u}_j(t) = 0$ for all t , so we have:

$$\dot{\eta}_j(t) = iq_j^*(t)\dot{q}_j(t),$$

from which it follows that:

$$\eta_j(1) - \eta_j(0) = i \int_0^1 q_j^*(t)\dot{q}_j(t)dt,$$

where $\eta_j(1)$ is, modulo 2π , the principle phase associated to λ_j defined as α_j in (2.1).

Finally, we show that (2.2) is independent of the periodic factor Q_γ . Let \tilde{Q}_γ be another smooth 1-periodic unitary factor in the eigendecomposition of A_γ , with $\tilde{Q}_\gamma(0) = Q_\gamma(0)$. Then, since the eigenvalues are distinct, \tilde{Q}_γ and Q_γ differ by a phase matrix, and, since both are periodic, then we have $\tilde{Q}_\gamma(t) = Q_\gamma(t) \text{diag}(e^{i\beta_j(t)}, j = 1, \dots, n)$ for all $t \in [0, 1]$, where the function β_j is smooth, $\beta_j(1) = \beta_j(0) + 2k_j\pi$, for some $k_j \in \mathbb{Z}$, and $\beta_j(0) = 0 \pmod{2\pi}$. Differentiating the relation $\tilde{q}_j(t) = q_j(t)e^{i\beta_j(t)}$, we will get

$$\tilde{q}_j^*\dot{\tilde{q}}_j = q_j^*\dot{q}_j + i\dot{\beta}_j,$$

and from this as above we obtain

$$\eta_j(1) - \eta_j(0) = i \int_0^1 \tilde{q}_j^*(t)\dot{\tilde{q}}_j(t)dt + \beta_j(1) - \beta_j(0),$$

where $\eta_j(1)$ is, modulo 2π , the principal phase associated to λ_j as before. \square

Remark 2.2. To further elucidate the relationship between MVD unitary factors and periodic unitary factors for a periodic Hermitian function A , we show here how a 1-periodic eigendecomposition can be directly constructed starting from a given MVD. Let $A \in \mathcal{C}_1^1(\mathbb{R}, \mathbb{C}^{n \times n})$ be Hermitian with distinct eigenvalues for all $t \in \mathbb{R}$, and let

$$U^*(t)A(t)U(t) = \Lambda(t)$$

be a MVD for A . For all $j = 1, \dots, n$, let α_j be the Berry phase associated to the eigenvalue λ_j of A . Then a simple choice to obtain a smooth 1-periodic unitary factor of A is given by:

$$Q(t) = U(t) \text{diag}(e^{-it\alpha_j}, j = 1, \dots, n).$$

Remark 2.3. The definition of *geometric phase factor* of Berry, see [1, Eq. (6)], in our notation (see (2.1)) is given by

$$u_j^*(0)u_j(1) = q_j^*(0)q_j(1)e^{i\alpha_j} = e^{i\alpha_j}, \quad (2.3)$$

where q_j 's are the periodic eigenvectors² and u_j 's are the MVD decomposition ones.

² These correspond to the *no phase condition* of Berry (see [1, Eq. (6), and again just below equation (2)]) who considered the eigenvectors as function of the spatial variable ξ and required the eigenvectors to be single valued in a parameter domain enclosing the circuit Γ .

As it turns out, the Berry phase is a property of the curve Γ , and not of the adopted parametrization for it. This fundamental result will be a consequence of a more general result – which we give next – that essentially states that two different parametrizations of the same curve will lead to the same unitary factors at all points of the curve if and only if they are both MVDs.

Theorem 2.4. *Let $A \in C^k(\Omega, \mathbb{C}^{n \times n})$, $k \geq 1$, Hermitian. Let $\Gamma \subset \Omega$ be a smooth simple arc and assume that at all points $\xi \in \Gamma$, A has distinct eigenvalues. Let $\gamma_1 \in C^k([0, T_1], \Gamma)$ and $\gamma_2 \in C^k([0, T_2], \Gamma)$ be two smooth parametrizations of Γ , so that any point $\xi \in \Gamma$ can be written as $\xi = \gamma_1(t) = \gamma_2(\tau)$, for some values $t \in [0, T_1]$, and $\tau \in [0, T_2]$. Finally, let $A(\gamma_1(\cdot)) \in C^k([0, T_1], \mathbb{C}^{n \times n})$, and $A(\gamma_2(\cdot)) \in C^k([0, T_2], \mathbb{C}^{n \times n})$, be the restrictions of A to Γ , in the two different parametrizations. We will write $A_1(t)$ for $A(\gamma_1(t))$, $t \in [0, T_1]$, and $A_2(\tau)$ for $A(\gamma_2(\tau))$, $\tau \in [0, T_2]$, and similarly $U_1^*(t)A_1(t)U_1(t) = \Lambda_1(t)$, $t \in [0, T_1]$, and $U_2^*(\tau)A_2(\tau)U_2(\tau) = \Lambda_2(\tau)$, $\tau \in [0, T_2]$, for the two C^k Schur decompositions of $A(\gamma_1(\cdot))$ and $A(\gamma_2(\cdot))$, with $U_1(0) = U_2(0)$ and where $\Lambda_{1,2}$ contain the ordered eigenvalues.*

*Then, at any point $\xi \in \Gamma$, letting t and τ be such that $\xi = \gamma_1(t) = \gamma_2(\tau)$, we have $U_1(t) = U_2(\tau)$ if and only if U_1 and U_2 are associated to two MVDs. In particular, in this case we have $U_1(0)^*U_1(T_1) = U_2(0)^*U_2(T_2)$.*

Proof. All points $\xi \in \Gamma$ can be written as $\xi = \gamma_1(t) = \gamma_2(\tau)$, for $t \in [0, T_1]$, $\tau \in [0, T_2]$, and we always have a diffeomorphic change of variables on Γ between t and τ .

Therefore, at ξ , we have $A(\xi) = U_1(t)\Lambda_1(t)U_1^*(t)$ and also $A(\xi) = U_2(\tau)\Lambda_2(\tau)U_2^*(\tau)$, for some t and τ , with $\Lambda_1(t) = \Lambda_2(\tau)$, and where U_1 and U_2 satisfy (1.2):

$$\partial_t U_1 = U_1 H(A_1(t), U_1), \quad \partial_\tau U_2 = U_2 H(A_2(\tau), U_2), \quad U_1(0) = U_2(0),$$

and H is defined as in (1.2) (with the diagonal entries $H_{jj}(A_1, \cdot)$ and $H_{jj}(A_2, \cdot)$, $j = 1, \dots, n$, not yet specified, but otherwise equal).

We make these observations:

- (a) $\partial_\tau A_2 = (\partial_t A_1) \frac{\partial t}{\partial \tau}$ and further, if $H_{jj} = 0$, for all $j = 1, \dots, n$, then we also have $H(A_2(\tau), \cdot) = H(A_1(t), \cdot) \frac{\partial t}{\partial \tau}$;
- (b) $e^{-i\Phi} H(A_2(\tau), U_2) e^{i\Phi} = H(A_2(\tau), U_2 e^{i\Phi})$.

Since the eigenvalues of A along Γ are distinct, at any given point $\xi \in \Gamma$ we know that $U_1 = U_2 e^{i\Phi}$, where Φ is diagonal, $\Phi = \text{diag}(\phi_j, j = 1, \dots, n)$.

Now, consider the relation $U_1(t) = U_2(\tau(t))e^{i\Phi(t)}$ and differentiate it with respect to t . We have

$$\partial_t U_1 = (\partial_t U_2) e^{i\Phi} + i U_2(t) e^{i\Phi} \partial_t \Phi = (\partial_t U_2) e^{i\Phi} + i U_1(t) \partial_t \Phi,$$

and since $(\partial_t U_2) = (\partial_\tau U_2) \frac{\partial \tau}{\partial t}$, we get

$$\partial_t U_2 = U_2 H(A_2(\tau), U_2) \frac{\partial \tau}{\partial t}$$

and so

$$\partial_t U_1 = U_2 e^{i\Phi} (e^{-i\Phi} H(A_2(\tau), U_2) e^{i\Phi}) \frac{\partial \tau}{\partial t} + i U_1(t) \partial_t \Phi,$$

or

$$\partial_t U_1 = U_1 H(A_2(\tau), U_1) \frac{\partial \tau}{\partial t} + i U_1(t) \partial_t \Phi. \quad (2.4)$$

We claim that $U_1 = U_2$, at all $\xi \in \Gamma$, when $H_{jj}(A_1, \cdot) = H_{jj}(A_2, \cdot) = 0$, $j = 1, \dots, n$. In fact, in this case, from (a) we get $H(A_2(\tau), U_2) \frac{\partial \tau}{\partial t} = H(A_1(t), U_2)$, and so (2.4) rewrites as

$$\partial_t U_1 = U_1 H(A_1(t), U_1) + i U_1(t) \partial_t \Phi.$$

But, since $\partial_t U_1 = U_1 H(A_1(t), U_1)$, then we have $\partial_t \Phi = 0$, and we must have $\Phi(t)$ constant for all t . Thus, since $\Phi(0) = 0, \mod (2\pi)$, $\Phi(t) = 0, \mod (2\pi)$, for all t , from which we get $U_1 = U_2$, at all $\xi \in \Gamma$.

On the other hand, suppose that U_1 and U_2 are not MVDs, so that $H_{jj}(A_1, U_1), H_{jj}(A_2, U_2) \neq 0$ (for at least some $j = 1, \dots, n$). The relation (2.4) still holds, which gives

$$\partial_t U_1 = U_1 \left[H(A_2(\tau), U_1) \frac{\partial \tau}{\partial t} + i \partial_t \Phi \right].$$

From this, and $\partial_t U_1 = U_1 H(A_1(t), U_1)$, we must have $U_1 [H(A_2(\tau), U_1) \frac{\partial \tau}{\partial t} + i \partial_t \Phi - H(A_1(t), U_1)] = 0$, which shows that we cannot have $\partial_t \phi_j = 0$, for all $j = 1, \dots, n$, and so $\Phi(\cdot)$ cannot be a constant function and $U_1 \neq U_2$ at some $\xi \in \Gamma$. \square

In other words, what we have is that: *If we choose the MVD along the curve Γ , then the decomposition is independent of the parametrization, otherwise it is not.* Of course, if (at least one of) the decompositions U_1, U_2 , in the Theorem is not a MVD, then we will not have $U_1(\xi) = U_2(\xi)$ at all $\xi \in \Gamma$, though this may happen at some point.

As a consequence of Theorem 2.4, the MVD (and only the MVD) allows for a definition of phase along a loop that is independent of how the loop is parametrized. This is the anticipated result:

Corollary 2.5. *The Berry phase is a property of the circuit Γ and not of a parametrization γ of Γ .*

Proof. For a given parametrization γ of the simple closed curve Γ , the Berry phase is the phase factor accrued by the MVD of A_γ (see (2.1)). By Theorem 2.4, the latter is independent of the parametrization of the circuit Γ and so the result follows. \square

We complete this section with the following equivalence result of the three “different” choices for unitary factors done in the works [3,5,20]. Recall that we are looking at a (smooth) unitary decomposition of a (smooth) Hermitian matrix valued function $A \in \mathcal{C}_1^k([0, 1], \mathbb{C}^{n \times n})$, whose eigenvalues are distinct for all $t \in [0, 1]$. In such case, see Section 1.1, we know that any unitary decomposition of A will be determined only up to a smooth diagonal phase matrix. The above mentioned three choices are ways to fix this phase matrix. Let us recall, in our language, what each of them amounts to.

- (i) *Diagonal of H equal to 0*; see [5]. This is the choice resulting from taking $H_{jj} = 0$ in (1.3)–(1.2).
- (ii) *Minimum variation decomposition*; see [3]. The choice here is to select the unitary factor Q in the eigendecomposition of A which minimizes the total variation

$$\text{Vrn}(Q(t)) = \int_0^1 \|\dot{Q}(t)\|_F dt, \quad (2.5)$$

over all possible choices of unitary factors Q . Here, for a matrix B , $(\|B\|_F)^2 = \sum_{i,j} |b_{ij}|^2$ is the Frobenius norm of B . [The Frobenius norm is the choice made in [3].]

- (iii) *2nd order in imaginary part*; see [20]. Stone (see [20, Eq. (1)]) assumed that $A \in \mathcal{C}^2$ and selected the smooth \mathcal{C}^2 eigenvectors $q_j, j = 1, \dots, n$, for which the following condition is satisfied

$$\text{Im}(q_j^*(t)q_j(t+dt)) = \mathcal{O}(dt^2), \quad j = 1, \dots, n. \quad (2.6)$$

Theorem 2.6. *The above choices (i)–(iii) are equivalent, that is they all lead to the same uniquely defined unitary factor.*

Proof. We will show that (ii) and (iii) are equivalent to (i).

The equivalence of (ii) and (i) is a consequence of the fact that the choice (2.5) is obtained by solving the ODEs (1.2) with $\text{diag}(H) = (0, \dots, 0)$. In fact, any smooth Q is the solution of the equation $\dot{Q} = QH$, where the diagonal of H is as yet undetermined. We always have

$$\|\dot{Q}\|_F = \|QH\|_F = \|H\|_F,$$

so that we need to look at $\|H\|_F^2$. We have

$$\|H\|_F^2 = \sum_{k=1}^n |H_{kk}|^2 + 2 \sum_{k,j: j=2,\dots,n, k < j} |H_{kj}|^2,$$

where $H_{kj} = q_k^* \dot{q}_j$. Now, every Q is of the form $Q = Ue^{i\Phi}$ and so (for $k \neq j$) $q_k^* \dot{q}_j = e^{i(\phi_j - \phi_k)} u_k^* \dot{u}_j$, and thus $|q_k^* \dot{q}_j| = |u_k^* \dot{u}_j|$ and therefore $|H_{kj}|$ is invariant with respect to the unitary matrix we select. Thus, clearly $\|H\|_F$, and hence the total variation, is minimized by the choice $H_{11} = \dots = H_{nn} = 0$.

The equivalence of (iii) and (i) is by the following argument. Let q_j be a smooth eigenvector of A . (Presently, we assume –as does Stone– that the eigenvectors are C^2 .) By Taylor's expansion, we have

$$q_j(t + dt) = q_j(t) + \dot{q}_j(t)dt + \mathcal{O}(dt^2).$$

Left-multiplying by q_j^* we get:

$$q_j^*(t)q_j(t + dt) = 1 + q_j^*(t)\dot{q}_j(t)dt + \mathcal{O}(dt^2).$$

Finally, taking the imaginary part of both sides, we obtain:

$$\text{Im}(q_j^*(t)q_j(t + dt)) = q_j^*(t)\dot{q}_j(t)dt + \mathcal{O}(dt^2) = H_{jj}dt + \mathcal{O}(dt^2),$$

and thus (2.6) is equivalent to $H_{jj} = 0$, that is case (iii) is equivalent to case (i). \square

Remark 2.7. As a consequence of the results in Section 2.1 and of Theorem 2.6, the geometric phase factor of Berry coincides with the phase factor of Stone.

2.2. Phase rotating and phase preserving surfaces.

In this section, we see how to characterize surfaces with respect to (the MVD of) smooth Hermitian functions defined on the surface.

First, we collect some results of differential geometry which we need.

Definition 2.8. Let $f: \mathbb{S}^2 \rightarrow \mathbb{R}^3$ be a C^k map, $k \geq 1$. We say that f is a (C^k -) *embedding* if its Jacobian matrix is full-rank everywhere on \mathbb{S}^2 and f maps \mathbb{S}^2 (C^k -) diffeomorphically onto its image. We call $f(\mathbb{S}^2)$ the *embedded image* of \mathbb{S}^2 .

Throughout this paper, unless otherwise stated, we will always consider surfaces in \mathbb{R}^3 which are embedded images of \mathbb{S}^2 under some embedding f . Such surfaces will be referred to as *2-spheres*, and will be denoted by the letter S . We remark that the term 2-sphere will refer to the embedded image and not to one particular embedding, as the same surface is the image of \mathbb{S}^2 under infinitely many embeddings (think of $f \circ g$, where g is an arbitrary diffeomorphism of \mathbb{S}^2).

Below, we will need a result which says that if we have two smooth 2-spheres, one strictly inside the other, then there is a smooth homotopy from one to the other. The following theorem will be a fundamental tool for the construction of such homotopy.

Theorem 2.9 (Annulus Theorem).³ For any $k \in \{0, \dots, \infty\}$, let S_0 and S_1 be two C^k -smooth 2-spheres, with S_0 contained in the compact region bounded by S_1 . Then, the region co-bounded by S_0 and S_1 is C^k -diffeomorphic to $\mathbb{S}^2 \times [0, 1]$.

³ We are grateful to Prof. John Etnyre, of Georgia Tech, for having clarified to us how this result follows from the C^k -Schönflies theorem proved by Hatcher [9].

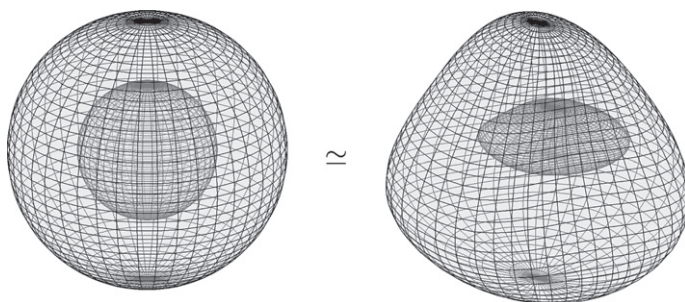


Fig. 1. Picture illustrating the thesis of Theorem 2.9.

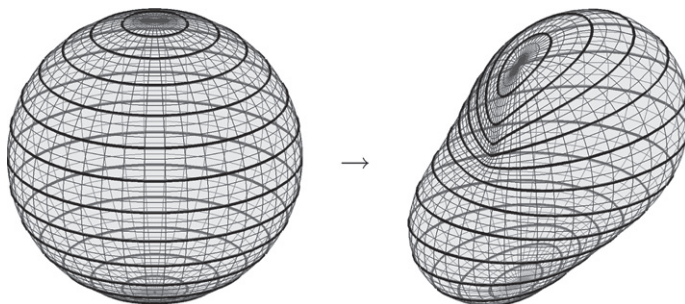


Fig. 2. The 2-sphere S (right) inherits a Γ -covering from \mathbb{S}^2 (left).

See Fig. 1 for a geometric illustration of this fact.

Now, on \mathbb{S}^2 let us consider the following normalized geographical coordinates:

$$\begin{cases} x(s, t) = \sin(\pi s) \cos(2\pi t) \\ y(s, t) = \sin(\pi s) \sin(2\pi t) \\ z(s, t) = \cos(\pi s) \end{cases}$$

with $s, t \in [0, 1]$ representing, respectively, latitude and longitude. We can think of \mathbb{S}^2 as covered by the family of loops $\{C_s\}_{s \in [0, 1]}$, where each loop represents a parallel, i.e. it consists of all points of \mathbb{S}^2 sharing the same latitude. More precisely, each loop C_s is parametrized as

$$\gamma_s(\cdot) = (x(s, \cdot), y(s, \cdot), z(s, \cdot)).$$

Note that γ_0 and γ_1 are constant functions that represent, respectively, north pole and south pole of \mathbb{S}^2 . We will refer to $\{C_s\}_{s \in [0, 1]}$ as the *standard covering* of \mathbb{S}^2 (see left picture in Fig. 2).

Let S be a 2-sphere and f be an embedding such that $S = f(\mathbb{S}^2)$. Then S inherits through f a covering of loops from \mathbb{S}^2 in a natural way. Namely, S is the following disjoint union of loops:

$$S = \bigcup_{s \in [0, 1]} \Gamma_s, \quad (2.7)$$

where $\Gamma_s = f(C_s)$ for all $s \in [0, 1]$. As s goes through the interval $[0, 1]$, the loops Γ_s trace out the surface S , originating from, and ending at, two distinct points on S . We will call a covering of the form (2.7) a Γ -covering for S (see right picture in Fig. 2). Similarly, S also inherits through f a smooth system of coordinates from \mathbb{S}^2 , such that points on S are parametrized as $\xi = f(\gamma_s(t))$, with $(s, t) \in [0, 1]^2$. We will refer to such system of coordinates as the *system of coordinates for S associated to the Γ -covering* (2.7).

Smooth Berry Phases for a Γ -covering. Now, let $S \subset \Omega$ be a 2-sphere and $\{\Gamma_s\}_{s \in [0,1]}$ be a Γ -covering for S . Let $A \in \mathcal{C}^1(\Omega, \mathbb{C}^{n \times n})$ be Hermitian with distinct eigenvalues on S . For all $s \in [0, 1]$, any loop Γ_s of the Γ -covering can be parametrized by a 1-periodic variable t . Therefore, along each loop we have a smooth MVD of A (which is independent of the parametrization of the loop) and for each loop we can unambiguously define the principal (Berry) phases associated to each eigenvalue, according to (2.1), that is the phase α_j obtained by comparing the eigenvectors of the MVD at the beginning and end of the current loop. Now, recall that although the geometric phase factor $e^{i\alpha_j}$ is well defined, the phase itself is only defined modulo 2π , a fact which prompted us to select the principal phase, that is the argument of the logarithm was chosen in $(-\pi, \pi]$. However, we now want to select a phase which varies smoothly in s . Therefore, as s varies in $[0, 1]$, we will let the phase move from a branch of the logarithm to an adjacent one continuously. So doing, for any $\Gamma_s, s \in [0, 1]$, we will consider Berry phases $\alpha_j(s)$'s, smooth in s , associated to each of the eigenvalues, namely n smooth maps $\alpha_j : s \in [0, 1] \mapsto \alpha_j(s) \in \mathbb{R}$, for $j = 1, \dots, n$. Since the loops Γ_0 and Γ_1 are in fact points in Ω , on which the matrix A will be constant, we will fix $\alpha_j(0) = 0$ for all $j = 1, \dots, n$, and we will necessarily have $\alpha_j(1) = 2\pi k_j$, for some values $k_j \in \mathbb{Z}, j = 1, \dots, n$.

Definition 2.10. With $S, \{\Gamma_s\}_{s \in [0,1]}, A$ and α_j 's as above, we say that S is *phase-preserving* for A if

$$\alpha_j(1) = 0, \quad \forall j = 1, \dots, n.$$

We say that S is *phase-rotating* if it is not phase-preserving.

In other words, relatively to a given Hermitian function A as above, we call phase-rotating a surface S for which, as Γ_s traces out S , the phase factor $e^{i\alpha_j(s)}$ associated to one of the eigenvalues of A completes a loop around the origin in the complex plane.

Remark 2.11. For a Γ -covering, any possible choice of smooth (in s) Berry phase for $s \in [0, 1]$ must assume values multiple of 2π at the end points of this interval. We have selected the most natural choice, denoted by $\alpha_j(s)$, for which $\alpha_j(0) = 0, j = 1, \dots, n$. This has allowed us to write the definition of phase-preserving/rotating solely in terms of the values $\alpha_j(1)$'s, but (strictly speaking) it is not necessary to consider the branch of smooth Berry phases which goes through the origin. Equivalently, one could say that S is phase-rotating for A if one (and hence any) smooth branch of Berry phases associated to some eigenvalue of A undergoes an increment of $2k\pi, k \neq 0$ integer, over the interval $[0, 1]$.

The concept of phase-rotating and phase-preserving surface was first introduced by Stone [20] nearly 40 years ago. As far as we can tell, however, a rigorous clarification that this is a property of the surface (i.e., that it is independent of the covering chosen for S) is still lacking. We will prove this fact here below.

Theorem 2.12 (Phase-rotating independent of Γ -covering). *Let $A \in \mathcal{C}^1(\Omega, \mathbb{C}^{n \times n})$ and let $S \subset \Omega$ be a 2-sphere. Consider two distinct Γ -coverings of S :*

$$S = \{\Gamma_s^0\}_{s \in [0,1]} = \{\Gamma_s^1\}_{s \in [0,1]}.$$

For each covering consider the Berry phase functions associated to each eigenvalue of A : $\alpha_j^m(s)$, with $m = 0, 1, j = 1, \dots, n$. Then we have:

$$|\alpha_j^0(1)| = |\alpha_j^1(1)| \text{ for all } j = 1, \dots, n.$$

Proof. Let f_0, f_1 be the embeddings that define, respectively, the two Γ -coverings above. Let $\psi = f_0^{-1} \circ f_1$. The map ψ is a diffeomorphism of \mathbb{S}^2 , hence (see [14]) it must be smoothly isotopic⁴ either to the identity map on \mathbb{S}^2 or to the antipodal map on \mathbb{S}^2 . Let us first assume ψ is isotopic to the identity

⁴ We recall that an isotopy is a homotopy $H_\zeta(\cdot), \zeta \in [0, 1]$, such that each H_ζ is a homeomorphism.

$id : \mathbb{S}^2 \rightarrow \mathbb{S}^2$. This means that there exist a smooth family of diffeomorphisms $H_\zeta : \mathbb{S}^2 \rightarrow \mathbb{S}^2$, $\zeta \in [0, 1]$, such that $H_0 \equiv id$ and $H_1 \equiv \psi$.

Now let (s, t) be normalized geographical coordinates on \mathbb{S}^2 , and let us define $\tilde{A}(s, t, \zeta) = A(f_0 \circ H_\zeta(s, t))$, for all $(s, t, \zeta) \in [0, 1]^3$. The matrix \tilde{A} is smooth and has distinct eigenvalues for all $(s, t, \zeta) \in [0, 1]^3$. Appealing to smooth dependence with respect to parameters, let us take a smooth Schur decomposition $\tilde{U}^* \tilde{A} \tilde{U} = \tilde{\Lambda}$ on $[0, 1]^3$, such that

$$\tilde{U}^*(s, \cdot, \zeta) \tilde{A}(s, \cdot, \zeta) \tilde{U}(s, \cdot, \zeta) = \tilde{\Lambda}(s, \cdot, \zeta)$$

is a minimum variation decomposition for all s, ζ . Let us denote the columns of $\tilde{U}(s, t, \zeta)$ with $\tilde{u}_j(s, t, \zeta)$, $j = 1, \dots, n$.

For any fixed $\zeta \in [0, 1]$, let us define the n smooth (in s) phases $\alpha_j^\zeta(s)$ through the identity:

$$\tilde{u}_j^*(s, 0, \zeta) \tilde{u}_j(s, 1, \zeta) = e^{i\alpha_j^\zeta(s)}, \quad s \in [0, 1].$$

Finally, let us consider the following functions of ζ : $\varphi_j(\zeta) = \alpha_j^\zeta(1)$. All functions are smooth and take values in $2\pi\mathbb{Z}$, hence they must be constant. This shows that $\alpha_j^0(1) = \alpha_j^1(1)$, for all $j = 1, \dots, n$.

In case ψ is isotopic to the antipodal map, a similar argument shows that $\alpha_j^0(1) = -\alpha_j^1(1)$, for all $j = 1, \dots, n$. \square

Corollary 2.13. *For a 2-sphere S , relatively to a Hermitian function $A \in \mathcal{C}^1(\Omega, \mathbb{C}^{n \times n})$ with distinct eigenvalues on S , the property of being phase-rotating does not depend on the covering for S .*

3. One pair coalescing: the 2×2 case

In this section we consider the case of a Hermitian function A taking values in $\mathbb{C}^{2 \times 2}$. This will serve as stepping stone for the general case to be presented in Section 4.

Let $A \in \mathcal{C}^1(\Omega, \mathbb{C}^{2 \times 2})$ be Hermitian and let λ_1, λ_2 be its continuous eigenvalues, labeled so that $\lambda_1(\xi) \leq \lambda_2(\xi)$ for all $\xi \in \Omega$. We say that ξ is a *coalescing point* for A if we have $\lambda_1(\xi) = \lambda_2(\xi)$.

Now, write:

$$A(\xi) = \begin{bmatrix} a(\xi) & b(\xi) + ic(\xi) \\ b(\xi) - ic(\xi) & d(\xi) \end{bmatrix}$$

with $a, b, c, d \in \mathcal{C}^1(\Omega, \mathbb{R})$. Let $F : \Omega \rightarrow \mathbb{R}^3$ be defined as follows:

$$F(\xi) = \begin{bmatrix} \frac{a(\xi) - d(\xi)}{2} \\ b(\xi) \\ c(\xi) \end{bmatrix}. \quad (3.1)$$

Note that ξ is a coalescing point for A if and only if $F(\xi) = 0$, i.e. if and only if $A(\xi)$ is a scalar multiple of the identity. We call a point ξ_0 a *generic coalescing point* for A if $F(\xi_0) = 0$ and the Jacobian $DF(\xi_0)$ is invertible. (This is called “normal singular point” in [18].)

Theorem 3.1. *Let $A \in \mathcal{C}^1(\Omega, \mathbb{C}^{2 \times 2})$ be Hermitian. Let λ_1, λ_2 be its continuous eigenvalues. Let $\xi_0 \in \Omega$ be a generic coalescing point for A in Ω , and suppose that ξ_0 is the only coalescing point in Ω . Let $S \subset \Omega$ be a 2-sphere. If the interior part of S contains ξ_0 , then S is phase-rotating.*

Proof. The proof will go as follows. We will first prove the result for a small 2-sphere S_0 that contains ξ_0 and is contained in S . Then we will show, through the same homotopy argument used in Theorem 2.12, that the result is true also for S .

Without loss of generality, let us assume that A satisfies the condition:

$$d(\xi) = -a(\xi) \quad \text{for all } \xi \in \Omega$$

as this can be easily enforced through a shift of A by the diagonal matrix

$$\frac{a(\xi) + d(\xi)}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

leaving F unchanged and preserving eigenvectors and generic coalescing points.

In virtue of the Inverse Function Theorem, F is a local diffeomorphism of a neighborhood \mathcal{U} of ξ_0 onto a neighborhood $F(\mathcal{U})$ of the origin. Let us consider the restriction, call it f_0 , of F^{-1} to a small sphere $B_\rho(0) = \{\xi \in \mathbb{R}^3 : \|\xi\|_2 = \rho\} \subset F(\mathcal{U})$. If we choose ρ small enough, the embedding f_0 properly defines a 2-sphere $S_0 = f_0(B_\rho(0))$ that is contained in S and contains ξ_0 in its interior. We now show, by direct computation, that S_0 is phase-rotating. We do this by considering on S_0 the Γ -covering inherited through f_0 by the standard covering of $B_\rho(0)$.

Parametrizing $B_\rho(0)$ through normalized geographical coordinates allows us to rewrite A on S_0 in a very simple form:

$$A = \rho \begin{bmatrix} \sin(\pi s) \cos(2\pi t) & \sin(\pi s) \sin(2\pi t) + i \cos(\pi s) \\ \sin(\pi s) \sin(2\pi t) - i \cos(\pi s) & -\sin(\pi s) \cos(2\pi t) \end{bmatrix} \quad (3.2)$$

with $s, t \in [0, 1]$. The matrix A has two constant eigenvalues for all s, t : $\lambda_\pm = \pm\rho$. The following eigenvector associated to λ_+ can be easily obtained by direct computation:

$$q_s^+(t) = \frac{1}{\sqrt{2 + 2 \sin(\pi s) \cos(2\pi t)}} \begin{bmatrix} 1 + \sin(\pi s) \cos(2\pi t) \\ \sin(\pi s) \sin(2\pi t) - i \cos(\pi s) \end{bmatrix}$$

defined for all $(s, t) \in [0, 1] \times [0, 1] \setminus (1/2, 1/2)$. Since each $q_s^+(\cdot)$, $s \in [0, 1] \setminus \{1/2\}$, has unit length and is 1-periodic, formula (2.2) can be used to derive the Berry phase function $\alpha^+(s)$. Direct computation yields the following expressions:

$$\int_0^1 (q_s^+(t))^* \partial_t q_s^+(t) dt = \begin{cases} \pi - \pi \cos(\pi s) & \text{if } s \in [0, 1/2) \\ -\pi - \pi \cos(\pi s) & \text{if } s \in (1/2, 1] \end{cases}.$$

These expressions deliver, modulo 2π , and invoking the continuity of $\alpha^+(\cdot)$ over $[0, 1]$, the desired Berry phase function:

$$\alpha^+(s) = \pi(1 - \cos(\pi s)), \quad \text{for all } s \in [0, 1].$$

Note that the value assumed by α^+ at $s = 1/2$ could have been predicted through [7, Theorem 2.2], since in this case A is real-valued and symmetric.

The Berry phase function α^+ computed above satisfies the following conditions: $\alpha^+(0) = 0$, $\alpha^+(1) = 2\pi$. Hence, by Definition 2.10, S_0 is phase-rotating. A similar argument shows that $\alpha^-(0) = 0$, $\alpha^-(1) = -2\pi$.

Now let us consider the compact region $S \setminus S_0$. By Theorem 2.9, there exist a diffeomorphism h that maps $S \setminus S_0$ onto $\mathbb{S}^2 \times [0, 1]$. The annulus $\mathbb{S}^2 \times [0, 1]$ can be trivially identified with the compact region \mathcal{A} bounded by two concentric spheres in \mathbb{R}^3 centered at the origin:

$$\mathbb{S}^2 \times [0, 1] \equiv \mathcal{A} = \{x \in \mathbb{R}^3 : 1 \leq \|x\|_2 \leq 2\}.$$

Let us consider the linear scaling T_ζ that deforms $T_0 = \mathbb{S}^2 \times \{0\} \equiv B_1(0)$ into $T_1 = \mathbb{S}^2 \times \{1\} \equiv B_2(0)$. We will think of each sphere T_ζ as parametrized by normalized geographical coordinates (i.e.

$T_\zeta = T_\zeta(s, t)$ and covered by the standard covering for \mathbb{S}^2 . Finally, let us consider the composition $H_\zeta(s, t) = h^{-1}(T_\zeta(s, t))$, with $(s, t, \zeta) \in [0, 1]^3$. Through the “pull-back” map h^{-1} , the compact region $S \setminus S_0$ inherits from $\mathbb{S}^2 \times [0, 1]$ a differentiable family of Γ -coverings that swipes all of $S \setminus S_0$, moving from S_0 to S .

Similarly to what was done in Theorem 2.12, let us define $\tilde{A}(s, t, \zeta) = A(H_\zeta(s, t))$, for all $(s, t, \zeta) \in [0, 1]^3$. Being \tilde{A} smooth with distinct eigenvalues for all $(s, t, \zeta) \in [0, 1]^3$, we can take a smooth Schur decomposition $\tilde{U}^* \tilde{A} \tilde{U} = \tilde{\Lambda}$ on $[0, 1]^3$, such that

$$\tilde{U}^*(s, \cdot, \zeta) \tilde{A}(s, \cdot, \zeta) \tilde{U}(s, \cdot, \zeta) = \tilde{\Lambda}(s, \cdot, \zeta)$$

is a MVD for all s, ζ . Let us denote the two eigenvectors of $\tilde{U}(s, t, \zeta)$ with $\tilde{u}^\pm(s, t, \zeta)$.

Finally, for any $\zeta \in [0, 1]$, let us define the two smooth (in s) phases $\alpha_\zeta^\pm(s)$ through the identity:

$$\tilde{u}^*(s, 0, \zeta) \tilde{u}(s, 1, \zeta) = e^{i\alpha_\zeta^\pm(s)}, s \in [0, 1].$$

The two functions $\varphi^\pm(\zeta) = \alpha_\zeta^\pm(1)$ are smooth and take values in $2\pi\mathbb{Z}$, hence they must be constant. Having already showed that S_0 is phase-rotating, we have that $\varphi^\pm(1) = \varphi^\pm(0) = \pm 2\pi$, which finally allows us to conclude that also S is phase-rotating. \square

4. Generalizations: generic coalescing for $n \times n$ matrices. Multiple coalescing of eigenvalues

Let $A \in \mathcal{C}^1(\Omega, \mathbb{C}^{n \times n})$ be Hermitian. Let $\lambda_1, \dots, \lambda_n$ be its continuous eigenvalues, labeled so that $\lambda_1(\xi) \leq \lambda_2(\xi) \leq \dots \leq \lambda_n(\xi)$ for all $\xi \in \Omega$.

We say that ξ is a *coalescing point* for A if we have $\lambda_k(\xi) = \lambda_{k+1}(\xi)$, for some $k = 1, \dots, n-1$.

Below, we consider the case when a pair of eigenvalues coalesce in a *generic way*. To properly define this situation, we will need the fundamental result below, adapted from [11, 17], which will allow us to isolate, locally, a coalescing pair of eigenvalues from the rest of the spectrum.

Theorem 4.1 (Block-diagonalization). *Let R be a closed pluri-rectangular region in \mathbb{R}^3 . Suppose that the eigenvalues of $A \in \mathcal{C}^k(R, \mathbb{C}^{n \times n})$, $k \geq 1$, can be labeled so that they belong to two disjoint sets for all $\xi \in R$: $\lambda_1(\xi), \dots, \lambda_p(\xi)$ in $\Lambda_1(\xi)$ and $\lambda_{p+1}(\xi), \dots, \lambda_n(\xi)$ in $\Lambda_2(\xi)$, $\Lambda_1(\xi) \cap \Lambda_2(\xi) = \emptyset$ for all $\xi \in R$. Then, there exists $M \in \mathcal{C}^k(R, \mathbb{C}^{n \times n})$, invertible, such that*

$$M^{-1}(\xi)A(\xi)M(\xi) =: S(\xi) = \begin{bmatrix} S_1(\xi) & 0 \\ 0 & S_2(\xi) \end{bmatrix}, \quad \text{for all } \xi \in R,$$

where $S_1 \in \mathcal{C}^k(R, \mathbb{C}^{p \times p})$, $S_2 \in \mathcal{C}^k(R, \mathbb{C}^{(n-p) \times (n-p)})$, and the eigenvalues of $S_j(\xi)$ are those in $\Lambda_j(\xi)$, for all $\xi \in R$ and $j = 1, 2$.

Remarks 4.2. The following facts are easily proven in a similar way to what was done in [7, Remark 1.5 and Theorem 1.6].

- (i) The Theorem above can be refined to an arbitrary number of disjoint groups of eigenvalues, resulting in a block-diagonal matrix S having several blocks, one for each group. Simple eigenvalues lead to 1-dimensional blocks, with the possibility of a full smooth diagonalization of A in case all eigenvalues are distinct in R .
- (ii) If A is Hermitian, which is the case of interest for us, then M can be chosen to be unitary.
- (iii) In general, M (and consequently the S_j 's) is not uniquely determined. In the Hermitian case, a unitary M is determined only up to right-multiplication by a smooth block-diagonal unitary matrix having the same block-structure as S .

With the aid of Theorem 4.1, we are ready to define a generic coalescing.

Definition 4.3. Let $A \in \mathcal{C}^k(\Omega, \mathbb{C}^{n \times n})$, $k \geq 1$, be Hermitian with continuous eigenvalues $\lambda_1(\xi), \dots, \lambda_n(\xi)$, $\xi \in \Omega$, satisfying

$$\lambda_1(\xi) < \lambda_2(\xi) < \dots < \lambda_h(\xi) \leq \lambda_{h+1}(\xi) < \dots < \lambda_n(\xi), \quad \forall \xi \in \Omega$$

and

$$\lambda_h(\xi) = \lambda_{h+1}(\xi) \iff \xi = \xi_0 \in \Omega.$$

Let R be a pluri-rectangular region $R \subseteq \Omega$ containing ξ_0 in its interior. Moreover, let

- (1) $U \in \mathcal{C}^k(R, \mathbb{C}^{n \times n})$ be a \mathcal{C}^k unitary function achieving the reduction (see Theorem 4.1 and Remarks 4.2)

$$U^*(\xi)A(\xi)U(\xi) = \begin{bmatrix} \Lambda_1(\xi) & 0 & 0 \\ 0 & P(\xi) & 0 \\ 0 & 0 & \Lambda_2(\xi) \end{bmatrix}, \quad \forall \xi \in R,$$

where $\Lambda_1 \in \mathcal{C}^k(R, \mathbb{C}^{(h-1) \times (h-1)})$ and $\Lambda_2 \in \mathcal{C}^k(R, \mathbb{C}^{(n-h-1) \times (n-h-1)})$, such that, for all $\xi \in R$,

$$\Lambda_1(\xi) = \text{diag}(\lambda_1(\xi), \dots, \lambda_{h-1}(\xi)), \quad \Lambda_2(\xi) = \text{diag}(\lambda_{h+2}(\xi), \dots, \lambda_n(\xi)).$$

Moreover, $P \in \mathcal{C}^k(R, \mathbb{C}^{2 \times 2})$ is Hermitian, with eigenvalues $\lambda_h(\xi)$, $\lambda_{h+1}(\xi)$ for each $\xi \in R$;

- (2) for all $\xi \in R$, write $P(\xi) = \begin{bmatrix} a(\xi) & b(\xi) + ic(\xi) \\ b(\xi) - ic(\xi) & d(\xi) \end{bmatrix}$, and define the function F as in (3.1),
for $\xi \in R$.

Then, we call ξ_0 a *generic coalescing point of eigenvalues* for A if the Jacobian $DF(\xi_0)$ is nonsingular.

Remark 4.4. Notice that the definition of generic coalescing point is tantamount to require that – locally – the zero-set of F is given by three surfaces ($a - d = 0$, $b = 0$, $c = 0$) which intersect transversally at ξ_0 . In other words, for a coalescing point of eigenvalues to be a generic coalescing point is a generic property.

Before proceeding, we must show that Definition 4.3 is independent of the \mathcal{C}^k unitary function U that achieves the block diagonalization of Definition 4.3. We will resort to an explicit verification.

Theorem 4.5. Let A be as in Definition 4.3 and let U be a given \mathcal{C}^k unitary function achieving the reduction:

$$U^*(\xi)A(\xi)U(\xi) = \begin{bmatrix} \Lambda_1(\xi) & 0 & 0 \\ 0 & P(\xi) & 0 \\ 0 & 0 & \Lambda_2(\xi) \end{bmatrix}, \quad \forall \xi \in R,$$

as in Definition 4.3, with $P(\xi) = \begin{bmatrix} a(\xi) & b(\xi) + ic(\xi) \\ b(\xi) - ic(\xi) & d(\xi) \end{bmatrix}$. Let $V \in \mathcal{C}^k(R, \mathbb{C}^{n \times n})$ be another unitary function achieving a similar block reduction:

$$V^*(\xi)A(\xi)V(\xi) = \begin{bmatrix} \Lambda_1(\xi) & 0 & 0 \\ 0 & \tilde{P}(\xi) & 0 \\ 0 & 0 & \Lambda_2(\xi) \end{bmatrix}, \quad \forall \xi \in R.$$

Write $\tilde{P}(\xi) = \begin{bmatrix} \alpha(\xi) & \beta(\xi) + i\gamma(\xi) \\ \beta(\xi) - i\gamma(\xi) & \delta(\xi) \end{bmatrix}$, which is of course similar to P , and consider the function

$$G = \begin{bmatrix} \frac{1}{2}(\alpha - \delta) \\ \beta \\ \gamma \end{bmatrix}, \text{ which has a unique zero (the unique coalescing point of eigenvalues) at } \xi_0. \text{ Then, } DF(\xi_0)$$

is nonsingular if and only if $DG(\xi_0)$ is.

Proof. We know (see Remark 4.2-(iii)) that $\tilde{P}(\xi) = Q^*(\xi)P(\xi)Q(\xi)$, where $Q \in C^k(R, \mathbb{C}^{2 \times 2})$ is unitary. Write $Q(\xi) = [q_1(\xi), q_2(\xi)]$, for all $\xi \in R$. We also have the following equalities:

$$q_j^*(\xi)q_j(\xi) = 1 \Rightarrow q_j^*(\xi)(\partial_{x,y,z}q_j(\xi)) + (\partial_{x,y,z}q_j(\xi))^*q_j(\xi) = 0, \quad j = 1, 2, \quad \forall \xi \in R,$$

and

$$q_1^*(\xi)q_2(\xi) = 0 \Rightarrow q_1^*(\xi)(\partial_{x,y,z}q_2(\xi)) + (\partial_{x,y,z}q_1(\xi))^*q_2(\xi) = 0, \quad \forall \xi \in R.$$

As a consequence of these relations, and since $P(\xi_0)$ is a scalar multiple of the identity, direct computation shows that

$$\nabla(\alpha - \delta)|_{\xi_0} = \begin{bmatrix} q_1^*P_xq_1 - q_2^*P_xq_2 & q_1^*P_yq_1 - q_2^*P_yq_2 & q_1^*P_zq_1 - q_2^*P_zq_2 \end{bmatrix}_{\xi_0},$$

$$\nabla\beta|_{\xi_0} = \frac{1}{2} \begin{bmatrix} q_1^*P_xq_2 + q_2^*P_xq_1 & q_1^*P_yq_2 + q_2^*P_yq_1 & q_1^*P_zq_2 + q_2^*P_zq_1 \end{bmatrix}_{\xi_0},$$

$$\nabla\gamma|_{\xi_0} = \frac{1}{2i} \begin{bmatrix} q_1^*P_xq_2 - q_2^*P_xq_1 & q_1^*P_yq_2 - q_2^*P_yq_1 & q_1^*P_zq_2 - q_2^*P_zq_1 \end{bmatrix}_{\xi_0},$$

and therefore $DG(\xi_0)$ is nonsingular if and only if the following matrix is nonsingular:

$$M_1 := \begin{bmatrix} \nabla(\alpha - \delta) \\ \nabla(\beta + i\gamma) \\ \nabla(\beta - i\gamma) \end{bmatrix}_{\xi_0} = \begin{bmatrix} q_1^*P_xq_1 - q_2^*P_xq_2 & q_1^*P_yq_1 - q_2^*P_yq_2 & q_1^*P_zq_1 - q_2^*P_zq_2 \\ q_1^*P_xq_2 & q_1^*P_yq_2 & q_1^*P_zq_2 \\ q_2^*P_xq_1 & q_2^*P_yq_1 & q_2^*P_zq_1 \end{bmatrix}_{\xi_0},$$

whereas $DF(\xi_0)$ is nonsingular if and only if the following matrix is:

$$M_2 := \begin{bmatrix} (a-d)_x & (a-d)_y & (a-d)_z \\ (b+ic)_x & (b+ic)_y & (b+ic)_z \\ (b-ic)_x & (b-ic)_y & (b-ic)_z \end{bmatrix}_{\xi_0}.$$

Now, we are going to show that $M_1 = MM_2$, with M invertible, and the result will follow.

Let $q_1 = \begin{bmatrix} \sigma \\ \tau \end{bmatrix}$, $q_2 = \begin{bmatrix} \rho \\ \eta \end{bmatrix}$, and let $M = (m_{ij})_{i,j=1}^3$. Lengthy, but simple, calculations give:

$$m_{11} = |\sigma|^2 - |\rho|^2 = -|\tau|^2 + |\eta|^2, \quad m_{12} = \bar{\sigma}\tau - \bar{\rho}\eta, \quad m_{13} = \bar{m}_{12}$$

$$m_{21} = \bar{\sigma}\rho = -\bar{\tau}\eta, \quad m_{22} = \bar{\sigma}\eta, \quad m_{23} = \bar{\tau}\rho, \quad m_{31} = \bar{m}_{21}, \quad m_{32} = \bar{m}_{23}, \quad m_{33} = \bar{m}_{22}.$$

Therefore, explicit computation of $\det(M)$ gives:

$$\det(M) = (|\sigma|^2 + |\rho|^2)(|\sigma|^2|\eta|^2 - \sigma\eta\bar{\tau}\bar{\rho} - \tau\rho\bar{\sigma}\bar{\eta} + |\rho|^2|\tau|^2).$$

The first factor in this determinant is 1, since Q is unitary. The second factor can be recognized as $\det Q \det Q^*$ which is again 1, so the result follows. \square

We are now ready to deal with the case of a coalescing pair of eigenvalues for a $(n \times n)$ function.

Theorem 4.6. Let $A \in C^1(\Omega, \mathbb{C}^{n \times n})$ be Hermitian. Let $\lambda_1(\xi), \lambda_2(\xi), \dots, \lambda_n(\xi)$ be its continuous eigenvalues, with

$$\lambda_1(\xi) < \lambda_2(\xi) < \dots < \lambda_h(\xi) \leq \lambda_{h+1}(\xi) < \dots < \lambda_n(\xi),$$

for all $\xi \in \Omega$. Let $\xi_0 \in \Omega$ be a generic coalescing point for A such that $\lambda_h(\xi_0) = \lambda_{h+1}(\xi_0)$, and suppose ξ_0 is the only coalescing point for A in Ω . Let $S \subset \Omega$ be a 2-sphere. If the interior part of S contains ξ_0 , then S is phase-rotating.

Proof. Let us consider a pluri-rectangle $R \subseteq \Omega$ whose interior part contains ξ_0 , and let $S_0 \subset R$ be a sphere centered at ξ_0 . Let us think of S_0 as endowed with the standard covering $\{C_s\}_{s \in [0,1]}$ for spheres, i.e. smoothly parametrized in terms of latitude/longitude $(s, t) \in [0, 1]^2$.

In virtue of Theorem 4.1, let us consider a smooth unitary matrix function V such that:

$$V^*(\xi)A(\xi)V(\xi) = \begin{bmatrix} \Lambda(\xi) & 0 \\ 0 & P(\xi) \end{bmatrix}, \quad \text{for all } \xi \in R, \quad (4.1)$$

where $P \in C^1(R, \mathbb{C}^{2 \times 2})$ is Hermitian and $\Lambda \in C^1(R, \mathbb{R}^{(n-2) \times (n-2)})$ is diagonal, with $\text{diag}(\Lambda(\xi)) = (\lambda_1(\xi), \dots, \lambda_{h-1}(\xi), \lambda_{h+2}(\xi), \dots, \lambda_n(\xi))$ for all $\xi \in R$. Let $V = [V_1 V_2]$, with V_1 of size $n \times (n-2)$ and V_2 of size $n \times 2$.

Let us consider the restriction of A to S_0 , write it $A(\xi(s, t)) =: \hat{A}(s, t)$, and similarly we will write $\hat{V}(s, t)$, $\hat{\Lambda}(s, t)$ and $\hat{P}(s, t)$ for $V(\xi(s, t))$, $\Lambda(\xi(s, t))$ and $P(\xi(s, t))$. In this notation, we can rewrite Eq. (4.1) in terms of parameters s and t :

$$\hat{V}^*(s, t)\hat{A}(s, t)\hat{V}(s, t) = \begin{bmatrix} \hat{\Lambda}(s, t) & 0 \\ 0 & \hat{P}(s, t) \end{bmatrix}, \quad \text{for all } (s, t) \in [0, 1]^2,$$

where all matrices are now 1-periodic with respect to t , for all $s \in [0, 1]$.

Similarly to how is done in Remark 2.2, it is possible to construct a smooth eigendecomposition:

$$Q^*(s, t)\hat{P}(s, t)Q(s, t) = \begin{bmatrix} \hat{\lambda}_h(s, t) & 0 \\ 0 & \hat{\lambda}_{h+1}(s, t) \end{bmatrix}, \quad \text{for all } (s, t) \in [0, 1]^2, \quad (4.2)$$

with $Q = [q_h \ q_{h+1}]$ unitary, such that $q_j(s, \cdot)$ is 1-periodic for all $s \in [0, 1]$ and $j = h, h+1$. By Theorem 3.1, S_0 is phase-rotating for P , so, as a consequence of Lemma 2.1, we have that the following (smooth) integral function:

$$G_j(s) = \int_0^1 q_j^*(s, t) \partial_t q_j(s, t) dt$$

undergoes an increment of 2π or -2π over $[0, 1]$, for $j = h, h+1$.

Now let us consider the following eigenvector of A associated to λ_j :

$$w_j(s, t) = \hat{V}_2(s, t)q_j(s, t), \quad \text{for all } (s, t) \in [0, 1]^2, \quad j = h, h+1,$$

and let us use formula (2.2) to compute the increment in Berry phase associated to the Γ -covering under consideration. Let:

$$Z_j(s) = \int_0^1 w_j^*(s, t) \partial_t w_j(s, t) dt, \quad \text{for all } s \in [0, 1], \quad j = h, h+1.$$

We have:

$$Z_j(s) = \int_0^1 q_j^*(s, t) \widehat{V}_2^*(s, t) \partial_t \widehat{V}_2(s, t) q_j(s, t) dt + G_j(s), \text{ for all } s \in [0, 1], j = h, h + 1.$$

Now we simply observe that $\widehat{V}_2(0, t)$ and $\widehat{V}_2(1, t)$ are constant with respect to t (since they are eigendecompositions at points, the South and North poles), so the first term on the right-hand side of the equation above is a smooth function of s that assumes value zero for $s = 0, 1$. It follows that $Z_j(1) - Z_j(0) = G_j(1) - G_j(0)$, so S_0 is phase-rotating for A . Finally, the same homotopy argument used in the proof of Theorem 3.1 allows us to conclude that also S is phase-rotating for A . \square

Remark 4.7. In the proof above, we have restricted our attention to the eigenvectors of A associated to the coalescing pair of eigenvalues. However, similar considerations could have been applied to the remaining eigenvectors, leading to the conclusion that the Berry phase functions associated to the non-coalescing eigenvalues do not undergo any increment as a Γ -covering swipes S . A straightforward, but nonetheless fundamental, consequence of this fact is the following theorem.

Theorem 4.8. *Let $A \in C^1(\Omega, \mathbb{C}^{n \times n})$ be Hermitian. Let $S \subseteq \Omega$ be a 2-sphere. Suppose all eigenvalues of A are distinct on Ω . Then S is phase-preserving.*

From Theorem 4.8 it follows immediately the following fundamental result, which goes in the opposite direction of Theorem 4.6. In essence, this is the result of Stone (see [20]).

Corollary 4.9. *Let $A \in C^1(\Omega, \mathbb{C}^{n \times n})$ be Hermitian. Let $S \subseteq \Omega$ be a 2-sphere. Suppose S is phase-rotating. Then there is a coalescing point for A inside S .*

Our next task is to consider the case when inside the region Ω there are several generic coalescing points. The following result will be useful in identifying the cases which can occur, and it is of independent interest. It establishes a conservation property satisfied by the sum of all the (smooth) Berry phases associated to the eigenvalues of a Hermitian matrix A as the loops of a Γ -covering swipe a 2-sphere S .

Theorem 4.10. *Let $S \subset \Omega$ be a 2-sphere and $\{\Gamma_s\}_{s \in [0, 1]}$ be a Γ -covering for S . Let $A \in C^1(\Omega, \mathbb{C}^{n \times n})$ be Hermitian, with distinct eigenvalues $\lambda_1 < \dots < \lambda_n$ on S . For $j = 1, \dots, n$, let $\alpha_j(s)$ be the Berry phase function associated to λ_j . Then we have that:*

$$\sum_{j=1}^n \alpha_j(s) = 0, \text{ for all } s \in [0, 1].$$

Proof. Let (s, t) be the coordinates system for S associated to $\{\Gamma_s\}_{s \in [0, 1]}$. Let $Q^* A Q = \Lambda$ be a smooth Schur decomposition on $[0, 1]^2$ such that $Q(s, t)$ is 1-periodic in t for all $s \in [0, 1]$. Let q_j denote the j th column of Q . Then, as a consequence of Lemma 2.1, we have the following equality:

$$\sum_{j=1}^n \alpha_j(s) = \sum_{j=1}^n i \int_0^1 q_j^*(s, t) \partial_t q_j(s, t) dt = i \int_0^1 \text{trace}(Q^*(s, t) \partial_t Q(s, t)) dt.$$

Let us recall the following formula for the derivative of the logarithm of the determinant of an invertible matrix valued function $Y(t)$ (e.g., see [13, p. 127]):

$$\frac{d}{dt} \log(\det Y(t)) = \text{trace}(Y^{-1} \frac{d}{dt} Y).$$

Next, observe that as a special case of this formula we can rewrite

$$\text{trace}(Q^*(s, t) \partial_t Q(s, t)) = \text{trace}(Q^{-1}(s, t) \partial_t Q(s, t)) = \partial_t \log(\det Q(s, t)).$$

Therefore, we obtain

$$\sum_{j=1}^n \alpha_j(s) = i \int_0^1 \partial_t (\log \det(Q(s, t))) dt = 0. \quad \square$$

Next, we consider the case of two distinct generic coalescing points inside Ω , relative to either different pairs of eigenvalues or the same pair.

Theorem 4.11. *Let $A \in C^1(\Omega, \mathbb{C}^{n \times n})$ be Hermitian. Let $\lambda_1(\xi), \dots, \lambda_n(\xi)$ be its continuous eigenvalues, labeled in ascending order. Suppose they are distinct for all $\xi \in \Omega$, except for two generic coalescing points $\xi_1, \xi_2 \in \Omega$, $\xi_1 \neq \xi_2$, such that:*

$$\lambda_{h_1}(\xi) = \lambda_{h_1+1}(\xi) \iff \xi = \xi_1, \quad \lambda_{h_2}(\xi) = \lambda_{h_2+1}(\xi) \iff \xi = \xi_2$$

with $h_1 \leq h_2$. Let $S \subset \Omega$ be a 2-sphere and $\{\Gamma_s\}_{s \in [0,1]}$ be a Γ -covering for S . For each $j = 1, \dots, n$, let $\alpha_j(s)$ be the Berry phase function associated to λ_j . Suppose the interior part of S contains ξ_1 and ξ_2 . Then we have one of the following three possibilities:

$$\begin{aligned} \text{(i)} \quad & (\alpha_{h_1}(1), \alpha_{h_1+1}(1), \alpha_{h_2}(1), \alpha_{h_2+1}(1)) = \begin{cases} \pm(2\pi, 2\pi, -2\pi, -2\pi) \\ \pm(2\pi, -2\pi, 2\pi, -2\pi) & \text{if } h_1 + 1 < h_2 \\ \pm(-2\pi, 2\pi, 2\pi, -2\pi) \end{cases} \\ \text{(ii)} \quad & (\alpha_{h_1}(1), \alpha_{h_1+1}(1), \alpha_{h_1+2}(1)) = \begin{cases} \pm(2\pi, -4\pi, 2\pi) \\ \pm(2\pi, 0, -2\pi) \end{cases} & \text{if } h_1 + 1 = h_2 \\ \text{(iii)} \quad & (\alpha_{h_1}(1), \alpha_{h_1+1}(1)) = \begin{cases} (0, 0) \\ \pm(4\pi, -4\pi) \end{cases} & \text{if } h_1 = h_2. \end{aligned} \tag{4.3}$$

Proof. The idea of the proof is to “cut” the 2-sphere S through a meridian in two regions which are further smoothly embedded in two 2-spheres, having only this meridian in common, and so that the points ξ_1 and ξ_2 will each belong to one of these 2-spheres.

So, we construct a 2-sphere $\tilde{S} \subset \mathbb{R}^3$ that satisfies the following properties (see Fig. 3):

- \tilde{S} is contained in the compact region bounded by S ,
- $\tilde{S} \cap S = \Gamma_{\tilde{s}}$ for a unique $\tilde{s} \in (0, 1)$,
- ξ_1 and ξ_2 belong each to a different connected component of the set of points of Ω that are interior to S and exterior to \tilde{S} .

To verify that this construction is always possible, consider the following. Let S be a 2-sphere, f be an embedding such that $S = f(\mathbb{S}^2)$, and B be the unit ball in \mathbb{R}^3 . By virtue of the C^k -Schönflies Theorem, f can be extended to a smooth embedding $\tilde{f} : B \rightarrow \mathbb{R}^3$ such that $\tilde{f}|_{\mathbb{S}^2} \equiv f$. Let $D = \{\xi = (x, y, z) \in B : z = 0\}$. Without loss of generality, we can assume that $f^{-1}(\xi_1)$ and $f^{-1}(\xi_2)$ belong to distinct connected components of $B \setminus D$ (if this is not the case, we could simply replace f by $f \circ g$ where g is an appropriate rigid rotation of \mathbb{S}^2 about the origin). Now consider the following family of ellipsoids:

$$\mathcal{E}_a = \left\{ \xi = (x, y, z) \in \mathbb{R}^3 : x^2 + y^2 + \left(\frac{z}{a}\right)^2 = 1 \right\}$$

with $0 < a < 1$. Pick $a > 0$ small enough such that $f^{-1}(\xi_1)$ and $f^{-1}(\xi_2)$ are exterior to \mathcal{E}_a , and define $\tilde{S} = \tilde{f}(\mathcal{E}_a)$. Clearly \tilde{S} is a 2-sphere that satisfies all the required properties.

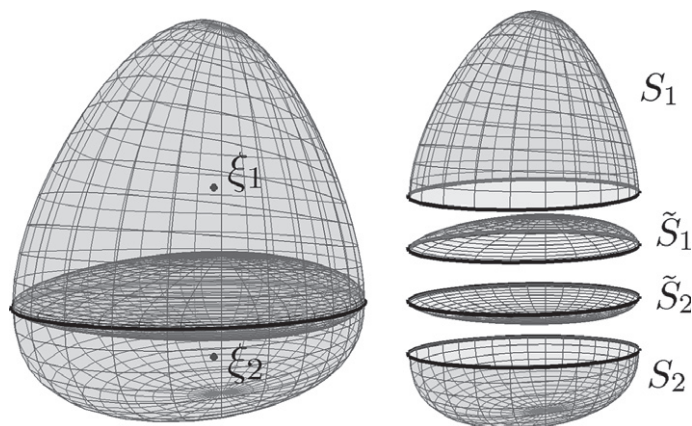


Fig. 3. Reference picture for proof of Theorem 4.11.

Let us consider a Γ -covering $\{\tilde{\Gamma}_s\}_{s \in [0,1]}$ for \tilde{S} such that $\Gamma_{\tilde{s}} = \tilde{\Gamma}_{\tilde{s}}$. The loop $\Gamma_{\tilde{s}}$ separates S into two surfaces with boundary:

$$S_1 = \bigcup_{s \in [0, \tilde{s}]} \Gamma_s, \quad S_2 = \bigcup_{s \in [\tilde{s}, 1]} \Gamma_s,$$

and similarly for \tilde{S} :

$$\tilde{S}_1 = \bigcup_{s \in [0, \tilde{s}]} \tilde{\Gamma}_s, \quad \tilde{S}_2 = \bigcup_{s \in [\tilde{s}, 1]} \tilde{\Gamma}_s.$$

Now, \tilde{S}_1 (and analogously for \tilde{S}_2) can be joined smoothly with either S_1 or S_2 , along $\Gamma_{\tilde{s}}$, in order to obtain two 2-spheres. Without loss of generality, let us assume that $S_1 \cup \tilde{S}_2$ is the 2-sphere whose interior part contains ξ_1 , and that $\tilde{S}_1 \cup S_2$ is the 2-sphere whose interior part contains ξ_2 ; again, see Fig. 3.

Let us now consider the following continuous family of loops:

$$\Delta_s = \begin{cases} \Gamma_s & \text{for } 0 \leq s \leq \tilde{s} \\ \tilde{\Gamma}_s & \text{for } \tilde{s} \leq s \leq 1 \\ \tilde{\Gamma}_{2-s} & \text{for } 1 \leq s \leq 2 \\ \tilde{\Gamma}_{s-2} & \text{for } 2 \leq s \leq 2 + \tilde{s} \\ \Gamma_{s-2} & \text{for } 2 + \tilde{s} \leq s \leq 3 \end{cases}.$$

Note that we have:

$$S_1 \cup \tilde{S}_2 = \bigcup_{s \in [0,1]} \Delta_s, \quad \tilde{S} = \bigcup_{s \in [1,2]} \Delta_s, \quad \tilde{S}_1 \cup S_2 = \bigcup_{s \in [2,3]} \Delta_s. \quad (4.4)$$

Just like before, consider the n continuous Berry phase functions $\beta_j : s \in [0, 3] \mapsto \beta_j(s) \in \mathbb{R}$, with $\beta_j(0) = 0$ for all $j = 1, \dots, n$, where each $\beta_j(s)$ corresponds, modulo 2π , to the Berry phase associated to λ_j along the loop Δ_s .

By applying Theorems 4.6 and 4.8 to the three 2-spheres in (4.4), we have that $S_1 \cup \tilde{S}_2$ and $\tilde{S}_1 \cup S_2$ are phase-rotating whereas \tilde{S} is phase-preserving. Theorem 4.6, and Remark 4.7, allow us to recast this information in terms of properties of the maps β_j 's:

$$\begin{aligned}\beta_j(1) &= \beta_j(0) \pm 2\pi, \quad \text{for } j = h_1, h_1 + 1, \\ \beta_j(3) &= \beta_j(2) \pm 2\pi, \quad \text{for } j = h_2, h_2 + 1, \\ \beta_j(s+1) &= \beta_j(s), \quad \text{in all other cases with } s = 0, 1, 2 \text{ and } j = 1, \dots, n.\end{aligned}$$

Now we simply need to observe that the loops $\{\Delta_s\}_{s \in [\bar{s}, 2+\bar{s}]}$ have no effect on the accumulation of Berry phase for the β_j 's, i.e. $\beta_j(\bar{s}) = \beta_j(2 + \bar{s})$ for all $j = 1, \dots, n$, and hence $\alpha_j(s) = \beta_j(2 + s)$ for all $j = 1, \dots, n$ and $s \in [\bar{s}, 1]$. In particular, we have:

$$\alpha_j(1) = \beta_j(3), \quad \text{for all } j = 1, \dots, n.$$

This gives

$$\begin{aligned}\text{(i)} \quad & \alpha_{h_1}(1), \alpha_{h_1+1}(1), \alpha_{h_2}(1), \alpha_{h_2+1}(1) \in \{\pm 2\pi\} && \text{if } h_1 + 1 < h_2 \\ \text{(ii)} \quad & \alpha_{h_1}(1), \alpha_{h_1+2}(1) \in \{\pm 2\pi\}, \alpha_{h_1+1}(1) \in \{0, \pm 4\pi\} && \text{if } h_1 + 1 = h_2 \\ \text{(iii)} \quad & \alpha_{h_1}(1), \alpha_{h_1+1}(1) \in \{0, \pm 4\pi\} && \text{if } h_1 = h_2.\end{aligned}$$

But, by virtue of Theorem 4.10, there are fewer possibilities than what this expression might suggest, namely only those of (4.3). \square

Remark 4.12. As a consequence of Theorem 4.11, a 2-sphere that contains two (distinct) generic coalescing points for the same pair of eigenvalues may, or may not, be phase-rotating. In other words, Theorem 4.11 shows that the impact of each (of two) generic coalescing points leads to an accumulation of the Berry phases in a “nice”, though not completely predictable, way.

We are now ready for the general result, which considers what happens when there are several generic coalescing points, relative to different or repeated pairs of eigenvalues.

Theorem 4.13. Let $A \in \mathcal{C}^1(\Omega, \mathbb{C}^{n \times n})$ be Hermitian. Let $\lambda_1(\xi), \dots, \lambda_n(\xi)$ be its continuous eigenvalues, labeled in ascending order. Suppose that, for any $j = 1, \dots, n-1$, we have:

$$\lambda_j = \lambda_{j+1}$$

solely at d_j distinct generic coalescing points in Ω , and that there is a total of $N = \sum_{j=1}^{n-1} d_j$ distinct coalescing points for A in Ω . Let $S \subset \Omega$ be a 2-sphere and $\{\Gamma_s\}_{s \in [0,1]}$ be a Γ -covering for S . For each $j = 1, \dots, n$, let $\alpha_j(s)$ be the Berry phase function associated to λ_j . Suppose the interior part of S contains all coalescing points for A in Ω . Then we have that:

$$\begin{aligned}\text{(i)} \quad & \alpha_1(1) = 0 \text{ (resp. } 2\pi) \pmod{4\pi} \text{ if } d_1 \text{ is even (resp. odd)} \\ \text{(ii)} \quad & \alpha_j(1) = 0 \text{ (resp. } 2\pi) \pmod{4\pi} \text{ if } d_{j-1} + d_j \text{ is even (resp. odd)} \\ & \text{and } j = 2, \dots, n-1 \\ \text{(iii)} \quad & \alpha_n(1) = 0 \text{ (resp. } 2\pi) \pmod{4\pi} \text{ if } d_{n-1} \text{ is even (resp. odd)}\end{aligned}$$

with $|\alpha_1(1)| \leq 2d_1\pi$, $|\alpha_n(1)| \leq 2d_{n-1}\pi$, and $|\alpha_j(1)| \leq 2(d_{j-1} + d_j)\pi$ for $j = 2, \dots, n-1$.

Proof. We will prove the result by induction on the total number of coalescing points for A in Ω . The argument will follow closely the one used in the proof of Theorem 4.11, to which we refer for notation.

Let $\tilde{S} \subset R$ be a 2-sphere that separates, similarly to the proof of Theorem 4.11, the interior of S into three regions in such a way that all coalescing points for A are exterior to \tilde{S} , and one coalescing point (call it ξ_N) belongs to a different region with respect to the remaining $N-1$ coalescing points. Similarly to the proof of Theorem 4.11, let us define $\{\tilde{\Gamma}_s\}_{s \in [0,1]}$, $\tilde{\Gamma}_{\tilde{s}}$, $S_1, S_2, \tilde{S}_1, \tilde{S}_2$, $\{\Delta_s\}_{s \in [0,3]}$ and β_j 's, for $j = 1, \dots, n$.

Now, the claim is true for 2-spheres enclosing 0, 1 or 2 coalescing points, see Theorems 4.8, 4.6 and 4.11. Let us assume that the claim is true for 2-spheres enclosing $N - 1$ distinct coalescing points. Without loss of generality, assume that ξ_N is a coalescing point such that $\lambda_{n-1}(\xi_N) = \lambda_n(\xi_N)$. By induction hypothesis, we have:

- (i) $\beta_1(1) = 0 \text{ (resp. } 2\pi) \pmod{4\pi}$ if d_1 is even (resp. odd)
- (ii) $\beta_j(1) = 0 \text{ (resp. } 2\pi) \pmod{4\pi}$ if $d_{j-1} + d_j$ is even (resp. odd)
and $j = 2, \dots, n - 2$
- (iii) $\beta_{n-1}(1) = 0 \text{ (resp. } 2\pi) \pmod{4\pi}$ if $d_{n-2} + d_{n-1} - 1$ is even (resp. odd)
- (iv) $\beta_n(1) = 0 \text{ (resp. } 2\pi) \pmod{4\pi}$ if $d_{n-1} - 1$ is even (resp. odd)

with $|\beta_1(1)| \leq 2d_1\pi$, $|\beta_j(1)| \leq 2(d_{j-1} + d_j)\pi$ for $j = 2, \dots, n - 2$, $|\beta_{n-1}(1)| \leq 2(d_{n-2} + d_{n-1} - 1)\pi$ and $|\beta_n(1)| \leq 2(d_{n-1} - 1)\pi$.

Subsequently, by applying, in the given order, Theorems 4.8 and 4.6, we obtain:

$$\begin{aligned}\beta_j(2) &= \beta_j(1) \quad \text{for } j = 1, \dots, n \\ \beta_j(3) &= \beta_j(2) \quad \text{for } j = 1, \dots, n - 2 \\ \beta_j(3) &= \beta_j(2) \pm 2\pi \quad \text{for } j = n - 1, n.\end{aligned}$$

Finally, recalling that $\alpha_j(1) = \beta_j(3)$, for all $j = 1, \dots, n$, we sum up all the information above as:

- (i) $\alpha_1(1) = 0 \text{ (resp. } 2\pi) \text{ modulo } 4\pi$ if d_1 is even (resp. odd)
- (ii) $\alpha_j(1) = 0 \text{ (resp. } 2\pi) \text{ modulo } 4\pi$ if $d_{j-1} + d_j$ is even (resp. odd)
and $j = 2, \dots, n - 2$
- (iii) $\alpha_{n-1}(1) = 2\pi \text{ (resp. } 0) \text{ modulo } 4\pi$ if $d_{n-2} + d_{n-1} - 1$ is even (resp. odd)
- (iv) $\alpha_n(1) = 2\pi \text{ (resp. } 0) \text{ modulo } 4\pi$ if $d_{n-1} - 1$ is even (resp. odd)

with $|\beta_1(1)| \leq 2d_1\pi$, $|\beta_j(1)| \leq 2(d_{j-1} + d_j)\pi$ for $j = 2, \dots, n - 1$ and $|\beta_n(1)| \leq 2d_{n-1}\pi$. Now we simply observe that the points (i)–(iv) and the bounds on $|\beta_j(1)|$ show that the result is true for N points, and the theorem follows. \square

5. Nongeneric coalescings: what to expect

The following examples show some situations which can occur when there are non-generic coalescing points. In particular, we see how the results of Sections 3 and 4 can be violated.

In the first example, we have a Hermitian matrix function A with a unique coalescing point (non-generic) and a 2-sphere S that is phase-preserving for A .

Example 5.1. Let $\varphi \in C^1([0, +\infty), [0, 1])$ be such that:

$$\varphi(t) = 1 \text{ for } t \leq t_1, \quad \varphi(t) = 0 \text{ for } t \geq t_2, \quad \varphi \text{ is strictly decreasing on } [t_1, t_2],$$

with $0 < t_1 < t_2 < 1$. Let $f(\xi) = \varphi(x^2 + y^2 + z^2)$, for all $\xi = (x, y, z) \in \mathbb{R}^3$. For any $\varepsilon \in \mathbb{R}$, let:

$$A_\varepsilon(\xi) = \begin{bmatrix} x^2 & y + iz \\ y - iz & -x^2 \end{bmatrix} + f(x, y, z) \begin{bmatrix} \varepsilon & 0 \\ 0 & -\varepsilon \end{bmatrix},$$

for all $\xi \in \mathbb{R}^3$. Clearly, we have $A_\varepsilon \in C^1(\mathbb{R}^3, \mathbb{C}^{2 \times 2})$ Hermitian, for all ε . Now observe that:

- there exists a unique coalescing point for A_0 in \mathbb{R}^3 : $\xi_0 = (0, 0, 0)$; furthermore, ξ_0 is a non-generic coalescing point ($\text{rank } DF(\xi_0) = 2$, where F is defined in (3.1));
- for any $\varepsilon > 0$, there are no coalescing points for A_ε in \mathbb{R}^3 ;
- for any $\varepsilon < 0$, there are precisely two (distinct) coalescing points for A_ε in \mathbb{R}^3 ; both are generic coalescing points.

Let us consider the 2-sphere \mathbb{S}^2 . In virtue of Theorem 4.8, \mathbb{S}^2 is phase-preserving for all A_ε with $\varepsilon > 0$. On the other hand, all matrix functions A_ε coincide on $\{(x, y, z) \in \mathbb{R}^3 : x^2 + y^2 + z^2 \geq t_2\}$, and in particular on \mathbb{S}^2 ; therefore \mathbb{S}^2 must be phase-preserving also for all A_ε with $\varepsilon \leq 0$ (but small enough so that \mathbb{S}^2 still encloses the coalescing points). In particular, we have that \mathbb{S}^2 is phase-preserving for A_0 . \square

The above example highlights that a non-generic coalescing point may go undetected by the criteria presented in Sections 3 and 4 of this work. It is easy to construct more instances of non-generic coalescing points analogously to the above. For example, by considering suitable perturbations of the matrices

$$A(\xi) = \begin{bmatrix} x^p & y + iz \\ y - iz & -x^p \end{bmatrix}$$

with $p \geq 3$ integer, for which \mathbb{S}^2 would be phase-preserving (respectively, phase-rotating) whenever p is even (respectively, odd).

Our second example exhibits a different kind of non-generic coalescing points, an infinity of them, all lying on a surface.

Example 5.2. Let $A_\varepsilon \in C^1(\mathbb{R}^3, \mathbb{C}^{2 \times 2})$ be defined as follows:

$$A_\varepsilon(\xi) = \begin{bmatrix} x^2 + y^2 + z^2 - \varepsilon & 0 \\ 0 & -(x^2 + y^2 + z^2 - \varepsilon) \end{bmatrix}, \quad \text{for all } \xi \in \mathbb{R}^3 \text{ and } \varepsilon \in \mathbb{R}.$$

We have that:

- there exist a unique, non-generic, coalescing point for A_0 in \mathbb{R}^3 , namely $\xi_0 = (0, 0, 0)$.
- For any $\varepsilon > 0$, the whole surface $\sqrt{\varepsilon}\mathbb{S}^2$ (i.e. the sphere of radius $\sqrt{\varepsilon}$ centered at the origin) is made of coalescing points for A_ε . Obviously, these points are not isolated, hence not generic.
- For any $\varepsilon < 0$, there are no coalescing points for A_ε in \mathbb{R}^3 .

On the other hand, for all $\varepsilon \in \mathbb{R}$, A_ε is constant over all spheres centered at ξ_0 , therefore the Berry phase associated to any loop that belongs to one of such spheres must be zero. It follows that any sphere centered at ξ_0 is phase-preserving for A_ε . \square

6. Conclusions

In this work, we considered geometrical criteria to detect when a Hermitian function depending on three parameters has coalescing eigenvalues inside a 2-sphere. Our theoretical results translate nicely into numerical methods to locate the points in parameter space where the eigenvalues coalesce; see [6].

In future extensions of the present work, we anticipate considering the case of coalescing singular values of complex valued functions depending on three parameters.

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