QUANTITATIVE $K$-THEORY AND SPIN CHERN NUMBERS

TERRY A. LORING

Abstract. We examine the various indices defined on pairs of almost commuting unitary matrices that can detect pairs that are far from commuting pairs. We do this in two symmetry classes, that of general unitary matrices and that of self-dual matrices, with an emphasis on quantitative results. We determine what values of the norm of the commutator guarantee that the indices are defined, where they are equal, and what quantitative results on the distance to a pair with a different index are possible.

We validate a method of computing spin Chern numbers that was developed with Hastings and only conjectured to be correct. Specifically, the Pfaffian-Bott index can be computed by the “log method” for commutator norms up to a specific constant.

1. Introduction

A natural question regarding a pair of unitary matrices that almost commute is: how close is this to a pair that actually commutes? The answer to this question necessarily involves the $K$-theory of the two-torus. Before we get to new results, let us review how this connection arose.

There is a particularly practical formula for the projection $e$ in $M_2(C(T^2))$ that has rank one and first Chern class one. The formula is similar to that of the Rieffel projections $[21]$ in the irrational rotation algebras, specifically

$$e(z, w) = \begin{bmatrix} f(z) & g(z) + h(z)w \\ g(z) + h(z)\bar{w} & 1 - f(z) \end{bmatrix}$$

where $f$, $g$ and $h$ are certain real functions defined on the unit circle. The straight-forward plan in $[14]$ was to compute the $K$-theory of a $\ast$-homomorphism $\varphi : C(T^2) \rightarrow A$ by examining the associated commuting unitary elements $U = \varphi(u_0)$ and $V = \varphi(v_0)$ of the AF algebra $A$ and the projection

$$\begin{bmatrix} f(V) & g(z) + h(U)U \\ g(V) + U^*h(V) & 1 - f(V) \end{bmatrix}$$

where $u_0$ and $v_0$ are the canonical generating unitaries in $C(T^2)$. This formula applies also to a pair of almost commuting unitary matrices, $U$ and $V$ that approximate $\varphi(u_0)$ and $\varphi(v_0)$, leading not to a projection, but a hermitian matrix with a large gap at zero in its spectrum. The spectrum of $e(U_n, V_n)$ then determines the $K$-theory of $\varphi$, but it was also used in $[14]$ to define the Bott index of the pair $(U_n, V_n)$. This index can distinguish pairs of commuting matrices close to commuting pairs from those that are far from commuting pairs. This fact turned out to be more interesting than the $K$-theory of the specific $\varphi$ being studied at the time.

2000 Mathematics Subject Classification. 19M05, 46L60, 46L80.

Key words and phrases. $K$-theory, topological insulators, time reversal symmetry, $C^*$-algebras, matrices.
There is ambiguity in the choice of $f$, $g$ and $h$. There are other ambiguities, discussed in [3], such that the fact that $h(z)w$ could just as well been interpreted as

$$\frac{1}{2} \{h(V), U\} = \frac{1}{2} (h(V)U + Uh(V)).$$

To get good quantitative results about the distance to the closest commuting pair of unitary matrices, we will select our functions and formulas very carefully.

In 1986 the only numerical computation of the Bott index that was practical involved relatively small matrices where $V$ was diagonal. Today we have from physics [17, 12, 7] large matrices where neither is diagonal. The cost of computing $f(V)$, $g(V)$ and $h(V)$ depends heavily on the choices in the scalar functions on the circle.

We end up with choices for $f$, $g$ and $h$ that are very similar to the smooth functions illustrated in [14], although we don’t select them to have rapidly decreasing Fourier coefficients. We select functions that are well approximated by degree-five trigonometric polynomials and where the Fourier series are relatively easy to calculate.

Soon after the Bott index was introduced, we found in joint work with Exel [6] that a simpler formula based on winding numbers can be used. We only proved that this formula worked for sufficiently small commutator norms. Here we will find a concrete $\delta_0$ so that $\| [U, V]\| \leq \delta_0$ implies the two invariants are equal.

We begin with a survey, and some improved theorems, of the winding number index of [6]. Our expectation is that quantitative results regarding almost commuting matrices will be useful in applications, especially in relation to topological insulators [17, 12, 7].

We follow mathematical conventions, so $U^*$ refers to the conjugate-transpose when $U$ is a matrix. To accommodate time reversal invariance in physics, we need to consider what in physics is called the dual operation,

$$\left[ \begin{array}{cc} A & B \\ C & D \end{array} \right] \overset{\#} = \left[ \begin{array}{cc} D^T & -B^T \\ -C^T & A^T \end{array} \right].$$

Our main result, from the standpoint of physics, is Theorem 6.2. It relates the spin Chern number of a finite system in 2D as follows. As discussed in length in [12], the position operators, assume the geometry of the model is the torus, are two commuting unitary matrices, but the band-compressed position operators are almost commuting matrices acting on low-energy space that are almost unitary. If the signalization of the Hamiltonian is done preserving symmetry, if we start in class AI we end up with matrices $A$ and $B$ so that $A^\sharp = A$ and $B^\sharp = B$ and only have approximate relation

$$AB \approx BA$$

$$A^* A \approx I$$

$$B^* B \approx I$$

If we compute any approximate self-dual logarithm $iK$ of $B$, meaning

$$-\pi \leq K \leq \pi$$

and $K^2 = K$ and $e^{iK} \approx B$, then the spin Chern number of the system will be even or odd depending on the sign of

$$\text{Pf} \left( Q^* \left( \frac{1}{2} \left\{ \frac{1}{\pi} K, U^* \right\} \sqrt{I - \frac{1}{\pi} K^2, U} \right) \right).$$
where $Q$ is a specific matrix discussed below that creates anti-symmetry in the formula so that that Pfaffian makes sense.

Of course the logarithm, as a matrix function, will be discontinuous as we cannot assume anything about the spectrum of $A$ and $B$ beyond Kramers doubling. Put another way, the various self-dual approximate logarithms of $B$ are far apart, so it is not even clear that the sign of the Pfaffian is well defined. There is a separate issue of how to compute approximate logarithms of almost unitary matrices, and how to be sure to get a self-dual output given a self-dual input. That is discussed in a separate paper [15].

In practice, it is feasible to simply compute the unitary parts of $A$ and $B$ before computing further, so

$$U = A (A^*A)^{-\frac{1}{2}}$$

which is unitary and self-dual, as is

$$V = B (B^*B)^{-\frac{1}{2}}.$$  

The comparison of $\|[U, V]\|$ with $\|[A, B]\|$ is not hard. For the rest of the paper we discuss self-dual matrices. We discuss the Pfaffian-Bott index, which depends only on $U$ and $V$ (or $A$ and $B$) but was shown [12, Lemma 5.8] to equal the spin Chern index, at least for large systems and other mild assumptions.

Our results on the Pfaffian-Bott index are quantitative, but the correspondence with spin Chern numbers is not quantitative. This will be possible once certain new quantitative results concerning localization of Wannier functions or concerning approximation by commuting matrices are developed.

Our results are principally stated in terms of unitary matrices. However, the study of almost commuting unitary element of $C^*$-algebras is not that different. We know this because we know that the soft-torus is RFD [2]. We are not prepared to make such a statement about unitary elements in real $C^*$-algebras, in part because the theory of generators and relations for real $C^*$-algebras [23] is still rather new and unfamiliar.

2. The winding number invariant

Given two unitary matrices $U$ and $V$ with $\delta = \|[U, V]\|$, we find

$$\|[VUV^*U^* - I]\| = \|[U, V]\|$$

and so by the spectral theorem

$$\sigma(VUV^*U^*) \subseteq \{ z \in \mathbb{T} | |z - 1| \leq \delta \}.$$  

Thus when $\delta < 2$ we can define $(VUV^*U^*)^t$ for $t$ between 0 and 1, using a branch of $x^t$ with discontinuity on the negative $x$-axis. This is a continuous path of unitary matrices from $I$ to $VUV^*U^*$ and

$$\det(VUV^*U^*) = \det(I) = 1$$

so

$$t \mapsto \det((VUV^*U^*)^t)$$

is a loop on the unit circle. We define $\omega(U, V)$ to be the winding number of this path.

This winding number invariant is very computable. There are a few alternate formulas, including

$$\omega(U, V) = \text{Tr} \left( \frac{1}{2\pi i} \log(VUV^*U^*) \right)$$  

where
which we easily prove: since in some basis \( V U V^* U^* \) is diagonal and unitary,
\[
V U V^* U^* = \begin{pmatrix}
e^{i\theta_1} & \cdots & \cdots & e^{i\theta_n}
\end{pmatrix}
\]
for some \(-\pi < \theta_j < \pi\) and
\[
\text{Tr} \left( \frac{1}{2\pi i} \log (V U V^* U^*) \right) = \frac{1}{2\pi i} \text{Tr} \left( \begin{pmatrix} i\theta_1 & \cdots & \cdots & i\theta_n \\
\end{pmatrix} \right) = \frac{1}{2\pi} \sum \theta_j
\]
and
\[
\text{det} \left( (V U V^* U^*)^t \right) = \text{det} \left( \begin{pmatrix} e^{it\theta_1} & \cdots & \cdots & e^{it\theta_n} \\
\end{pmatrix} \right) = \prod e^{it\theta_j}
\]
and this path has winding number
\[
\omega(U, V) = \frac{1}{2\pi} \sum \theta_j.
\]

**Lemma 2.1.** When \( U \) and \( V \) are commuting unitary matrices, \( \omega(U, V) = 0 \).

*Proof.* In this case the path of determinants is the constant path. \( \Box \)

**Lemma 2.2.** For
\[
U = \begin{pmatrix} 0 & 1 & 1 \\
1 & 0 & 1 \\
1 & \cdots & 0 \\
\end{pmatrix}, \quad V = \begin{pmatrix} e^{i\pi/n} & e^{2i\pi/n} \\
e^{2i\pi/n} & e^{-i\pi/n} \\
\end{pmatrix}
\]
we have \( \omega(U, V) = -1 \).

*Proof.* We find \( V U V^* U^* = e^{-\frac{2\pi i}{n}} I \) and so
\[
\frac{1}{2\pi i} \text{Tr} \left( \log (V U V^* U^*) \right) = \frac{1}{2\pi i} \text{Tr} \left( -\frac{2\pi i}{n} I \right) = -1.
\]
\( \Box \)

It is easy to modify the example in Lemma 2.2 to get a pair of unitary matrices with
\( \| [U, V] \| = \delta \) and \( \omega(U, V) = n \) for any \( 0 < \delta < 2 \) and any \( n \).

**Theorem 2.3.** Consider a pair of unitary matrices with \( \| [U, V] \| = \delta < 2 \). If \( \omega(U, V) \neq 0 \) then the distance to a commuting pair of unitary matrices exceeds 1, meaning
\[
\| U - U_1 \| + \| V - V_1 \| > 1,
\]
whenever \( U_1 \) and \( V_1 \) are unitary matrices with \( U_1 V_1 = V_1 U_1 \). Indeed,
\[
\| U - U_1 \| + \| V - V_1 \| \geq 1 + \sqrt{1 - \frac{1}{4}\delta^2}.
\]

The proof of this will be broken into lemmas and propositions. Theorem 2.3 is a slight improvement on the results obtained with Exel \cite{exel}. 

Figure 2.1. The solid curve shows the minimum radius in the gap at $-1$ in with spectrum of $VU^*V^*$ for unitaries $U$ and $V$, as a function of $\delta = \|[U, V]\|$.

The lower curve show the minimum distance one must go to find a pair with winding number index either undefined or different.

Lemma 2.4. Suppose $\|[U_0, V_0]\| < 2$. If $\|[U_1, V_1]\| < 2$ and

$$\omega(U_0, V_0) \neq \omega(U_1, V_1)$$

then for any path $U_s, V_s$ of unitary matrices, there must be at least one $s_0$ so that

$$\|[U_{s_0}, V_{s_0}]\| = 2.$$  

Proof. We will use a homotopy argument. If no such $s_0$ existed then

$$(s, t) \mapsto \det \left( (V_sU_s^*V_s^*U_s)^t \right)$$

is a homotopy between the path that determines $\omega(U_0, V_0)$ and the path that determines $\omega(U_1, V_1)$. Therefore the winding numbers of these paths are equal. \hfill \Box

Proposition 2.5. Suppose $\|[U, V]\| < 2$. If $\|[U_1, V_1]\| = 2$ or if $\|[U_1, V_1]\| < 2$ and

$$\omega(U_1, V_1) \neq \omega(U, V)$$

then

$$\|U - U_1\| + \|V - V_1\| \geq \sqrt{1 - \frac{1}{4} \|[U, V]\|^2 + \sqrt{1 - \frac{1}{4} \|[U_1, V_1]\|^2}}.$$ 

Proof. The general case follows from the case $\|[U_1, V_1]\| = 2$ by Lemma 2.4. Since this invariant in zero for commuting pairs, this proposition implies Theorem 2.3.

Since $-1$ is in the spectrum of $V_1U_1V_1^*U_1^*$ then, by a spectral variation result $[1]$, similar to Weyl’s estimate on Hermitian operators,

$$\|V_1U_1V_1^*U_1^* - VUV^*U^*\| \geq \text{dist} \left( -1, \sigma(VUV^*U^*) \right).$$

We also have

$$\|V_1U_1V_1^*U_1^* - VUV^*U^*\| \leq 2 \|U - U_1\| + 2 \|V - V_1\|$$

and

$$\delta = \text{dist} \left( 1, \sigma(VUV^*U^*) \right).$$
A little basic geometry shows

\[(\text{dist}(-1, \sigma(VUV^*U^*)))^2 + (\text{dist}(-1, \sigma(VUV^*U^*)))^2 = 4\]

and so

\[\|U - U_1\| + \|V - V_1\| \geq \sqrt{1 - \frac{1}{4}\delta^2}.\]

□

We now get to a difficult question. Is the winding number invariant the only obstruction to closely approximating \(U\) and \(V\) by commuting unitary matrices? It is important here that we stick with the operator norm in defining “close approximation” as the answers to these sort of questions can change dramatically if considering the Frobenius norm [8, 9, 20, 22]. (In particular, see the discussion in section III in [20].) Results such as this also change dramatically when the matrices come from different symmetry classes, as seen in [18].

There is an answer, but it is only a non-quantitative, nonconstructive result for small \(\delta\). This is Theorem 6.15 in [4] and we repeat it here. Also it matters that we are only interested in results for unitaries in \(\mathbf{M}_d(\mathbb{C})\) that are independent of \(d\) [10, 13].

**Theorem 2.6.** For any \(\epsilon > 0\), there is a \(\delta\) in \((0, 2)\) so that, whenever \(U\) and \(V\) are unitary matrices in \(\mathbf{M}_d(\mathbb{C})\) with \(\|[U, V]\| \leq \delta\) and \(\omega(U, V) = 0\), there exist unitary matrices \(U_1\) and \(V_1\) in \(\mathbf{M}_d(\mathbb{C})\) so that

\[\|U - U_1\| + \|V - V_1\| \leq \epsilon\]

and \([U_1, V_1] = 0\).

A serious limitation of the invariant \(\omega(U, V)\) is that it does not generalize to unitaries in general \(C^*\)-algebras, as it depends crucially on the determinant. Another limitation is that we don’t know how to modify it to work in other symmetry classes. For example if we have self-dual unitary matrices, so \(U^\sharp = U\) and \(V^\sharp = V\), where \(\sharp\) is a specific generalized involution detailed below, we find

\[(VUV^*U^*)^\sharp = U^*V^*UV\]

and so generally \(VUV^*U^*\) is not self-dual.

### 3. A direct \(K\)-theory invariant — the Bott index

We need functional calculus of unitary matrices, also called matrix functions in applied mathematics. An example is above where we applied the logarithm to a unitary matrix. Generally speaking, for the functional calculus \(f(V)\) to be define for a unitary matrix we need \(f\) defined on the circle. One diagonalizes \(V\) via another unitary \(Q\) and applies \(f\) on the diagonal, so

\[V = Q \begin{pmatrix} e^{i\theta_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{i\theta_d} \end{pmatrix} Q^* \implies f(V) = Q \begin{pmatrix} f(e^{i\theta_1}) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & f(e^{i\theta_d}) \end{pmatrix} Q^*.

However, most of our calculations will involve Fourier series, and traditionally those are defined in terms of scalar functions that are periodic.
Definition 3.1. Assume then that $f$ is periodic of period $2\pi$ we define $f[V]$ as $\tilde{f}(V)$ where $\tilde{f} = f \circ \log$. In other words,

$$V = Q \begin{pmatrix} e^{i\theta_1} & \cdots & e^{i\theta_d} \end{pmatrix} Q^* \implies f[V] = Q \begin{pmatrix} f(\theta_1) & \cdots \ f(\theta_1) \end{pmatrix} Q^*.$$ 

When $f$ has uniformly convergent Fourier series, this is easier:

$$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{inx} \implies f[V] = \sum_{n=-\infty}^{\infty} a_n V^n. \tag{3.1}$$

Definition 3.2. Define

$$f(x) = \frac{1}{128} (150 \sin(x) + 25 \sin(3x) + 3 \sin(5x))$$

and $g$ and $h$:

$$g = \begin{cases} 0 & x \in \left[ -\frac{\pi}{2}, \frac{\pi}{2} \right] \\ \sqrt{1 - f^2} & x \notin \left[ -\frac{\pi}{2}, \frac{\pi}{2} \right] \end{cases}$$

and

$$h = \begin{cases} \sqrt{1 - f^2} & x \in \left[ -\frac{\pi}{2}, \frac{\pi}{2} \right] \\ 0 & x \notin \left[ -\frac{\pi}{2}, \frac{\pi}{2} \right] \end{cases}$$
Figure 3.2. In both: solid curve on top is the guaranteed spectral gap in $B(U,V)$ for a given $\delta$. The dashed curve is the distance one can move where it is proven the gap will not close. The dotted curve in the left plot is $\frac{19}{20} \sqrt{1 - 5\delta}$. The dotted curve on the right is $\frac{1}{5} \sqrt{1 - 5\delta}$.

which are shown in Figure 3.1. For any unitaries set

$$B(U,V) = \begin{pmatrix} f[V] + \frac{1}{2} \{h[V], U^*\} & g[V] + \frac{1}{2} \{h[V], U\} \\ g[V] + \frac{1}{2} \{h[V], U\} & -f[V] \end{pmatrix}$$

and if $\|[U,V]\| \leq 0.206007$ define $\kappa(U,V)$ as the integer

$$\kappa(U,V) = \frac{1}{2} \text{Sig}(B(U,V)).$$

For an invertible, hermitian matrix $A$ we define its signature $\text{Sig}(A)$ as the number (with multiplicity) of positive eigenvalues minus the number of negative eigenvalues. We will prove that $\|[U,V]\| \leq 0.206007$ forces $B(U,V)$ to be invertible.

It should be noted that

$$\gamma_1 = f(\theta)$$
$$\gamma_2 = g(\theta) + h(\theta) \cos(\theta_1)$$
$$\gamma_3 = h(\theta) \sin(\theta_1)$$

defines the coordinates of a map from $T^2 \to S^2 \subseteq \mathbb{R}^3$ that has mapping degree one. Also notice $gh = 0$ and $f^2 + g^2 + h^2 = 1$.

**Theorem 3.3.** Suppose $U$ and $V$ are unitaries and

$$\delta = \|[U,V]\| \leq 0.206007.$$

(1) The hermitian matrix $B(U,V)$ has a spectral gap at 0 of radius at least $\frac{19}{20} \sqrt{1 - 5\delta}$. Indeed, the gap is at least as large as the function of $\delta$ plotted as a solid curve in Figure 3.2.
Figure 3.3. Upper bound on the gap radius, as $\| [V, U] \|$ varies from 0 to about 0.21.

(2) The distance $\| U - U_1 \| + \| V - V_1 \|$ needed so that $B(U_1, V_1)$ has 0 in its spectrum is at least $\frac{1}{2} \sqrt{1 - 5\delta}$. Indeed, this distance is at least as large as the function of $\delta$ plotted as a dashed curve in Figure 3.2.

We will prove Theorem 3.3 in Section 5 and it will be a lot of work to prove. Moreover, the gap here is much smaller than we saw for $VUV^*U^*$. Why do we bother? The point is symmetry.

Suppose $U^\sharp = U$ and $V^\sharp = V$ for unitaries in $M_{2d}(\mathbb{C})$ and with $\sharp$ the generalized involution discussed in the next section, that physicists call the dual. Then $B(U, V)$ is in $M_{2d}(\mathbb{C}) \otimes M_2(\mathbb{C})$ which has on it the generalized involution $\tau = \sharp \otimes \sharp$. In terms of real $C^*$-algebras, this is a copy of $M_{2d+2}(\mathbb{C})$ with the transpose operation. In physics language, we are tensoring two half-odd-integer spin systems to get a system with integer spin, in a non-standard basis. We find

$$B(U, V)^\tau = -B(U, V)$$

and so $B(U, V)$ defines a class in

$$K_2(\mathbb{R}) \cong K_{-2}(\mathbb{H}) \cong \mathbb{Z}/2$$

that is computed directly in terms of the a Pfaffian, hence the Pfaffian-Bott index studied in [17]. In return for a small gap, indeed no guaranteed gap if $\| [U, V] \|$ is too large, we get a construction that is amenable to symmetries.

An easy upper bound on the gap radius can be found, using the example in Lemma 2.2 shown in Figure 3.3. This shows we cannot get a big a gap using $B(U, V)$ as was possible with $VUV^*U^*$, but that the situation is likely not as bad as Figure 3.2 indicates.

Fortunately $B(U, V)$ is readily computable since $f$, $g$ and $h$ we chosen to have rather fast decay in their Fourier coefficients. Thus we were able to replace (3.1) by the simpler evaluation of order-5 trig polynomials. For applications to index studies, the following is the most useful. We will later have a version of this for the Pfaffian-Bott index.
Proposition 3.4. Suppose \( \| [U, V] \| \leq 0.206007 \). If \( \| [U_1, V_1] \| \leq 0.206007 \) and 
\[ \kappa(U_1, V_1) \neq \kappa(U, V) \]
then
\[ \| U - U_1 \| + \| V - V_1 \| \geq \frac{1}{5} \sqrt{1 - 5 \| [U, V] \|^2} + \frac{1}{5} \sqrt{1 - 5 \| [U_1, V_1] \|^2}. \]

Another consequence of Theorem 3.3 is the following.

Theorem 3.5. Suppose \( U \) and \( V \) are unitary matrices. If \( \| [U, V] \| \leq 0.206007 \) then
\[ \kappa(U, V) = \omega(U, V). \]

Proof. Exel [5] showed that for \( \| [U, V] \| < 2 \) the winding invariant equals an abstract \( K \)-theory invariant. In the notation of [5], this is defined in terms of \( b_\epsilon \) in \( K_0(A_\epsilon) \). It is easy to check that as long \( B(u, v) \) has a spectral gap, where \( u \) and \( v \) are the generators of the soft torus \( A_\epsilon \), the \( K \)-theory class of \( B(u, v) \) is \( b_\epsilon \). \( \square \)

4. Defining the Pfaffian-Bott index

The Pfaffian of skew-symmetric matrices is not the most familiar object, and it it not clear at the outset how it applies to a problem involving self-dual matrices. Let us start by recalling the dual operation.

We fix 
\[ Z = Z_N = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \]
in \( M_{2N}(\mathbb{C}) \) and this specifies the dual operation
\[ X^\sharp = -ZX^TZ \]
as above in (1.1).

When we discuss \( M_2(M_{2N}(\mathbb{C})) = M_{2N}(\mathbb{C}) \otimes M_2(\mathbb{C}) \) we require the unitary 
\[ Q = \frac{1}{\sqrt{2}} \begin{bmatrix} I & -iZ \\ iZ & I \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} I & 0 & 0 & -iI \\ 0 & I & iI & 0 \\ 0 & iI & I & 0 \\ -iI & 0 & 0 & I \end{bmatrix} \]
which has the convenient property [12, Lemma 1.3]
\[ Q^* X^\sharp \otimes Q = (Q^* X Q)^T. \]

Here
\[ \begin{bmatrix} A & B \\ C & D \end{bmatrix}^\sharp \otimes \sharp = \begin{bmatrix} D^\sharp & -B^\sharp \\ -C^\sharp & A^\sharp \end{bmatrix} \]
or
\[ \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix}^\sharp \otimes \sharp = \begin{bmatrix} A_{11}^T & -A_{24}^T & -A_{24}^T & A_{14}^T \\ -A_{43}^T & A_{13}^T & A_{13}^T & -A_{13}^T \\ -A_{43}^T & A_{13}^T & A_{13}^T & -A_{13}^T \\ A_{14}^T & -A_{31}^T & -A_{21}^T & A_{11}^T \end{bmatrix}. \]
Recall the Pfaffian is defined for all skew-symmetric, complex $2n$-by-$2n$ matrices by
\[
\text{Pf}\begin{pmatrix}
0 & a_1 & a_2 & a_3 & \cdots & a_{2n-1} \\
-a_1 & 0 & a_3 & 0 & \cdots & a_{2n-1} \\
-a_2 & -a_3 & 0 & \cdots & \cdots & \cdots \\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots \\
\end{pmatrix} = \det(O) a_1 a_3 \cdots a_{2n-1}.
\]
for $O$ real orthogonal. (All skew-symmetric matrices have such a factorization, a modified Hessenberg decomposition.) The essential properties are that
\[\text{Pf}(Y XY^T) = \det(Y) \text{Pf}(X)\]
for arbitrary $Y$, that the Pfaffian varies continuously, and
\[(\text{Pf}(X))^2 = \det(X)\]
so is zero exactly on the set of skew-symmetric, singular matrices.

For matrices with the symmetry $X^{\sigma_2} = -X$ we can define a modified Pfaffian
\[
\tilde{\text{Pf}}(X) = \text{Pf} (Q^* X Q).
\]
We still have
\[\left(\tilde{\text{Pf}}(X)\right)^2 = \det(X)\]
and that this varies continuously. The sign of the Pfaffian can be used to prove a homotopy result, in the same way we use the determinant to detect that the real orthogonal matrices fall into two connected parts.

**Proposition 4.1.** Suppose $B$ is in $M_{4N}(\mathbb{C})$ and $B^* = B$ and $B^T = -B$ and $B$ is invertible. Then
\[\text{Pf}(B) \in \mathbb{R} \setminus \{0\}.\]

If $B_1$ and $B_2$ are elements of
\[\mathcal{H} = \{ B \in M_{4N}(\mathbb{C}) | B^* = B = -B^T \text{ is invertible} \},\]
then they can be connected by a path in $\mathcal{H}$ if and only if with $\text{Pf}(B_1)$ and $\text{Pf}(B_2)$ have the same sign.

**Proof.** We can apply Theorem 8.7 in [12] to $iB$ and learn that there is a real orthogonal matrix $O$ so that $\det(O) = 1$ and
\[
B = O \begin{pmatrix}
0 & i\lambda_1 & 0 & \cdots & 0 \\
-i\lambda_1 & 0 & i\lambda_2 & \cdots & 0 \\
& \ddots & \ddots & \ddots & \cdots \\
\end{pmatrix} O^T
\]
and all the real numbers $\lambda_j$ are positive except $\lambda_1$ which as the same sign as $\text{Pf}(B)$. It is clear from this form that two such matrices with Pfaffian of the same sign will be connected. The spectrum of $B$ is $\{\pm \lambda_1, \ldots, \pm \lambda_{2N}\}$. Thus there will be an even number of negative eigenvalues, so $\det(B) > 0$. Since the square of the Pfaffian is the determinant, we find $\text{Pf}(B)$ is real, and as $B$ is invertible, the Pfaffian cannot be zero. Since the Pfaffian varies
continuously, it is not possible to connect two matrices in $\mathcal{H}$ that have Pfaffians of opposite signs. □

Now we explain the Pfaffian-Bott index.

**Definition 4.2.** Let $f$, $g$, $h$ and $B(U,V)$ be as in §3. If $\| [U, V] \| \leq 0.206007$ define $\kappa(U,V)$ as the value in $\{\pm 1\}$ given by

$$\kappa_2(U,V) = \text{Sign} \left( \widetilde{\text{Pf}}(B(U,V)) \right).$$

**Lemma 4.3.** When $U$ and $V$ are commuting unitary matrices, $\omega(U,V) = 1$.

**Proof.** One proof is to use Lemma 6.4 of [11]. Here is another.

One easily checks that $\kappa_2$ remains constant along a path so long as $\| [U, V] \| \leq 0.206007$. One can use functional calculus, and so keep the self-dual condition, to deform a commuting pair $U_0$ and $V_0$ that is self-dual over to $U_1 = I$ and $V_1 = I$. One can then compute that

$$B(I, I) = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$$

and

$$\widetilde{\text{Pf}} \left( \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \right) = \text{Pf} \left[ \begin{pmatrix} iZ & 0 \\ 0 & -iZ \end{pmatrix} \right] = \text{Pf} (iZ) \text{Pf} (-iZ) = i^n(-i)^n = 1.$$ □

**Proposition 4.4.** Suppose $\| [U, V] \| \leq 0.206007$ and that $U$, $V$, $U_1$, $V_1$ are self-dual unitary matrices. If $\| [U_1, V_1] \| \leq 0.206007$ and

$$\kappa_2(U_1, V_1) \neq \kappa_2(U, V)$$

then

$$\| U - U_1 \| + \| V - V_1 \| \geq \frac{1}{5} \sqrt{1 - 5 \| [U, V] \|^2} + \frac{1}{5} \sqrt{1 - 5 \| [U_1, V_1] \|^2}.$$ 

**Proposition 4.5.** Suppose $\| [U, V] \| \leq 0.206007$ and that $U$, $V$, $U_1$, $V_1$ are self-dual unitary matrices. If $U_1$ commutes with $V_1$ and $\kappa_2(U, V) = -1$ then

$$\| U - U_1 \| + \| V - V_1 \| \geq \frac{1}{5} + \frac{1}{5} \sqrt{1 - 5 \| [U, V] \|^2}.$$ 

5. Proof that the gap persists

Now we prove Theorem 3.3, finding a lower bound on the size of the gap in $B(U,V)$ along as $\delta = \| [U, V] \|$ is not too small. We do so by finding an upper bound on the norm of $B(U,V)^2 - I$. It is then a routine application of the spectral mapping theorem to get lower bound on the size of the gap.

We will need some results about commutators and the functional calculus. There is the folklore estimate

$$\| [f[V], U] \| \leq ||f'||_F \| [U, V] \|$$

where $||f'||_F$ is the $\ell^1$-norm of the sequence of Fourier coefficients of $f$. This estimate is really only helpful for very small commutators.
**Definition 5.1.** Suppose $f$ is continuous and $2\pi$-periodic. Following [19] we define $\eta_f : [0, \infty) \to [0, \infty)$ by

$$\eta_f(\delta) = \sup \{ \| f[V], A \| \mid V \text{ unitary, } \| A \| \leq 1, \| [V, A] \| \leq \delta \}$$

where the supremum is taken over all $V$ and $A$ in every unital $C^*$-algebra.

Once we have a bound on $\eta_f$ we can use it to bound more than just commutators. Indeed, by [19, Lemma 1.2], for any two unitaries $V_1$ and $V_2$ we have

$$\| f[V] - f[V_1] \| \leq \eta_f (\| V - V_1 \| ).$$

We need a special case of a Lemma in [19].

**Lemma 5.2.** Suppose $f$ is continuous, real-valued and periodic, and that $f_1$ is the trigonometric polynomial

$$f_1(x) = \sum_{k=-n}^{n} a_k e^{ikx}.$$ 

Let $f_2 = f - f_1$. Then

$$\eta_f(\delta) \leq m\delta + b$$

where

$$m = \sum_{k=-n}^{n} |ka_k|$$

and

$$b = \max f_2(x) - \min f_2(x).$$

Before we focus on our choice of the three functions $f, g$ and $h$ to use in the Bott invariant, we look at the terms we need to control when bounding $B(U, V)^2 - I$.

**Lemma 5.3.** Suppose $f, g$ and $h$ are continuous, real-valued functions that are $2\pi$-periodic, and with

$$f^2 + g^2 + h^2 = 1$$

and

$$gh = 0.$$

Suppose $U$ and $V$ are unitary matrices and define

$$S = \begin{bmatrix} f[V] & g[V] + \frac{1}{2} \{ h[V], U \} \\ g[V] + \frac{1}{2} \{ h[V], U^* \} & -f[V] \end{bmatrix}.$$ 

Then $S^* = S$ and

$$\| S^2 - I \| \leq 2 \| [h[V], U] \| + \| [f[V], U] \| .$$

**Proof.** Since $f, g$ and $h$ are real-valued, the matrices $f[V], g[V]$ and $h[V]$ are hermitian. Let us write $f$ for $f[V], g$ for $g[V], etc. We see easily $S^* = S$ and

$$\begin{bmatrix} f + \frac{1}{2} \{ h, U \} & g + \frac{1}{2} \{ h, U \} \\ g + \frac{1}{2} \{ h, U^* \} & -f \end{bmatrix}^2 = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix}$$

where

$$A = f^2 + g^2 - I + \frac{1}{4} \{ h, U \} \{ h, U^* \} + \frac{1}{2} g \{ h, U^* \} + \frac{1}{2} \{ h, U \} g$$

$$= -h^2 + \frac{1}{4} \{ h, U \} \{ h, U^* \} + \frac{1}{2} g \{ h, U^* \} + \frac{1}{2} \{ h, U \} g$$
and

\[ B = fg + \frac{1}{2} f \{ h, U \} - gf - \frac{1}{2} \{ h, U \} f \]

\[ = \frac{1}{2} f \{ h, U \} - \frac{1}{2} \{ h, U \} f. \]

We have

\[ \| S^2 - I \| \leq \left\| \begin{bmatrix} A & 0 \\ 0 & A^* \end{bmatrix} \right\| + \left\| \begin{bmatrix} 0 & B \\ B^* & 0 \end{bmatrix} \right\| \]

\[ = \| A \| + \| B \|. \]

Notice \( f^2 + g^2 + h^2 = 1 \) forces these functions to take value in \([-1, 1]\) so \( \| f[V] \| \leq 1 \), etc. Therefore

\[ \| A \| \leq \frac{1}{4} \| UhU^* + UhU^*h - 3h^2 \| + \frac{1}{2} \| gU^*h - ghU^* + hUg - Uhg \| \]

\[ \leq \frac{1}{2} \| h \| \| Uh - hU \| + \frac{1}{4} \| Uh^2 - h^2U \| + \| g \| \| Uh - hU \| \]

\[ \leq 2 \| Uh - hU \| \]

and

\[ \| B \| = \frac{1}{2} \| hfU + fUh - hUf - fh \| \]

\[ \leq \frac{1}{2} \| h[f, U] \| + \frac{1}{2} \| [f, U] h \| \]

\[ \leq \| [f, U] \| \]

so

\[ \| S^2 - I \| \leq 2 \| [h, U] \| + \| [f, U] \|. \]

Now we let \( f, g \) and \( h \) be the functions from Definition 3.2. Here we start needing a computer algebra package. It shows us that

\[ f(x)^2 + \frac{407}{512} \cos^6(x) \left( 1 + \frac{96}{407} \cos(2x) + \frac{9}{407} \cos(4x) \right) = 1 \]

which means

\[ g(x) = \sqrt{\frac{407}{512} \cos^3(x)} \sqrt{1 + \frac{96}{407} \cos(2x) + \frac{9}{407} \cos(4x)} \left( 1 - \chi_{[-\frac{\pi}{2}, \frac{\pi}{2}]}(x) \right) \]

\[ h(x) = \sqrt{\frac{407}{512} \cos^3(x)} \sqrt{1 + \frac{96}{407} \cos(2x) + \frac{9}{407} \cos(4x)} \chi_{[-\frac{\pi}{2}, \frac{\pi}{2}]}(x) \]

A handy formula here is

\[ \frac{407}{320} \left( 1 + \frac{96}{407} \cos(2x) + \frac{9}{407} \cos(4x) \right) = \left( 1 + \frac{15}{40} \cos^2(x) + \frac{9}{40} \cos^4(x) \right) \]

and we get alternate expression for \( g \) and \( h \), in particular

\[ h(x) = \sqrt{\frac{10}{4} \cos^3(x)} \sqrt{1 + \frac{15}{40} \cos^2(x) + \frac{9}{40} \cos^4(x)} \chi_{[-\frac{\pi}{2}, \frac{\pi}{2}]}(x). \]

We now bound the derivative of \( g \) and \( h \), computing

\[ \frac{d}{dx} \left( \sqrt{\frac{10}{4} \cos^3(x)} \sqrt{1 + \frac{15}{40} \cos^2(x) + \frac{9}{40} \cos^4(x)} \right) = \frac{p(\sin(x))}{16 \sqrt{q(\sin(x))}} \]
where 

\[ p(x) = 30(x - 1)(x + 1)(3x^4 - 10x^2 + 15) \]

and 

\[ q(x) = 9x^4 - 33x^2 + 64. \]

On \([-1, 1]\) the max of \(p(x)\) is 150 and the min of \(q(x)\) is 64 so we find 

\[ |h'(x)| \leq \frac{150}{128} \]

and the same for \(g'\).

We need \(h\) as a cosine or Fourier series so need

\[
c_n = \frac{1}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos(nx) \sqrt{\frac{407}{512}} \cos^3(x) \sqrt{1 + \frac{96}{407} \cos (2x) + \frac{9}{407} \cos (4x)} \, dx.
\]

We computed these with numerical integration, and without checking error estimates, in [17]. We compute these a little more carefully here. The code for doing the needed We find

\[
c_n = \frac{1}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos(nx) \sqrt{\frac{407}{512}} \cos^3(x) \sum_{k=0}^{\infty} \left(\frac{1}{2k}\right) \left( \frac{96}{407} \cos (2x) + \frac{9}{407} \cos (4x) \right) dx
\]

\[
= \sum_{k=0}^{\infty} \frac{1}{2\pi} \sqrt{\frac{407}{512}} \left(\frac{1}{2k}\right) \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos(nx) \cos^3(x) \left( \frac{96}{407} \cos (2x) + \frac{9}{407} \cos (4x) \right)^k \, dx
\]

\[
= \sum_{k=0}^{\infty} I_{n,k},
\]

where the \(I_{n,k}\) were defined in-line and are easy to compute with a computer algebra package. The convergence here is rather rapid, as

\[
I_{n,k} \leq \frac{1}{2\pi} \sqrt{\frac{407}{512}} \left(\frac{1}{2k}\right) (-1)^k \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \left| \cos(nx) \cos^3(x) \left( \frac{96}{407} \cos (2x) + \frac{9}{407} \cos (4x) \right) \right|^k \, dx
\]

\[
\leq \frac{1}{2\pi} \sqrt{\frac{407}{512}} \left(\frac{1}{2k}\right) \left( \frac{-105}{407} \right)^k.
\]

Letting \(T_K\) denote the the Taylor polynomial

\[ T_K(x) \approx \sqrt{1 + x} \]

of degree \(K\) expanded at 0, we have

\[
\sum_{k=K+1}^{\infty} |I_{n,k}| \leq \frac{1}{2\pi} \sqrt{\frac{407}{512}} \sum_{k=K+1}^{\infty} \left(\frac{1}{2k}\right) \left( \frac{-105}{407} \right)^k
\]

\[
= \frac{1}{2\pi} \sqrt{\frac{407}{512}} \left( \sum_{k=0}^{\infty} \left(\frac{1}{2k}\right) \left( \frac{-105}{407} \right)^k \right) - \sum_{k=0}^{K} \left(\frac{1}{2k}\right) \left( \frac{-105}{407} \right)^k
\]

\[
= \frac{1}{2\pi} \sqrt{\frac{407}{512}} \left( \sqrt{1 - \frac{105}{407}} - T_K \left( \frac{-105}{407} \right) \right)
\]
Table 1. These are approximations to the first coefficients in the Fourier expansions of the $f$, $g$ and $h$ used to define the Bott index. Extend these to negative indices by the rules $a_{-n} = \overline{a_n}$ and $b_{-n} = b_n$ and $c_n = -c_n$.

This means we need $K = 7$ to get six digits absolute accuracy, with the results shown in Table 1. The integration was done symbolically in Matlab, with code [16] that is available from a repository hosted by the University of New Mexico.

Using the values in the table to define

$$h_5(x) = \sum_{n=-5}^{5} c_n e^{inx}$$

or

$$h_5(x) = c_0 + 2c_2 \cos(x) + 2c_2 \cos(2x) + 2c_3 \cos(3x) + 2c_4 \cos(4x) + 2c_5 \cos(5x)$$

and we find,

$$\left| \frac{d}{dx} (h - h_5) \right| \leq \frac{150}{128} + 1.48498 = 2.656855.$$ 

and so we can estimate to six decimal places the maximum of $|h - h_5|$ by simply plugging in values between $-\pi$ and $\pi$ with an even spacing of a little less than $10^{-7}$. Keeping track of the errors and rounding up, we find

$$\text{diam} (h(x) - h_5(x)) \leq 0.004110$$

and we note

$$\|h'_5\|_F = \sum_{n=-5}^{5} n|c_n| = 1.48498.$$

The other estimates of this sort, for $h_0, \ldots, h_4$, are summarized in Table 2.

We also can use brute force to find

$$\sup_x |h(x) - h_5(x)| \leq 0.002338.$$

Lemma 5.4. For any unitary matrix $V$,

$$\|h_5[V] - h[V]\| \leq 0.002338$$

We get the same error estimate on using only $b_{-5}$ through $b_5$ when numerically computing $g[V]$.

Lemma 5.5. For $h$ as in Definition 3.2 we have

$$\|h'\|_F \leq 2.99208.$$
Proof. We check that
\[
h'(x) = \frac{-1}{\sqrt{3256}} \left( 45 \cos^4(x) + 60 \cos^2(x) + 120 \right) \sqrt{1 + \frac{96}{407} \cos(2x) + \frac{9}{407} \cos(4x)} \sin(x) \cos^2(x) \chi_{[-\frac{\pi}{2}, \frac{\pi}{2}]}(x)
\]
and attack this as three factors. It is easy to see
\[
\left\| \frac{1}{\sqrt{3256}} \left( 45 \cos^4(x) + 60 \cos^2(x) + 120 \right) \right\|_F = \frac{225}{\sqrt{3256}}
\]
and the next factor is not so bad, as we see
\[
\left\| \frac{1}{\sqrt{1 + \frac{96}{407} \cos(2x) + \frac{9}{407} \cos(4x)}} \right\|_F \leq \sum_{k=0}^{\infty} \left( \frac{-1/2}{k} \right) \left\| \frac{96}{407} \cos(2x) + \frac{9}{407} \cos(4x) \right\|_F^k
\]
\[
= \sum_{k=0}^{\infty} \left( \frac{-1/2}{k} \right) (-1)^k \left( \frac{105}{407} \right)^k
\]
\[
= \frac{1}{\sqrt{1 - \frac{105}{407}}} = \sqrt{\frac{407}{302}}.
\]
We estimate
\[
\left\| \sin(x) \cos^2(x) \chi_{[-\frac{\pi}{2}, \frac{\pi}{2}]}(x) \right\|_F
\]
as follows. The Fourier series of \(-i \sin(x) \cos^2(x) \chi_{[-\frac{\pi}{2}, \frac{\pi}{2}]}(x)\) is
\[
\ldots \frac{16}{3465 \pi}, 0, \frac{4}{315 \pi}, \frac{1}{15 \pi}, \frac{8}{16}, -\frac{8}{16}, -\frac{1}{16}, \frac{8}{16}, -\frac{1}{16}, \frac{8}{16}, -\frac{8}{16}, \frac{4}{315 \pi}, 0, -\frac{16}{3465 \pi} \ldots
\]
with terms beyond \(n = 3\) being given by
\[
-\cos \left( \frac{n \pi}{2} \right) \left( \frac{1}{(n-1)^3 - 4(n-1)} + \frac{1}{(n+1)^3 - 4(n+1)} \right).
\]

| \(n\) | \(m = \text{bound on } \|h_n'\|_F\) | \(b = \text{bound on } \text{diam}(h_n(x) - h_n(x))\) |
|---|---|---|
| 0 | 0 | 1 |
| 1 | 0.359880 | 0.732237 |
| 2 | 0.862500 | 0.350141 |
| 3 | 1.258560 | 0.106619 |
| 4 | 1.446120 | 0.017509 |
| 5 | 1.484980 | 0.004110 |
| \(\infty\) | 2.992080 | 0 |

Table 2. Bounds on \(\eta_n\) as a slope and an offset.
\[ n \quad m = \text{bound on } \| f_n \|_F \quad b = \text{bound on } \text{diam}(f(x) - f_n(x)) \]

| n | m | b |
|---|---|---|
| 0 | 0 | 2 |
| 1 | 1.171875 | 0.4375 |
| 2 | 1.7578125 | 0.04687 |
| \infty | 1.875 | 0 |

**Table 3.** Bounds on \( \eta_f \) as a slope and an offset.

Therefore
\[
\left\| \sin(x) \cos^2(x) \chi_{[-\frac{\pi}{2}, \frac{\pi}{2}]} \right\|_F \\
= \frac{1}{4} + \frac{16}{15\pi} + \frac{18}{105\pi} + \frac{4}{\pi} \sum_{n=3}^{\infty} \frac{1}{(2n+1)^3 - 4(2n+1)} \\
\leq \frac{1}{4} + \frac{16}{15\pi} + \frac{18}{105\pi} + \frac{4}{315\pi} + \frac{16}{3465\pi} + \frac{4}{315\pi} \int_{\frac{1}{4}}^{\infty} \frac{1}{8x^3 + 12x^2 - 2x - 3} \, dx \\
= \frac{1}{4} + \frac{16}{15\pi} + \frac{18}{105\pi} + \frac{4}{315\pi} + \frac{16}{3465\pi} + \frac{1}{4\pi} \ln \left( \frac{81}{77} \right)
\]

and so
\[
\| h' \|_F \leq \frac{225}{\sqrt{3256}} \sqrt{\frac{407}{302}} \left( \frac{1}{4} + \frac{16}{15\pi} + \frac{18}{105\pi} + \frac{4}{315\pi} + \frac{16}{3465\pi} + \frac{1}{4\pi} \ln \left( \frac{81}{77} \right) \right) < 2.992076
\]

We approximate \( f \) the same way, but this is just arithmetic since \( f \) is already a trigonometric polynomial.

**Lemma 5.6.** Let \( f \) and \( g \) and \( h \) be as in Definition 3.2. Then
\[
\eta_f(\delta) \leq m\delta + b
\]
for each of the values in Table 3 and
\[
\eta_g(\delta) \leq m\delta + b
\]
and
\[
\eta_h(\delta) \leq m\delta + b
\]
for each of the values in Table 2.

Let
\[
\beta(\delta) = 2\eta_h(\delta) + \eta_f(\delta)
\]
which is shown in Figure 5.1.

**Theorem 5.7.** Suppose \( U \) and \( V \) are unitary matrices. Then
\[
\| B(U,V)^2 - I \| \leq \beta(\|[U,V]\|)
\]
and for \( \|[U,V]\| \leq 0.206007 \) the gap at 0 in the spectrum of \( B(U,V) \) has radius at least
\[
\sqrt{1 - \beta(\|[U,V]\|)}.
\]

The other key thing we have is how \( B(U,V) \) varies.
Figure 5.1. The function $\beta(\delta)$ that bounds $\|B(U, V)^2 - I\|$ in terms of $\delta = \|[U, V]\|$.

Theorem 5.8. If $U_j$ and $V_j$ are unitary matrices then

$$\|B(U_0, V_0) - B(U_0, V_0)\| \leq \beta (\|V_0 - V_1\|) + \|U_0 - U_1\|$$

and so

$$\|B(U_0, V_0) - B(U_0, V_0)\| \leq \beta (\|V_0 - V_1\| + \|U_0 - U_1\|)$$

All our main theorems now follow.

6. The log method

An alternate way to compute the Bott index was considered in [6]. One replaces $B(U, V)$ with

$$B_L(U, V) = \begin{pmatrix} \frac{1}{\pi} K & \frac{1}{2} \left\{\sqrt{I - \frac{1}{\pi^2} K^2}, U\right\} \\ \frac{1}{2} \left\{\sqrt{I - \frac{1}{\pi^2} K^2}, U^*\right\} & -\frac{1}{\pi} K \end{pmatrix}$$

where $iK$ is the logarithm of $V$, meaning $-\pi \leq K < \pi$ and $e^{iK} = V$. Numerical evidence in [17] suggests that, for small commutators, the Pfaffian-Bott index can be computed using $B_L(U, V)$. We validate this here.

Since the logarithm is not continuous, numerical errors will mean we might accidentally compute the wrong branch of logarithm on $V$, or indeed any logarithm at all.

We note that when $q$ is periodic,

$$q(K) = q[V].$$

Lemma 6.1. Suppose $f, g$ and $h$ are real-valued Borel functions on $[-\pi, \pi]$ satisfying

$$f^2 + g^2 + h^2 = 1$$

and

$$gh = 0.$$ 

Let $q(x) = f(x)h(x)$ and assume further that $q$ and $h$ are continuous and $2\pi$-periodic. Suppose $U$ and $V$ are unitary matrices and $-iK$ is a logarithm of $V$ and define

$$S = \begin{bmatrix} f(K) & g(K) + \frac{i}{2} \{h(K), U\} \\ g(K) + \frac{i}{2} \{h(K), U^*\} & -f(K) \end{bmatrix}.$$
Then \( S^* = S \) and
\[
\| S^2 - I \| \leq (\| g \| + 1) \| [h[V], U] \| + \frac{1}{4} \| [h[V], U] \|^2 + \frac{1}{2} \| [h^2[V], U] \| + \| [g[V], U] \|.
\]

**Proof.** We write \( f \) for \( f(K) \) and compute a bit more carefully than before. We find
\[
\frac{1}{4} \| hUhU^* + Uh^2U^* + Uh^*h - 3h^2 \|
\]
\[
= \frac{1}{4} \| hUhU^* - h^2 + Uh^*h - Uh^2U^* + 2Uh^2U^* - 2h^2 \|
\]
\[
= \frac{1}{4} \| -[h, U][h, U]^* + 2(Uh^2U^* - h^2) \|
\]
\[
\leq \frac{1}{4} \| [h, U] \|^2 + \frac{1}{2} \| [h^2, U] \|
\]
and
\[
\frac{1}{2} \| g\{h, U^*\} + \{h, U\}g \| = \frac{1}{2} \| gU^*h + hUg \|
\]
\[
= \frac{1}{2} \| g[U^*, h] + [h, U]g \|
\]
\[
\leq \| g \| \|[h, U]\|
\]
and
\[
\frac{1}{2} \| f\{h, U\} - \{h, U\}f \| = \frac{1}{2} \| fhU - Ufh + fUh - hUf \|
\]
\[
= \frac{1}{2} \| 2fhU - 2Ufh + fUh - fUf + Uhf \|
\]
\[
\leq \| fhU - Uhf \| + \frac{1}{2} \| fUh - fUf \| + \frac{1}{2} \| Uhf - Uhf \|
\]
\[
\leq \| fhU - Uhf \| + \frac{1}{2} \| Uh - hU \| + \frac{1}{2} \| hU - Uh \|
\]
\[
= \|[f, h]U\| + \|[h, U]\|
\]
\[
= \|[q, U]\| + \|[h, U]\|.
\]

\[\Box\]

**Theorem 6.2.** Suppose \( U \) and \( V \) are unitary matrices, if \( \|[U, V]\| \leq \frac{1}{8} \), then for any choice of \( K \) with \( -\pi \leq K \leq \pi \) and \( e^{iK} = V \), there is a path \( B_t \) of invertible self-adjoint matrices between \( B(U, V) \) and
\[
\left( \begin{array}{cc}
\frac{1}{\pi} K & \frac{1}{2} \left\{ \sqrt{I - \frac{1}{\pi^2} K^2}, U \right\} \\
\frac{1}{2} \left\{ \sqrt{I - \frac{1}{\pi^2} K^2}, U^* \right\} & -\frac{1}{\pi} K
\end{array} \right)
\]
and, if \( U \) and \( V \) are self-dual, then the path may be chosen with the symmetry \( B_t^\otimes = B_t \).

**Proof.** We can select paths \( f_t \), \( g_t \) and \( h_t \) from
\[
(f_0, g_0, h_0) = (f, g, h),
\]
the standard triple, as in Definition \ref{def:standard_triple} to \( (f_1, g_1, h_1) \) where
\[
f_1(x) = \frac{1}{\pi} x, \quad g_1(x) = 0, \quad h_1(x) = \sqrt{1 - \frac{1}{\pi^2} x^2}
\]
and the conditions $f^2 + g^2 + h^2 = 1$ and $gh = 0$ hold along the way. This gives us paths of matrices

$$B_t(U, V) = \begin{bmatrix} f_t(K) & g_t(K) + \frac{1}{2} \{h_t(K), U^*\} \\ g_t(K) + \frac{1}{2} \{h_t(K), U\} & -\bar{f}_t(K) \end{bmatrix}$$

with the needed symmetries. It remains to show these are invertible. One needs to compute

$$\|g_t\| + 1, \eta_{h_t}(\delta) + \frac{1}{4} (\eta_{h_t}(\delta))^2 + \frac{1}{2} \eta_{h_t^2}(\delta) + \eta_{h_t}(\delta)$$

(6.2)
and check that this takes value less than 1 at $\delta = \frac{1}{8}$. This is a to much to do by hand, so use a computer [16] to repeatedly calculate the constant needed in Lemma 6.1. We find that (6.2) takes value less than 0.95 at $\delta = \frac{1}{8}$ for all $t$ in a mesh $t_1, \ldots, t_w$ selected so that

$$\|f_t - f_{t+1}\|_{\infty} + \|g_t - g_{t+1}\|_{\infty} + \|h_t - h_{t+1}\|_{\infty} \leq \sqrt{1 - 0.95} \approx 0.2236.$$ 

We can keep $f_t$ fixed at

$$f_t(x) = \begin{cases} 
-1 & -\frac{\pi}{2} \leq x \leq -\frac{\pi}{4} \\
\frac{1}{128} (150 \sin(x) + 25 \sin(3x) + 3 \sin(5x)) & -\frac{\pi}{4} \leq x \leq \frac{\pi}{4} \\
1 & 1\frac{\pi}{4} \leq x \leq \pi
\end{cases}$$

while altering $g_t$ from the standard $g$ to 0. The more interesting part of the path interpolates $f_t$ from the above to $\frac{1}{\pi}x$ while keeping $g_t = 0$ and

$$h_t(x) = \sqrt{1 - f_t(x)}.$$

The graphs of the computed bounds are shown in Figure 6.3. These bounds have been rounded up to accommodate the various errors in computing offset terms when applying Lemma 5.2. The errors in computing Fourier coefficients lead to sub-optimal results, but do not need to be accounted for as it is the computed coefficients that are used when applying Lemma 5.2. The analysis of the error bounds is dull and omitted.

It is apparent that that the limitation on the constant in this result comes from the functions used in the log method (6.1). The computed bounds are shown in Figure 6.4. $\square$

7. Acknowledgments

The author wishes to thank Matt Hastings and Fredy Vides for discussions, both useful and entertaining. Also he wishes to thank Robert Israel and Nick Weaver for help via MathOverflow. This work was partially supported by a grant from the Simons Foundation (208723 to Loring).

References

[1] R. Bhatia and C. Davis, A bound for the spectral variation of a unitary operator, Linear and Multi-linear Algebra, 15 (1984), pp. 71–76.
Figure 6.4. Bounds on $\|B_1(U,V)^2 - I\|$.

[2] S. Eilers and R. Exel, Finite-dimensional representations of the soft torus, Proc. Amer. Math. Soc., 130 (2002), pp. 727–731.

[3] S. Eilers and T. A. Loring, Computing contingencies for stable relations, Internat. J. Math., 10 (1999), pp. 301–326.

[4] S. Eilers, T. A. Loring, and G. K. Pedersen, Morphisms of extensions of $C^*$-algebras: pushing forward the Busby invariant, Adv. Math., 147 (1999), pp. 74–109.

[5] R. Exel, The soft torus and applications to almost commuting matrices, Pacific J. Math., 160 (1993), pp. 207–217.

[6] R. Exel and T. A. Loring, Invariants of almost commuting unitaries, J. Funct. Anal., 95 (1991), pp. 364–376.

[7] I. Fulga, F. Hassler, and A. Akhmerov, Scattering theory of topological insulators and superconductors, Physical Review B, 85 (2012), p. 165409.

[8] L. Glebsky, Almost commuting matrices with respect to normalized Hilbert-Schmidt norm, (2010).

[9] F. Gygi, J. Fattebert, and E. Schwegler, Computation of maximally localized Wannier functions using a simultaneous diagonalization algorithm, Computer Physics Communications, 155 (2003), pp. 1–6.

[10] P. R. Halmos, Some unsolved problems of unknown depth about operators on Hilbert space, Proc. Roy. Soc. Edinburgh Sect. A, 76 (1976/77), pp. 67–76.

[11] M. B. Hastings and T. A. Loring, Almost commuting matrices, localized Wannier functions, and the quantum Hall effect, J. Math. Phys., 51 (2010), p. 015214.

[12] M. B. Hastings and T. A. Loring, Topological insulators and $C^*$-algebras: Theory and numerical practice, Ann. Physics, 326 (2011), pp. 1699–1759.

[13] H. Lin, Almost commuting selfadjoint matrices and applications, in Operator algebras and their applications (Waterloo, ON, 1994/1995), vol. 13 of Fields Inst. Commun., Amer. Math. Soc., Providence, RI, 1997, pp. 193–233.

[14] T. A. Loring, The torus and noncommutative topology, PhD thesis, University of California, Berkeley, 1986.

[15] T. A. Loring, Computing a logarithm of a unitary matrix with general spectrum, Numer. Linear Algebra Appl., (to appear).

[16] Code for creating most of the tables and figures in this paper is available at the Lobo Vault, hosted by the University of New Mexico, repository.unm.edu/handle/1928/23494.

[17] T. A. Loring and M. B. Hastings, Disordered topological insulators via $C^*$-algebras, Europhys. Lett. EPL, 92 (2010), p. 67004.

[18] T. A. Loring and A. P. W. Sørensen, Almost commuting unitary matrices related to time reversal, Comm. Math. Phys., 323 (2013), pp. 859–887.

[19] T. A. Loring and F. Vides, Estimating norms of commutators. arXiv:1301.4252.

[20] N. Marzari, I. Souza, and D. Vanderbilt, An introduction to maximally-localized Wannier functions, Highlight the Month, Psi-K Newsletter, 57 (2003), pp. 129–68.
[21] M. A. Rieffel, *C*-algebras associated with irrational rotations, Pacific J. Math., 93 (1981), pp. 415–429.

[22] A. Ruhe, Closest normal matrix finally found!, BIT, 27 (1987), pp. 585–598.

[23] A. Sørensen, Semiprojectivity and the geometry of graphs, PhD thesis, University of Copenhagen, 2012. www.math.ku.dk/noter/filer.

Department of Mathematics and Statistics, University of New Mexico, Albuquerque, NM 87131, USA.