Quantitative K-Theory Related to Spin Chern Numbers*

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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 which 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.

Key words: K-theory; C^*-algebras; matrices

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Dedicated to Marc A. Rieffel, whose lectures
on Morita equivalence inspired all this

1 Introduction

In the past decade, in condensed matter physics, certain systems with gapped Hamiltonians were found to fall into two basic types. Some were perturbations of completely trivial systems, and some were found to be far from all completely trivial systems. These are now called "ordinary insulators" and "topological insulators" respectively. It is observed that a path of systems perturbing a topological insulator to an ordinary insulator must at some point have closed the gap. Physicists use K-theory, both real and complex, to determine which insulators are which.

An older mathematical situation springs to mind here. Given C^*-relations [14] in a form where they can hold exactly and also hold approximately, it was found that these approximate solutions fell into two basic types. Some are close to exact solutions, and others are far away from all exact solutions. The latter were called "phantom approximate solutions" [2]. These approximate solutions were often found in matrix algebras $\mathbf{M}_n(\mathbb{C})$, but also in C^*-algebras. In either case, the main tools for distinguishing phantom from ordinary approximate solutions were constructions in complex K-theory.

The most basic set of C^*-relations are the relations, in the unital category,

$$u^*u = 1, \qquad uu^* = 1, \qquad v^*v = 1, \qquad vv^* = 1, \qquad uv = vu.$$

There is generally no big distinction between u being "almost unitary" and being unitary, so we often study almost commuting unitaries in C^*-algebras, meaning unitaries u and v with $\|[u,v]\| \leq \delta$ for some small δ greater than zero.

There is a direct connection between almost commuting unitary matrices and certain classes of finite models of topological insulators, explored in [11, 16, 17]. In that research, many interesting mathematical conjectures and questions were raised, some of which we address here. Any serious numerical study of topological insulators must take into account the scattering method [7] of Fulga and his coauthors, which utilizes the sparseness of the matrices modeling both position observables and the Hamiltonian. That method still utilizes the Pfaffian–Bott index [16], discussed below, but as a secondary calculation after a dimension reduction from 3D to 2D.

What we wish to emphasize here are aspects of phantom approximate solutions that are similar to the behavior in topological insulators. The connection between these two fields of study is certainly greater than what has been explored to date.

Most of the theorems regarding approximate solutions to C^*-relations are completely non-quantitative. There is often an constant δ_0, unknown except for the fact that it is positive, so that nice things happen with relations hold to within at most δ_0. One of the goals in this context is to develop efficient numerical algorithms. When working numerically, a constant like 10^{-10} can act effectively like zero. Thus the desire for quantitative results.

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. Let us review how this connection arose.

There is a particularly practical equation for the projection e in $\mathbf{M}_2(C(\mathbb{T}^2))$ that has rank one and first Chern class one. The formula is similar to that of the Rieffel projections [20] in the irrational rotation algebras, specifically

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

where f, g and h are certain real functions defined on the unit circle.

The straight-forward plan in [13] was to compute the K-theory of a $*$-homomorphism $\varphi : C(\mathbb{T}^2) \to A$ by examining the associated commuting unitary elements $U = \varphi(u_0)$ and $V = \varphi(v_0)$ of the AF algebra A and the projection

$$e(U,V) = \begin{bmatrix} f(V) & g(z) + h(V)U \\ g(V) + U^*h(V) & 1 - f(V) \end{bmatrix} \tag{1.1}$$

where u_0 and v_0 are the canonical generating unitaries in $C(\mathbb{T}^2)$. Unitaries in an AF algebra are well-known to be the limits of direct sums of unitary matrices, and so commuting unitaries are determined by sequences of almost commuting matrices. In the specific situation of [13], $U = \lim(U_n \oplus A_n)$ and $V = \lim(V_n \oplus B_n)$ where A_n, B_n were commuting unitary matrices and U_n, V_n were unitary matrices with $\|[U_n, V_n]\| \to 0$.

Equation (1.1) applies also to a pair of almost commuting unitary matrices such as U_n and V_n. The result is not a projection, but a hermitian matrix with a large gap at $\frac{1}{2}$ in its spectrum. The K-theory of φ was easily evaluated once the spectrum of $e(U_n, V_n)$ and $e(A_n, B_n)$ were understood.

The more interesting discovery in [13] was that formula (1.1) can be used to define what is now called the Bott index of a pair of almost commuting unitary matrices. This index can distinguish pairs of commuting matrices close to commuting pairs from those that are far from commuting pairs.

There is ambiguity in the choice of f, g and h. There are other ambiguities, discussed in [2], 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 [7, 11, 16] 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 [13], 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 δ_0 so that $\|[U,V]\| \le \delta_0$ 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 [7, 11, 16].

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

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^\sharp = \begin{bmatrix} D^{\mathrm{T}} & -B^{\mathrm{T}} \\ -C^{\mathrm{T}} & A^{\mathrm{T}} \end{bmatrix}. \tag{1.2}$$

Specific unitary matrices that can be studied in the context of a free particle system on a finite lattice on a two-torus are essentially complex-valued position operators that have been compressed to low energy space. These are actually not quite unitary, but one can consider the unitary parts of their polar decomposition. These then are almost commuting unitary matrices that carry a lot of information about the original system [11, § 1.1].

When the system has fermionic time reversal symmetry, the resulting unitary matrices will be self-dual. The correct matrix problem to study is then almost commuting self-dual matrices. The invariant [16] that can be used to show that some pairs are bounded away from commuting self-dual unitary pairs is the sign of

$$\mathrm{Pf}(Q^*(2e(U,V) - I)Q),$$

where Q is a specific matrix discussed below that creates anti-symmetry in the formula so that the Pfaffian makes sense. The resulting index we called the Pfaffian–Bott index [16].

The Pfaffian–Bott index of the unitary matrices associated to certain 2D systems has, for large system size, been proven [11, Lemma 5.8.] to equal the spin Chern number of that system. It is perhaps more accurate to say that this Pfaffian–Bott index equals Kitaev's $\mathbb{Z}/2$ index for finite 2D systems in class AII.

An alternate way to compute a Bott index [6, Definition 2.1], equal to the Bott index for small commutators, involves taking the logarithm of one of the unitaries. It was surprising to find that this method, when adapted to the self-dual case, seemed to generate better data in a numerical study of disordered topological insulators [16, 17].

We show in the final section that this method of computing the Pfaffian–Bott index gives the correct answer for commutator norms up to a specific constant. 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].

Our results are principally stated in terms of unitary matrices. However, the study of almost commuting unitary elements of C^*-algebras is not that different. We know this because we know that the soft-torus is RFD (residually finite-dimensional) [1].

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

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

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

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

due to Exel [4, Lemma 3.1]. This we easily prove: since in some basis VUV^*U^* is diagonal and unitary,

$$VUV^*U^* = \begin{pmatrix} e^{i\theta_1} & & \\ & \ddots & \\ & & e^{i\theta_n} \end{pmatrix}$$

for some $-\pi < \theta_j < \pi$ and

$$\mathrm{Tr}\left(\frac{1}{2\pi i} \log\left(VUV^*U^*\right)\right) = \frac{1}{2\pi i}\mathrm{Tr}\begin{pmatrix} i\theta_1 & & \\ & \ddots & \\ & & i\theta_n \end{pmatrix} = \frac{1}{2\pi}\sum \theta_j$$

and

$$\det\left((VUV^*U^*)^t\right) = \det\begin{pmatrix} e^{it\theta_1} & & \\ & \ddots & \\ & & e^{it\theta_n} \end{pmatrix} = \prod e^{it\theta_j}$$

and this path has winding number

$$\omega(U, V) = \frac{1}{2\pi}\sum \theta_j.$$

Lemma 2.1 ([6, p. 367]). *When U and V are commuting unitary matrices, $\omega(U, V) = 0$.*

Proof. In this case the path of determinants is the constant path. ∎

Lemma 2.2 ([5]). *For*

$$
U = \begin{pmatrix} 0 & & & & 1 \\ 1 & 0 & & & \\ & 1 & \ddots & & \\ & & \ddots & 0 & \\ & & & 1 & 0 \end{pmatrix}, \qquad V = \begin{pmatrix} e^{i\pi/n} & & & & \\ & e^{2i\pi/n} & & & \\ & & \ddots & & \\ & & & e^{-i\pi/n} & \\ & & & & 1 \end{pmatrix}
$$

we have $\omega(U, V) = -1$.

Proof. We find $VUV^*U^* = e^{-\frac{2\pi i}{n}}I$ and so

$$
\frac{1}{2\pi i}\mathrm{Tr}(\log(VUV^*U^*)) = \frac{1}{2\pi i}\mathrm{Tr}\left(-\frac{2\pi i}{n}I\right) = -1.
$$
∎

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 $\sqrt{2}$, meaning*

$$
\|U - U_1\| + \|V - V_1\| > \sqrt{2},
$$

whenever U_1 and V_1 are unitary matrices with $U_1 V_1 = V_1 U_1$. Indeed,

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

The proof of this will be broken into lemmas and propositions. Theorem 2.3 is a variation on the main result in [5]. That result had a smaller lower bound, but the bound applied to the distance to any pair of commuting matrices, not just commuting unitary matrices.

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 continuous path U_s of unitary matrices from U_0 to U_1, and for any continuous path V_s of unitary matrices from V_0 to V_1, 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 exists then

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

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. ∎

Proposition 2.5. *Suppose $\|[U, V]\| < 2$. If $\|[U_1, V_1]\| = 2$, then*

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

If $\|[U_1, V_1]\| < 2$ and $\omega(U_1, V_1) \neq \omega(U, V)$, then

$$
\|U - U_1\| + \|V - V_1\| \geq \sqrt{4 - \left(\max(\|[U, V]\|, \|[U_1, V_1]\|)\right)^2}.
$$

More generally, $\|U - U_1\| + \|V - V_1\|$ is greater than or equal to

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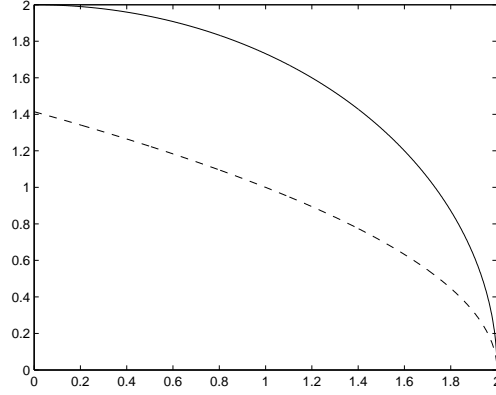$$

Figure 1. The solid curve shows the minimum radius in the gap at -1 in with spectrum of VUV^*U^* 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.

Proof. We can connect $U = U_0$ to U_1 by an analytic path of unitary matrices U_t of length $2\arcsin(\frac{1}{2}\|U_0 - U_1\|)$. Similarly we have an analytic path V_t from $V = V_0$ to V_1 of length $2\arcsin(\frac{1}{2}\|V_0 - V_1\|)$. We now bound the length of the path $W_t = V_t U_t V_t^* U_t^*$ in two ways. We compute the derivative W_t' of $t \mapsto W_t$, and since $\|W_t'\| \le 2\|U_t'\| + 2\|V_t'\|$ we see that

$$\text{Length}(W_t) \le 4\arcsin\left(\frac{1}{2}\|U_0 - U_1\|\right) + 4\arcsin\left(\frac{1}{2}\|V_0 - V_1\|\right).$$

On the other hand, if $\mu_k(t)$ is an analytic choice of eigenvalues for W_t then we know from [6, p. 374] that $|\mu_k'(t)| \le \|W_t'\|$. One of these paths of eigenvalues must hit -1, and yet

$$|\mu_k(t) - 1| \le \|[U_t, V_t]\|$$

for $t = 0$ and $t = 1$, so

$$\text{Length}(W_t) \ge 2\pi - 2\arcsin\left(\frac{1}{2}\|[U_0, V_0]\|\right) - 2\arcsin\left(\frac{1}{2}\|[U_1, V_1]\|\right).$$

Therefore

$$4\arcsin\frac{\|U_0 - U_1\|}{2} + 4\arcsin\frac{\|V_0 - V_1\|}{2} \ge 2\pi - 2\arcsin\frac{\|[U_0, V_0]\|}{2} - 2\arcsin\frac{\|[U_1, V_1]\|}{2}.$$

We need to know the smallest value of $\|U_0 - U_1\| + \|V_0 - V_1\|$ that can be achieved, and for this it suffices to minimize these subject to the constraint

$$4\arcsin\frac{\|U_0 - U_1\|}{2} + 4\arcsin\frac{\|V_0 - V_1\|}{2} = 2\pi - 2\arcsin\frac{\|[U_0, V_0]\|}{2} - 2\arcsin\frac{\|[U_1, V_1]\|}{2}.$$

This is the problem of placing 6 chords that are adjacent to each other that go around the unit circle, with two chords fixed of length $\|[U_0, V_0]\|$ and $\|[U_1, V_1]\|$, while the other four come in pairs, two of length x and two of length y. The minimizing of $2x + 2y$ occurs when we set one length, say y, to zero, with the other the arc length corresponding to arc length π minus half the arc length occupied by the two fixed chords, so

$$2\arcsin\left(\frac{1}{2}x\right) = \pi - \arcsin\left(\frac{1}{2}\|[U_0, V_0]\|\right) - \arcsin\left(\frac{1}{2}\|[U_1, V_1]\|\right).$$

We conclude

$$\|U_0 - U_1\| + \|V_0 - V_1\| \geq 2\sin\left(\frac{1}{2}\left(\pi - \arcsin\left(\frac{1}{2}\|[U_0, V_0]\|\right) - \arcsin\left(\frac{1}{2}\|[U_1, V_1]\|\right)\right)\right).$$

We find

$$2\sin\left(\frac{1}{2}\left(\pi - \arcsin\left(\frac{1}{2}\|[U_0, V_0]\|\right) - \arcsin\left(\frac{1}{2}\|[U_1, V_1]\|\right)\right)\right)$$

$$= \sqrt{2}\sqrt{1 - \cos\left(\pi - \arcsin\left(\frac{1}{2}\|[U_0, V_0]\|\right) - \arcsin\left(\frac{1}{2}\|[U_1, V_1]\|\right)\right)}$$

$$= \sqrt{2}\sqrt{1 + \cos\left(\arcsin\left(\frac{1}{2}\|[U_0, V_0]\|\right) + \arcsin\left(\frac{1}{2}\|[U_1, V_1]\|\right)\right)}$$

$$= \sqrt{2 + 2\sqrt{1 - \frac{1}{4}\|[U_0, V_0]\|^2}\sqrt{1 - \frac{1}{4}\|[U_1, V_1]\|^2} - \frac{1}{2}\|[U_0, V_0]\|\|[U_1, V_1]\|}$$

and so, setting $\Delta = \max(\|[U_0, V_0]\|, \|[U_1, V_1]\|)$, we find

$$\|U_0 - U_1\| + \|V_0 - V_1\| \geq \sqrt{2 + 2\sqrt{1 - \frac{1}{4}\Delta^2}\sqrt{1 - \frac{1}{4}\Delta^2} - \frac{1}{2}\Delta^2} = \sqrt{4 - \Delta^2}. \qquad \blacksquare$$

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, 19, 21]. (In particular, see the discussion in Section III in [19].) Results such as this also change dramatically when the matrices come from different symmetry classes, as seen in [17].

There is an answer, but it is only a non-quantitative, nonconstructive result for small δ. This we proven in joint work with Eilers and Pederson and we restate 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, 12].

Theorem 2.6 ([3, Theorem 6.15]). *For any $\epsilon > 0$, there is a δ 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 defined 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

$$V = Q \begin{pmatrix} e^{i\theta_1} & & \\ & \ddots & \\ & & e^{i\theta_d} \end{pmatrix} Q^* \implies f(V) = Q \begin{pmatrix} f(e^{i\theta_1}) & & \\ & \ddots & \\ & & f(e^{i\theta_2}) \end{pmatrix} Q^*.$$

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 2π we define $f[V]$ as $\tilde{f}(V)$ where $\tilde{f}(z) = f(-i\log(z))$. In other words,

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

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

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

and

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

which are shown in Fig. 2. For any unitaries set

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

We have in mind unitary matrices, but let us look briefly at the more abstract situation. If we have commuting unitary matrices u and v in a unital C^*-algebra A then we have, by the spectral theorem, a $*$-homomorphism $\varphi : C(\mathbb{T}^2) \to B$.

Let us adopt the convention that K_0 will be defined by hermitian elements with spectrum within $\{-1, 1\}$ instead of the usual description using projections, which are just hermitian elements with spectrum within $\{0, 1\}$. Then φ pushes forward the Bott element

$$\beta = [B(z,w)] - \left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \qquad \text{to} \qquad [B(u,v)] - \left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right].$$

If we have $\|[u,v]\| = \delta$ for small delta, then we can imagine something weaker than a $*$-homomorphism, $\psi : C(\mathbb{T}^2) \to B$, and attempt the push-forward.
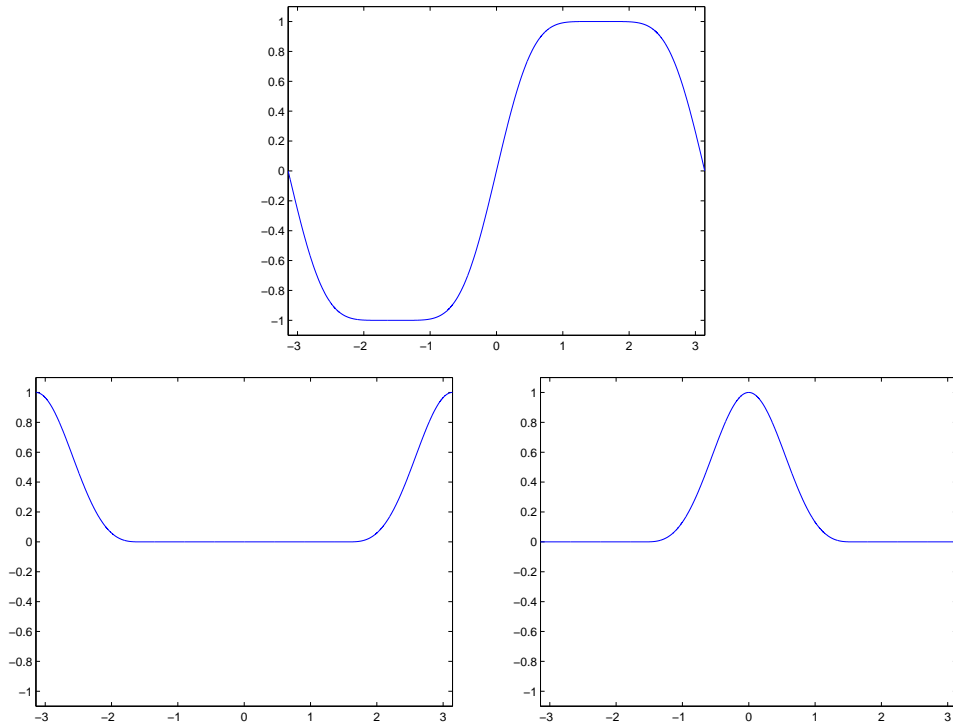
Figure 2. Functions for the standard Bott index (trig method).

Working heuristically, we simply create $[B(u, v)]$ and expect that this will be hermitian and with spectrum close to being contained in $\{-1, 1\}$. Now we apply functional calculus $\chi(B(u, v))$ (this is spectral flattening in physics) and define the Bott index of this pair as

$$\chi(B(u, v)) - \left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right]$$

in $K_0(B)$.

This construction can be formalized in many ways. Exel [4] defined the soft torus A_δ as the universal unital C^*-algebra generated by two elements u_δ and v_δ subject to being unitary with $\|[u_\delta, v_\delta]\| \leq \delta$. The only restriction on δ is $\delta < 2$. He calculated the K-theory of A_δ, showing that the natural map ρ_δ onto $C(\mathbb{T}^2) = A_0$ is an isomorphism on K-theory. From u and v we get a commuting diagram

$$
\begin{array}{ccc}
A_\delta & & \\
\downarrow{\scriptstyle \rho_\delta} & \searrow{\scriptstyle \gamma} & \\
C(\mathbb{T}^2) & & B
\end{array}
$$

and can defined a very abstract index of (u, v) as $\gamma_* \circ ((\rho_\delta)_*)^{-1}(\beta)$.

Computationally, spectrally flattening an invertible matrix can be expensive. Most importantly, doing so will destroy sparseness, should it initially exist. Therefore, in the special case $B = \mathbf{M}_n(\mathbb{C})$ we use the signature. Abstractly this is counting eigenvalues, but numerically there are many options for algorithms.

Now we resume discussion of the special case of unitary matrices. For an invertible, hermitian matrix A we define its *signature* $\mathrm{Sig}(A)$ 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. Notice that if A is in $M_n(\mathbb{C})$ and if n is even then $\mathrm{Sig}(A)$ must be even.
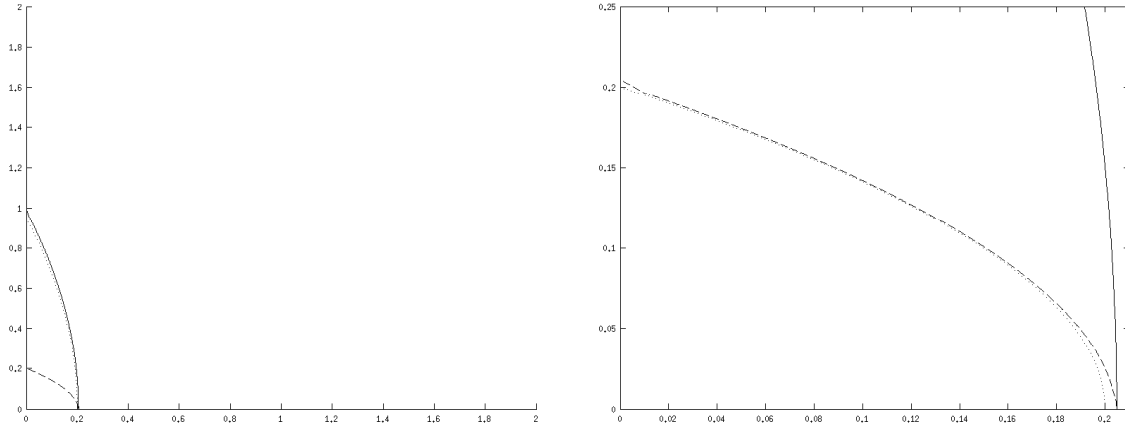
Figure 3. In both: solid curve on top is the guaranteed spectral gap in $B(U,V)$ for a given δ. The dashed curve is the distance one can move where it is proven the gap will not close. The dotted curve in the left plot is $\frac{19}{20}\sqrt{1-5\delta}$. The dotted curve on the right is $\frac{1}{5}\sqrt{1-5\delta}$.

Remark 3.3. Monte Carlo methods have generated numerical evidence that the gap in $B(U,V)$ actually closes at about $\delta = 0.85$.

Definition 3.4. If $\|[U,V]\| \leq 0.206007$ define $\kappa(U,V)$, the *Bott index* of (U,V), as the integer

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

It should be noted that setting

$$\gamma_1 = f(\theta_2), \qquad \gamma_2 = g(\theta_2) + h(\theta_2)\cos(\theta_1), \qquad \gamma_3 = h(\theta_2)\sin(\theta_1)$$

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

Theorem 3.5. *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 δ plotted as a solid curve in Fig. 3.*

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 $\frac{1}{5}\sqrt{1-5\delta}$. Indeed, this distance is at least as large as the function of δ plotted as a dashed curve in Fig. 3.*

We will prove Theorem 3.5 in Section 5, and it will be a lot of work. 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 $\mathbf{M}_{2d}(\mathbb{C})$ and with $\sharp$ the generalized involution discussed in the next section, that physicists call the dual. Then $B(U,V)$ is in $\mathbf{M}_{2d}(\mathbb{C}) \otimes \mathbf{M}_2(\mathbb{C})$ which has on it the generalized involution $\tau = \sharp \otimes \sharp$. In terms of real C^*-algebras, this is a copy of $\mathbf{M}_{2d+2}(\mathbb{C})$ 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 Pfaffian, hence the Pfaffian–Bott index studied in [16]. 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.
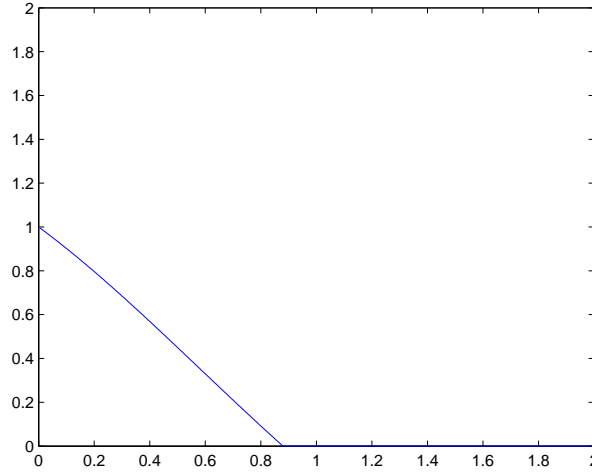
Figure 4. Upper bound on the gap radius, as $\|[V, U]\|$ varies from 0 to about 0.21.

An easy upper bound on the gap radius can be found, using the example in Lemma 2.2, shown in Fig. 4. This shows we cannot get as big a gap using $B(U, V)$ as was possible with VUV^*U^*, but that the situation is likely not as bad as Fig. 3 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 3.6. *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 3.5 is the following.

Theorem 3.7. *Suppose* U *and* V *are unitary matrices. If* $\|[U, V]\| \leq 0.206007$ *then*

$$\kappa(U, V) = \omega(U, V).$$

Proof. Exel [4] showed that for $\|[U, V]\| < 2$ the winding invariant equals an abstract K-theory invariant. In the notation of [4], this is defined in terms of b_δ in $K_0(A_\delta)$. 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_δ, the K-theory class of $B(u, v)$ is b_δ. ∎

Remark 3.8. The smallest $\delta = \|[U, V]\|$ for which these invariants have been observed to differ, in numerical examples, is $\delta \approx 0.85$.

Remark 3.9. There is ambiguity in how we define the Bott index when $\|[U, V]\|$ is large. Exel's abstract index in terms of the soft torus is not really computable, as there are no known explicit formulas for b_δ when $\delta > 0.206007$. Certainly the estimates above are not optimal so we are not sure for which δ a different formula is needed. In general, when computing the K-theoretical obstructions to approximate representations of relations being close to exact representations, there is ambiguity when the error in the relations is large. Ultimately, the ambiguity does not generally matter, as was discussed at length in [2]. In the case of almost commuting unitary matrices, both the winding number invariant and the Bott index as in Definition 3.4 give computable invariants that, when the commutator is small, are stable in a sizable region around the pair. More importantly, when either index is non-trivial, we know there is a considerable distance to any pair of commuting unitary matrices.

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 $\mathbf{M}_{2N}(\mathbb{C})$ and this specifies the dual operation

$$X^\sharp = -ZX^\mathrm{T}Z$$

as above in (1.2).

When we discuss $\mathbf{M}_2(\mathbf{M}_{2N}(\mathbb{C})) = \mathbf{M}_{2N}(\mathbb{C}) \otimes \mathbf{M}_2(\mathbb{C})$ 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 [11, Lemma 1.3]

$$Q^* X^{\sharp\otimes\sharp} Q = (Q^* X Q)^\mathrm{T}.$$

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

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix}^{\sharp\otimes\sharp} = \begin{bmatrix} A_{44}^\mathrm{T} & -A_{34}^\mathrm{T} & -A_{24}^\mathrm{T} & A_{14}^\mathrm{T} \\ -A_{43}^\mathrm{T} & A_{33}^\mathrm{T} & A_{23}^\mathrm{T} & -A_{13}^\mathrm{T} \\ -A_{42}^\mathrm{T} & A_{32}^\mathrm{T} & A_{22}^\mathrm{T} & -A_{12}^\mathrm{T} \\ A_{41}^\mathrm{T} & -A_{31}^\mathrm{T} & -A_{21}^\mathrm{T} & A_{11}^\mathrm{T} \end{bmatrix}.$$

Recall the Pfaffian is defined for all skew-symmetric, complex $2n$-by-$2n$ matrices by

$$\mathrm{Pf}\left(O \begin{bmatrix} 0 & a_1 & & & \\ -a_1 & 0 & a_2 & & \\ & -a_2 & 0 & a_3 & \\ & & -a_3 & 0 & \ddots \\ & & & \ddots & \ddots \end{bmatrix} O^\mathrm{T} \right) = \det(O) a_1 a_3 \cdots a_{2n-1}$$

for O real orthogonal. (All skew-symmetric matrices have such a factorization, a modified Hessenberg decomposition.) The essential properties are that

$$\mathrm{Pf}\left(YXY^\mathrm{T}\right) = \det(Y)\mathrm{Pf}(X)$$

for arbitrary Y, that the Pfaffian varies continuously, and

$$(\mathrm{Pf}(X))^2 = \det(X)$$

so the Pfaffian is zero exactly on the set of skew-symmetric, singular matrices.

For matrices with the symmetry $X^{\sharp \otimes \sharp} = -X$ we can define a modified Pfaffian

$$\widetilde{\mathrm{Pf}}(X) = \mathrm{Pf}(Q^* X Q).$$

We still have

$$\left(\widetilde{\mathrm{Pf}}(X)\right)^2 = \det(X)$$

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 $\mathbf{M}_{4N}(\mathbb{C})$ and $B^* = B$ and $B^{\mathrm{T}} = -B$ and B is invertible. Then $\mathrm{Pf}(B) \in \mathbb{R} \setminus \{0\}$. If B_1 and B_2 are elements of*

$$\mathcal{H} = \left\{ B \in \mathbf{M}_{4N}(\mathbb{C}) \,\middle|\, B^* = B = -B^{\mathrm{T}} \text{ is invertible} \right\},$$

then they can be connected by a path in $\mathcal{H}$ if and only if with $\mathrm{Pf}(B_1)$ and $\mathrm{Pf}(B_2)$ have the same sign.

Proof. We can apply Theorem 8.7 in [11] to iB and learn that there is a real orthogonal matrix O so that $\det(O) = 1$ and

$$B = O \begin{bmatrix} 0 & i\lambda_1 & & & & \\ -i\lambda_1 & 0 & & & & \\ & & 0 & i\lambda_2 & & \\ & & -i\lambda_2 & 0 & & \\ & & & & \ddots & \ddots \\ & & & & \ddots & \ddots \end{bmatrix} O^{\mathrm{T}}$$

and all the real numbers λ_j are positive except λ_1 which as the same sign as $\mathrm{Pf}(B)$. 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 $\mathrm{Pf}(B)$ 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 Section 3. If $\|[U,V]\| \leq 0.206007$ define $\kappa_2(U,V)$ as the value in $\{\pm 1\}$ given by

$$\kappa_2(U,V) = \mathrm{Sign}\big(\widetilde{\mathrm{Pf}}(B(U,V))\big).$$

Lemma 4.3. *When U and V are commuting unitary matrices, $\kappa_2(U,V) = 1$.*

Proof. This is a special case of Theorem 8.8 of [11]. Here is that proof in less technical language for this special case.

One easily checks that κ_2 remains constant along a path so long as $\|[U_t, V_t]\| \leq 0.206007$. One can use joint functional calculus (for commuting normal operators), 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

$$\widetilde{\mathrm{Pf}} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} = \mathrm{Pf} \begin{bmatrix} iZ & 0 \\ 0 & -iZ \end{bmatrix} = \mathrm{Pf}\,(iZ)\,\mathrm{Pf}\,(-iZ) = i^n(-i)^n = 1. \qquad \blacksquare$$

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*

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

Remark 4.6. We can describe the Pfaffian–Bott index more generally if we use the language of real C^*-algebras. Suppose we are given a real C^*-algebra as a complex C^*-algebra B along with an anti-multiplicative linear involution τ on B. Then a nice picture of $K_{-2}(B, \tau)$ (ignoring details with higher matrices) is in terms of

$$\{x \in \mathrm{GL}(B \otimes \mathbf{M}_2(\mathbb{C})) \,\big|\, x^* = x, \; x^{\tau \otimes \sharp} = -x\},$$

as was proven in [11, § 8]. Then $B(z, w)$ is an element in $C(\mathbb{T}^2) \otimes \mathbf{M}_2(\mathbb{C})$ that is hermitian, with spectrum $\{-1, 1\}$ and, with τ the identity on $C(\mathbb{T}^2)$, also $B(z, w)^{\tau \otimes \sharp} = -B(z, w)$. Therefore $B(z, w)$ determines an element in $K_{-2}(C(\mathbb{T}^2))$. Given U and V self-dual unitary matrices in some unital real C^*-algebra (B, τ), we can define, for now informally, the push-forward by something that is "almost a morphism" $\psi : (C(\mathbb{T}^2), \tau) \to (B, \tau)$, to produce the element $[B(U, V)]$ in $K_{-2}(B, \tau)$. We can define a real structure on the soft-torus A_δ by setting $u_\delta^\tau = u_\delta$ and $v_\delta^\tau = v_\delta$ (see [22, Chapter 5] for details on why this is well-defined) and consider $\beta_\delta = [B(u_\delta, v_\delta)]$. Then, for small δ, we have a real $*$-homomorphism

$$\gamma : \; (A_\delta, \tau) \to (B, \tau)$$

and the Pfaffian–Bott element is then $\gamma_*(\beta_\delta)$ in $K_{-2}(B, \tau)$. For larger δ we can proceed, but need an analysis of $K_{-2}(A_\delta, \tau)$ that is best left for another paper. In the special case of (B, τ) equal to $(\mathbf{M}_{2n}(\mathbb{C}), \sharp)$ we used first the isomorphism

$$K_{-2}(\mathbf{M}_{2n}(\mathbb{C}), \sharp) \cong K_2(\mathbf{M}_{2n+2}(\mathbb{C}), \mathrm{T})$$

induced by conjugation by a set unitary, and then the isomorphism

$$K_2(\mathbf{M}_{2n+2}(\mathbb{C}), \mathrm{T}) \to \mathbb{Z}/2$$

induced by the sign of the Pfaffian. So

$$\big(C(\mathbb{T}^2), \mathrm{id}\big) \leftarrow (A_\delta, \tau) \to (\mathbf{M}_{2n}(\mathbb{C}), \sharp)$$

leads to

$$K_{-2}(C(\mathbb{T}^2), \mathrm{id}) \leftarrow K_{-2}(A_\delta, \tau) \to K_{-2}(\mathbf{M}_{2n}(\mathbb{C}), \sharp) \to K_2(\mathbf{M}_{2n+2}(\mathbb{C}), \mathrm{T}) \to \mathbb{Z}/2$$

with the right-most arrow given by the Pfaffian. The remaining issue is showing the left-most arrow is surjective, which we have done here for small δ by explicitly defining $B(u_\delta, v_\delta)$.

5   Proof that the gap persists

Now we prove Theorem 3.5, finding a lower bound on the size of the gap in $B(U, V)$ as long as $\delta = \|[U, V]\|$ is not too big. 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 $\|[f[V], U]\| \leq \|f'\|_{\mathrm{F}} \|[U, V]\|$ where $\|f'\|_{\mathrm{F}}$ is the ℓ^1-norm of the sequence of Fourier coefficients of f. On its own, this estimate is really only helpful for very small commutators.

Definition 5.1. Suppose f is continuous and 2π-periodic. Following [18] we define $\eta_f : [0, \infty) \to [0, \infty)$ by

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

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

Once we have a bound on η_f we can use it to bound more than just commutators. Indeed, by [18, 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 [18].

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

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

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 2π-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

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

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 $f[V]$, etc. We see easily $S^* = S$ and

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

where

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

and

$$B = fg + \tfrac{1}{2}f\{h,U\} - gf - \tfrac{1}{2}\{h,U\}f = \tfrac{1}{2}f\{h,U\} - \tfrac{1}{2}\{h,U\}f.$$

We have

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

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

$$\|A\| \leq \tfrac{1}{4}\left\|hUhU^* + Uh^2U^* + UhU^*h - 3h^2\right\| + \tfrac{1}{2}\left\|gU^*h - ghU^* + hUg - Uhg\right\|$$
$$\leq \tfrac{1}{2}\|h\|\|Uh - hU\| + \tfrac{1}{4}\left\|Uh^2 - h^2U\right\| + \|g\|\|Uh - hU\| \leq 2\|Uh - hU\|$$

and

$$\|B\| = \tfrac{1}{2}\|hfU + fUh - hUf - Ufh\| \leq \tfrac{1}{2}\|h[f,U]\| + \tfrac{1}{2}\|[f,U]h\| \leq \|[f,U]\|,$$

so

$$\left\|S^2 - I\right\| \leq 2\|[h,U]\| + \|[f,U]\|. \qquad \blacksquare$$

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

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

and

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

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

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

We new bound the derivative of g and h, computing

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

where

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

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 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 [16]. We compute these a little more carefully here. Thus Table 1 is a slightly more accurate replacement for Table 11 in [11]. We find

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

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

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

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

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

Letting T_K denote the Taylor polynomial $T_K(x) \approx \sqrt{1+x}$ of degree K expanded at 0, we have

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

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

$$= \frac{1}{2\pi} \sqrt{\frac{407}{512}} \left(\sqrt{1 - \frac{105}{407}} - T_K \left(-\frac{105}{407} \right) \right).$$

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[1].

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[1] Code assisting with tables and figures and calculations is available at http://repository.unm.edu/handle/1928/23494.

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 $c_n = -c_n$.

n	0	1	2	3	4	5
a_n	0	$-\frac{150i}{256}$	0	$-\frac{25i}{256}$	0	$-\frac{3i}{256}$
b_n	0.202047	-0.179940	0.125655	-0.066010	0.023445	-0.003886
c_n	0.202047	0.179940	0.125655	0.066010	0.023445	0.003886

Using the values in the table to define

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

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 π 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

$$\left\| h_5' \right\|_{\text{F}} = \sum_{n=-5}^{5} n|c_n| = 1.48498.$$

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*

$$\|h'\|_{\text{F}} \leq 2.99208.$$

Proof. We check that

$$h'(x) = \frac{-\frac{1}{\sqrt{3256}}\left(45\cos^4(x) + 60\cos^2(x) + 120\right)}{\sqrt{1 + \frac{96}{407}\cos(2x) + \frac{9}{407}\cos(4x)}} \sin(x)\cos^2(x)\chi_{[-\frac{\pi}{2},\frac{\pi}{2}]}(x)$$

Table 2. Bounds on η_h as a slope and an offset.

n	$m =$ bound on $\|h'_n\|_{\mathrm{F}}$	$b =$ bound on $\mathrm{diam}(h(x) - h_n(x))$
0	0	1
1	0.359880	0.732237
2	0.862500	0.350141
3	1.258560	0.106619
4	1.446120	0.017509
5	1.48498	0.004110
∞	2.99208	0

and attack this as three factors. It is easy to see

$$\left\| -\frac{1}{\sqrt{3256}}\left(45\cos^4(x) + 60\cos^2(x) + 120\right) \right\|_{\mathrm{F}} = \frac{225}{\sqrt{3256}}$$

and the next factor is not so bad, as we see

$$\left\| \frac{1}{\sqrt{1 + \frac{96}{407}\cos(2x) + \frac{9}{407}\cos(4x)}} \right\|_{\mathrm{F}} \leq \sum_{k=0}^{\infty} \left|\binom{-1/2}{k}\right| \left\| \frac{96}{407}\cos(2x) + \frac{9}{407}\cos(4x) \right\|_{\mathrm{F}}^{k}$$

$$= \sum_{k=0}^{\infty} \binom{-1/2}{k}(-1)^k \left(\frac{105}{407}\right)^k = \frac{1}{\sqrt{1 - \frac{105}{407}}} = \sqrt{\frac{407}{302}}.$$

We estimate

$$\left\| \sin(x)\cos^2(x)\chi_{[-\frac{\pi}{2},\frac{\pi}{2}]}(x) \right\|_{\mathrm{F}}$$

as follows. The Fourier series of $-i\sin(x)\cos^2(x)\chi_{[-\frac{\pi}{2},\frac{\pi}{2}]}$ is

$$\ldots, \frac{16}{3465\pi}, 0, \frac{-4}{315\pi}, 0, \frac{8}{105\pi}, \frac{1}{16}, \frac{-8}{15\pi}, \frac{-1}{16}, 0, \frac{1}{16}, \frac{8}{15\pi}, \frac{-1}{16}, \frac{-8}{105\pi}, 0, \frac{4}{315\pi}, 0, \frac{-16}{3465\pi}, \ldots$$

with terms beyond $n = 3$ being given by

$$-\cos\left(\frac{\pi n}{2}\right)\left(\frac{1}{(n-1)^3 - 4(n-1)} + \frac{1}{(n+1)^3 - 4(n+1)}\right).$$
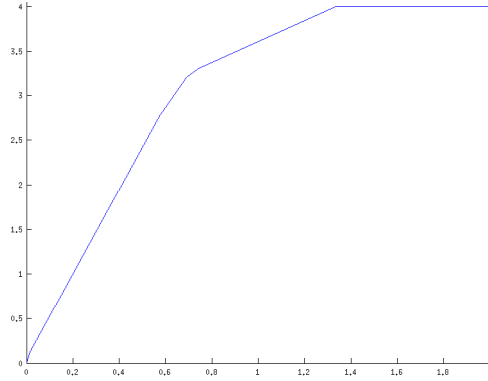
Therefore

$$\left\| \sin(x)\cos^2(x)\chi_{[-\frac{\pi}{2},\frac{\pi}{2}]} \right\|_{\mathrm{F}} = \frac{1}{4} + \frac{16}{15\pi} + \frac{18}{105\pi} + \frac{4}{\pi}\sum_{n=3}^{\infty} \frac{1}{(2n+1)^3 - 4(2n+1)}$$

$$\leq \frac{1}{4} + \frac{16}{15\pi} + \frac{18}{105\pi} + \frac{4}{315\pi} + \frac{16}{3465\pi} + \frac{4}{\pi}\int_4^{\infty} \frac{1}{8x^3 + 12x^2 - 2x - 3}\,dx$$

$$= \frac{1}{4} + \frac{16}{15\pi} + \frac{18}{105\pi} + \frac{4}{315\pi} + \frac{16}{3465\pi} + \frac{1}{4\pi}\ln\left(\frac{81}{77}\right)$$

and so

$$\|h'\|_{\mathrm{F}} \leq \frac{225}{\sqrt{3256}}\sqrt{\frac{407}{302}}\left(\frac{1}{4} + \frac{16}{15\pi} + \frac{18}{105\pi} + \frac{4}{315\pi} + \frac{16}{3465\pi} + \frac{1}{4\pi}\ln\left(\frac{81}{77}\right)\right) < 2.992076. \quad \blacksquare$$

Table 3. Bounds on η_f as a slope and an offset.

n	$m = $ bound on $\|f_n'\|_{\mathrm{F}}$	$b = $ bound on $\mathrm{diam}(f(x) - f_n(x))$
0	0	2
1	1.171875	0.4375
2	1.7578125	0.04687
∞	1.875	0

Figure 5. The function $\beta(\delta)$ that bounds $\|B(U,V)^2 - I\|$ in terms of $\delta = \|[U,V]\|$.

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 $\eta_f(\delta) \le m\delta + b$ for each of the values in Table 3, and $\eta_g(\delta) \le m\delta + b$ and $\eta_h(\delta) \le m\delta + b$ for each of the values in Table 2.*

Let $\beta(\delta) = 2\eta_h(\delta) + \eta_f(\delta)$ which is shown in Fig. 5.

Theorem 5.7. *Suppose U and V are unitary matrices. Then*

$$\left\|B(U,V)^2 - I\right\| \le \beta(\|[U,V]\|)$$

and for $\|[U,V]\| \le 0.206007$ 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 must show is how $B(U,V)$ varies as U and V vary. After this, all our main theorems will follow.

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

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

and so

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

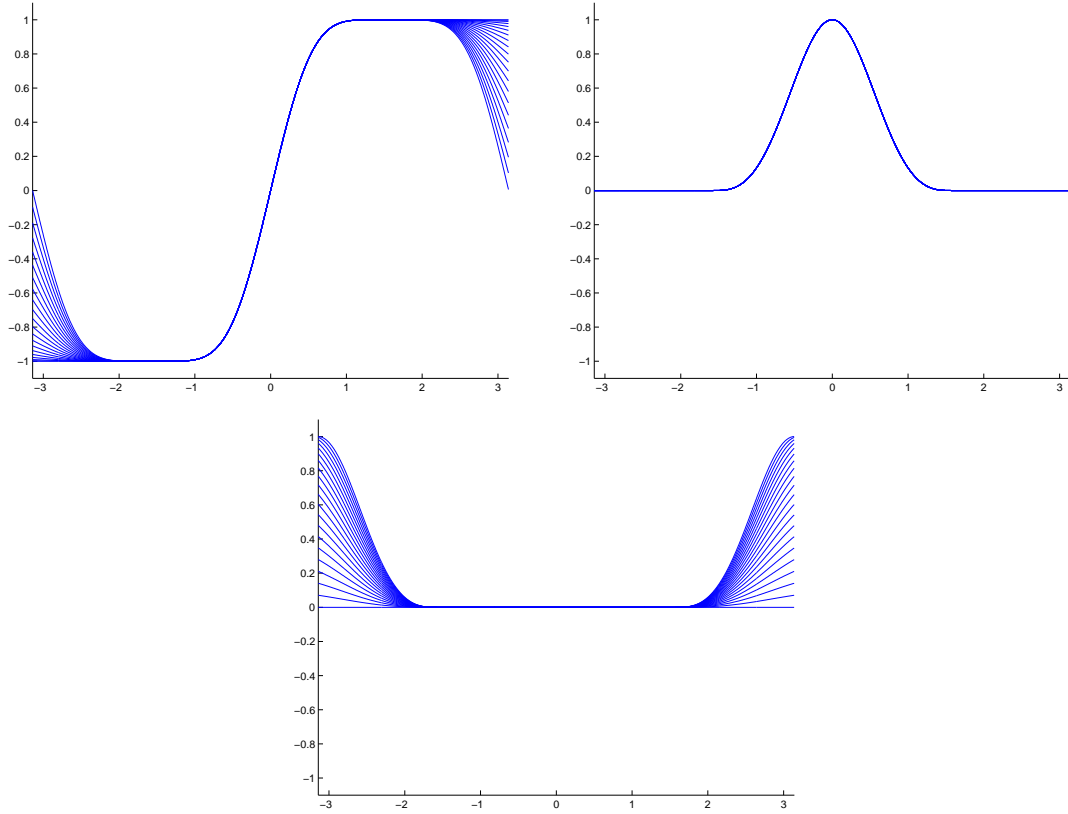**Proof.** This follows easily from Lemma 5.6 and [18, Lemma 1.2].   ■

Figure 6. First part of the path, showing f_t then h_t then g_t.

6 The log method

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

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

where iK is the logarithm of V, meaning $-\pi \le K < \pi$ and $e^{iK} = V$. Numerical evidence in [16] suggests that, for small commutators, the Pfaffian–Bott index can be computed using $B_{\mathrm{L}}(U, V)$. 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 of V whatsoever.

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 2π-periodic. Suppose U and V are unitary matrices and $-iK$ is a logarithm of V and define*

$$S = \begin{bmatrix} f(K) & g(K) + \frac{1}{2}\left\{h(K), U\right\} \\ g(K) + \frac{1}{2}\left\{h(K), U^*\right\} & -f(K) \end{bmatrix}.$$

Then $S^* = S$ and

$$\left\|S^2 - I\right\| \le (\|g\| + 1)\|[h[V], U]\| + \frac{1}{4}\|[h[V], U]\|^2 + \frac{1}{2}\left\|[h^2[V], U]\right\| + \|[q[V], U]\|.$$
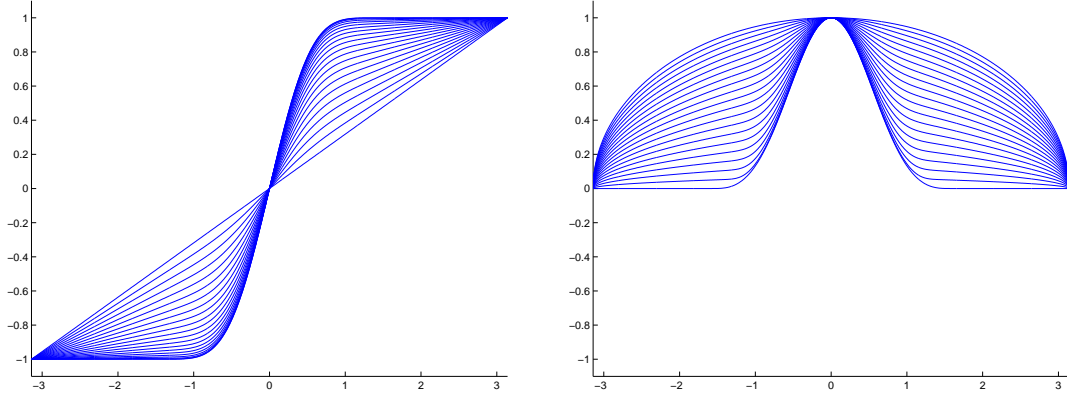
Figure 7. Second part of the path, showing only f_t then h_t. Here g_t is zero.

Proof. We write f for $f(K)$, etc., and estimate a bit more carefully than before. We find

$$\frac{1}{4}\|hUhU^* + Uh^2U^* + UhU^*h - 3h^2\|$$

$$= \frac{1}{4}\|hUhU^* - h^2 + UhU^*h - Uh^2U^* + 2Uh^2U^* - 2h^2\|$$

$$= \frac{1}{4}\| - [h,U][h,U]^* + 2(Uh^2U^* - h^2)\| \le \frac{1}{4}\|[h,U]\|^2 + \frac{1}{2}\|[h^2,U]\|$$

and

$$\frac{1}{2}\|g\{h,U^*\} + \{h,U\}g\| = \frac{1}{2}\|gU^*h + hUg\| = \frac{1}{2}\|g[U^*,h] + [h,U]g\| \le \|g\|\|[h,U]\|$$

and

$$\frac{1}{2}\|f\{h,U\} - \{h,U\}f\| = \frac{1}{2}\|2fhU - 2Ufh + fUh - fhU - hUf + Uhf\|$$

$$\le \|fhU - Uhf\| + \frac{1}{2}\|fUh - fhU\| + \frac{1}{2}\|hUf - Uhf\|$$

$$\le \|fhU - Uhf\| + \frac{1}{2}\|Uh - hU\| + \frac{1}{2}\|hU - Uh\|$$

$$= \|[fh,U]\| + \|[h,U]\| = \|[q,U]\| + \|[h,U]\|. \qquad \blacksquare$$

Lemma 6.2. *Suppose U and V are unitary matrices. If $\|[U,V]\| \le \frac{1}{8}$ then for any choice of K with $-\pi \le K \le \pi$ and $e^{iK} = V$, there is a path B_t of invertible self-adjoint matrices between $B(U,V)$ and*

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

and, if U and V are self-dual, then the path may be chosen with the symmetry $B_t^{\sharp\otimes\sharp} = B_t$.

Proof. We can select paths, illustrated in Figs. 6 and 7, f_t, g_t and h_t, from the standard triple $(f_0, g_0, h_0) = (f, g, h)$, in Definition 3.2, to (f_1, g_1, h_1) where

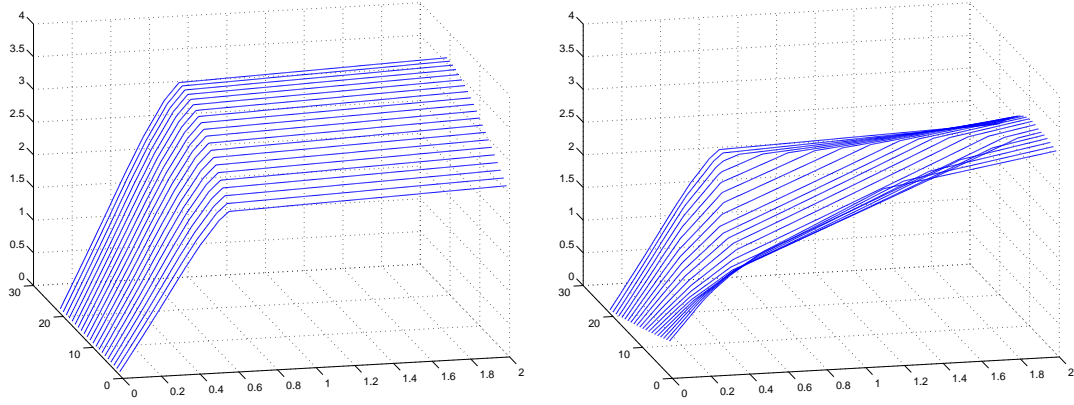$$f_1(x) = \frac{1}{\pi}x, \qquad g_1(x) = 0, \qquad h_1(x) = \sqrt{1 - \frac{1}{\pi^2}x^2}. \qquad (6.1)$$

Figure 8. Bounds on $\left\|B_t(U,V)^2 - I\right\|$.
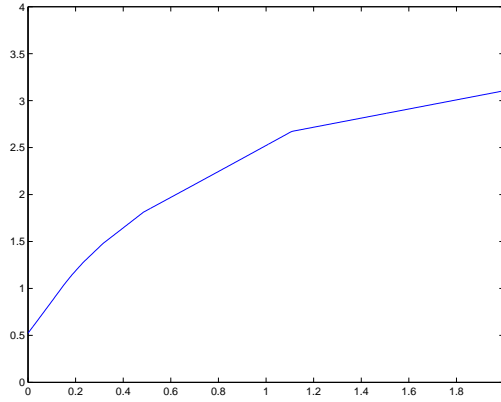

Figure 9. Bounds on $\|B_L(U,V)^2 - I\|$.

The conditions $f^2 + g^2 + h^2 = 1$ and $gh = 0$ hold along the path. This gives us paths of matrices

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

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

$$(\|g_t\| + 1)\eta_{h_t}(\delta) + \frac{1}{4}(\eta_{h_t}(\delta))^2 + \frac{1}{2}\eta_{h_t^2}(\delta) + \eta_{q_t}(\delta) \tag{6.2}$$

and check that this takes value less than 1 at $\delta = \frac{1}{8}$. This is too much to do by hand, so use a computer[2] to repeatedly calculate the constants 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

$$\|f_{t_j} - f_{t_{j+1}}\|_\infty + \|g_{t_j} - g_{t_{j+1}}\|_\infty + \|h_{t_j} - h_{t_{j+1}}\|_\infty \le \sqrt{1 - 0.95} \approx 0.2236.$$

We can keep f_t fixed at

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

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[2]See code at http://repository.unm.edu/handle/1928/23494.

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 Fig. 8. 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 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 Fig. 9.

Theorem 6.3. *Suppose U and V are self-dual unitary matrices. If $\|[U,V]\| \leq \frac{1}{8}$ then, for any K with $-\pi \leq K \leq \pi$ and $e^{iK} = V$,*

$$\kappa_2(U,V) = \text{Sign}\left(\widetilde{\text{Pf}}\left(\begin{pmatrix} \frac{1}{\pi}K & \frac{1}{2}\left\{\sqrt{I - \frac{1}{\pi^2}K^2}, U\right\} \\ \frac{1}{2}\left\{\sqrt{I - \frac{1}{\pi^2}K^2}, U^*\right\} & -\frac{1}{\pi}K \end{pmatrix}\right)\right).$$

Acknowledgements

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