EXCITON SCATTERING VIA ALGEBRAIC TOPOLOGY

MICHAEL J. CATANZARO, VLADIMIR Y. CHERNYAK, AND JOHN R. KLEIN

Abstract. This paper introduces an intersection theory problem for maps into a smooth manifold equipped with a stratification. We investigate the problem in the special case when the target is the unitary group $U(n)$ and the domain is a circle. The first main result is an index theorem that equates a global intersection index with a finite sum of locally defined intersection indices. The local indices are integers arising from the geometry of the stratification.

The result is used to study a well-known problem in chemical physics, namely, the problem of enumerating the electronic excitations (excitons) of a molecule equipped with scattering data. We provide a lower bound for this number. The bound is shown to be sharp in a limiting case.

Contents

1. Introduction 1
2. The stratification of $U(n)$ 10
3. Intersection Theory in $U(n)$ 12
4. The proof of Theorem A 19
5. The proof of Theorem B 19
6. The proof of Addendum C 20
References 21

1. Introduction

This paper has two objectives. The first objective is to apply algebraic topology to a problem in chemical physics. The problem, when translated into topology, is a special case of a more general problem which is both natural and elementary to state. Our other objective
is an investigation of the general problem, which we hope will be of
independent interest to mathematicians.

In its barest form, the chemical physics problem involves calculating
the set of solutions to a system of linear equations parametrized by the
circle. The equations are derived from a finite graph equipped with
additional structure, where the graph is a mathematical representation
of a molecule. The set of nontrivial solutions of the system of equations
is finite and the problem is to enumerate them, taking multiplicity into
account. The solutions are called *excitons*. We refer the reader to the
end of this section for some of the historical background and to the
chemical physics paper [C] for a more extensive treatment.

To translate to problem into algebraic topology, the equations first
need to be converted to a compact form. The requisite form is a
parametrized (+1)-eigenvalue problem
\[ \Gamma(z) \psi = \psi, \quad \text{for } z \in S^1, \Gamma(z) \in U(n), \psi \in \mathbb{C}^n. \]
Quantum mechanics suggests that for all but finitely many points \( z \),
equation (1) has no non-trivial solutions, and this will be taken as an
axiom. Consequently, the solution to the problem is reduced to that
of enumerating with multiplicity the set of points \( z \in S^1 \) for which (1)
has a non-trivial solution.

From the perspective of algebraic topology, an advantage of equa-
tion (1) is that it recasts the problem as a kind of intersection the-
ory question in the unitary group \( U(n) \): the number of excitons is
just the intersection number of the curve \( \Gamma(S^1) \) with the subspace
\( D_1 U(n) \subset U(n) \) consisting of unitary matrices having non-trivial (+1)-
eigenspace. However, there is a catch: for \( n \geq 2 \), the space \( D_1 U(n) \)
is not a manifold. Nevertheless, \( D_1 U(n) \) is a stratified space and the
intersection problem turns out to be tractable.

1.1. An intersection problem. The intersection problem alluded to
above is a special case of a more general problem, whose investigation
is the other goal of this paper. Suppose \( M \) is a closed smooth oriented
manifold of dimension \( m \) equipped with a filtration
\[ \emptyset = M^{(-1)} \subset M^{(0)} \subset M^{(1)} \subset \cdots \subset M^{(m)} = M \]
giving an oriented stratifold structure [Kr, chap. 2]. In particular, the
open strata \( M_j := M^{(j)} \setminus M^{(j-1)} \) are smooth manifolds of dimension \( j \).
Concretely, one encounters such a filtration if \( M \) is equipped with the
structure of a CW complex, the filtration is given by the skeleta and
the characteristic maps for the cells satisfy a smoothness condition.
Examples of this kind arise in Morse theory [Q1], [Q2].
For a fixed degree $q$, set $Q := M^{(q)}$. On occasion, the singular homology group $H_q(Q; \mathbb{Z})$ is found to be infinite cyclic.\(^1\) When this happens, the stratifold orientation determines a preferred generator. Denote the generator by $\mu_q$.

Suppose that $f : P \to M$ is a smooth map where $P$ is a closed oriented manifold of dimension $p := m - q$. Let $[P] \in H_p(P; \mathbb{Z})$ denote the fundamental class. Then the homological intersection number (or global intersection index) is defined as

\[
\alpha_f := \mu_q \cdot f_*([P]) \in \mathbb{Z},
\]

where $\cdot : H_q(M; \mathbb{Z}) \otimes H_p(M; \mathbb{Z}) \to \mathbb{Z}$ is the intersection pairing.

Henceforth, assume that the preimage

\[
\Sigma := f^{-1}(Q)
\]

is a finite set of points.

**Question.** Is there a description of the homological intersection number (2) given in terms of the restriction of $f$ to an arbitrarily small neighborhood of $\Sigma$?

Stated another way, the question asks for a formula for the global invariant (2) in terms of local invariants coming from the differential topology of the map $f$ near the set $\Sigma$.

In certain cases, the answer to the above question is well-known and classical. For example, if $Q \subset M$ happens to be a closed submanifold with fundamental class $\mu_q$ and $f$ happens to be transverse to $Q$, then the homological intersection number is just the sum over the points of $\Sigma$ counted with sign. However, in the case addressed in this paper, $Q$ is not a manifold and the function $f$ is not assumed to satisfy any transversality.

In the case considered in the paper, $M$ is $U(n)$, the unitary group of $n \times n$ matrices, a manifold of dimension $n^2$. We equip $U(n)$ with a CW decomposition whose $(n^2 - 1)$-skeleton is the space $Q := D_1 U(n)$ described above. Then $H_q(Q; \mathbb{Z})$ (for $q = n^2 - 1$) is infinite cyclic with preferred generator $\mu$. If $n \geq 2$, then $Q$ is not a manifold; see Example 2.1 below.

A main result (Theorem A) of this paper is a kind of index theorem. The crucial difference with the classical case is that the sign of a point $\zeta \in \Sigma$ is now replaced by a local index $\iota_\zeta$, given by the net change in the number of eigenvalues of $f(z)$ passing through $+1 \in U(1)$ as nearby

\(^1\) This phenomenon is not as infrequent as one might initially suppose: For example, it occurs when the stratum $M_q = \tilde{Q}$ is connected and the boundary homomorphism $H_q(M^{(q)}, M^{(q-1)}; \mathbb{Z}) \to H_{q-1}(M^{(q-1)}; \mathbb{Z})$ has non-trivial kernel.
Figure 1. Left: an example of the actual molecular geometry. Right: the metric graph on which it is based. The length of an edge is given by the number of repeat units it contains.

points $z \in S^1$ pass through $\zeta$ in a counterclockwise direction (see §3.3 for details).

**Theorem A** (Index Theorem). Assume $f : S^1 \to U(n)$ is smooth and the preimage $\Sigma = f^{-1}(D_1 U(n))$ is discrete. Then the global intersection index (2) of $f$ equals the sum of the local indices, i.e.,

$$\alpha_f = \sum_{\zeta \in \Sigma} \iota_{\zeta} .$$

In summary, Theorem A provides a description of the homological intersection number as a sum over local indices in the particular case of $f : S^1 \to U(n)$. The extent to which a result of this kind applies in other instances remains open.

1.2. **Exciton scattering.** The molecules we investigate possess discrete, 1-dimensional translational symmetry which is broken only in a finite number of places. The molecules are mathematically represented by simple metric graphs whose edge lengths are positive integers (cf. Figure 1).

Let $Y$ be a connected, finite, simple graph. Let $Y_0$ denote the set of vertices and $Y_1$ the set of edges. The graph $Y$ models the geometry of our molecule. Since $Y$ is simple, there is at most one edge for each pair of distinct vertices. If $a, b \in Y_0$ are distinct vertices joined by an edge, we often refer to the edge by $\{a, b\}$.

Associated with $Y$ is a directed graph $X$ called the double of $Y$, whose set of vertices is $Y_0$ and where a directed edge is given by a pair $(a, e) \in Y_0 \times Y_1$ such that $a$ is incident to $e$. Each directed edge is uniquely represented by an ordered pair of distinct vertices $(a, b)$ and we often specify $e$ as $ab$ (the arrows of Figure 1 depict the directed edges of $X$).
The lengths of the edges are given by a function
\[ L : Y_1 \rightarrow \{1, 2, 3, \ldots \} . \]
By slight abuse of notation, consider this as a function defined on \( X_1 \)
defined by \( ab \mapsto L_{ab} \), with \( L_{ba} = L(a, b) = L_{ab} \). From the viewpoint of
chemical physics, the value \( L_{ab} \) is the number of repeat units of the edge \( ab \) and corresponds to the number of periods of the discrete
symmetry on the edge.

If \( a \in X_0 = Y_0 \) is a vertex, let \( X_{a,-}^a \) denote the set of incoming edges
at \( a \), and similarly let \( X_{a,+}^a \) be the set of outgoing edges at \( a \). There
are canonical bijections \( X_{a,+}^a \cong Y_a \), where \( Y_a \) is the set of edges of \( Y_1 \)
that meet \( a \). The bijection \( X_{a,+}^a \cong Y_a \) is given by by \( ab \mapsto \{a, b\} \) and
the bijection \( X_{a,-}^a \cong Y_a \) is given by \( ba \mapsto \{a, b\} \).

Notation 1.1. For a finite set \( T \), let \( C[T] \) be the complex vector space
with basis \( T \). Let
\[ U(T) \]
denote the unitary group of \( C[T] \) consisting of \( C \)-linear transformations
\( A : C[T] \rightarrow C[T] \), such such that \( AA^* = I \), where \( A^* \) is the conjugate transpose of \( A \).

The vertices of \( X \) break the discrete symmetry, and hence, cause the
excitons to scatter (vertices are often referred to simply as scattering
centers for this reason). Associated to each vertex \( a \in X_0 \), and each
real number \( k \in \mathbb{R} \), there is a scattering matrix
\[ \tilde{\Gamma}^a(k) : C[X_{a,-}^a] \rightarrow C[X_{a,+}^a] \]
that describes the outgoing waves in terms of the incoming ones.\(^2\)

The scattering matrix is invertible and the function \( k \mapsto \tilde{\Gamma}^a(k) \) is
\((2\pi)\)-periodic. In view of the canonical bijections \( X_{a,+}^a \cong Y_a \), the
scattering matrix at \( k \in \mathbb{R} \) can equally be regarded an invertible self-map
\( \tilde{\Gamma}^a(k) : C[Y_a] \rightarrow C[Y_a] \).

Hypothesis 1.2. For each \( a \in X_0 \) and \( k \in \mathbb{R} \), the operator of \( (3) \) is
unitary. Furthermore, the map \( \tilde{\Gamma}^a : \mathbb{R} \rightarrow U(Y_a) \) given by \( k \mapsto \tilde{\Gamma}^a(k) \)
is real analytic. In particular, the map
\[ \mathbb{R} \times C[Y_a] \rightarrow C[Y_a] , \]
given by \( (k, \psi) \mapsto \tilde{\Gamma}^a(k)\psi \), is real analytic.

\(^2\)The real number \( k \) is known as quasimomentum; it appears as a consequence of
translational invariance.
The hypothesis, which we take as an axiom, is suggested by quantum mechanics [LL]. It has been substantiated in a variety of cases. Periodicity implies that $\tilde{\Gamma}^a$ factors as a map through the circle. I.e.,

$$\Gamma^a(e^{ik}) := \tilde{\Gamma}^a(k),$$

where $\Gamma^a : S^1 \to U(Y^a_1)$ is also real analytic.

Excitons satisfy time-reversal symmetry (Kramers’ symmetry):

$$(4) \quad \tilde{\Gamma}^a(k)^* = \tilde{\Gamma}^a(-k).$$

In terms of $\Gamma^a$, this equation translates to $(\Gamma^a)(z) = \Gamma^a(\bar{z})$, which means that $\Gamma^a$ is $\mathbb{Z}/2\mathbb{Z}$-equivariant with respect to conjugation on the circle and inversion on $U(Y^a_1)$.

The scattering matrices are computed using quantum chemistry methods, and we treat these as known.

1.3. The Exciton Scattering Equations. For a vector $\psi \in \mathbb{C}[X_1]$ and a directed edge $ab \in X_1$, let $\psi_{ab} \in \mathbb{C}$ be the component of $\psi$ along $ab$. Hence, $\psi = \sum \psi_{ab}ab$.

Exciton scattering theory implies the following two equations, which are taken here as axioms [Wu1, eqns. (3),(4)]:

$$(5) \quad \psi_{ba} = e^{ikL_{ab}}\psi_{ab},$$

$$\psi_{ba} = \sum_{ac \in X_1} \Gamma^a_{ba,ac}(e^{ik})\psi_{ac},$$

where in the indexing for the sum the vertex $a$ is fixed. There is such a pair of equations for every edge in $X$. The entire system is referred to as the ES equations.

The matrix entries $\Gamma^a_{ba,ac}$ can be interpreted as the amplitude of the wave function $\psi$ on edge $ba$ as the result of scattering a Gaussian plane wave from edge $ac$ onto vertex $a$ [LL].

**Remark 1.3.** The first equation in (5) expresses the fact that when an exciton wave propagates along a linear segment, it acquires a phase change. The phase change depends on both the length of the segment and $e^{ik}$. The second equation in (5) connects the amplitude of outgoing waves to those of the incoming.

**Remark 1.4.** The ES equations of [Wu1, eqns. (3),(4)] are written in a slightly different notation than the equations of (5). The notation in the former case is intended for an audience of chemists and physicists, whereas (5) is geared toward mathematicians.
To bring algebraic topology into the picture, the equations need to be put into a compact form. Let \( \tilde{\Gamma}_0 \) be the composition

\[
\mathbb{R} \xrightarrow{\Delta} \prod_{a \in X_0} \mathbb{R} \xrightarrow{\Pi_a \tilde{\Gamma}_a} \prod_{a \in X_0} U(Y_1^a) \xrightarrow{\oplus_a} U(X_1),
\]

where \( \Delta \) is the diagonal and the map \( \oplus_a \) is defined by block sum of matrices (here, we used the canonical bijection \( X_1 \cong \bigsqcup_a Y_1^a \)).

Choose once and for all a linear ordering on \( Y_0 \). Then the lexicographical ordering on ordered pairs identifies \( X_1 \) with the standard ordered basis for \( \mathbb{C}^n \) where \( n = |X_1| \). In this way, \( \tilde{\Gamma}_0 \) becomes a \((2\pi)\)-periodic real analytic map \( \mathbb{R} \to U(n) \).

Passing to the circle, one obtains a map \( \Gamma_0 : S^1 \to U(n) \) defined by

\[
\Gamma_0(z) := \tilde{\Gamma}_0(k), \quad \text{for } z = e^{ik}.
\]

Let

\[
\hat{L} : \mathbb{C}[X_1] \to \mathbb{C}[X_1]
\]

be the length rescaling operator given by \( \hat{L}(ab) = L_{ab}ab \). Finally, define a map \( \Gamma : S^1 \to U(n) \) by

\[
\Gamma(z) := e^{ik\hat{L}} \cdot \Gamma_0(e^{ik}), \quad z = e^{ik}.
\]

One verifies by direct calculation that the full set of exciton scattering equations is equivalent to the single parametrized eigenvector equation

\[
(6) \quad \Gamma(z)\psi = \psi, \quad z \in S^1,
\]

where \( \Gamma : S^1 \to U(n) \) is real analytic, and \( 0 \neq \psi \in \mathbb{C}^n \) is a vector. Henceforth, we resort to this version of the ES equations throughout the paper.

### 1.4. Enumeration of excitons

The analyticity of \( \Gamma \) implies that equation (6) can hold only for finitely many points \( z \in S^1 \). Specifically, let \( S^{2n-1} \subset \mathbb{C}^n \) be the unit sphere. By Hypothesis 1.2, the map

\[
F : S^1 \times S^{2n-1} \to \mathbb{C}^n
\]

given by \( F(e^{ik}, v) = \Gamma(e^{ik})v - v \) is analytic. By the principle of permanence and the compactness of \( S^1 \times S^{2n-1} \), the set of zeros \( F^{-1}(0) \subset S^1 \times S^{2n-1} \) is finite. The image of the first factor projection \( p_1 : F^{-1}(0) \to S^1 \) is then a finite set of points

\[
e^{ik_1}, e^{ik_2}, \ldots, e^{ik_\ell} \in S^1, \quad 0 \leq k_1 < k_2 < \cdots < k_\ell < 2\pi.
\]

This is just the set of points \( z \in S^1 \) where \( \Gamma(z)\psi = \psi \) has a non-trivial solution. Let \( z_j = e^{ik_j} \).

For \( 1 \leq j \leq \ell \), let \( m_j \) denote the dimension of the \((+1)\)-eigenspace of \( \Gamma(z_j) \). Then \( m_j \) is the number of linearly independent solutions of the
ES equations at $z_j$. Recall the problem is to count the total number of excitons weighted with their multiplicities, i.e., $m = \sum m_j$. The following result, which is an application Theorem A, provides a lower bound for $m$.

**Theorem B (Exciton Lower Bound).** Let $m$ denote the total number of solutions of the ES equations (5), weighted with their multiplicities. Then

$$m \geq \sum_{ab \in X_1} L_{ab} + \sum_{a \in X_0} w(\Gamma^a),$$

where $\Gamma^a$ is the scattering matrix at the vertex $a$ and $w(\Gamma^a)$ is the degree of the map $\det \circ \Gamma^a : S^1 \to U(1)$.

There is evidence that the inequality of Theorem B is sharp. In fact, for molecules with large segment lengths, one has the following result.

**Addendum C (The Long-Arm Limit).** Up to second order approximation and for sufficiently large segment lengths, the bound of Theorem B becomes an equality.

**Remark 1.5.** “Up to second order approximation” refers to exchanging the one-parameter family of operators $\Gamma(z)$ with its associated 1-jet at the solution set. Empirical evidence from physics indicates that the addendum is valid even without resorting to the approximation.

1.5. **Historical background.** The theory of excitons was launched by Frenkel, Peierls, and Wannier in the 1930s [F, P, Wa]. In its early years the subject grew slowly and sporadically. The theory blossomed in the 1950s as a result of an increase in technology as well as the drive for a better understanding of the optical properties of solids [O]. For an early survey, see the introduction to [Kn].

The sort of excitations considered here are produced when an organic structure, like chlorophyll, absorbs light of a certain wavelength. The absorbed photon excites an electron into a higher energy state and the excited electron can form a bound state with the “hole” it leaves behind. The pair consisting of the excited electron and the hole is known as an exciton. Finding a method to accurately enumerate excitons in an organic molecule has consequences for engineering. For example, it plays an important role in the design of more efficient organic solar cells.

The exciton scattering (ES) approach, introduced in [Wu] (see also [Wu1]), was a dramatic improvement over previous attempts to study electronic excitations in branched conjugated molecules for a number of reasons (for an extensive bibliography, see [Wu1, Wu2, Wu3]). The ES
approach has shown itself to be more powerful than traditional quantum chemistry methods, such as Time Dependent-Density Functional Theory (TDDFT): the computational time of electronic excitations with the ES approach is on the order of seconds, whereas the same computations with traditional methods are on the order of hours or days.

In earlier papers, the ES approach was only applied to molecules with perfect symmetries, e.g. an ‘X’ or ‘Y’ joint with the same number of repeat units on each arm [Li]. For example, the molecule displayed in Figure 1 fails to have perfect symmetry and is therefore not capable of study using previous techniques. The symmetric case was done by studying the equations (5) using the full symmetry group of the molecule (and the representation theory thereof). Rewriting the ES equations in the form (6) above allows for the analysis of electronic excitations of general branched, conjugated molecules done in this paper, as well as in [C], regardless of symmetry. Stated differently, this paper is the result of analyzing the ES equations for generic molecules, in a mathematically rigorous way.

Theorem B exhibits an estimate for $m$, the number of solutions to the ES equations weighted by their multiplicities. Chemical physicists are interested instead in a number, denoted by $N$, which is the number of excitations that lie in a fixed energy range, called the exciton band. The two numbers are related by the formula

$$2N = m + d_0 + d_\pi,$$

where $d_k = d^+_k - d^-_k$ and $d^+_k$ is the dimension of the $(\pm 1)$-eigenspace of $\tilde{\Gamma}(k)$ for $k = 0, \pi$. (cf. [C, eqn. (12)]). The formula (7) is a reflection of the observation that the solutions of the ES equations with $k \neq 0, \pi$ come in pairs, by time-reversal symmetry (4). The appearance of the terms $d_k$ account for the identity $\tilde{\Gamma}(k)^2 = I$, when $k = 0, \pi$, which is again a consequence of time-reversal symmetry. The fundamental domain $[-\pi, \pi]$ is known as the Brillouin zone.

1.6. Remark on the exposition. We have written the paper so that it is accessible to readers with a modest background in algebraic and differential topology. The material from chemical physics—especially the technical jargon—has been kept to a bare minimum and is usually relegated to remarks or footnotes in an effort to make the paper accessible to a broad mathematical audience.

---

3TDDFT and all other quantum chemistry methods consist of approximation schemes for solving the Schrödinger equation for a many-electron system.
Outline. The CW decomposition of $U(n)$ is described in §2. The technical results required for the proof of Theorem A appear in §3. An exposition of the proof Theorem A appears in §4. The proof of Theorem B appears in §5 and the proof of Addendum C appears in §6.

Acknowledgements. The authors wish to thank Tian Shi for helpful discussions and for assistance with the figures. The authors also wish to thank a diligent referee whose numerous suggestions improved the readability of this document. This material is based upon work supported by the National Science Foundation Grant CHE-1111350 and the Simons Foundation Collaboration Grant 317496.

2. The stratification of $U(n)$

We describe the CW decomposition of $U(n)$ appearing in Steenrod’s book [St]. The decomposition is attributed to Miller [Mi] and Yokota [Y].

Following [St, ch. IV], let $E_{2(n-1)} \subset S^{2n-1} \subset \mathbb{C}^n$ be the subspace consisting of vectors whose final coordinates are real and nonnegative, where we are using the standard ordered basis on $\mathbb{C}^n$. The circle $S^1 \subset \mathbb{C}$ acts freely on $S^{2n-1}$ by $\nu \cdot (z_1, \ldots, z_n) = (\nu z_1, \ldots, \nu z_n)$. Let $Q_n$ be the quotient space of $S^1 \times S^{2n-1}$ where $(\lambda, x) \sim (\lambda, \nu \cdot x)$ for $\nu \in S^1$, and $(1, x) \sim (1, y)$ for all $x, y \in \mathbb{C}^n$. The space $Q_n$ is homeomorphic to the reduced suspension $\Sigma(\mathbb{C}P_n^{n-1})$, where $\mathbb{C}P^{n-1}$ is the projective space of $\mathbb{C}^n$ and $X_+$ denotes the effect of adding a disjoint basepoint to a space $X$. A point of $Q_n$ will be written as an equivalence class $[\lambda, v]$, where $\lambda \in S^1 \subset \mathbb{C}$ and $v \in S^{2n-1} \subset \mathbb{C}^n$.

For each $j \leq n$, there is a natural map

$$E^{2j-1} := E^{2(j-1)} \times [0, 1] \to S^{2j-1} \times S^1 \to Q_j,$$

where the second displayed map is the projection onto orbits, and the first is the product of the inclusion $E^{2(j-1)} \subset S^{2j-1}$ with the map $[0, 1] \to S^1$ given by $t \mapsto e^{2\pi it}$. The displayed map defines a relative homeomorphism

$$ (E^{2j-1}, S^{2j-2}) \to (Q_j, Q_{j-1}).$$

The maps (8) define a CW decomposition of $Q_n$ which is just the suspension of the usual CW structure of $\mathbb{C}P_n^{n-1}$.

An embedding of $Q_n$ into $U(n)$ is given by sending an equivalence class $[\lambda, v] \in Q_n$ to the transformation which fixes the orthogonal complement of $v \in \mathbb{C}^n$ and multiplies any point on the line $\mathbb{C}v$ by $\lambda$ (by convention, $Q_0$ maps to the identity transformation). This gives rise to embeddings $Q_j \to U(n)$ for $j \leq n$ using the inclusion $U(j) \to U(n)$,
given by including the first \( j \) coordinates. Multiplying the cells leads to normal cells: for any ordered subset

\[
I = \{ i_1 < i_2 < \cdots < i_r \} \subset \{ 1 < 2 < \cdots < n \},
\]

there is a map

\[
E^{2i_1-1} \times E^{2i_2-1} \times \cdots \times E^{2i_r-1} \to Q_{i_1} \times Q_{i_2} \times \cdots \times Q_{i_r} \to U(n)
\]

where the first map of (9) is the product of the maps (8) and the second map is given by multiplication. The normal cells (together with the 0-cell corresponding to the identity) give a CW decomposition of \( U(n) \) [St, ch. IV, thm. 2.1]. By construction, the interior of normal cells are identified with unitary transformations characterized by a fixed number of eigenvalues. Identifying \( Q_j \) with its image under the embedding \( Q_j \to U(n) \) implies that \( Q_j \) consists of matrices with +1 along the diagonal, except in the \((j,j)\) entry. More generally, taking products of such yields \( Q_{i_1} \times \cdots \times Q_{i_r} \), corresponding to matrices with +1 along the diagonal, except in the \((i_1,i_1), \ldots, (i_r,i_r)\) entries.

The above equips \( U(n) \) with a CW decomposition whose \((n^2 - 1)\)-skeleton is given by the transformations having nontrivial \((+1)\)-eigenspace, i.e., \( D_1U(n) \). In particular, the cell \( Q_2 \times Q_3 \times \cdots \times Q_n \) is the unique \((n^2 - 1)\)-cell.

**Example 2.1.** Let \( n = 2 \). The above equips \( U(2) \) with a CW structure with a single cell in dimensions 0, 1, 3 and 4. The 3-skeleton in this case is given by \( D_1U(2) \cong \Sigma(\mathbb{CP}^1) \), where \( \Sigma \) denotes the reduced suspension. The space \( \Sigma(\mathbb{CP}^1) \) can be thought of as the quotient space of \( S^3 \) obtained by identifying a single pair of antipodal points, as shown in Figure 2 below.

There is another CW structure on \( U(2) \) which uses the well-known homeomorphism \( U(2) \cong S^1 \times S^3 \). This CW structure also has a single cell in dimensions 0, 1, 3 and 4, and the 3-skeleton in this case is \( S^1 \vee S^3 \). Although \( \Sigma(\mathbb{CP}^1) \) is homotopy equivalent to \( S^1 \vee S^3 \), the two spaces are not homeomorphic. Hence the two CW structures are distinct (in fact, \( SU(2) \) fails to be a subcomplex of the first CW structure).

Blurring the distinction between the two CW structures in this paper invariably leads to unrecoverable errors. In particular, the proof of \( n = 2 \) case of Proposition 3.10 goes wildly wrong were we to use \( S^1 \vee S^3 \) in place of \( D_1U(2) \).

**Remark 2.2.** In a previous version of this manuscript, the above CW decomposition was derived from Morse theory. The standard height function \( f_a(x) = \operatorname{Re} \operatorname{Tr}(ax) \) on \( U(n) \) is a Morse function for almost all \( a \in M_n(\mathbb{C}) \). In a private communication, Liviu Nicolaescu pointed out
that for $a \in U(n)$ diagonal with distinct, real entries, the flow generated by $f$ satisfies the Morse-Smale condition and leads to the above CW decomposition [N, Q1, Q2]. He also pointed out that in the Lagrangian interpretation of the intersections we are considering, $D_1 U(n)$ can be interpreted as the Maslov variety and the global intersection index $\alpha_f$ (defined below) is known as the Maslov index. However, we will not pursue this interpretation here.

3. Intersection Theory in $U(n)$

3.1. The global index. The CW decomposition of $U(n)$ given in §2 has one top cell and its $(n^2 - 1)$-skeleton is $D_1 U(n)$. The top cell of $D_1 U(n)$ defines a generator $\mu \in H_{n^2-1}(D_1 U(n))$ (with integer coefficients being understood). Alternatively, the generator can be obtained by means of Poincaré duality: the fundamental class $[U(n)] \in H_{n^2}(U(n))$ defined by the top cell of $U(n)$ gives an isomorphism $H_{n^2-1}(D_1 U(n)) \cong H_{n^2}(U(n)) \cong \mathbb{Z}$, where the first displayed map is induced by the inclusion $j : D_1 U(n) \to U(n)$ and the second displayed map is Poincaré duality. The generator of $H^1(U(n))$ comes from the determinant map $\det : U(n) \to S^1$. The map $j_*$ is an isomorphism by the homology long exact sequence of the pair $(U(n), D_1 U(n))$. Let $[S^1] \in H_1(S^1)$ be the fundamental class.

Definition 3.1. The global intersection index of a map $f : S^1 \to U(n)$ is the homological intersection number

$$\alpha_f = j_*(\mu) \cdot f_*([S^1]) \in H_0(U(n); \mathbb{Z}) \cong \mathbb{Z}.$$

Definition 3.2. The intersection set is the fiber product

$$\mathcal{I}_f := \{(A,z) \in D_1 U(n) \times S^1 | A = f(z)\}.$$

Hypothesis 3.3. The set $\mathcal{I}_f$ is discrete, i.e., $\Sigma = f^{-1}(D_1 U(n))$ is a finite set.

It will be convenient to express the global intersection index in terms of orientation classes [Sp, p. 294].

Notation 3.4. For a subset $A \subset X$, let

$$(X | A) := (X, X \setminus A).$$

Note the case $A = X$ is the pair $(X, \emptyset)$. The case $A = p$ is a point gives rise to the local (singular) homology at $p$, i.e., $H_*(X | p) := H_*(X, X \setminus p)$. 
Definition 3.5. Let $X$ be a smooth $m$-manifold and let $\Delta \subset X \times X$ be the diagonal. An orientation for $X$ is a (singular cohomology) class $x \in H^m(X \times X \mid \Delta)$ such that for all $p \in X$, the class $i^*_p(x)$ generates $H^m(X \mid p) \cong \mathbb{Z}$, where $i_p$ is the inclusion $(X \times p \mid p \times p) \subset (X \times X \mid \Delta)$.

Remark 3.6. The terminology is not universal. An orientation in the above sense is equivalent to choosing a Thom class for the tangent bundle $TX$. In [MS, p. 123], $x$ is called a fundamental cohomology class. A choice of orientation class $x \in H^{n^2}(U(n) \times U(n) \mid \Delta)$ is equivalent to a choice of fundamental class for $H^{n^2}(U(n))$. Henceforth, $x$ is chosen to correspond to the class $[U(n)]$ defined above.

Lemma 3.7. The global intersection index coincides with the Kronecker index, i.e., $\alpha_f = \langle x, b_*(j \times f)_*(\mu \times [S^1]) \rangle$.

Proof. This follows immediately from the standard description of the intersection number as a slant product (cf. [Sp, chap. 6], [Mc, §4]). □

3.2. The local multiplicity. The local multiplicity, defined below, counts the dimension of the solution space of the equation

$$f(z)\psi = \psi, \quad \psi \in \mathbb{C}^n,$$

at a given $z \in S^1$.

Definition 3.8. Let $p = (A, z) \in \mathcal{I}_f$ be any point. The local multiplicity of $p$, denoted $m_p$, is the dimension of the $(+1)$-eigenspace of $f(z) = A$. In particular, $m_p \geq 1$.

The local multiplicity of $f$ is the number

$$m = \sum_p m_p,$$

where the sum is indexed over all points $p \in \mathcal{I}_f$.

The local multiplicity of $f$ enumerates the entire set of solutions to equation (10), where each solution $p$ is counted with multiplicity $m_p$. 

3.3. The local intersection index. For \( p = (A,z) \in \mathcal{I}_f \), let \( k_p \in [0, 2\pi) \) be the unique point such that \( z = e^{ik_p} \). By hypothesis, the non-trivial solutions to the equation \( f(z)\psi = \psi \) occur at isolated points \( z \in S^1 \).

Choose a small arc \( J \) containing \( +1 \in S^1 \) such that the eigenvalues of \( f(z) \) other than \( +1 \) lie outside \( J \). Consider an interval \( I \subset \mathbb{R} \) centered at \( k_p \). If \( k \in I \), then the number of eigenvalues of \( f(e^{ik}) \) which lie in \( J \) is constant in \( k \) provided that \( I \) is chosen sufficiently small. If \( k \in I \setminus \{k_p\} \) then the number of eigenvalues of \( f(e^{ik}) \) lying in \( J \) and having positive imaginary part is a constant function on each component.

**Definition 3.9.** With respect to the above assumptions, let \( \iota^-_p \) be the number of eigenvalues lying in \( J \) having positive imaginary part taken at \( k < k_p \) with \( k \in I \). Similarly, let \( \iota^+_p \) be the number of eigenvalues lying in \( J \) having positive imaginary part taken at some \( k > k_p \) with \( k \in I \).

The **local intersection index** at \( p \in \mathcal{I}_f \) is the integer

\[
\iota_p := \iota^+_p - \iota^-_p .
\]

The **local intersection index** of \( f : S^1 \to U(n) \) is the sum

\[
q_f := \sum_{p \in \mathcal{I}_f} \iota_p .
\]

Intuitively, \( \iota_p \) is the number of eigenvalues passing through \( 1 \in U(1) \cong S^1 \) counterclockwise, as \( k \) passes through \( k_p \) from left to right.

The definition trivially implies the inequalities

\[
m_p \geq \iota_p ,
\]

\[
m \geq q_f
\]

(cf. Definition 3.8).

The following result plays a key role of the proof of Theorem A.

**Proposition 3.10.** There is a preferred isomorphism

\[
H_{n^2}(D_1U(n) \times S^1 | p) \cong \mathbb{Z}^{m_p} .
\]

In particular, \( H_{n^2}(D_1U(n) \times S^1 | p) \) is free abelian of rank \( m_p \), so the local multiplicity of \( p \in \mathcal{I}_f \) is detected by local homology.

**Proof.** Assume that \( n \geq 2 \), as the \( n = 1 \) case is trivial. Let \( g \in D_1U(n) \) be a point having multiplicity \( m_p \), i.e., the dimension of the \((+1)\)-eigenspace of \( g \) is \( m_p \). By the K"unneth theorem of pairs, it will be enough to exhibit a preferred isomorphism

\[
H_{n^2-1}(D_1U(n) | g) \cong \mathbb{Z}^{m_p} .
\]
(cf. Fig. 2).

Fix $\epsilon > 0$ and take a standard neighborhood $\{ A \in u(n) : ||A|| < \epsilon \}$ using the standard operator norm on the Lie algebra $u(n)$ (i.e. $n \times n$ matrices $A$ satisfying $A^* = -A$). Let

$$U_\epsilon(g) = \{ g \cdot \exp(A) : ||A|| \leq \epsilon \}$$

where $\exp : u(n) \rightarrow U(n)$ is the exponential map. This produces a neighborhood of any $g \in U(n)$. Define $V_\epsilon(g) = D_1U(n) \cap U_\epsilon(g) \subset D_1U(n)$, to obtain a neighborhood of $g \in D_1U(n)$. The closure of $D_1U(n) \setminus V_\epsilon(g)$ is contained in the interior of $D_1U(n) \setminus g$, so excision applies in this situation and produces an isomorphism

$$H_*(D_1U(n) \setminus g) \cong H_*(V_\epsilon(g) \setminus g).$$

By definition, $\partial U_\epsilon(g) = \{ g \cdot \exp(a) : ||a|| = \epsilon \}$ is a sphere of radius $\epsilon$ in $U(n)$ centered at $g$ (since $\exp$ is a local diffeomorphism), so $\partial V_\epsilon(g) \subset S^{n^2-1}$. Apply Alexander duality to obtain a preferred isomorphism

$$H_{n^2-1}(V_\epsilon(g) \setminus g) \cong H_{n^2-2}(\partial V_\epsilon(g)) \cong \tilde{H}^0(S^{n^2-1} \setminus \partial V_\epsilon(g)),$$

where $\tilde{H}^*$ denotes reduced cohomology. In (12), we are using that $\partial V_\epsilon(g) \setminus \{ g \}$ is homotopy equivalent to $V_\epsilon(g)$, and that $V_\epsilon(g)$ is contractible for every $g \in D_1U(n)$.

The unreduced cohomology group $H^0(S^{n^2-1} \setminus \partial V_\epsilon(g))$ is free abelian on the number of components of $S^{n^2-1} \setminus \partial V_\epsilon(g)$. Let $\chi$ denote the set of these components. We will first show that $|\chi| = m_p + 1$.

The space $X(g) := \partial U_\epsilon(g) \setminus \partial V_\epsilon(g)$ consists of transformations with no eigenvalues equal to one, and is open in $\partial U_\epsilon$ (since $\partial V_\epsilon$ is closed). Recall the arc $J$ associated to $p$ defined at the beginning of this subsection. Each point $a \in X(g)$ has precisely $m_p$ eigenvalues in the arc $J$, none of which are equal to 1. Let $c : X(g) \rightarrow \{0, 1, \ldots, m_p \}$ be the function which assigns to each $a \in X(g)$ the number of eigenvalues lying in the arc $J$ with positive imaginary part. Then

$$X(g)_j := c^{-1}(j)$$

is connected and non-empty since it contains $g \cdot \exp(A_j)$, where $A_j = \text{diag}(i\epsilon, \ldots, i\epsilon, -i\epsilon, \ldots, -i\epsilon)$ is a diagonal, skew-symmetric matrix whose first $j$ entries are $i\epsilon$. Then

$$X(g) = \prod_{j=0}^{m_p} X(g)_j$$

These statements follow from the natural contractions of $J \setminus \{1\}$ to $\partial J$, and $J$ to $\{0\}$, respectively.
Figure 2. A rendering of $D_1U(2) = \Sigma(\mathbb{C}P^1_+)$ in one dimension less. The point $p$ corresponds to the identity matrix and has multiplicity $m_p = 2$. The two small cones emanating from $p$ generate the local homology at $p$ (cf. the proof of Proposition 3.10).

(see Figure 3). Hence, $X(g)$ has $m_p + 1$ components. The subspaces $X(g)_j$ determine a set of preferred generators $\{\delta_j\}$ for $H^0(X(g))$. We infer that the classes $\{\delta_j - \delta_0\}_{j \geq 1}$ form a basis for the reduced cohomology group $\tilde{H}^0(X(g))$.

Let $\mu_j \in H_{n^2-1}(D_1U(n) | g)$ with $1 \leq j \leq m_p$ be the homology class corresponding to $\delta_j - \delta_0$ via Alexander duality. Then

$$\{\mu_j\}_{j=1}^{m_p}$$

is a basis for $H_{n^2-1}(D_1U(n) | g)$. This basis gives the identification $H_{n^2-1}(D_1U(n) | g) \cong \mathbb{Z}^{m_p}$. \qed

Remark 3.11. With respect to the isomorphism of Proposition 3.10 and the identification $H_{n^2}(D_1U(n) \times S^1) \cong \mathbb{Z}$, it is straightforward to check that the evident homomorphism

$$H_{n^2}(D_1U(n) \times S^1) \to H_{n^2}(D_1U(n) \times S^1 | p)$$

corresponds to the diagonal homomorphism $\mathbb{Z} \to \mathbb{Z}^{m_p}$.

Construction 3.12. Suppose that

$$F: (X, A) \to (Y, B)$$

is a map of pairs such that $B \subset Y$ is a closed subspace and $F^{-1}(B) = A \amalg A'$, where $A'$ is disjoint from $A$. Suppose also that $X$ is a normal space. Then there is an open neighborhood $U$ of $A$ which is disjoint from an open neighborhood of $A'$. It follows that $F$ determines a map of pairs $(U \mid A) \to (Y \mid B)$. By excision, $H_*(U \mid A) \cong H_*(X \mid A)$. Hence there is an induced homomorphism

$$(F \mid A)_*: H_*(X \mid A) \to H_*(Y \mid B).$$
Let $p = (f(z), z) \in \mathcal{J}_f$. Apply the construction to the map of pairs
\[ j \times f : (D_1U(n) \times S^1, p) \to (U(n) \times U(n), \Delta) \]
to obtain a homomorphism
\[ (j \times f)_* : H_n^2(D_1U(n) \times S^1 | p) \to H_n^2(U(n) \times U(n) | \Delta). \]
Consider the composition
\begin{equation}
H_n^2(D_1U(n) \times S^1) \longrightarrow H_n^2(U(n) \times S^1 | p)
\downarrow_{(j \times f)_*}
\longrightarrow H_n^2(U(n) \times U(n) | \Delta) \xrightarrow{\langle x, - \rangle \sim} \mathbb{Z},
\end{equation}
where $x \in H_n^2(U(n) \times U(n) | \Delta)$ is the orientation class. The unlabeled arrow is induced by the evident map $(D_1U(n) \times S^1 | D_1U(n) \times S^1) \to (D_1U(n) \times S^1 | p)$.

**Proposition 3.13.** The homomorphism (14) maps the class $\mu \times [S^1]$ to the local intersection index $\iota_p$.

**Proof.** The unlabeled homomorphism appearing in the displayed composition (14) is identified with the diagonal $\mathbb{Z} \to \mathbb{Z}^m$ (cf. Remark 3.11). We need to identify the homomorphism $(j \times f)_*$ of (13), which is of the form $\mathbb{Z}^m \to \mathbb{Z}$. If $u_i$ generates the $i$-th factor of $\mathbb{Z}^m$, $1 \leq i \leq m$, then the value of this homomorphism on $u_i$ is an integer $s_i$. It suffices to show $\sum s_i = \iota_p$. An artifact of the argument given below is that $s_i \neq 0$ for at most two of the indices.

Recall the neighborhoods $U_\epsilon(g)$ and $V_\epsilon(g)$ from the proof of Proposition 3.10. To avoid notational clutter, eliminate the argument $g$ from the notation and write $U_\epsilon$ and $V_\epsilon$ respectively. For $z = e^{ik} \in S^1$ with $f(z) = g$, define $W \subset S^1$ to be an open arc of length $2\gamma$ centered at $z$, where $\gamma$ is chosen sufficiently small so that $f(W) \subset U_\epsilon$.

Consider the homomorphism
\begin{equation}
(j \times f)_*: H_n^2(V_\epsilon \times W | p) \to H_n^2(U(n) \times U(n) | \Delta)
\end{equation}
Clearly, it will be enough to identify (15) since it is a localized form of (13).

If $w: W \to S^1$ is the inclusion, then the pushforward of the fundamental class of the circle, i.e.,
\[ \mu_W := w_!(\{S^1\}) \in H_1(W | z) \cong \mathbb{Z}, \]
is a generator.

By the proof of Proposition 3.10, the domain of (15) has a preferred isomorphism to $\mathbb{Z}^{m_p}$, where $m_p$ is the multiplicity of $f(e^{ik})$. Following
that proof, there are generators \((\mu_i \times \mu_W)_{i=1,\ldots,m_p}\) for the domain. Applying the orientation class to the image of these generators yields the intersection product \(j_* (\mu_t) \cdot f_* (\mu_W)\). To analyze this product, we make use of the fact that the homological intersection product is equivalent to a linking number \([Sp, p. 361, Ex. 2, 3]\). Therefore, \(j_* (\mu_t) \cdot f_* (\mu_W)\) is non-zero only when the curve \(f(W)\) links with \(j_* (\mu_t)\), which occurs when \(f(W)\) has non-trivial intersection with the path component of \(S^{n^2-1} \setminus \partial V\) corresponding to the class \(\mu_t\) via Alexander duality. In general, this intersection index will only be non-zero on at most two of the generators (see Figure 3). Let \(A\) be the arc \(\{e^{ik} | 0 < k < \epsilon\}\). The orientation of the arc \(W\) is induced by the counter-clockwise orientation of \(S^1\). The counterclockwise orientation of \(S^1\) implies that the intersection index will be given by the number of eigenvalues of \(f(e^{i(k+\gamma)})\) in \(A\) minus the number of eigenvalues of \(f(e^{i(k-\gamma)})\) in \(A\). But this is the definition of the local intersection index \(\iota_p\).  \(\Box\)
4. The proof of Theorem A

The proof of Theorem A relies on the commutative diagram

\[
\begin{array}{ccc}
H_n^2(D_1U(n) \times S^1) & \xrightarrow{(j \times f)_*} & H_n^2(U(n) \times U(n)) \\
\downarrow & & \downarrow \\
\oplus_{p \in \mathcal{I}_f} H_n^2(D_1U(n) \times S^1 | p) & \xrightarrow{\oplus(j \times f|p)_*} & H_n^2(U(n) \times U(n) | \Delta)
\end{array}
\]

where the \( p \)-th component of the arrow \( a_* \) is induced by the evident map

\[
(D_1U(n) \times S^1|D_1U(n) \times S^1) \to (D_1U(n) \times S^1|p).
\]

and \( b_* \) is as in Lemma 3.7.

By Lemma 3.7, the composite \( b_* \circ (j \times f)_* \) maps \( \mu \times [S^1] \) to a class which, when paired with the orientation class, yields \( \alpha_f \). By Proposition 3.10, Proposition 3.13, and Remark 3.11, the composite \( \oplus(j \times f|p)_* \circ a_* \) maps \( \mu \times [S^1] \) to a class which pairs to \( q = \sum \iota_p \).

Invoking the commutativity of the diagram completes the proof. □

5. The proof of Theorem B

Recall the scattering matrix \( \Gamma^a : S^1 \to U(Y_1^a) \) defined in §1.

**Definition 5.1.** The **winding number** \( w(\Gamma^a) \) of a vertex \( a \in Y_0 \) is the degree of the composition

\[
S^1 \xrightarrow{\Gamma^a} U(Y_1^a) \xrightarrow{\det} U(1) \cong S^1.
\]

The following proposition identifies the global intersection index in terms of the winding numbers and the length function \( L \).

**Proposition 5.2.**

\[
\alpha_\Gamma = \sum_{ab \in X_1} L_{ab} + \sum_{a \in X_0} w(\Gamma^a).
\]

**Proof.** By Poincaré duality, the class \( \Gamma_*([S^1]) \in H_1(U(n)) \) is given by \( \alpha_{\Gamma*} \), where \( \iota \) is the generator which hits the fundamental class of \( S^1 \) under \( \det_* : H_1(U(n)) \to H_1(S^1) \). The result now follows from the calculation

\[
\det_* \Gamma_*[S^1] = \det_*(\alpha_\Gamma \iota) = \alpha_\Gamma \det_*(\iota) = \alpha_\Gamma[S^1].
\]
The displayed formula involves a computation of the determinant of $\Gamma$. For $z = e^{ik} \in S^1$, the homomorphism property of the determinant implies the equation
\begin{equation}
\det \Gamma(z) = \det e^{ik\hat{L}} \cdot \det \Gamma_0(z).
\end{equation}

The number $\alpha_{\Gamma}$ is therefore just the degree of the map $\det \Gamma : S^1 \to S^1$, and is given by the sum of the degrees of the two maps appearing on the right side of eqn. (16).

Since $\hat{L}$ is a diagonal operator, the term $\det e^{ik\hat{L}}$ is given by $\prod_{ab} e^{ikL_{ab}}$. Its degree is therefore the sum $\sum_{ab \in X_1} L_{ab}$. The determinant of $\Gamma_0(k)$ is the product of $w(\Gamma^a)$ indexed over the vertices of $X$, so its degree is $\sum_{a \in X_0} w(\Gamma^a)$. It follows that the degree of $\det \Gamma : S^1 \to S^1$ is given by the expression
\[ \sum_{ab \in X_1} L_{ab} + \sum_{a \in X_0} w(\Gamma^a). \]

**Proof of Theorem B.** By the inequality (11) in conjunction with Theorem A, we infer $m \geq q = \alpha_{\Gamma}$.

The result now follows by Proposition 5.2. \qed

6. **The Proof of Addendum C**

Let $\zeta = e^{i\ell} \in S^1$ be a point for which $\Gamma(\zeta) := \tilde{\Gamma}(\ell)$ has an eigenvalue equal to $+1$. Set $p := (\Gamma(\zeta), \zeta) \in I_{\Gamma}$.

Set $f(k) := e^{ik\hat{L}}$. Then, taking the first Taylor approximation of $\tilde{\Gamma}$ at $\ell$, we obtain
\begin{equation}
(17) \quad \tilde{\Gamma}(k) = \tilde{\Gamma}(\ell) + (k-\ell)f'(\ell)\tilde{\Gamma}_0(\ell) + f(\ell)\tilde{\Gamma}'_0(\ell) + o \left( (k-\ell)^2 \right),
\end{equation}

for $|k - \ell| < \delta$ and for some $\delta > 0$ sufficiently small. Observe that the first term $\tilde{\Gamma}(\ell)$ is length independent (since $|e^{i\ell\hat{L}}| = 1$). The third term, which contains $\tilde{\Gamma}'_0(\ell)$, measures the dependence of scattering on $k$, which is a local phenomenon. It too is length independent. On the other hand, the second term
\[ (k-\ell)f'(\ell)\tilde{\Gamma}_0(\ell) = (k-\ell)i\hat{L}\tilde{\Gamma}(\ell) \]

is length dependent. When the edge lengths are large, the second term of the approximation dominates the third.
Hence, we omit the third term of (17) to obtain the approximation, valid up to the second order

$$\tilde{\Gamma}(k) \approx (I + i(k - \ell)\hat{L})\tilde{\Gamma}(\ell)$$

for $|k - \ell| < \delta$ and sufficiently large edge lengths. Since $\hat{L}$ is given by rescaling the edge lengths, we see that each of its eigenvalues must exceed the minimal edge length, which we denote by $\mu$, of the weighted graph. Consequently, if the edge lengths are sufficiently large, the eigenvalues of the 1-jet $J_1^\ell \tilde{\Gamma}(k)$ are bounded below by the operator

$$J_1^\ell ((I + i(k - \ell)\mu)\tilde{\Gamma}(\ell)).$$

We infer that the imaginary part of any eigenvalue of $J_1^\ell \tilde{\Gamma}(k)$ is positive if $k > \ell$ and negative if $k < \ell$ for $k$ lying in a sufficiently small neighborhood of $\ell$.

Hence, ignoring the distinction between $\tilde{\Gamma}(k)$ and $J_1^\ell \tilde{\Gamma}(k)$, it follows by Definition 3.9 that $\iota_p^- = 0$ and

$$\iota_p = \iota_p^+ = m_p$$

when the edge length is large. Summing up over all $p$ completes the proof. □

REFERENCES

[C] Catanzaro, M.J., Shi, T., Tretiak, S., Chernyak, V. Y.: Counting the number of excited states in organic semiconductor systems using topology. J. Chem. Phys., 142, 084113 (2015)

[F] Frenkel, I. J.: On the Transformation of light into Heat in Solids. Phys. Rev. 37, p. 17 (1931).

[Kn] Knox, R. S.: Theory of Excitons. (Solid State Physics, Supplement 5) Academic Press, New York and London, 1963.

[Kr] Kreck, M.: Differential algebraic topology. From stratifolds to exotic spheres. Graduate Studies in Mathematics, 110. American Mathematical Society, Providence, RI, 2010.

[LL] Landau, L.D.; Lifshitz, L.M: Quantum Mechanics: Non-Relativistic Theory. Pergamon Press, Oxford, 1977.

[Li] Li, H.; Wu, S.; Malinin, S. V.; Tretiak, S.; Chernyak, V. Y.: Exciton Scattering on Symmetric Branching Centers in Conjugated Molecules. J. Phys Chem B 115, 5465–5475 (2011)

[Mc] McCrory, C.: A characterization of homology manifolds. J. London Math. Soc. 16, 149–159 (1977)

[Mi] Miller, C. E.: The topology of rotation groups. Ann. of Math. 57, 90–114 (1953)

[MS] Milnor, J. W.; Stasheff, J. D.: Characteristic classes. Annals of Mathematics Studies, No. 76, Princeton University Press, 1974.

[Mo] Moiseiwitsch, B. L.: Variational principles. Dover Publications, Mineola, NY, 2004.
[N] Nicolaescu, L.: Schubert calculus on the Grassmannian of Hermitian La-
grangian spaces. *Adv. Math.* 224, 2361–2434 (2010)

[O] Overhauser A. W.: Multiplet Structure of Excitons in Ionic Crystals. *Phys. Rev.* 101, 1702 (1956)

[P] Peierls, R. E.: Theory of the absorption spectra of solid bodies. *Ann. Physik* 13, p. 905 (1932)

[Q1] Qin, L.: On moduli spaces and CW structures arising from Morse theory on Hilbert manifolds. *J. Topol. Anal.* 2, 469–526 (2010)

[Q2] Qin, L.: An application of topological equivalence to Morse theory. arXiv:1102.2838

[Sc] Schiff, L. I.: Quantum Mechanics, 3rd ed., McGraw-Hill, New York, 1968.

[Sp] Spanier, E. H.: Algebraic Topology. McGraw-Hill, New York-Toronto, Ont.-London, 1966.

[St] Steenrod, N.E.: Cohomology Operations. Princeton University Press. Princeton, New Jersey, 1962.

[Wa] Wannier, G.H.: The Structure of Electronic Excitation Levels in Insulating Crystals. *Phys. Rev.* 52, p. 191 (1937)

[Wu] Wu, C., Malinin S.V., Tretiak, S., Chernyak, V. Y.: Exciton scattering and localization in branched dendrimeric structures. *Nature Physics* 2, 631–635 (2006)

[Wu1] Wu, C., Malinin S.V., Tretiak, S., Chernyak, V. Y.: Exciton scattering approach for branched conjugated molecules and complexes I. Formalism. *J Chem Phys* 129, 174111 (2008)

[Wu2] Wu, C., Malinin S.V., Tretiak, S., Chernyak, V. Y.: Exciton scattering approach for branched conjugated molecules and complexes II. Extraction of the exciton scattering parameters from quantum-chemical calculations. *J Chem Phys* 129, 174112 (2008)

[Wu3] Wu, C., Malinin S.V., Tretiak, S., Chernyak, V. Y.: Exciton scattering approach for branched conjugated molecules and complexes III. Applications. *J Chem Phys* 129, 174113 (2008)

[Y] Yokota, I.: On the cellular decompositions of unitary groups. *J. Inst. Polytech. Osaka City Univ. Ser. A.* 7, 39–49 (1956)

Dept. of Mathematics, Wayne State University, Detroit, MI 48202
E-mail address: mike@math.wayne.edu

Dept. of Chemistry, Wayne State University, Detroit, MI 48202
E-mail address: chernyak@chem.wayne.edu

Dept. of Mathematics, Wayne State University, Detroit, MI 48202
E-mail address: klein@math.wayne.edu