Exciton Scattering for Topologists

Michael J. Catanzaro

University of Florida

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Outline

1. The Exciton Scattering Problem
2. CW structure of $U(n)$
3. The Index Theorem
   - Global Intersection theory
   - Local Intersection theory
4. Relation to Actual Excitations

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Mathematical Overview

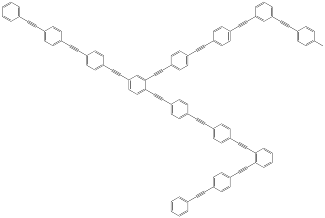
- We're interested in an intersection problem inside the unitary group $U(n)$.
- We want to count intersections of $f : S^1 \to U(n)$ with a stratified space $D_j U(n) \subset U(n)$.
- Intersections are weighted with multiplicity instead of a usual ± 1.
- We do so by using an index theorem, relating these multiplicities to local indices, which are much easier to compute.

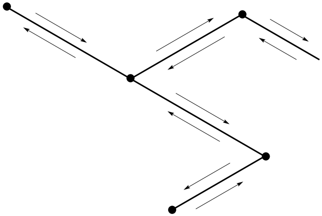
Excitons

- In organic semiconductors and insulators, excited electrons form bound states, comprised of the excited electron and the 'hole' it leaves behind.
- These *excitons* behave like actual particles, moving along the linear segments and getting scattered near the vertices.
- Excitons posess a momentum like quantity known as quasi-momentum k.

Molecules under study

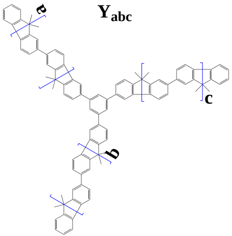
- We're interested in branched, conjugated molecules.
- These posess discrete, 1-dimensional translational symmetry, which is only broken near the vertices ($k \in S^1$).





- We formulate the problem on a metric graph, whose edges are weighted by integers known as *repeat units*.

- Away from the vertices, excitons are described by a superposition of two plane waves.
- The scattering at a degree n vertex a is described by an $n \times n$ unitary matrix, referred to as the scattering matrix, dependent upon k: $\Gamma^a(k)$.
- The calculation of $\Gamma(k)$ is done via quantum chemistry calculations, and we treat these matrices as known.
- $\Gamma(k)$ is an analytic function of k.

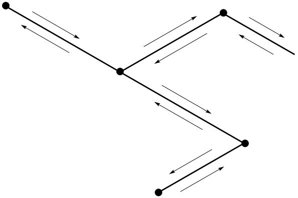


ES equations

Let X_1 denote the edges on our graph, so that a solution to the ES equations lies in $\mathbb{C}[X_1]$. Letting ab denote the oriented edge $b \to a$, and writing ψ^+_{ab} for the wave function incoming to a from the edge ab:

$$\psi^+_{ba} = e^{ikL_{ab}} \psi^-_{ba}$$

$$\psi^-_{ba} = \sum_{c \in X_0}^{(a,c) \in X_1} \Gamma_{ba,ac}(k) \psi^+_{ac},$$



To simplify the analysis:

- introduce $\sigma : X_1 \to X_1$, sending $ab \mapsto ba$,
- define $\hat{L} : X_1 \to X_1$, sending $ab \mapsto L_{ab}ab$, and
- combine the scattering data

$$\Gamma_0(k) = \bigoplus_{a \in X_0} \Gamma^a(k).$$

Finally, define

$$\Gamma(k) = e^{ik\hat{L}} \sigma \Gamma_0(k).$$

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Now the ES equations read

$$\Gamma(k)\psi = \psi$$

Solutions

- A solution to the ES equations corresponds to $k \in S^1$ and $\psi \in \mathbb{C}[X_1]$ so that $\Gamma(k)\psi = \psi$.

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- $\Gamma : S^1 \to U(n)$ should have at least one unit eigenvalue.
- Let $D_1 U(n)$ denote the set of all such matrices.
- We look for intersections of S^1 (under Γ) with $D_1 U(n)$ inside of $U(n)$.

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- Let $D_1 U(n)$ denote the set of all such matrices.
- We look for intersections of S^1 (under Γ) with $D_1 U(n)$ inside of $U(n)$.
- If m_j denotes the multiplicity of a solution k_j, then $m = \sum m_j$ is referred to as the number of solutions to the ES equations.

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3 The Index Theorem
   Global Intersection theory
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4 Relation to Actual Excitations

Morse theory

- Milnor proved that every differentiable manifold has the homotopy type of a CW complex by showing $f_a : M \to \mathbb{R}$, defined by $f_a(x) = ||x - a||^2$ is a Morse function for almost all $a \in \mathbb{R}^n$, using Whitney's embedding theorem.

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$$\frac{\partial f_a}{\partial u_i} = 2\frac{\partial x}{\partial u_i}(x - a)$$

Thus x_0 is a critical point iff $x_0 - a$ is normal to M at x_0.

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- Let $M = U(n)$. For fixed $x_0 \in U(n)$, $M_n(\mathbb{C})$ admits the decomposition

$$M_n(\mathbb{C}) = \{u | u^* x_0 = -x_0^* u\} \oplus \{u | u^* x_0 = x_0^* u\}$$

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  A simple calculation shows

$$T_{x_0} U(n) = \{u \in M_n(\mathbb{C}) | u^* x_0 = -x_0^* u\}.$$

Morse theory

- The first summand lies in $T_{x_0}U(n)$, and therefore the second must be normal to $U(n)$ at x_0.
- Therefore, x_0 is a critical point iff $(x_0 - a)^* x_0 = x_0^*(x_0 - a)$, or equivalently $x_0^* a = a^* x_0$.

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- Take a to be a diagonal matrix, with distinct real entries. This implies x_0 must be of the form $x_0 = \mathrm{diag}(\pm 1, \pm 1, \ldots, \pm 1)$.
- If $I = [i_1, \ldots, i_r]$ denotes the indices corresponding to -1, then

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- $D_1 U(n)$ is the $n^2 - 1$ skeleton of $U(n)$ (replacing f_a by $-f_a$).

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Global Intersection Index

The aforementioned CW decomposition of $U(n)$ has $D_1 U(n)$ as its $(n^2 - 1)$-skeleton.

- The top cell of $D_1 U(n)$ defines a generator $\mu \in H_{n^2-1} D_1 U(n)$.
- Let $[S^1]$ be a generator for $H_1(S^1)$.
- Let $j : D_1 U(n) \to U(n)$ be the inclusion.

Definition

The *global intersection index* of Γ is the integer

$$\alpha_\Gamma = j_*(\delta) \cdot \Gamma_*([S^1]) \in H_0 U(n) \cong \mathbb{Z}\,.$$

Definition

Let $\mathfrak{I}_\Gamma = \{(x, y) \in D_1U(n) \times S^1 | x = \Gamma(y)\}$ *denote the set of* intersection points*.*

For $A \subset X$, let $(X|A) = (X, X \setminus A)$.

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The global intersection index can be phrased in terms of applying homology to the following diagram

$$\begin{array}{ccc} D_1U(n) \times S^1 & \xrightarrow{j \times \Gamma} & U(n) \times U(n) \\ \downarrow & & \downarrow \\ (D_1U(n) \times S^1 | \mathfrak{I}_\Gamma) & \longrightarrow & (U(n) \times U(n) | \Delta U(n)) \end{array}$$

Following $(\delta, [S^1])$ around either side and then applying an orientation class of $U(n)$, yields the intersection pairing, or global intersection index.

Winding number

Proposition

The global intersection index equals the winding number of Γ*,*

$$\alpha_\Gamma = w(\Gamma) = 2 \sum_{(a,b)\in X_1} L_{ab} + \sum_{a\in X_0} w(\Gamma^{(a)})$$

where $w(\Gamma^{(a)})$ *is the winding number of the vertex* a*.*

Proof.

Show $(\det\Gamma)_*[S^1] = \det_* \Gamma_*[S^1] = \alpha_\Gamma[S^1]$ and compute. □

Local Intersection theory

Definition

The multiplicity m_p *of* $p \in \mathfrak{I}_\Gamma$ *is defined to be the dimension of the (+1)-eigenspace of the matrix corresponding to p.*

In general, the computation of m_p can be difficult. What is much easier to compute is the local intersection index for a point $p \in \mathfrak{I}_\Gamma$. While this is only an approximation, its calculable, and when the lengths in the graph are long enough, this approximation becomes exact.

Local Intersection Index

- Let $k_p \in S^1$ correspond to a solution of the ES equations of mulitplicity m_p.
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- If we perturb k slightly all m_p eigenvalues will no longer be 1.
- Define $m_p^{\pm}$ to be the number of eigenvalues with positive imaginary parts for $k \in (k_p, k_p \pm \Delta k]$

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- If we perturb k slightly all m_p eigenvalues will no longer be 1.
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Definition

The local intersection index at $p \in \mathfrak{I}_\Gamma$ *is* $q_p := m_p^+ - m_p^-$. *The* local intersection index *is defined to be the sum of* q_p *taken over all* $p \in \mathfrak{I}_\Gamma$.

Obviously, $|q_p| \leq m_p$.

For $A \subset X$, let $H_*(X|A) = H_*(X, X \setminus A)$.

Proposition

The multiplicity of $p \in \mathfrak{I}_\Gamma$ is realized in homology. That is,

$$H_{n^2}(D_1 \times S^1|\{p\}) \cong \mathbb{Z}^{m_p}.$$

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Proposition

The map in homology

$$H_{n^2}(D_1 U(n) \times S^1|\{p\}) \to H_{n^2}(U(n) \times U(n)|\{p\})$$

after evaluating on an orientation class for $U(n)$ yields the local intersection index q_p.

Proof.

- The map in question is $j \times \Gamma$, restricted to this pair of spaces.
- The codomain of this map (in n^2-dimensional homology) is $\mathbb{Z}$, so we'll obtain an integer.
- Working locally with excisive neighborhoods,

$$\overline{(\delta_i, [S^1])} \mapsto (j \times \Gamma)_*(\overline{\delta_i, [S^1]}).$$

- Evaluating on an orientation class α, yields $\alpha(\Gamma(k_j + \Delta k) - \Gamma(k_j - \Delta k))$, which is precisely the local intersection index at p.

□

Index theorem

Theorem (Index theorem)

The global intersection index is equal to the sum of all the local intersection indices. That is,

$$\alpha_\Gamma = \sum_p q_p.$$

Proof of Index theorem

Proof.

$$\begin{array}{ccc}
D_1 U(n) \times S^1 & \xrightarrow{\;j\times\Gamma\;} & U(n) \times U(n) \\
\downarrow & & \downarrow \\
(D_1 U(n) \times S^1 | \mathfrak{I}_\Gamma) & \longrightarrow & (U(n) \times U(n) | \Delta U(n)) \\
\uparrow{\scriptstyle \text{excis.}} & & \uparrow{\scriptstyle \text{excis.}} \\
\coprod_{p \in \mathfrak{I}_\Gamma} (D_1 U(n) \times S^1 | \{p\}) & \longrightarrow & \coprod_{p=(x,y) \in \mathfrak{I}_\Gamma} (U(n) \times U(n) | \{(x,y)\})
\end{array}$$

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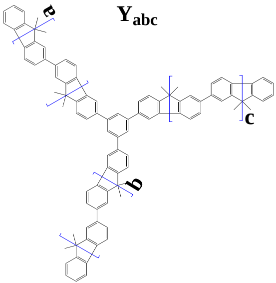
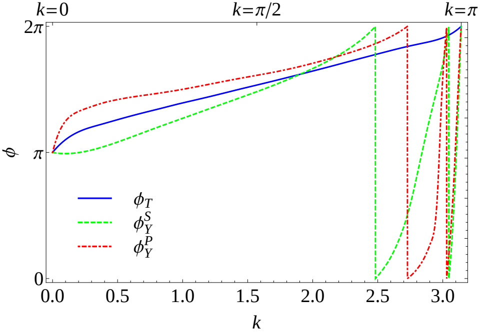
- These two solutions correspond to the same standing wave, i.e. exciton.
- The $k = 0, \pi$ case requires more care (since $k = -k$, incoming/outgoing waves are the same). Let $d_k^\pm$ denote the number of independent solutions to $\Gamma(k)\psi = \pm\psi$ for $k = 0, \pi$.
- Thus

$$N = \frac{1}{2}(m + (d_0^+ - d_0^-) + (d_\pi^+ - d_\pi^-)).$$

- In generic cases, $d_{0/\pi}^- = n/2$ and $d_{0/\pi}^+ = 0$.





$$w(\Gamma) = 2(j+m+n) + 3w(\Gamma_T) + w(\Gamma_Y)$$
$$= 2(j+m+n) + 18$$
$$N = (w(\Gamma) - 6)/2 = j + m + n - 6$$