Quantum Snowflake

Bachelor's Thesis Presentation

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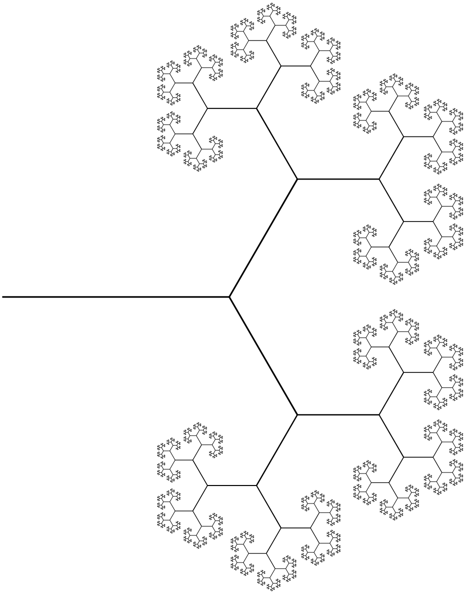
May 19, 2015

Table of Contents

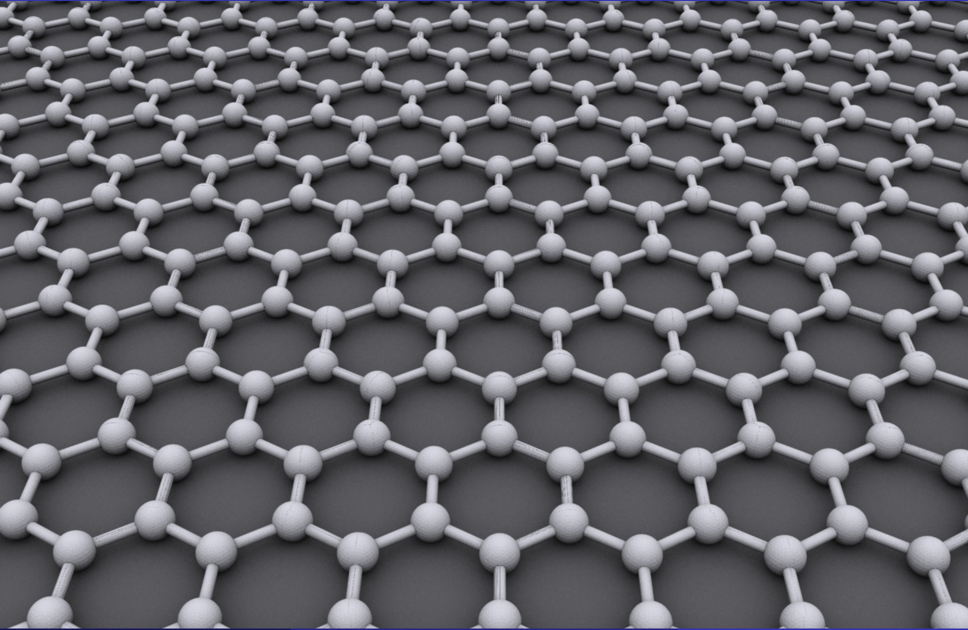
Illustration of a Quantum Snowflake



Intuitive Picture of Quantum Graphs

- Collection of thin (approximately one-dimensional) conductive wires, called *edges*.
- Edges are connected at points, called *vertices*.
- Electric and/or magnetic potential may be present on the edges.
- Study propagation of conductive particles, say electrons, through the graph, modeled by the Schrödinger equation.

Gaphene Modeled as a Quantum Graph



Example

One-dimensional time-independent Schrödinger equation with no potential

$$-u''(x) = \lambda u(x) \iff u(x) = A\overrightarrow{e^{ikx}} + B\overleftarrow{e^{-ikx}}, \quad k^2 = \lambda.$$

A and B are determined by the boundary conditions.

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Example (Particle in a Box)

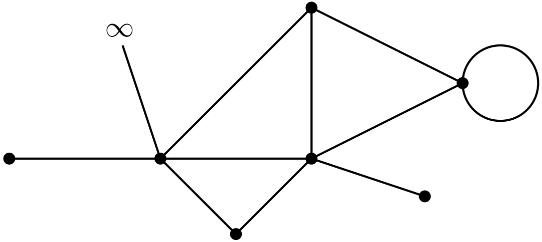
Infinite potential in the region $x < 0, x > \ell$ is modeled by allowing the particle to exist only on the interval $[0, \ell]$.

Figure : Finite line graph of length ℓ, parametrized from 0 to ℓ.

Boundary conditions $u(0) = u(\ell) = 0$ gives

$$u(x) = A \sin kx, \quad \lambda = k^2 = \frac{\pi^2}{\ell^2} n^2, \quad n = 1, 2, \ldots.$$

This discussion applies only to single-line graphs.



How to "connect" the equations at the vertices? *Matching conditions.*

Table of Contents

Formal definition of a Quantum Graph

Definition

A *quantum graph* is a triple (Γ, L, MC), where

- Γ is a *metric graph*,
- L is a *differential expression* defined on functions on Γ, and
- MC (*matching conditions*) is a set of conditions relating the limit values of the functions defined on the edges of Γ.

Metric Graph

Definition

A *metric graph* is a tuple (E, V) where:

- $E = \{e_n\}_{n=1}^{N}$ is a set of edges (intervals) $[x_{2n-1}, x_{2n}] \subset \mathbb{R}$.
- $V = \{v_m\}_{m=1}^{M}$ is a partition of the set $\{x_j\}_{j=1}^{2N}$.
  Each element in V is called a *vertex*.

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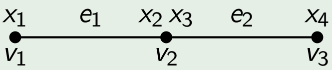
Example



$$E = \{e_1, e_2\} = \{[x_1, x_2], [x_3, x_4]\}$$
$$V = \{v_1, v_2, v_3\} = \{\{x_1\}, \{x_2, x_3\}, \{x_4\}\}$$

Functions on Metric Graphs

Definition

Metric graph Γ, define the Hilbert space $L_2(\Gamma)$ by

$$L_2(\Gamma) = \bigoplus_{e \in E} L_2(e), \qquad \langle f, g \rangle^2_{L_2(\Gamma)} = \int_\Gamma f(x)\overline{g}(x)\, dx.$$

Differential Expressions

Electric potential $q(x)$ and magnetic potential $a(x)$.
Magnetic Schrödinger Operator

$$L_{q,a} = \left(i \frac{d}{dx} + a(x) \right)^2 + q(x).$$

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Laplace Operator

$$L = L_{0,0} = -\frac{d^2}{dx^2}.$$

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The equation

$$Lu = \lambda u.$$

Differential Operators

In order to define a self-adjoint differential operator one must determine the domain of the associated differential expression.
[Technical, see Section 2.2.2]

Put shortly,

$$0 = \langle Lu, v \rangle - \langle u, Lv \rangle.$$

Implies that the energy of the system is preserved since the eigenvalues of L are real, and the corresponding eigenfunctions form an orthonormal basis.

Matching Conditions

Conditions that the functions must satisfy at each vertex so that the differential operator is self-adjoint:

$$0 = \langle Lu, v\rangle - \langle u, Lv\rangle = \sum_{m=1}^{M} \sum_{x_j \in v_m} \partial u(x_j)\overline{v}(x_j) - u(x_j)\partial\overline{v}(x_j).$$

Matching Conditions

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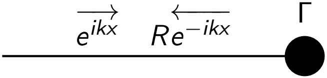
Definition

The *standard matching conditions*, for a vertex v, are given by

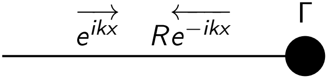
$$\begin{cases} u(x_j) = u(x_i) \text{ for all } x_j, x_i \in v \\ \displaystyle\sum_{x_j \in v} \partial u(x_j) = 0. \end{cases}$$

Scattering



$$|R|^2 = 1$$

Scattering



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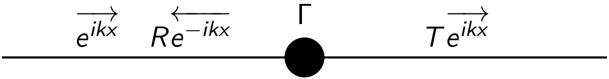


$$|R|^2 + |T|^2 = 1$$

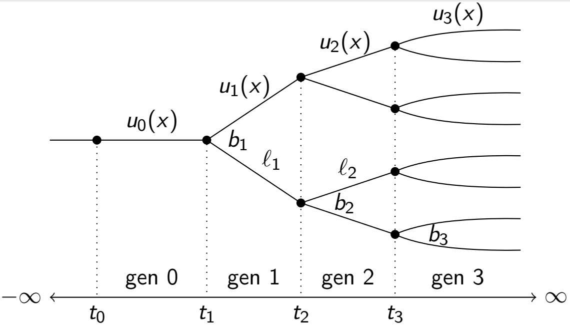
Table of Contents

Radial Tree Graphs

Definition

A *radial tree graph* Γ is a tree where all properties depend only on the distance from the root vertex.

- The n:th *generation* is the set of all edges being $n-1$ edges away from the root vertex.
- The *branching number* b_n of the n:th generation is the number of edges connected to each edge in generation $n-1$.



Scattering from 2-generation radial tree graph

Theorem

Let Γ be a 2-gen radial tree with standard matching conditions. The reflection coefficient and reflection probability are, respectively, given by

$$R(k) = -\frac{(b_1 - 1)(b_2 + 1) + (b_1 + 1)(b_2 - 1)e^{2ik\ell_1}}{(b_1 + 1)(b_2 + 1) + (b_1 - 1)(b_2 - 1)e^{2ik\ell_1}}.$$

Scattering from 2-generation radial tree graph

Proof.

Find the eigenfunctions on each edge

$$u(x) = \begin{cases} e^{ikx} + Re^{-ikx} & \text{generation } 0 \\ Ae^{ikx} + Be^{-ikx} & \text{generation } 1 \\ Te^{ikx} & \text{generation } 2. \end{cases}$$

Write down the equations given by the standard matching conditions

$$\begin{cases} 1 + R = A + B \\ -ik(1 - R) + b_1 ik(A - B) = 0 \end{cases}$$

$$\begin{cases} Ae^{ik\ell_1} + Be^{-ik\ell_1} = Te^{ik\ell_1} \\ -ik(Ae^{ik\ell_1} - Be^{-ik\ell_1}) + b_2 ikTe^{ik\ell_1} = 0. \end{cases}$$

Solve for R. □

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Theorem

Let Γ be a 2-gen radial tree with standard matching conditions. The reflection coefficient and reflection probability are, respectively, given by

$$R(k) = -\frac{(b_1-1)(b_2+1)+(b_1+1)(b_2-1)e^{2ik\ell_1}}{(b_1+1)(b_2+1)+(b_1-1)(b_2-1)e^{2ik\ell_1}},$$

$$|R(k)|^2 = \frac{(b_1-b_2)^2\sin^2(k\ell_1)+(b_1b_2-1)^2\cos^2(k\ell_1)}{(b_1+b_2)^2\sin^2(k\ell_1)+(b_1b_2+1)^2\cos^2(k\ell_1)}.$$

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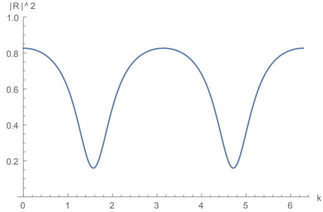
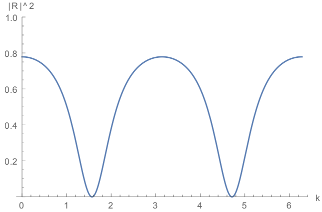
Corollary

- $R(0) = \frac{2}{b_1b_2+1} - 1$, *low-energy waves do not "see" the middle edges.*
- *Let $\widehat{\Gamma}$ be Γ with b_1 and b_2 interchanged, since $|R(k)|^2$ is invariant when interchanging b_1 and b_2, the graphs $\widehat{\Gamma}$ and Γ cannot be distinguished by measuring the reflection probability from the root of the graphs.*
- *Zero reflection is possible only when $b_1 = b_2$.*

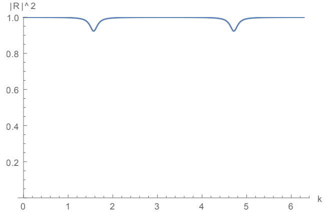
Scattering from 2-generation radial tree



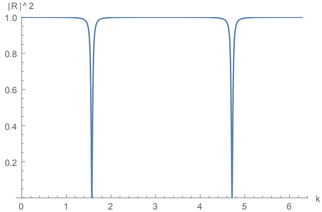
a $b_1 = 7, b_2 = 3$



b $b_1 = b_2 = 4$



c $b_1 = 500, b_2 = 10$



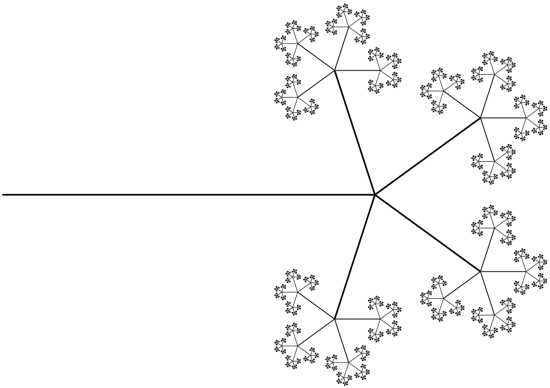
d $b_1 = b_2 = 100$

Figure : Reflection $|R|^2$ from 2 generation radial quantum tree graph with inner edge length $\ell_1 = 1$ and varying branching numbers b_1 and b_2.

Defining the snowflake graph

Definition

A *quantum snowflake* graph Γ is a radial quantum tree graph with infinite number of generations, all with branching number m. Furthermore, the length of all edges in generation k is $\ell\beta^k$ where ℓ and β are constant.



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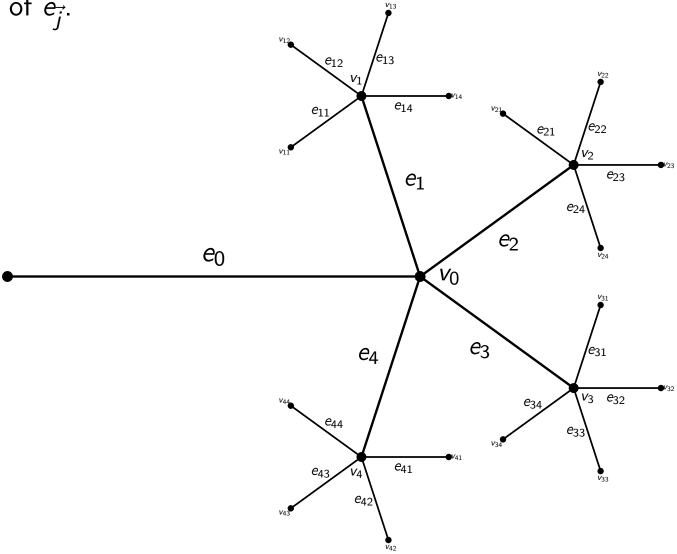
- If $0 < \beta < 1$ the graph has finite depth $\sum_{k=0}^{\infty} \ell\beta^k = \frac{\ell}{1-\beta}$.
- Waves disperse in the infinite structure.

Illustration of notation

Index edges by $e_{j_1, j_2, \ldots, j_n} = e_{\vec{j}}$, similarly vertex $v_{\vec{j}}$ is given by the right end-point of $e_{\vec{j}}$.



Rotation Operator

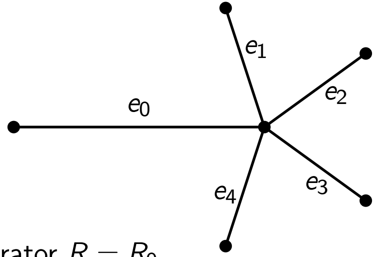
For $\vec{k} = (k_1, k_2, \ldots, k_n)$ and $\vec{j} = (j_1, j_2, \ldots, j_m)$ we define the rotation $R_{\vec{k}}$ as the cyclic permutation of edges

$$R_{\vec{k}} e_{\vec{j}} = \begin{cases} e_{j_1, j_2, \ldots, j_m}, & n > m \\ e_{j_1, j_2, \ldots, j_{n-1}, j_n + 1, j_{n+1}, \ldots, j_m}, & n \leq m. \end{cases}$$

Cyclic notation $e_{j_1, \ldots, j_k + m, \ldots, j_n} = e_{j_1, \ldots, j_k, \ldots, j_n}$.

Rotational symmetries on Γ_1

Because of the self-similarity of Γ, it suffices to consider a 1-generation sub-graph Γ_1 to study the rotational symmetries.



Only one rotation operator $R = R_0$

$$\begin{cases} Re_j = e_{j+1}, & j = 1, 2, \ldots, m \\ Re_0 = e_0 \end{cases} \qquad \begin{cases} (Rf)_j = f_{j+1}, & j = 1, 2, \ldots, m \\ (Rf)_0 = f_0. \end{cases}$$

Rotation-eigenfunctions

- In general $Rf \neq f$, but $R^m f = f$, hence R^m has eigenvalue 1.
- R has eigenvalues $z^n, 0 \leq n \leq m-1$ where $z = e^{i2\pi/m}$.
- Let f^n be the corresponding eigenfunction,

$$Rf^n = z^n f^n.$$

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- Let f^n be the corresponding eigenfunction,

$$Rf^n = z^n f^n.$$

Lemma

Every eigenfunction f^n of R, except f^0, vanishes everywhere on the root edge e_0.

Proof.

In generation 0 rotations do nothing, hence $Rf_0^n = f_0^n = z^n f_0$, implying $f_0^n \equiv 0$ for $1 \leq n \leq m-1$. □

Quasi rotation invariant component

Definition

The n-th quasi rotation invariant component f^n of a function f on Γ_1 is defined by

$$f_j^n = \frac{1}{m} \sum_{k=0}^{m-1} z^{-nk} f_{j+k}, \quad j = 1, 2, \dots, m$$

on the first generation, where $z = e^{\frac{2\pi}{m} i}$, and on the root edge e_0 it is defined by

$$\begin{cases} f_0^n = 0, & 0 \leq n \leq m-1 \\ f_0^0 = f_0 \end{cases}$$

where f_j denotes the restriction of f to the edge e_j.

- Generalization of even and odd functions.
- There are m such components, since $f^{n+m} = f^n$, because $z^{-(n+m)k} = z^{-nk}(z^m)^{-k}$ and $z^m = 1$.

The notation is consistent

Theorem

Let f^n for $n = 1, 2, \ldots, m-1$ be the quasi rotation invariant components of an arbitrary functions f defined on the graph. Then

(a) *f^n is an eigenfunction of R with the corresponding eigenvalue z^n,*

(b) *f is the sum of its quasi rotation invariant components.*

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(a) *f^n is an eigenfunction of R with the corresponding eigenvalue z^n,*

(b) *f is the sum of its quasi rotation invariant components.*

Corollary

By repeated rotations we have

$$f_j^n = z f_{j-1}^n = \ldots = z^{n(j-1)} f_1^n, \quad j = 1, 2, \ldots, m,$$

together with (b) *this shows that f on one entire generation can be reconstructed from the values of f^n on just one edge in the same generation.*

Collapsing the snowflake

Definition

Quantum snowflake Γ with edges $e_{j_1,j_2,\dots}$ define collapsed line-graph $\widetilde{\Gamma}$ by

$$\widetilde{\Gamma} = e_0 \cup e_1 \cup e_{11} \cup e_{111} \cup \dots .$$

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$$\widetilde{\Gamma} = e_0 \cup e_1 \cup e_{11} \cup e_{111} \cup \ldots .$$

- Study Γ via $\widetilde{\Gamma}$.
- Matching conditions on $\widetilde{\Gamma}$ so that Γ and $\widetilde{\Gamma}$ have equal reflection.
- Self-similarity $\rightarrow$ suffices to consider Γ_1 and $\widetilde{\Gamma}_1 = e_0 \cup e_1$.

Transforming $L_2(\Gamma_1) \to L_2(\widetilde{\Gamma}_1)$

Theorem

Let f^n and g^m be eigenfunctions of R, i.e. $Rf^n = z^n f^n$ and $Rg^m = z^m g^m$, then f^n and g^m are orthogonal for $n \neq m$ and
$\langle f^n, g^n \rangle = \langle f_0^n, g_0^n \rangle + m \langle f_1^n, g_1^m \rangle$, where f_0^n is non-zero only for $n = 0$.

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Hence

$$\|f\|^2_{L_2(\Gamma_1)} = \|f_0\|^2 + m\,\|f_1\|^2$$
$$\|f\|^2_{L_2(\widetilde{\Gamma}_1)} = \|f_0\|^2 + \|f_1\|^2 .$$

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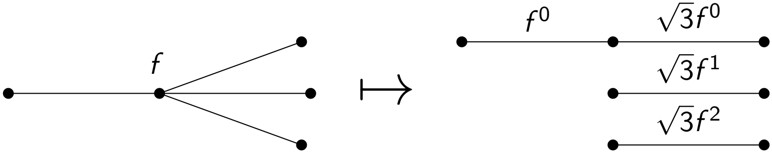
$\langle f^n, g^n \rangle = \langle f_0^n, g_0^n \rangle + m \langle f_1^n, g_1^m \rangle$, where f_0^n is non-zero only for $n = 0$.

Hence

$$\|f\|^2_{L_2(\Gamma_1)} = \|f_0\|^2 + m\,\|f_1\|^2$$
$$\|f\|^2_{L_2(\widetilde{\Gamma}_1)} = \|f_0\|^2 + \|f_1\|^2 .$$

There exists a unitary transformation, as illustrated, hence the graphs are isospectral. We cut off the redundant edges to get $\widetilde{\Gamma}_1$.



Matching Conditions on the Collapsed Snowflake

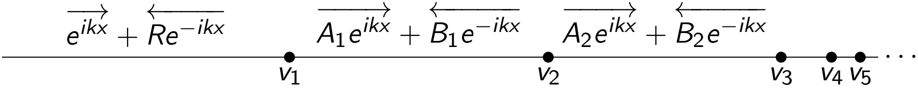
Theorem

Quantum snowflake Γ, branching number m, standard matching conditions. Corresponding collapsed graph $\widetilde{\Gamma}$. Then Γ and $\widetilde{\Gamma}$ have equal reflection if the matching conditions for $\widetilde{\Gamma}$ are chosen as

$$\begin{cases} f_{n+1}(v_{n+1}) = \sqrt{m} f_n(v_{n+1}) \\ f'_{n+1}(v_{n+1}) = \frac{1}{\sqrt{m}} f'_n(v_{n+1}) \end{cases}$$

for every vertex $v_1, v_2, \ldots$ in $\widetilde{\Gamma}$.

Problem reduced to finding reflection of



$$\begin{cases} A_n e^{ik\beta^n} + B_n e^{ik\beta^n} = \dfrac{1}{\sqrt{m}}(A_{n+1} + B_{n+1}) \\ A_n e^{ik\beta^n} - B_n e^{ik\beta^n} = \sqrt{m}(A_{n+1} - B_{n+1}). \end{cases}$$

Can no longer use self-similarity, reflection contribution from all edges; occurrence of $\beta^n \neq \beta^{n+1}$ in the n-th equation.

Step by Step: First step

Notation: S_{ij}, wave scattered towards direction i from direction j.
$i, j = \text{left}, \text{right}$.

wave incoming from left: $\overrightarrow{e^{ikx}} + \overleftarrow{S_{ll}e^{-ikx}}$ $\qquad$ $\overrightarrow{S_{rl}e^{ikx}}$

wave incoming from right: $\overleftarrow{S_{lr}e^{-ikx}}$ $\qquad 0 \qquad$ $\overleftarrow{e^{-ikx}} + \overrightarrow{S_{rr}e^{ikx}}$

Step by Step: First step

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$i, j = \text{left}, \text{right}$.

$$\begin{array}{lccc}
\text{wave incoming from left:} & \overrightarrow{e^{ikx}} + \overleftarrow{S_{ll}e^{-ikx}} & & \overrightarrow{S_{rl}e^{ikx}} \\
\hline
\text{wave incoming from right:} & \overleftarrow{S_{lr}e^{-ikx}} & 0 & \overleftarrow{e^{-ikx}} + \overrightarrow{S_{rr}e^{ikx}}
\end{array}$$

$$\text{wave incoming from left:} \begin{cases} 1 + S_{ll} = \dfrac{1}{\sqrt{m}} S_{rl} \\ 1 - S_{ll} = \sqrt{m} S_{rl} \end{cases} \implies \begin{cases} S_{ll} = \dfrac{1-m}{1+m} \\ S_{rl} = \dfrac{2\sqrt{m}}{1+m} \end{cases}$$

$$\text{wave incoming from right:} \begin{cases} S_{lr} = \dfrac{1}{\sqrt{m}} (1 + S_{rr}) \\ -S_{lr} = \sqrt{m}(-1 + S_{rr}) \end{cases} \implies \begin{cases} S_{rr} = -\dfrac{1-m}{1+m} \\ S_{lr} = \dfrac{2\sqrt{m}}{m+1}. \end{cases}$$

$S_{rr} = -S_{ll}$ and $S_{rl} = S_{lr}$.

Step by Step: Second step

$$\overrightarrow{e^{ikx}} + R\overleftarrow{e^{-ikx}} \qquad A\overrightarrow{e^{ikx}} + B\overleftarrow{e^{-ikx}} \qquad T\overrightarrow{e^{ikx}}$$

$$e_0 \qquad v_1 \qquad e_1 \qquad v_2 \qquad e_2$$

Total wave on e_1:

$$S_{rl}\overrightarrow{e^{ik(x-v_1)}} +$$

$$S_{rl}e^{ik(v_2-v_1)}S_{ll}\overleftarrow{e^{-ik(x-v_2)}} +$$

$$S_{rl}e^{ik(v_2-v_1)}S_{ll}e^{-ik(v_1-v_2)}S_{rr}\overrightarrow{e^{ik(x-v_1)}} +$$

$$S_{rl}e^{ik(v_2-v_1)}S_{ll}e^{-ik(v_1-v_2)}S_{rr}e^{ik(v_2-v_1)}S_{ll}\overleftarrow{e^{-ik(x-v_2)}} +$$

$$S_{rl}e^{ik(v_2-v_1)}S_{ll}e^{-ik(v_1-v_2)}S_{rr}e^{ik(v_2-v_1)}S_{ll}e^{-ik(v_1-v_2)}S_{rr}\overrightarrow{e^{ik(x-v_2)}} + \dots$$

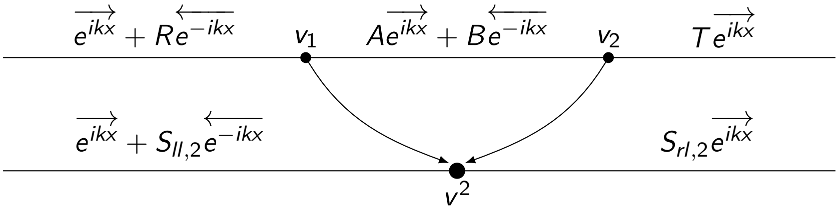
Step by Step: Second step

Converging geometric series for coefficients R, A, B, T.

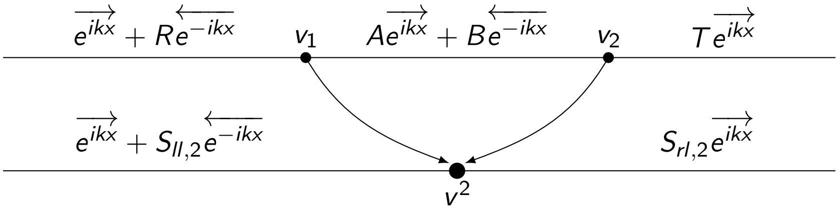
$$A = S_{rl}\left(1 + e^{2ik\ell_1} S_{ll} S_{rr} + \left(e^{2ik\ell_1} S_{ll} S_{rr}\right)^2 + \dots\right)$$

$$= \frac{S_{rl}}{1 - e^{2ik\ell_1} S_{ll} S_{rr}}$$

Merging vertices



Merging vertices



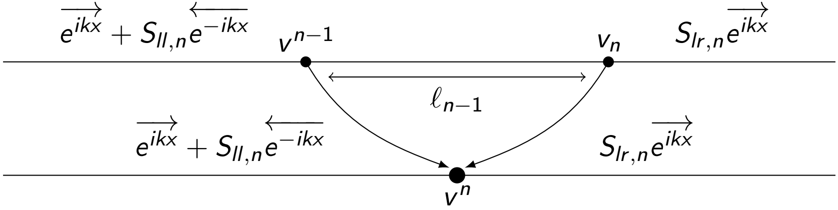
$$S_{ll,2} = S_{ll} + \frac{e^{2ik\ell_1} S_{rl} S_{ll} S_{lr}}{1 - e^{2ik\ell_1} S_{ll} S_{rr}}$$

$$S_{rl,2} = S_{rl,2} \frac{e^{ik\ell_1} S_{rl}^2}{1 - e^{2ik\ell_1} S_{ll} S_{rr}}$$

$$S_{rr,2} = S_{rl,2} S_{rr} + \frac{e^{2ik\ell_1} S_{lr} S_{rr} S_{rl}}{1 - e^{2ik\ell_1} S_{rr} S_{ll}}$$

$$S_{lr,2} = S_{rl,2} \frac{e^{ik\ell_1} S_{lr}^2}{1 - e^{2ik\ell_1} S_{rr} S_{ll}}$$

Recursive expression for reflection from n generations



Recursive expression for reflection from n generations

Theorem

Let Γ be a quantum snowflake graph with $n+1$ generations, branching number m and edge length $\ell_j = \ell\beta^j$ in generation j. Then the total reflection $R_{n+1}(k) = S_{ll,n+1}(k)$ is given by the recursion formula

$$\begin{cases} S_{ll,1} = \dfrac{1-m}{1+m} \\ S_{rl,1} = \dfrac{2\sqrt{m}}{1+m} \\ S_{rr,1} = -S_{ll,1} \\ S_{lr,1} = S_{rl,1} \end{cases} \qquad \begin{cases} S_{ll,n+1} = S_{ll,n} + \dfrac{e^{2ik\ell_n} S_{rl,n} S_{ll,1} S_{lr,n}}{1 - e^{2ik\ell_n} S_{rr,n} S_{ll,1}} \\ S_{rl,n+1} = \dfrac{e^{ik\ell_n} S_{rl,n} S_{rl,1}}{1 - e^{2ik\ell_n} S_{ll,1} S_{rr,n}} \\ S_{rr,n+1} = S_{rr,1} + \dfrac{e^{2ik\ell_n} S_{lr,1} S_{rr,n} S_{rl,1}}{1 - e^{2ik\ell_n} S_{ll,1} S_{rr,n}} \\ S_{lr,n+1} = \dfrac{e^{ik\ell_n} S_{lr,1} S_{lr,n}}{1 - e^{2ik\ell_n} S_{rr,n} S_{ll,1}} \end{cases}$$

Non-periodicity and irregularity

$$S_{3,II} = -\frac{(m-1)\left((m-1)^2 e^{2i\beta^{\mathbf{3}}k\ell} + (m+1)^2 e^{2i\beta^{\mathbf{2}}k\ell} + (m+1)^2 e^{2i\beta^{\mathbf{2}}(\beta+1)k\ell} + (m+1)^2\right)}{(m+1)\left((m-1)^2 e^{2i\beta^{\mathbf{3}}k\ell} + (m-1)^2 e^{2i\beta^{\mathbf{2}}k\ell} + (m-1)^2 e^{2i\beta^{\mathbf{2}}(\beta+1)k\ell} + (m+1)^2\right)}$$

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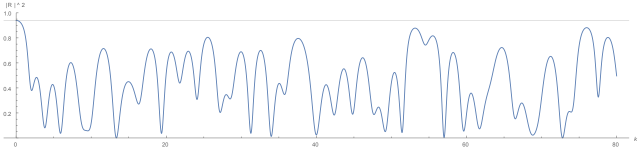
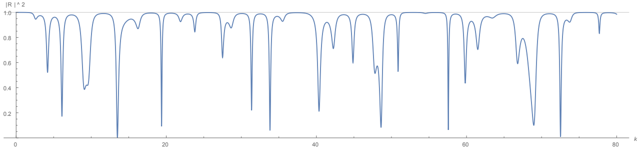
$$R(k;m,\beta) = \lim_{n\to\infty} S_{II,n}(k;m,\beta)$$

Closed-form expression? The seemingly irregular behavior makes this very difficult.

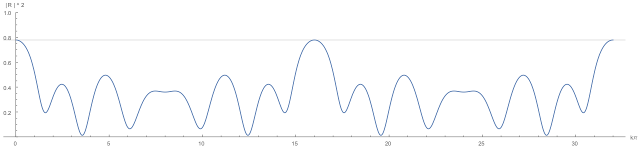
Plots of $|R|^2$ for Finite Snowflakes



a $n = 6, m = 2, \ell = 1, \beta = 0.7$



b $n = 6, m = 5, \ell = 1, \beta = 0.7$



c $n = 4, m = 2, \ell = 1, \beta = 0.5$

Band gap structure in the periodic snowflake

Consider the periodic snowflake graph: $\beta = 1$.

Band gap structure in the periodic snowflake

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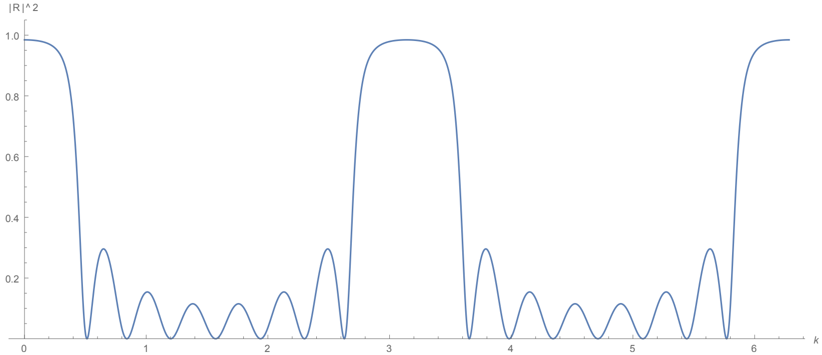
Theorem

Let Γ be a periodic quantum snowflake graph with edge lengths ℓ and branching number m. Only energies $\lambda = k^2$ satisfying

$$|\cos k\ell| < \frac{2\sqrt{m}}{m+1}$$

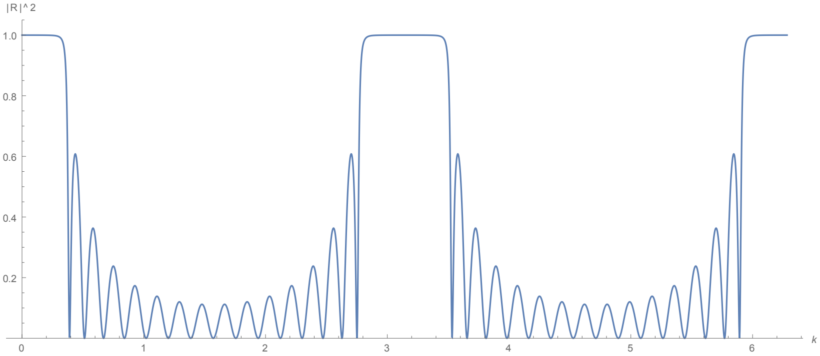
are realizable in the graph. Incoming waves with energies not satisfying this inequality are totally reflected.

Reflection from the periodic snowflake



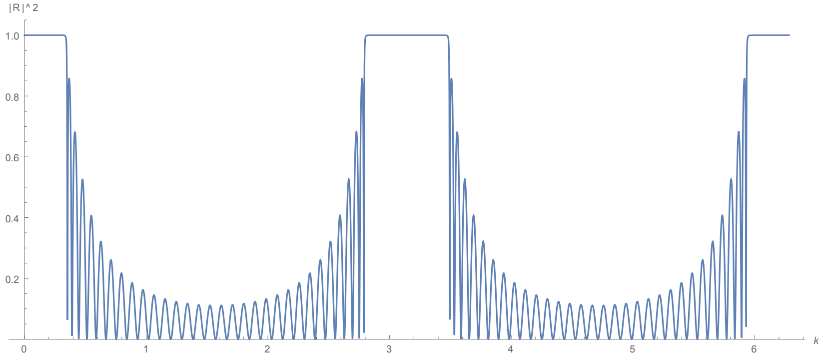
$$n = 8, m = 2, \ell = 1, \beta = 1$$

Reflection from the periodic snowflake



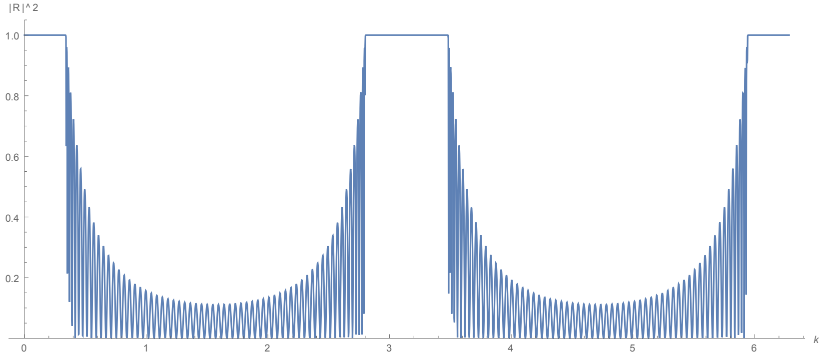
$$n = 16, m = 2, \ell = 1, \beta = 1$$

Reflection from the periodic snowflake



$$n = 32, m = 2, \ell = 1, \beta = 1$$

Reflection from the periodic snowflake



$$n = 64, m = 2, \ell = 1, \beta = 1$$

Average reflection

Average reflection in the periodic snowflake with branching number m

$$\frac{1}{2\pi\ell}\int_0^{2\pi\ell}|R(k)|^2\,dk = \frac{m-1}{m+1}.$$

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Results for average reflection of general snowflakes?

$$\frac{1}{k_1-k_0}\int_{k_0}^{k_1} R(k)\,dk.$$

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$$\begin{array}{c}\Gamma \\ \text{standard} \\ \text{conditions}\end{array} : \begin{cases} f(x_j) = f(x_i) & \forall x_j, x_i \in v \\ \sum_{x_j \in v} \partial f(x_j) = 0 \end{cases} \qquad \begin{array}{c}\widetilde{\Gamma} \\ \text{snowflake} \\ \text{conditions}\end{array} : \begin{cases} f_1(v) = \sqrt{m} f_0(v) \\ f_1'(v) = \frac{1}{\sqrt{m}} f_0'(v). \end{cases}$$

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- Recursive expression for reflection coefficient $R_n(k)$.