The Heat Kernel on the Diagonal for a Compact Metric Graph

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Abstract. We analyze the heat kernel associated with the Laplacian on a compact metric graph, with standard Kirchhoff–Neumann vertex conditions. An explicit formula for the heat kernel as a sum over loops, developed by Roth and Kostrykin–Potthoff–Schrader, allows for a straightforward analysis of small-time asymptotics. We show that the restriction of the heat kernel to the diagonal satisfies a modified version of the heat equation. This observation leads to an “edge” heat trace formula, expressing the sum over eigenfunction amplitudes on a single edge as a sum over closed loops containing that edge. The proof of this formula relies on a modified heat equation satisfied by the diagonal restriction of the heat kernel. Further study of this equation leads to explicit formulas for graphs which are symmetric about each vertex.

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1. Introduction

Let $G$ be a compact, connected metric graph. The Laplacian operator $-\Delta$ on $G$ is the self-adjoint operator on $L^2(G)$ associated with the quadratic form $\|u\|^2$ with domain $H^1(G)$. On each edge, $-\Delta$ acts as the differential operator $-d^2/dx^2$, subject to the standard Kirchhoff–Neumann vertex conditions, which require that the outward derivatives at each vertex sum to zero.

The paper is devoted to the study of the integral kernel of the heat operator $e^{t\Delta}$, which we denote by $H(t,\cdot,\cdot)$. Most of our results concern the restriction of heat kernel to the diagonal

$$h(t,q) := H(t,q,q).$$

We associate with $-\Delta$ an orthonormal basis of real-valued eigenfunctions $\psi_j$, with corresponding eigenvalues $\lambda_j$. Since $G$ is connected, $\lambda_1 = 0$ is a simple
eigenvalue. The eigenfunctions $\psi_j$ for $j > 1$ are generally not uniquely determined, because of multiplicities in the spectrum.

In terms of the eigenvalues and eigenfunctions, the heat kernel admits the expansion

$$H(t, q_1, q_2) = \sum_{j=1}^{\infty} e^{-\lambda_j t} \psi_j(q_1) \psi_j(q_2), \quad (1.1)$$

which converges uniformly on $G \times G$ for $t > 0$.

**Example 1.1.** Let $G$ be a star graph with $d$ equal edges of length $a$. Eigenfunctions which are nonzero at the central vertex must be symmetric and thus proportional to $\cos\left(\frac{\pi k}{a} x\right)$ for $k \in \mathbb{N}_0$, with $x$ the coordinate measured outward from the center on each edge.

The eigenfunctions which vanish at the center are given by $c_j \sin\left(\frac{\pi}{a} \left( k + \frac{1}{2}\right) x\right)$ for $k \in \mathbb{N}_0$, where $c_j$ is the coefficient for edge $j$. The vertex condition implies $\sum c_j = 0$, so this yields a $(d-1)$-dimensional eigenspace for each $k$.

Converting the eigenfunctions into an orthonormal basis yields the expansion, for the restriction to the diagonal,

$$h(t, x) = \frac{1}{ad} + \frac{2}{ad} \sum_{k=1}^{\infty} e^{-\left(\frac{\pi k}{a}\right)^2 t} \cos^2\left(\frac{\pi k}{a} x\right)$$
$$+ \frac{2(d-1)}{ad} \sum_{k=0}^{\infty} e^{-\left(\frac{\pi}{a} \left( k + \frac{1}{2}\right)\right)^2 t} \sin^2\left(\frac{\pi}{a} \left( k + \frac{1}{2}\right) x\right). \quad (1.2)$$

Observe that the value of $h(t, \cdot)$ at the central vertex is $1/d$ times the value at an endpoint of a Neumann interval of length $a$.

The small-time behavior of $h(t, \cdot)$ near vertices is illustrated in Fig. 1. Near a vertex of degree $d$, as $t \to 0$ the diagonal heat kernel approaches a value $2/d$ times its value at a generic edge point. A precise version of this statement can be derived from the heat kernel formulas of Roth [13] and Kostrykin–Potthoff–Schrader [12]; see Proposition 2.1. These asymptotics yield a local Weyl law (Theorem 4.1):
\[
\lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^{N} \psi_j(q)^2 = \frac{2}{d_q L},
\]

where \(L\) is the total length of \(G\) and \(d_q\) is the degree of \(q\), interpreted as 2 if \(q\) is an interior edge point.

We can also use the analysis of \(h(t, \cdot)\) to study the average concentration of eigenfunctions on an edge. To formulate this result, note that on an edge \(e\) of \(G\) parametrized by \(x \in [0, a]\), each (normalized) eigenfunction takes the form

\[
\psi_j(x) = b_j(e) \cos(\sigma_j x + \phi_j),
\]

where \(\lambda_j = \sigma_j^2\). The phases can be adjusted so that \(b_j > 0\), which makes \(b_j(e)\) uniquely determined by \(\psi_j\). In Sect. 4, we prove an edge version of the Weyl asymptotic

\[
\lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^{N} b_j(e)^2 = \frac{2}{L}
\]
on each edge.

The amplitudes \(b_j\) can also be used to prove an interesting variant of the heat trace formula. A trace formula expressing \(\text{tr} e^{t \Delta}\) as a sum over paths on \(G\) was established by Roth [13]. Theorem 5.2 gives an “edge” trace formula: for some constant \(c_e\) depending on the edge \(e\),

\[
\frac{1}{2} \sum_{j=1}^{\infty} e^{-\lambda_j t} b_j(e)^2 = \frac{1}{\sqrt{4 \pi t}} \sum_{\gamma \in P_e} \alpha(\gamma) e^{-\ell(\gamma)^2/4t} + c_e,
\]

where \(P_e\) is the collection of closed paths (including the trivial path) which start with a bond in \(e\).

Finally, we consider a modified heat equation satisfied by \(h\), which can be solved under certain conditions. We apply this approach to work out explicit formulas for \(h(t, q)\) for graphs with a high degree of symmetry.

### 2. Preliminaries

An expansion of the heat kernel on a metric graph as a sum over paths was first developed for compact graphs with Kirchhoff–Neumann vertex conditions by Roth [13, section III]. This was later generalized to infinite graphs in Cattaneo [6, Thm. 1] and to more general vertex conditions in Kostrykin–Potthoff–Schrader [12, Cor. 3.4]. An extension to more general convolution semigroups was given in Becker–Gregorio–Mugnolo [1, Thm. 1].

Our attention is restricted to the heat kernel of the Laplacian on a compact metric graph \(G\) with Kirchhoff–Neumann vertex conditions. The formula from [12] does not allow loops (tadpoles), where a single edge is attached to the same vertex at both ends. However, in the case of Kirchhoff–Neumann vertex conditions we could work around this issue by inserting an artificial (degree two) vertex into each loop. We will instead follow the approach from [13], which is to describe paths in terms of oriented edges.
In the terminology of [4], an oriented edge of $G$ is called a bond, so that each edge corresponds to exactly two bonds. (The corresponding term in the discrete graph literature is arc.) For each bond $\vec{e}$ we can identify an initial vertex $\partial^{-}(\vec{e})$ and final vertex $\partial^{+}(\vec{e})$. Note that a loop attached at vertex $v$ is associated with two bonds, both of which have $v$ as initial and final vertex.

Two bonds $\vec{e}_1$ and $\vec{e}_2$ are consecutive if $\partial^{+}(\vec{e}_1) = \partial^{-}(\vec{e}_2)$. A path $\gamma$ consists of a pair of vertices connected by an ordered sequence of consecutive bonds, i.e.,

$$\gamma = (v_{-}, \vec{e}_1, \ldots, \vec{e}_n, v_{+})$$

where $v_{-} = \partial^{-}(\vec{e}_1)$ and $v_{+} = \partial^{+}(\vec{e}_n)$. A path may “bounce” at a vertex, i.e., a bond may be followed by its inverse bond. Also, the trivial path connecting a vertex to itself is allowed and denoted by $\gamma = (v, v)$. The trivial path is not assigned a direction and hence counted only once. For any path $\gamma$, we denote the total length by

$$\ell(\gamma) := \sum_{j=1}^{n} \ell(\vec{e}_j)$$

To formulate the expansion for the heat kernel $H(t, \cdot, \cdot)$ in a way that includes vertex points, it is convenient to introduce artificial vertices at the evaluation points, if needed. Thus, in the formula for $H(t, q_1, q_2)$ we will assume that $q_1$ and $q_2$ are vertices, possibly of degree two if the original points were interior to an edge. With this convention, let $\mathcal{P}(q_1, q_2)$ denote the collection of paths with $v_{-} = q_1, v_{+} = q_2$. This includes the trivial path if $q_1 = q_2$.

To each path $\gamma$, we assign a coefficient $\alpha(\gamma)$ defined as follows. For the trivial path,

$$\alpha((v, v)) := \frac{2}{\deg(v)}. \quad (2.2)$$

For a path with at least one edge,

$$\alpha((v_{-}, \vec{e}_1, \ldots, \vec{e}_n, v_{+})) := \frac{4}{\deg(v_{-}) \deg(v_{+})} \prod_{j=1}^{n-1} \beta(\vec{e}_j, \vec{e}_{j+1}), \quad (2.3)$$

where $\beta$ is the bond-scattering matrix element, defined as

$$\beta(\vec{e}_j, \vec{e}_{j+1}) := \begin{cases} \frac{2}{\deg \partial^{+}(\vec{e}_j)}, & \partial^{-}(\vec{e}_j) \neq \partial^{+}(\vec{e}_{j+1}) \text{ (transfer)}, \\ \frac{2}{\deg \partial^{+}(\vec{e}_j)} - 1, & \partial^{-}(\vec{e}_j) = \partial^{+}(\vec{e}_{j+1}) \text{ (bounce)}. \end{cases}$$

Note that an artificial vertex contributes a factor of 0 for a bounce and 1 for a transfer. Thus, artificial vertices are essentially invisible except as potential terminal points for a path. Because of this, we may omit from $\mathcal{P}(q_1, q_2)$ any paths that bounce at artificial vertices.

We are now prepared to state the path sum formula for the heat kernel. The versions of this formula from [13] and [12] were restricted to points interior to the edges. The novel feature here is that the definitions of $\mathcal{P}(q_1, q_2)$ and of the path coefficient $\alpha$ have been adapted to account for general points on the graph.
Proposition 2.1. For points $q_1, q_2 \in G \times G$ (including vertices), the heat kernel for the Kirchhoff–Neumann Laplacian has the expansion

$$H(t, q_1, q_2) = \frac{1}{\sqrt{4\pi t}} \sum_{\gamma \in P(q_1, q_2)} \alpha(\gamma) e^{-\ell(\gamma)^2/4t},$$

which converges uniformly in $G \times G$ for all $t > 0$.

Proof. For interior edge points, (2.4) follows from either [13, section III] or [12, Cor. 3.4]. Our goal is thus to check the cases where either $q_j$ could be a vertex.

The behavior at vertex points can be derived from the general formula by continuity. Suppose that $q_1$ is interior to an edge with vertex $v_0$ (of degree $\geq 3$), and assume for the moment that $q_2$ is fixed and not equal to $v_0$. We will set $x = d(v_0, q_1)$ and consider the limit $x \to 0$. Paths in $P(q_1, q_2)$ may be divided into two types. A path $\gamma'$ of the first type consists of paths $\gamma$ whose first step is a transfer at $v_0$, as illustrated in Fig. 2. Truncating the first bond of $\gamma'$ gives a corresponding path $\gamma \in P(v_0, q_2)$, such that $\ell(\gamma') = \ell(\gamma) + x$. By (2.3) the path coefficients are equal

$$\alpha(\gamma) = \alpha(\gamma'),$$

because the transfer factor of $2/\deg(v_0)$ from $\alpha(\gamma')$ appears as the $2/\deg(v_-)$ in the expression for $\alpha(\gamma)$. We thus have

$$\lim_{x \to 0} \alpha(\gamma') e^{-\ell(\gamma')^2/4t} = \alpha(\gamma) e^{-\ell(\gamma)^2/4t}.$$

Paths of the second type either bounce at $v_0$ or first pass through $v_1$. These paths can be paired. For each path $\gamma' \in P(q_1, q_2)$ that does not initially pass through $v_0$, there is a partner $\gamma''$ which first passes through $q_1$, and then follows the same route thereafter. Associated with this pair is a unique path $\gamma \in P(v_0, q_2)$ which first hits $v_1$. The lengths of these paths are related by

$$\ell(\gamma) = \ell(\gamma') + x = \ell(\gamma'') - x,$$

and the coefficients by

$$\alpha(\gamma) = \frac{2}{\deg(v_0)} \alpha(\gamma'), \quad \alpha(\gamma'') = \left(1 - \frac{2}{\deg(v_0)}\right) \alpha(\gamma').$$
Figure 3. A pair of paths $\gamma', \gamma'' \in \mathcal{P}(q_1, q_2)$ of the second type and the corresponding $\gamma \in \mathcal{P}(v_0, q_2)$.

The limit of the contributions from to the heat kernel from $\gamma'$ and $\gamma''$ is thus accounted for by
\[
\lim_{x \to 0} \left[ \alpha(\gamma') e^{-\ell(\gamma')^2/4t} + \alpha(\gamma'') e^{-\ell(\gamma'')^2/4t} \right] = \frac{2}{\deg(v_0)} \alpha(\gamma') e^{-\ell(\gamma')^2/4t} = \alpha(\gamma) e^{-\ell(\gamma)^2/4t}.
\]

Similar considerations apply to the off-diagonal case where $q_2$ approaches a vertex.

For the diagonal case, assume that $q$ is an interior edge point approaching a vertex $v_0$, with $x = d(v_0, q)$. The trivial path $(v_0, v_0)$ is the limit of two paths in $\mathcal{P}(q, q)$, the trivial path $(q, q)$ and the path of length $2x$ which bounces off $v_0$. The limit of these two terms is given by
\[
\lim_{x \to 0} \left[ 1 + \left( \frac{2}{\deg(v_0)} - 1 \right) e^{-x^2/4t} \right] = \frac{2}{\deg(v_0)}.
\]

which agrees with $\alpha((v_0, v_0))$.

Finally, we consider a non-trivial path $\gamma \in \mathcal{P}(v_0, v_0)$, as the limit of paths in $\mathcal{P}(q, q)$. If neither the initial nor final bonds of $\gamma$ pass through $q$, then there is only one corresponding path $\gamma' \in \mathcal{P}(v_0, v_0)$, which transfers through $v_0$ in its first and last steps and follows $\gamma$ in between. This is similar to the first type shown in Fig. 2, except that $q_2 = q_1$ and $\ell(\gamma') = \ell(\gamma) + 2x$. The initial and final transfers of $\gamma'$ contribute a factor of $(2/\deg(v_0))^2$ to $\alpha(\gamma')$. These factors are included in $\alpha(\gamma)$ by the definition (2.3), so that
\[
\alpha(\gamma) = \alpha(\gamma').
\]

This accounts for the limit when $q$ does not lie on the initial or final edges of $\gamma$. If $q$ does lie on one or both of these edges, then the same factor occurs. This can be derived, as in the case shown in Fig. 3, by combining paths with a short bounce at $v_0$ with corresponding paths that terminate at $q$ directly.
The argument for uniform convergence was given in [12, Cor. 3.4]. Let $a_0$ denote the minimum edge length of $G$. The set $\mathcal{P}(q_1, q_2)$ contains at most 3 paths which do not contain a true edge (of the original graph without artificial vertices). If $G$ has $m$ edges, then the number of paths that contain $k$ full edges is bounded by $m^k$. The contribution to the sum from the paths that contain at least one true edge is bounded by

$$
\sum_{k=1}^{\infty} m^k e^{-k^2 a_0^2/4t} < \infty,
$$

independently of the choice of points.

Example 2.2. For the interval $[0, a]$, with Neumann boundary conditions, the eigenfunction expansion of the heat kernel is

$$
H(t, x, y) = \frac{1}{a} + \frac{2}{a} \sum_{j=1}^{\infty} e^{-(\frac{j\pi}{a})^2 t} \cos\left(\frac{j\pi}{a} x\right) \cos\left(\frac{j\pi}{a} y\right).
$$

The path sum formula of Proposition 2.1 yields the same result as the method of images:

$$
H(t, x, y) = \frac{1}{\sqrt{4\pi t}} \sum_{k \in \mathbb{Z}} \left[ e^{-(x-y+2ka)^2/4t} + e^{-(x+y+2ka)^2/4t} \right]. \quad (2.5)
$$

Restricting to the diagonal gives

$$
h(t, x) = \frac{1}{\sqrt{4\pi t}} \left[ 2 + 2 \sum_{k=1}^{\infty} e^{-(ka)^2/t} + 2 \sum_{k=1}^{\infty} e^{-(x+ka)^2/t} \right].
$$

For $h(t, 0)$, the sums combine to give a total coefficient of 4, which shows the factor $(2/\deg)^2$ from (2.3).

Example 2.3. Consider a two-petal flower graph (i.e., two loops joined at a point) of total length $L$. The graph is invariant under reflection of the petals keeping the vertex and the extreme point of the petals invariant. We can thus assume that the eigenfunctions are either even or odd with respect to the reflection. Suppose that the edge $e_1$ has length $a < L$ and is parametrized by $x \in [0, a]$. Then the even eigenfunctions are proportional to $\cos\left(\frac{2\pi k}{L}(x - a/2)\right)$ while the odd eigenfunctions vanish at the vertex. Consequently, the eigenfunction expansion for the heat kernel on the diagonal on this edge, denoted by $h_{e_1}(t, \cdot)$, can be written in the form

$$
h_{e_1}(t, x) = \frac{1}{L} + \frac{2}{L} \sum_{k=1}^{\infty} e^{-(2\pi k/L)^2 t} \cos^2\left(\frac{2\pi k}{L}(x - a/2)\right)
+ \frac{2}{a} \sum_{k=1}^{\infty} e^{-(2\pi k/a)^2 t} \sin^2\left(\frac{2\pi k x}{a}\right).
$$

Note that there is no contribution from the eigenfunctions with frequency $2\pi k/(L - a)$, because these are supported only on the edge $e_2$. 
The eigenvalue expansion of \( h_{e_1}(t, \cdot) \) can be rewritten in the form of (2.4) using Poisson summation. The result is

\[
h_{e_1}(t, x) = \frac{1}{\sqrt{4\pi t}} \sum_{n \in \mathbb{Z}} \left[ \frac{1}{2} e^{-(nL)^2/4t} + \frac{1}{4} e^{-(2x-a+nL)^2/4t} + \frac{1}{4} e^{-(2x-a-nL)^2/4t} \right] \\
+ \frac{1}{\sqrt{4\pi t}} \sum_{n \in \mathbb{Z}} \left[ \frac{1}{2} e^{-(na)^2/4t} - \frac{1}{4} e^{-(2x+na)^2/4t} - \frac{1}{4} e^{-(2x-na)^2/4t} \right]
\]

\[3. \text{ Small-Time Asymptotics}\]

Since our primary applications involve eigenvalue concentration, we will focus on restriction of the heat kernel to the diagonal, denoted by \( h(t, \cdot) \). From Proposition 2.1, we derive the following:

**Proposition 3.1.** Suppose that the compact metric graph \( G \) has \( m \) edges in total and minimum edge length \( a_0 \). For a point \( q \in G \), let \( v_0 \) be the nearest (non-artificial) vertex (possibly with \( q = v_0 \)), with \( d_0 \) the degree of \( v_0 \). Then, for any \( t_0 < a_0^2/(2\log m) \),

\[
h(t, q) = \frac{1}{\sqrt{4\pi t}} \left[ 1 + \left( \frac{2}{d_0} - 1 \right) e^{-d(q,v_0)^2/t} + O(me^{-a_0^2/4t}) \right], \quad (3.1)
\]

for \( t \in (0, t_0] \), where the constant in the error estimate depends only on \( t_0 \).

**Proof.** Suppose that \( q \) lies within the edge \( e \), with nearest vertex \( v_0 \). Let \( a \) denote the length of \( e \), so that the edge can be parametrized by \( x = d(q, v_0) \in [0, a] \). The set \( \mathcal{P}(q, q) \) contains, in addition to the trivial path, paths of length \( 2x \) and \( 2(a-x) \). All other paths contain at least one complete edge.

In this notation, the restriction of \( h(t, q) \) to \( e \) is given by the formula (2.4) as

\[
h_e(t, x) = \frac{1}{\sqrt{4\pi t}} \left[ 1 + \left( \frac{2}{d_0} - 1 \right) e^{-x^2/t} + \left( \frac{2}{d_1} - 1 \right) e^{-(a-x)^2/t} + R(t, x) \right],
\]

where \( R(t, x) \) contains the contributions from paths that transfer through \( v_0 \) or \( v_1 \). Suppose that such a path contains \( k \) complete edges, not counting the segments that connect \( q \) to a vertex. The length of this path is at least \( ka_0 \), where \( a_0 \) is the minimum edge length. Note that \( k \geq 1 \) since the path contains a transfer. The number of paths with \( k \) edges is bounded by \( m^k \), where \( m \) is the total number of edges of \( G \). We can thus estimate

\[
|R(t, x)| \leq \sum_{k=1}^{\infty} m^k e^{-(2x+ka_0)^2/4t}.
\]

For \( t < a_0^2/(2\log m) \), we have a linear estimate for \( k \geq 1 \),

\[
\frac{(ka_0)^2}{4t} + k \log m \geq -\frac{a_0^2}{4t} + \frac{ka_0^2}{2t} + k \log m.
\]

Applying this to the error term gives

\[
|R(t, x)| \leq \sum_{k=1}^{\infty} m^k e^{ka_0^2/4t-ka_0^2/2t} = \frac{me^{-a_0^2/4t}}{1 - me^{-a_0^2/2t}}.
\]

\[\square\]
Proposition 3.1 shows that the leading behavior of $h(t, \cdot)$ as $t \to 0$ depends only on the distance to the nearest vertex and the degree of that vertex. This is illustrated schematically in Fig. 4. Applying a Taylor approximation to (3.1) yields the following:

**Corollary 3.2.** Let $v_0$ be the vertex nearest $q$ and set $x = d(v_0, q)$. For $t$ sufficiently small and $x \lesssim \sqrt{t}$,

$$h(t, q) = \frac{1}{4\pi t} \left[ \frac{2}{d_0} + \frac{d_0 - 2x^2}{t} + O\left(\frac{x^4}{t^2}\right) + O(e^{-a_0^2/4t}) \right]$$

An analysis similar to that of Proposition 3.1 is possible in the off-diagonal case, yielding

$$H(t, q_1, q_2) \sim \frac{c}{\sqrt{4\pi t}} e^{-d(q_1, q_2)^2/4t},$$

for $q_1 \neq q_2$, where the constant is given by a sum over minimal paths connecting $q_1$ to $q_2$,

$$c = \sum_{\gamma \in \mathcal{P}(q_1, q_2): t(\gamma) = d(q_1, q_2)} \alpha(\gamma).$$

Minimal paths contain no bounces, so the coefficient $\alpha(\gamma)$ appearing here is the product of $2/\deg$ for the vertices along the path.

### 4. Eigenfunction Concentration

The Weyl asymptotic for compact metric graphs is standard (proofs may be found in [2,10]) and gives

$$\#\{\lambda_j \leq t\} \sim \frac{L}{\pi} t^{1/2},$$

where $L$ is the total length of $G$. From Proposition 3.1, we can deduce the following local Weyl law:
Theorem 4.1. For a point $q \in G$, the eigenfunctions satisfy, as $N \to \infty$,
\[
\lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^{N} \psi_j(q)^2 = \frac{2}{d_q L},
\]
where $d_q$ is the degree of $q$, interpreted as 2 if $q$ is an interior edge point.

Proof. From (3.1), we have the asymptotic
\[
\sum_{j=1}^{\infty} e^{-t \lambda_j} \psi_j(q)^2 \sim \frac{1}{\sqrt{4 \pi t d_q}}
\]
as $t \to 0$. By the Karamata Tauberian theorem (see, for example, [5, section 6.5.4]), this implies that
\[
\sum_{\lambda_j \leq \lambda} \psi_j(q)^2 \sim \frac{2}{\pi d_q} \lambda^{1/2}
\]
as $\lambda \to \infty$. The Weyl law (4.1) then allows us to replace $\lambda_j \leq \lambda$, by $j \leq N$, where $\lambda \sim (\pi N/L)^2$.

The result of Theorem 4.1 cannot be directly integrated over edges, because the convergence is not uniform at the vertices. However, we can derive the integrated version of the eigenfunction asymptotic from Proposition 3.1.

Proposition 4.2. Suppose the edge $e$ is parametrized by $x \in [0, a]$, and denote by $h_e(t, \cdot)$ the restriction of $h(t, \cdot)$ to $e$. For $f \in C[0, a]$, as $t \to 0$,
\[
\int_0^a f(x) h_e(t,x) \, dx = \frac{1}{\sqrt{4 \pi t}} \int_0^a f(x) \, dx + \left( \frac{2}{d_0} - 1 \right) \frac{f(0)}{4} + \left( \frac{2}{d_1} - 1 \right) \frac{f(a)}{4} + o(t),
\]
where $d_0$ and $d_1$ are the degrees of the vertices at $x = 0$ and $a$, respectively.

Proof. The leading term is clear from (3.1), and the contribution from the remainder $R(t, x)$ is $O(e^{-a_0^2/t})$. The vertex terms are easily calculated from
\[
\lim_{t \to 0} \frac{1}{\sqrt{4 \pi t}} \int_0^a f(x) e^{-x^2/t} \, dx = \frac{f(0)}{4}.
\]

Applying the Karamata theorem as above gives the following asymptotic for the average distribution of eigenfunctions:

Corollary 4.3. For an edge $e$ parametrized by $x \in [0, a]$, let $\psi_j|_e(x)$ denote the restriction of the $j$th eigenfunction. For a continuous function $f$ on $[0, a]$,
\[
\lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^{N} \int_0^a f(x) \psi_j|_e(x)^2 \, dx = \frac{1}{L} \int_0^a f(x) \, dx.
\]
The corresponding result is well known in the case of Riemannian manifolds, with no ergodicity assumptions [7, section 4]. The stronger condition of quantum ergodicity, i.e., the convergence of $\psi_j(x)^2 \, dx$ to uniform measure for sequences of eigenfunctions, is known to fail for quantum graphs in general [3,11].

The result of Corollary 4.3 could also be interpreted in terms of the amplitudes of eigenfunctions. Within a given edge each (normalized), eigenvalue takes the form

$$\psi_j|_e(x) = b_j(e) \cos(\sigma_j x + \phi_j),$$  \hspace{1cm} (4.2)

where $\lambda_j = \sigma_j^2$. We will assume that the phase is chosen that $b_j(e) > 0$, which fixes $b_j(e)$ uniquely (depending on the choice of basis $\{\psi_j\}$).

The semiclassical limit measures associated with sequences of eigenfunctions were studied by Colin de Verdière [8], who noted that a sequence of measures $\psi_j^2 \, dx$ has a weak limit if and only if the corresponding sequence $b_j(e)^2$ is convergent. This follows from the identity

$$\psi_j|_e(x)^2 = \frac{b_j(e)^2}{2} \left( 1 + \cos(2\sigma_j x + 2\phi_j) \right)$$

and the Riemann–Lebesgue lemma. The same reasoning applies to the average measure, so that Corollary 4.3 is equivalent to the statement that

$$\lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^N b_j(e)^2 = \frac{2}{L}. \hspace{1cm} (4.3)$$

### 5. Edge Trace Formula

In Roth’s statement of the heat trace formula [13], a cycle is defined as an equivalence class of closed, oriented paths on $G$, excluding trivial paths. A path is closed if its initial and final vertices match, and two paths are equivalent if they are related by cyclic permutation of the bonds. A cycle is primitive if it cannot be written as the iteration of a smaller cycle. Let $C$ denote the set of primitive cycles of $G$.

**Theorem 5.1.** (Roth) For a compact metric graph $G$ with $V$ vertices and $E$ edges,

$$\sum_{j=1}^\infty e^{-t\lambda_j} = \frac{L}{\sqrt{4\pi t}} + \frac{1}{2}(V-E) + \frac{1}{\sqrt{4\pi t}} \sum_{\gamma \in C} \sum_{k=1}^\infty \alpha(\gamma) \ell(\gamma) e^{-k^2 \ell(\gamma)^2/4t}.$$

Using the path sum formula for the heat kernel, we can develop a variant of the trace formula which is localized to a specific edge. As in the previous section, we focus on a single edge $e$ of length $a$, with eigenfunctions represented by (4.2) as functions of $x \in [0,a]$. In particular, the restrictions of the eigenfunctions to $e$ determine a sequence of amplitudes $b_j(e) > 0$.

Let $P_e$ denote the set of closed paths which begin with a bond contained in the edge $e$. The trivial path is included.
Theorem 5.2. (edge trace formula) For a fixed edge $e$, define the eigenfunction amplitudes $b_j(e)$ as in (4.2). There exists a constant $c_e$ such that for $t > 0$,

$$
\frac{1}{2} \sum_{j=1}^{\infty} e^{-\lambda_j t} b_j(e)^2 = \frac{1}{\sqrt{4\pi t}} \sum_{\gamma \in P_e} \alpha(\gamma) e^{-\ell(\gamma)^2/4t} + c_e.
$$

Proof. Let $q$ denote an interior point in $e$ corresponding to $x \in (0,a)$. In the expansion formula (2.4) for $h(t,q)$, we can subdivide

$$
P(q,q) = P_0(q,q) \cup P_1(q,q),
$$

where $P_0(q,q)$ consists of the trivial path along with the paths which return to $q$ from the opposite of the initial direction. The set $P_1(q,q)$ consists of paths whose final bond is the reverse of the initial. These classes are illustrated in Fig. 5, for a path of the form $(q, \vec{e}_1, \ldots, \vec{e}_n, q)$.

Note that the length of a path in $P_0(q,q)$ is independent of $x$. There is a length-preserving bijection from $P_0(q,q)$ to $P_e$ given by

$$(q, \vec{e}_1, \ldots, \vec{e}_n, q) \mapsto (v_0, \vec{e}_n + \vec{e}_1, \vec{e}_2, \ldots, \vec{e}_{n-1}, v_0),$$

where $v_0 := \partial_-(\vec{e}_n)$. The artificial vertex $q$ is deleted in this process, but since $q$ has degree 2, the coefficient $\alpha$ is preserved. The contribution to the path sum formula for $h_e(t, \cdot)$ from paths in $P_0(q,q)$ can thus be written as

$$h_0(t) := \frac{1}{\sqrt{4\pi t}} \sum_{\gamma \in P_e} \alpha(\gamma) e^{-\ell(\gamma)^2/4t}.
$$

For $\gamma \in P_1(q,q)$, the length takes the form

$$\ell(\gamma) = \pm (2x + c_\gamma),$$

for some $c_\gamma \in \mathbb{R}$. The contribution to $h_e(t, \cdot)$ from paths in $P_1(q,q)$ thus takes the form

$$h_1(t,x) := \frac{1}{\sqrt{4\pi t}} \sum_{\gamma \in P_1(q,q)} \alpha(\gamma) e^{-(2x+c_\gamma)^2/4t}.
$$

Note that the terms in the series expansion for $h_1$ individually satisfy the equation

$$\left(\partial_t - \frac{1}{4} \partial_x^2\right) \frac{1}{\sqrt{4\pi t}} e^{-(2x+c_\gamma)^2/4t} = 0.$$
The sum over \( P_1(q,q) \) is uniformly convergent on \([\epsilon, \infty) \times G\), for every \( \epsilon > 0 \), by the estimates used in the proof of Proposition 2.1, and the same is true of the series for its derivatives. Therefore, for all \( t > 0 \) the term \( h_1 \) satisfies a modified heat equation:

\[
(\partial_t - \frac{1}{4} \partial_x^2) h_1 = 0. \tag{5.1}
\]

With \( h_0 \) and \( h_1 \) defined as above,

\[
h_e(t, x) = h_0(t) + h_1(t, x). \tag{5.2}
\]

On the other hand, in the notation (4.2), the eigenfunction expansion gives

\[
h_e(t, x) = \frac{1}{2} \sum_{j=1}^{\infty} b_j(e) 2 e^{-\lambda_j t} \left( 1 + \cos(2(\sigma_j x + \phi_j)) \right). \tag{5.3}
\]

This expression admits a decomposition

\[
h_e(t, x) = \eta_0(t) + \eta_1(t, x),
\]

where

\[
\eta_0(t) := \frac{1}{2} \sum_{j=1}^{\infty} b_j(e) 2 e^{-\lambda_j t}
\]

and

\[
\eta_1(t, x) := \frac{1}{2} \sum_{j=1}^{\infty} b_j(e) 2 e^{-\lambda_j t} \cos(2(\sigma_j x + \phi_j)).
\]

By (4.3) and the Weyl law for \( \lambda_j \), the series for \( \eta_1 \) converges uniformly \([\epsilon, \infty) \times G\), for all \( \epsilon > 0 \), as do the series for its derivatives. Therefore, \( \eta_1 \) also satisfies the modified heat equation,

\[
(\partial_t - \frac{1}{4} \partial_x^2) \eta_1 = 0, \tag{5.4}
\]

for \( t > 0 \). From Eqs. (5.1) and (5.4), we deduce that

\[
\partial_t [h_0(t) - \eta_0(t)] = 0,
\]

which completes the proof. \( \square \)

### 6. Equation for the Kernel on the Diagonal

In this section, we will study the restriction of the heat kernel to the diagonal on a single edge of \( G \). As before, we assume that \( G \) is a compact metric graph, with standard Kirchhoff–Neumann conditions at the vertices.

Assume that the edge \( e \) is parametrized by \( x \in [0, a] \), and denote the restriction of \( h(t, \cdot) \) by \( h_e(t, \cdot) \). A useful property of \( h_e(t, \cdot) \), which we can see implicitly in the proof of Theorem 5.2, is that its spatial derivative satisfies a heat equation of its own.

**Proposition 6.1.** On each edge \( e \), \( \partial_x h_e \) satisfies a modified heat equation,

\[
(\partial_t - \frac{1}{4} \partial_x^2) \partial_x h_e(t, x) = 0. \tag{6.1}
\]

As a function on \( G \), \( h(t, \cdot) \) is continuous for \( t > 0 \) and satisfies Kirchhoff–Neumann conditions at the vertices.
Proof. Consider the local expansion for $h_e(t, \cdot)$ given by (5.3), using the notation (4.2) for the restriction of eigenfunctions to the edge. As noted in the proof of Theorem 5.2, this series converges uniformly, and the same is true for the series for its derivatives obtained by term-by-term differentiation. We thus calculate

\[(\partial_t - \frac{1}{4} \partial_x^2) h_e(t, x) = \frac{1}{2} \sum_j b_j(e)^2 e^{-\lambda_j t} \lambda_j. \tag{6.2}\]

The right side is independent of $x$, so this proves (6.1).

As to the vertex conditions, the continuity of $h(t, \cdot)$ at vertices is clear from (1.1), since the eigenfunctions are continuous. Differentiating (1.1) directly gives

\[\partial_x h_e(t, x) = -2 \sum_j b_j(e)^2 e^{-\lambda_j t} \sigma_j \cos(\sigma_j x + \phi_j) \sin(\sigma_j x + \phi_j).\]

Evaluating at $x = 0$ gives

\[\partial_x h_e(t, x) \big|_{x=0} = 2 \sum_j b_j(e)^2 e^{-\lambda_j t} \psi_j(v) \partial_e \psi_j(v),\]

where $v$ denotes the vertex at $x = 0$, and $\partial_e$ is the outward derivative in direction of edge $e$. Since $\psi_j(v)$ is independent of $e$, when this expression is summed over the edges incident to $v$, the result is 0 by the Kirchhoff–Neumann conditions on $\psi_j$. \qed

At a given vertex, we can arrange the parametrizations of outgoing edges so that $\partial_x h$ satisfies the anti-Kirchhoff–Neumann vertex condition, as described in [9, Def. 6]. However, $\partial_x h$ is not globally well defined because of the dependence on edge orientation. On a particular edge, the difficulty in solving the modified heat Eq. (6.1) lies in fact that the boundary conditions on $\partial_x h_e$ at the endpoints of $e$ are generally time dependent. Moreover, there is no apparent way to write the boundary values explicitly in the general case. The inhomogeneous Eq. (6.2) has the same problem; the source term is generally not calculable.

We can at least work out the initial condition for $\partial_x h_e$ at $t = 0$, from the following:

**Proposition 6.2.** For $f \in C^1[0, a]$, as $t \to 0$,

\[
\int_0^a f(x) \partial_x h_e(t, x) dx = \frac{1}{\sqrt{4\pi t}} \left[ \left( \frac{2}{d_1} - 1 \right) f(a) - \left( \frac{2}{d_0} - 1 \right) f(0) \right] + \frac{1}{4} \left( \frac{2}{d_0} - 1 \right) f'(0) + \frac{1}{4} \left( \frac{2}{d_1} - 1 \right) f'(a) + o(t).
\]

**Proof.** Integration by parts gives

\[
\int_0^a f(x) \partial_x h_e(t, x) dx = f(\cdot) h_e(t, \cdot) \big|_0^a - \int_0^a f'(x) h_e(t, x) dx.
\]

By Proposition 3.1, the first term has the asymptotic

\[f(\cdot) h_e(t, \cdot) \big|_0^a = \frac{1}{\sqrt{4\pi t}} \left[ \frac{2}{d_1} f(a) - \frac{2}{d_0} f(0) \right] + O(t^\infty).\]
For the second term, we apply Proposition 4.2 to deduce that
\[
\int_0^a f'(x)h_e(t,x) \, dx = \frac{1}{\sqrt{4\pi t}}[f(a) - f(0)] + \frac{1}{4} \left(\frac{2}{d_0} - 1\right) f'(0)
+ \frac{1}{4} \left(\frac{2}{d_1} - 1\right) f'(a) + o(t).
\]

\[\square\]

For certain graphs, such as equilateral complete graphs, star graphs, pumpkin graphs, etc., we can deduce that \(\partial_x h_e(t,\cdot)\) will vanish at the vertices. In these cases, Eq. (6.1) can be solved using Proposition 6.2.

**Proposition 6.3.** For an edge \(e\) parametrized by \(x \in [0,a]\), suppose that \(\partial_x h_e(t,0) = \partial_x h_e(t,a) = 0\).

Then, \(\partial_x h_e(t,\cdot)\) admits the expansion, for \(t > 0\),
\[
\partial_x h_e(t,x) = \sum_{n=1}^{\infty} c_n e^{-\left(\pi n/2a\right)^2 t} \sin\left(\frac{\pi nx}{a}\right),
\]
where
\[
c_n = \frac{\pi n}{2a^2} \left[\left(1 - \frac{2}{d_0}\right) + (-1)^n \left(1 - \frac{2}{d_1}\right)\right].
\]

**Proof.** Existence of the expansion (6.3) follows from Eq. (6.1) and the Dirichlet boundary conditions assumed for \(\partial_x h_e(t,\cdot)\). By the Fourier series coefficient formula,
\[
c_n e^{-\left(\pi n/2a\right)^2 t} = \frac{2}{a} \int_0^a \partial_x h_e(t,x) \sin\left(\frac{\pi nx}{a}\right) \, dx.
\]
Applying Proposition 6.2 and taking \(t \to 0\) then give the stated formula for \(c_n\). \[\square\]

### 7. Applications to Symmetric Graphs

As above, we continue to assume Kirchhoff–Neumann conditions on a compact graph \(G\). In this section, we assume that \(G\) has a high degree of symmetry and work out the consequences for the heat kernel.

**Definition 7.1.** A metric graph \(G\) is said to be **symmetric about a vertex** \(v\) if all edges incident to \(v\) have the same length and the graph is invariant under any permutation of those edges.

We first check that symmetry about a vertex will ensure that the hypothesis of Proposition 6.3 is satisfied at that vertex.

**Lemma 7.2.** The derivative of the diagonal heat kernel \(h_e(t,\cdot)\) vanishes at each vertex about which \(G\) is symmetric.
Figure 6. The Folkman graph is locally arc-transitive, but not vertex-transitive

Proof. As noted in Proposition 6.1, $h_e(t, \cdot)$ satisfies Kirchhoff–Neumann vertex conditions. Since the heat kernel is unique, symmetry about a vertex $v$ guarantees that value of its derivative at $v$ on any incident edge is the same. By the Kirchhoff–Neumann vertex conditions, that value must be 0.  \hfill \Box

An equilateral star graph is symmetric about each vertex, and so Proposition 6.3 applies to the star graph from Example 1.1. Setting $d_0 = d$, $d_1 = 1$ in (6.3) gives

$$
\partial_x h_e(t, x) = \frac{\pi(d-1)}{da^2} \sum_{n \text{ odd}} n e^{-(\pi n/2a)^2 t} \sin\left(\frac{\pi nx}{a}\right) - \frac{\pi}{da^2} \sum_{n \text{ even}} n e^{-(\pi n/2a)^2 t} \sin\left(\frac{\pi nx}{a}\right),
$$
in agreement with (1.2).

Symmetry about each vertex implies in particular that the discrete graph associated with $G$ is \textit{locally arc-transitive}. For simplicity, in the remainder of this section we restrict our attention to cases where $G$ is regular. Examples include complete graphs, cubes and hypercubes, flowers, pumpkins, periodic pumpkin chains, and (symmetric) torus grid graphs. A regular, locally arc-transitive graph need not be vertex-transitive, as illustrated by the Folkman graph shown in Fig. 6.

The spectrum of a general equilateral graph was worked out by von Below and Mugnolo [14]. If $a$ denotes the common edge length, then the eigenvalues
not contained in $(\pi/a)\mathbb{Z}$ are associated with eigenvalues of the discrete Laplacian of $G$. For a regular graph, the discrete Laplacian is equivalent to the adjacency matrix,

\[ A_{ij} := \begin{cases} 1, & v_i \text{ and } v_j \text{ are connected by an edge,} \\ 0, & \text{otherwise.} \end{cases} \]

**Theorem 7.3.** Let $G$ be a compact, regular, equilateral metric graph which is symmetric about each vertex. If $G$ has edge length $a$, vertex degree $d$, and $n$ vertices, then on each edge,

\[ h_e(t, x) = \frac{2}{dna} \sum_{k \in \mathbb{Z}} e^{-(c\pi k/a)^2 t} \left[ 1 - \cos \left( \frac{2\pi kx}{a} \right) \right] + \frac{2}{dna} \sum_{\sigma \in Q} \sum_{k \in \mathbb{Z}} \mu_\sigma e^{-(\sigma + 2\pi k/a)^2 t}, \]

where $c = 1$ if $G$ is bipartite and $2$ if not, and

\[ Q := \left\{ \sigma \in (0, \pi) : d\cos(\sigma a) \in \text{Spec}(A), \sigma \notin (\pi/a)\mathbb{N} \right\}, \]

with $\mu_\sigma$ the multiplicity of $d\cos(\sigma a)$ as an eigenvalue of $A$.

**Proof.** By Lemma 7.2, one ache have

\[ h_e(t, x) = h_0(t) - \frac{d}{da} \sum_{k=1}^{\infty} e^{-(\pi k/a)^2 t} \cos \left( \frac{2\pi kx}{a} \right), \quad (7.1) \]

for some function $h_0(t)$. Integrating over $x$ gives the heat trace

\[ \sum_{j=1}^{\infty} e^{-\lambda_j t} = \int_G h_e(t, x) \, dx = \frac{dna}{2} h_0(t). \]

To write the heat trace explicitly, we recall the spectrum from [14, Thm. 3.2]. The eigenvalues $\lambda_j$ are as follows:

1. $\lambda = (\sigma + 2\pi k/a)^2$ for $\sigma \in Q$ with multiplicity $\mu_q$.
2. $\lambda = k^2\pi^2/a^2$ for $k \in \mathbb{N}_0$, with multiplicities $m(0) = 1$ and

\[ m(k^2\pi^2/a^2) = \begin{cases} (d/2 - 1)n, & k \text{ odd,} \\ (d/2 - 1)n + 2, & k \text{ even.} \end{cases} \]

for $k \geq 1$ if $G$ is not bipartite. If $G$ is bipartite then $m(k^2\pi^2/a^2) = (d/2 - 1)n + 2$ for all $k \geq 1$.

The multiplicity $(d/2 - 1)n$ combines with the factor $2/dna$ to give the same coefficient $(d - 2)/da$ as the cosine term in (7.1). This leaves eigenvalues from (2) with multiplicity 2 for either $\lambda \in (\pi N/a)^2$ or $\lambda \in (2\pi N/a)^2$, depending on whether $G$ is bipartite.

The behavior of $h_e(t, \cdot)$ near the vertices is illustrated in Fig. 7. Note that the non-constant term in the formula $h_e(t, \cdot)$ depends only on $d$ and $a$ and is
otherwise independent of the graph. This term can be expressed in terms of the Jacobi theta function

\[ \vartheta_3(z; \tau) := \sum_{k \in \mathbb{Z}} e^{i \pi \tau k^2} \cos(2kz). \]

In particular,

\[ \sum_{k \in \mathbb{Z}} e^{-\left(\frac{\pi k}{a}\right)^2} \cos \left( \frac{2\pi k x}{a} \right) = \vartheta_3 \left( \frac{\pi x}{a}, \frac{i \pi t}{a^2} \right). \]

The expressions in Theorem 7.3 can be written in the form of Proposition 2.1 using the Poisson summation formula

\[ \sum_{k \in \mathbb{Z}} e^{-\left(\frac{c \pi k}{a}\right)^2} t = \frac{2a/c}{\sqrt{4 \pi t}} \sum_{l \in \mathbb{Z}} e^{-\left(\frac{la}{c}\right)^2}, \]

\[ \sum_{k \in \mathbb{Z}} e^{-\left(\frac{\pi k}{a}\right)^2} t \left[ 1 - \cos \left( \frac{2\pi k x}{a} \right) \right] = \frac{2a}{\sqrt{4 \pi t}} \sum_{l \in \mathbb{Z}} \left( e^{-\left(\frac{la}{t}\right)^2} - e^{-\left(\frac{la-x}{t}\right)^2} \right), \]

\[ \sum_{k \in \mathbb{Z}} e^{-\left(\frac{\sigma + 2\pi k}{a}\right)^2} t = \frac{a}{\sqrt{4 \pi t}} \sum_{l \in \mathbb{Z}} \cos(\sigma \alpha) e^{-\left(\frac{la}{2t}\right)^2}. \]

This yields the expansion

\[ h_e(t, x) = \frac{1}{\sqrt{4 \pi t}} \left[ \frac{4}{\sqrt{\pi}} \sum_{l \in \mathbb{Z}} A_l e^{-\left(\frac{la}{2t}\right)^2/c^2} + \frac{d-2}{d} \sum_{l \in \mathbb{Z}} \left( e^{-\left(\frac{la}{t}\right)^2} - e^{-\left(\frac{la-x}{t}\right)^2} \right) \right] \]

\[ + \frac{2}{dn} \sum_{\sigma \in Q} \sum_{l \in \mathbb{Z}} \mu_\sigma \cos(\sigma \alpha) e^{-\left(\frac{la}{4t}\right)^2}. \]

Note that the coefficients of \(1/\sqrt{4 \pi t}\) add up to 1, as required by Proposition 2.1, since \(Q\) has \(n - 2/c\) elements, counting multiplicities. Organizing the sum by lengths gives the following:

**Corollary 7.4.** For \(G\) as in Theorem 7.3,

\[ h_e(t, x) = \frac{1}{\sqrt{4 \pi t}} \left[ 1 + \sum_{l=2}^\infty A_l e^{-\left(\frac{la}{2t}\right)^2/c^2} - \frac{d-2}{d} \sum_{l \in \mathbb{Z}} e^{-\left(\frac{la-x}{t}\right)^2} \right]. \]
where, if $G$ is not bipartite,

$$A_l = \begin{cases} 
\frac{4}{dn} \left[ 1 + \sum_{\sigma \in Q} \mu_{\sigma} \cos(la\sigma) \right], & l \text{ odd}, \\
\frac{4}{dn} \left[ 1 + \sum_{\sigma \in Q} \mu_{\sigma} \cos(la\sigma) \right] + \frac{2(d-2)}{d}, & l \text{ even},
\end{cases}$$

and, if $G$ is bipartite,

$$A_l = \begin{cases} 
\frac{4}{dn} \sum_{\sigma \in Q} \mu_{\sigma} \cos(la\sigma), & l \text{ odd}, \\
\frac{4}{dn} \left[ 2 + \sum_{\sigma \in Q} \mu_{\sigma} \cos(la\sigma) \right] + \frac{2(d-2)}{d}, & l \text{ even},
\end{cases}$$

Example 7.5. Let $G$ be the complete regular graph with $n = d + 1$ vertices of degree $d$ and uniform edge length $a$. The adjacency matrix $A$ consists of zeros on the diagonal and ones off-diagonal. In this case, $Q$ consists of a single value $\sigma = \arccos(-1/d)$, with multiplicity $\mu_{\sigma} = d$.

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