Periodic-orbit evaluation of a spectral statistic of quantum graphs without the semiclassical limit

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Outline

All animals are equal, but some animals are more equal than others.

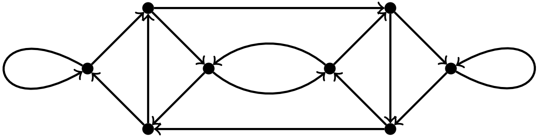
– George Orwell, Animal Farm

- Introduction to quantum graphs
- Dynamical formulas
- Coefficients of the characteristic polynomial
- Semiclassical limit

Dynamical approach to spectral statistics

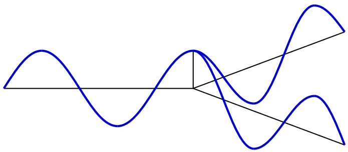
- '71 Gutzwiller's trace formula for the density of states in the semiclassical limit.
- '85 Berry - Diagonal approximation to the form factor using Hannay-Ozorio de Almeida sum rule.
- '99 Kottos and Smilansky - trace formula for the density of states of quantum graphs.
- '01 Sieber and Richter - 2nd order contribution to the small parameter asymptotics of the form factor from figure 8 orbits with one self-intersection.
- '03 Berkolaiko, Schanz and Whitney - 2nd and 3rd order contributions on quantum graphs.
- '04 Müller, Heusler, Braun, Haake and Altland - all higher order contributions.

Graphs



- A *directed graph* (graph) G is a set of *vertices* $\{0, \ldots, V-1\}$ connected by *bonds* $b = (i, j)$ with $i, j \in \{0, \ldots, V-1\}$.
- The *origin* and *terminus* of $b = (i, j)$ are $o(b) = i$ and $t(b) = j$.
- $b = (i, j)$ is *outgoing* at i and *incoming* at j.
- We consider 4-regular graphs with 2 incoming and 2 outgoing bonds at each vertex.
- The *degree* of vertex v is d_v the no. of bonds connected to v.

Quantum graphs



Quantum graphs model phenomena associated with complex quantum systems.

- Free electrons in organic molecules
- Superconducting networks
- Photonic crystals
- Nanotechnology
- Quantum chaos
- Anderson localization

Quantizing a graph

To quantize G;

- Assign length $L_b > 0$ to each bond b.
- Assign a unitary *vertex scattering matrix* $\sigma^{(v)}$ to each vertex v.

A democratic choice is the *discrete Fourier transform matrix*,

$$\boldsymbol{\sigma}^{(v)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} . \tag{1}$$

Bond scattering matrix,

$$\boldsymbol{\Sigma}_{b',b} = \begin{cases} \boldsymbol{\sigma}^{(v)}_{b',b} & v = t(b) = o(b') \\ 0 & \text{otherwise} \end{cases} , \tag{2}$$

Quantum evolution op. $\mathbf{U}(k) = \boldsymbol{\Sigma} \mathrm{e}^{\mathrm{i}k\mathbf{L}}$, with $\mathbf{L} = \mathrm{diag}\{L_1, \ldots, L_B\}$, defines a unitary stochastic matrix ensemble.

Graph spectrum

Neumann like (or standard) vertex conditions

Wavefunction continuous and outgoing derivatives sum to zero at vertices.

$$[\boldsymbol{\sigma}^{(v)}]_{ij} = \frac{2}{d_v} - \delta_{ij}$$

Eigenfunction defined by vector of coefficients of plane waves on the bonds $\overrightarrow{c}$ invariant under quantum evolution op.

$$\begin{aligned} \mathbf{U}(k)\overrightarrow{c} &= \overrightarrow{c} \\ \left(\mathbf{U}\left(k\right) - \mathbf{I}\right)\overrightarrow{c} &= 0 \\ \det\left(\mathbf{U}\left(k\right) - \mathbf{I}\right) &= 0 \end{aligned} \tag{3}$$

So if $k > 0$ is a root of the *secular equation* (3) then k^2 is an eigenvalue of the quantum graph.

Classical dynamics

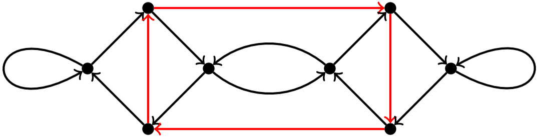
- Probability of transition from b to b' is $|\boldsymbol{\sigma}^{(v)}_{b',b}|^2$.
- 4-regular graphs $|\boldsymbol{\sigma}^{(v)}_{b',b}|^2 = 1/2$.
- Define *classical evolution op.* $\mathbf{M}$ where $\mathbf{M}_{b',b} = |\boldsymbol{\Sigma}_{b',b}|^2$.
- $\mathbf{M}$ is *doubly stochastic* $\sum_{b'} \mathbf{M}_{b',b} = \sum_b \mathbf{M}_{b',b} = 1$.
- Evolution is a Markov process.
- Evolution is *ergodic*, for $\overrightarrow{f}, \overrightarrow{g} \in \mathbb{R}^B$,

$$\lim_{N\to\infty} \frac{1}{N+1} \sum_{j=0}^{N} \overrightarrow{f} \cdot \mathbf{M}^j \overrightarrow{g} = \sum_b \frac{\overrightarrow{f}_b}{B} \ . \tag{4}$$

- For almost all graphs the evolution is *mixing*,

$$\lim_{j\to\infty} M^j \overrightarrow{g} = \frac{1}{B}(1, \ldots, 1)^T \ . \tag{5}$$

Periodic orbits



- A *periodic orbit* $\gamma = (b_1, \ldots, b_m)$ is the equivalence class of closed paths under cyclic shifts, $t(b_j) = o(b_{j+1})$.
- A *primitive periodic orbit* is a periodic orbit that is not a repetition of a shorter orbit.
- *Repetition number* r_γ the number of times a primitive periodic orbit is repeated to produce γ.
- *Topological length* of γ is m.
- *Metric length* of γ is $L_\gamma = \sum_{b_j \in \gamma} L_{b_j}$.
- *Stability amplitude* is $A_\gamma = \Sigma_{b_2 b_1} \Sigma_{b_3 b_2} \ldots \Sigma_{b_m b_{m-1}} \Sigma_{b_1 b_m}$.

Trace formulas

- '83 Trace of the heat kernel – Roth.
- '99 Trace formula for spectral density of Laplacian – Kottos and Smilansky.
- '07 Heat kernel with general vertex conditions – Kostrykin, Potthoff and Schrader.
- '09 Trace formula for general test functions – Bolte and Endres.

Trace formula for density of states

$$\sum_{j=1}^{\infty} \delta(k - k_j) = \frac{\operatorname{tr} \mathbf{L}}{2\pi} + \frac{1}{\pi} \mathrm{Re} \sum_{\gamma} \frac{L_\gamma}{r_\gamma} A_\gamma \mathrm{e}^{\mathrm{i}kL_\gamma}$$

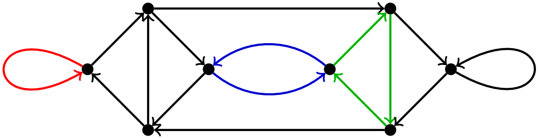
Characteristic polynomial

Characteristic polynomial of $\mathbf{U}(k)$

$$\det\left(\mathbf{U}\left(k\right)-\zeta\mathbf{I}\right)=\sum_{n=0}^{B}a_n(k)\zeta^{B-n}$$

- Secular equation $\det\left(\mathbf{U}\left(k\right)-\mathbf{I}\right)=0$.
- Riemann-Siegel lookalike formula, $a_n=a^*_{B-n}$ – Kottos and Smilansky '99.

Pseudo orbits



- A *pseudo orbit* $\bar{\gamma} = \{\gamma_1, \dots, \gamma_M\}$ is a set of periodic orbits.
- A *primitive pseudo orbit (PPO)* is a set of distinct primitive periodic orbits.
- $m_{\bar{\gamma}} = M$ no. of periodic orbits in $\bar{\gamma}$.
- $\mathcal{P}^n$ set of PPO with n bonds.
- *Metric length* $L_{\bar{\gamma}} = \sum_{j=1}^{M} L_{\gamma_j}$.
- *Stability amplitude* $A_{\bar{\gamma}} = \prod_{j=1}^{M} A_{\gamma_j}$.

Theorem 1 (Band-Harrison-Joyner '12)

Coefficients of the characteristic polynomial are given by,

$$a_n = \sum_{\bar{\gamma} \mid B_{\bar{\gamma}} = n} (-1)^{m_{\bar{\gamma}}} A_{\bar{\gamma}} e^{ikL_{\bar{\gamma}}} ,$$

where the sum is over all primitive pseudo orbits of topological length n.

Idea

- Expand $\det(\mathbf{U}(k) - \zeta \mathbf{I})$ as a sum over permutations.
- A permutation $\rho \in S_B$ can contribute iff $\rho(b)$ is adjacent to b for all b in ρ.
- Representing ρ as a product of disjoint cycles each cycle is a primitive periodic orbit.

Variance of coefficients of the characteristic polynomial

$$\langle a_n \rangle = \begin{cases} 1 & n = 0 \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{aligned} \langle |a_n|^2 \rangle_k &= \sum_{\bar{\gamma},\bar{\gamma}' | B_{\bar{\gamma}} = B_{\bar{\gamma}'} = n} (-1)^{m_{\bar{\gamma}} + m_{\bar{\gamma}'}} A_{\bar{\gamma}} \bar{A}_{\bar{\gamma}'} \lim_{K \to \infty} \frac{1}{K} \int_0^K \mathrm{e}^{\mathrm{i}k(L_{\bar{\gamma}} - L_{\bar{\gamma}'})} \mathrm{d}k \\ &= \sum_{\bar{\gamma},\bar{\gamma}' | B_{\bar{\gamma}} = B_{\bar{\gamma}'} = n} (-1)^{m_{\bar{\gamma}} + m_{\bar{\gamma}'}} A_{\bar{\gamma}} \bar{A}_{\bar{\gamma}'} \, \delta_{L_{\bar{\gamma}}, L_{\bar{\gamma}'}} \end{aligned} \quad (6)$$

Diagonal contribution

$$\langle |a_n|^2 \rangle_{\mathrm{diag}} = \sum_{\bar{\gamma} | B_{\bar{\gamma}} = n} |A_{\bar{\gamma}}|^2 = 2^{-n} |\mathcal{P}^n| \quad (7)$$

where $\mathcal{P}^n$ is the set of primitive pseudo orbits of n bonds.

Variance results

'99 Variance of coeffs of characteristic polynomial of quantum graphs – Kottos and Smilansky

'02 Variance of coeffs of characteristic polynomial of binary graphs in semiclassical limit – Tanner

'12 Pseudo orbit formula for the coefficients – Band, Harrison and Joyner

'19 Diagonal contribution for q-narry graphs – Band, Harrison and Sepanski

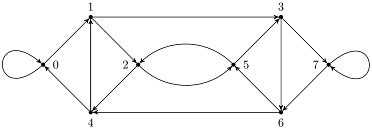
Proposition 2 (Harrison-Hudgins '22)

For a 4-regular quantum graph with $\{L_b\}$ incommensurate,

$$\langle |a_n|^2 \rangle = \frac{1}{2^n} \left(|\mathcal{P}_0^n| + \sum_{N=1}^{n} 2^N \, |\widehat{\mathcal{P}}_N^n| \right) \,, \tag{8}$$

where $\mathcal{P}_0^n$ is the set of PPO length n with no self-intersections and $\widehat{\mathcal{P}}_N^n$ is the set of PPO length n with N self-intersections, all of which are 2-encounters of length zero.

Example: Binary de Bruijn graph with $B = 2^4$



n	$\lvert\mathcal{P}_0^n\rvert$	$\lvert\widehat{\mathcal{P}}_1^n\rvert$	$\lvert\widehat{\mathcal{P}}_2^n\rvert$	$\langle \lvert a_n\rvert^2 \rangle$	Numerics	Error
0	1	0	0	1	1.000000	0.000000
1	2	0	0	1	0.999991	0.000009
2	2	0	0	1/2	0.499999	0.000001
3	4	0	0	1/2	0.499999	0.000001
4	8	0	0	1/2	0.499999	0.000001
5	8	8	0	3/4	0.749998	0.000002
6	8	20	0	3/4	0.749986	0.000014
7	16	16	8	5/8	0.624989	0.000011
8	16	16	24	9/16	0.562501	-0.000001

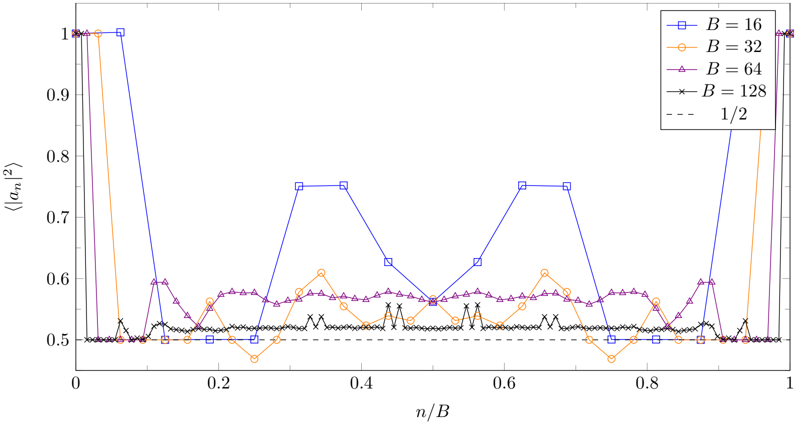
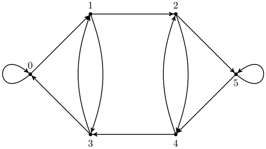


Figure 1: Variance of coefficients of the characteristic polynomial for the family of 4-regular binary de Bruijn graphs with 2^r vertices.

Example: Binary graph with $B = 3 \cdot 2^2$



n	$\lvert\mathcal{P}_0^n\rvert$	$\lvert\widehat{\mathcal{P}}_1^n\rvert$	$\langle\lvert a_n\rvert^2\rangle$	Numerics	Error
0	1	0	1	1.000000	0.000000
1	2	0	1	1.000000	0.000000
2	3	0	3/4	0.750001	-0.000001
3	6	0	3/4	0.750003	-0.000003
4	10	4	7/8	0.874999	0.000001
5	8	4	1/2	0.499998	0.000002
6	8	8	3/8	0.374999	0.000001

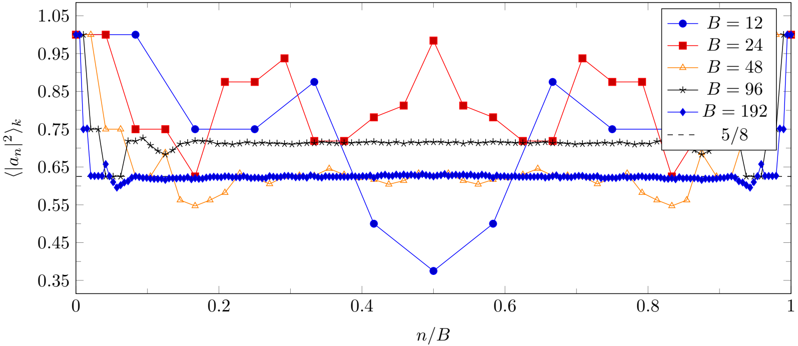
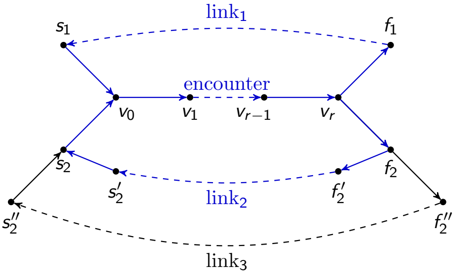


Figure 2: Variance of coefficients of the characteristic polynomial for the family of 4-regular binary graphs with $3 \cdot 2^r$ vertices.

Self-intersections

- A *self-intersection* is a section of a pseudo orbit that is repeated one or more times in the pseudo orbit.
- The maximally repeated section is the *encounter* $\mathrm{enc} = (v_0, \dots, v_r)$.
- The *length of the encounter* is r and an encounter has *length zero* when the encounter contains no bonds.
- If the encounter is repeated l times we refer to an *l-encounter*.
- The encounter can be repeated in a single periodic orbit or across multiple orbits in the pseudo orbit.
- An l-encounter with $l \geq 3$ has bonds preceding/following the encounter repeated 2 or more times as there are only 2 incoming/outgoing bonds at each vertex.

Examples of pseudo orbits with self-intersections

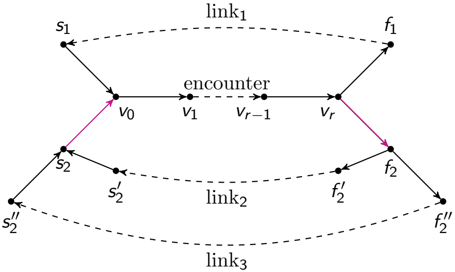


2-encounter: $\bar{\gamma} = (\gamma_1, \ldots, \gamma_m)$ with no self-intersections in $\gamma_2, \ldots, \gamma_m$ and

$$\gamma_1 = (f_1 \ldots, s_1, \mathrm{enc}, f_2, f_2' \ldots, s_2', s_2, \mathrm{enc}, f_1)$$

abbreviated $\gamma_1 = (1, 2)$ for link 1 followed by link 2.

Examples of pseudo orbits with self-intersections



3-encounter: Define $\bar{\gamma}$ similarly but with $\gamma_1 = (1, 2, 3)$.

Bonds (s_2, v_0) and (v_r, f_2) preceding and following the encounter are repeated twice.

Semiclassical limit

For quantum graphs the semiclassical limit is the limit of a sequence of graphs with $B \to \infty$. To take the semiclassical limit of the variance we fix n/B and consider long orbits on large graphs.

- In the semiclassical limit half of PPO with a single 2-encounter have encounter length zero, as the probability to follow the orbit at the initial encounter vertex is $1/2$.
- As the graph is mixing the proportion of orbits with 3-encounters is vanishingly small compared to 2-encounters.
- Let $\mathcal{P}_N^n$ denote the set of PPO length n with N encounters. Then $|\widehat{\mathcal{P}}_N^n| \approx 2^{-N}|\mathcal{P}_N^n|$.

$$\langle |a_n|^2 \rangle = 2^{-n}\left(|\mathcal{P}_0^n| + \sum_{N=1}^{n} 2^N \, |\widehat{\mathcal{P}}_N^n| \right) \approx 2^{-n} \sum_{N=0}^{n} |\mathcal{P}_N^n| = 2^{-n}\, |\mathcal{P}^n|$$

Sketch of a proof of theorem 2

The sum over PPO can be replaced by a sum over *irreducible pseudo orbits* length n where no bonds are repeated $\widehat{\mathcal{P}}^n$ – BHJ '12.

$$\langle |a_n|^2 \rangle = \sum_{\bar{\gamma}, \bar{\gamma}' \in \widehat{\mathcal{P}}^n} (-1)^{m_{\bar{\gamma}} + m_{\bar{\gamma}'}} A_{\bar{\gamma}} \bar{A}_{\bar{\gamma}'} \, \delta_{L_{\bar{\gamma}}, L_{\bar{\gamma}'}} = \sum_{\bar{\gamma} \in \widehat{\mathcal{P}}^n} C_{\bar{\gamma}} \qquad (9)$$

$$C_{\bar{\gamma}} = \sum_{\bar{\gamma}' \in \mathcal{P}_{\bar{\gamma}}} (-1)^{m_{\bar{\gamma}} + m_{\bar{\gamma}'}} A_{\bar{\gamma}} \bar{A}_{\bar{\gamma}'} \qquad (10)$$

where $\mathcal{P}_{\bar{\gamma}}$ is the set of PPO length $L_{\bar{\gamma}}$.

- If $\bar{\gamma}$ has no self-intersections $\mathcal{P}_{\bar{\gamma}} = \{\bar{\gamma}\}$ and $|A_{\bar{\gamma}}|^2 = 2^{-n}$ producing the 1st term in theorem 2.
- A PPO with an encounter of positive length is not irreducible.
- A PPO with an l-encounter with $l \geq 3$ is not irreducible as there are repeated bonds before and after the encounter.
- A PPO with a single 2-encounter length zero if $\bar{\gamma}' \neq \bar{\gamma}$ then $m_{\bar{\gamma}'} = m_{\bar{\gamma}} \pm 1$ and $\bar{A}_{\bar{\gamma}'} = -A_{\bar{\gamma}}$, hence $C_{\bar{\gamma}} = 2 \cdot 2^{-n}$.

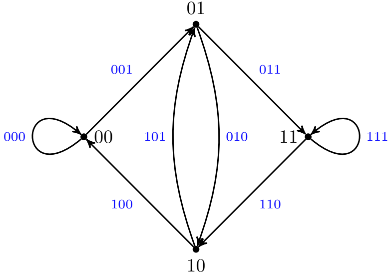
Binary graphs

- Introduced by Tanner '00, '01, '02.
- $V = p \cdot 2^r$ and $B = p \cdot 2^{r+1}$ with p odd.
- Adjacency matrix,

$$[\mathbf{A}_V]_{i,j} = \begin{cases} \delta_{2i,j} + \delta_{2i+1,j} & 0 \le i < V/2 \\ \delta_{2i-V,j} + \delta_{2i+1-V,j} & V/2 \le i < V \end{cases} \qquad (11)$$

Example: Binary graph with $V = 2^2$ and $B = 2^3$,

$$\mathbf{A} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$



Pseudo orbits on binary graphs

Proposition 3 (Harrison-Hudgins)

For a binary graph with $V = p \cdot 2^r$ vertices the number of PPO of length $n > p$ is

$$|\widehat{\mathcal{P}}^n| = C_p \cdot 2^{n-1} \ ,$$

where C_p is evaluated from the cycle decomposition of a generalized $p \times p$ permutation matrix, $1 \leq C_p \leq \frac{3}{2}(p-1)$ for $p > 1$. Note $C_1 = 1$ and $C_3 = 5/4$.

Corollary 4

For the family of binary graphs with $V = p \cdot 2^r$ vertices,

$$\lim_{r\to\infty} \langle |a_n|^2 \rangle_k = 2^{-n} \, |\mathcal{P}^n| = \frac{C_p}{2} \ .$$

Parity argument

Proposition 5 (Harrison-Hudgins)

If $\bar{\gamma}$ has an l-encounter of positive length or with $l \geq 3$ then $C_{\bar{\gamma}} = 0$.

Sketch of proof: assume $\bar{\gamma}$ has single l-encounter of positive length and no repeated links.

- $C_{\bar{\gamma}} = \sum_{\bar{\gamma}' \in \mathcal{P}_{\bar{\gamma}}} (-1)^{m_{\bar{\gamma}} + m_{\bar{\gamma}'}} A_{\bar{\gamma}} \bar{A}_{\bar{\gamma}'}$
- As the encounter has positive length $A_{\bar{\gamma}'} = A_{\bar{\gamma}}$.
- $C_{\bar{\gamma}} = (-1)^{m_{\bar{\gamma}}} 2^{-n} \sum_{\bar{\gamma}' \in \mathcal{P}_{\bar{\gamma}}} (-1)^{m_{\bar{\gamma}'}}$
- $\bar{\gamma}$ has l-links and elements of $\mathcal{P}_{\bar{\gamma}}$ correspond to $\rho_{\bar{\gamma}'} \in S_l$.
- $m_{\bar{\gamma}'}$ is no. of cycles in $\rho_{\bar{\gamma}'}$ (plus no. of periodic orbits with no self-intersections).
- As there are equal numbers of permutations with even/odd cycle decompositions $C_{\bar{\gamma}} = 0$.

Conclusions

- All pseudo orbits are equal – in the semiclassical limit the variance is determined by the total number of primitive pseudo orbits.
- Some pseudo orbits are more equal than others – the variance only depends on primitive pseudo orbits where all the self-intersections are 2-encounters of length zero.
- Parity argument shows $C_{\bar{\gamma}} = 0$ when $\bar{\gamma}$ has an l-encounter of positive length or with $l \geq 3$.
- Results use exact dynamical formulas for graphs and model where dynamical quantities can be evaluated.
- To extend results to q-narry graphs requires averaging over ways to assign the FFT scattering matrix at a vertex.
- For q-nary graphs variance depends on primitive pseudo orbits where all self-intersections are l-encounters of length zero with $l \leq q$.

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