# Quantum Graphs and Random-Matrix Theory

Hans A. Weidenmüller
MPI für Kernphysik
Heidelberg

In collaboration with
M. R. Zirnbauer, Universität zu Köln

RMT in High-Energy Physics and beyond (Workshop in honour of Jac Verbaarschot), Trento, August 2019

Contents:

1. Purpose
2. Approach
3. Chaotic Quantum Graphs. Supersymmetry
4. Coset Space
5. Universal Mode and Massive Modes
6. Effective Action
7. Gaussian Approximation
8. Order-of-Magnitude Estimates
9. Bounds
10. More Stringent Bounds
11. Discussion and Conclusions

# 1. Purpose

Bohigas, Giannoni and Schmit conjecture: Spectral fluctuation properties of Hamiltonian systems that are chaotic in the classical limit coincide with those of random-matrix ensemble in same symmetry class. Central element in understanding quantum chaos.

O. Bohigas, M. J. Giannoni, C, Schmit, Phys. Rev. Lett. 52 (1984) 1.

Substantial numerical evidence. Two analytical approaches to proof: Partial summation of Gutzwiller's semiclassical expansion of level density for general systems, and study of chaotic quantum graphs.

M. Sieber and K. Richter, Phys. Scr. T90 (2001) 128.

S. Müller, S. Heusler, A. Altland, P. Braun, F. Haake, New Journal of Physics 11 (2009) 103025

A. V. Andreev, O. Agam, B. D. Simons, B. L. Altshuler, Phys. Rev. Lett. 76 (1996) 3947 and Nucl. Phys. B 482 (1996) 536.

M. R. Zirnbauer, J. Math. Phys. 38 (1997) 2007, arXiv:cond.mat/9701024.

S. Gnutzmann, A. Altland, Phys. Rev. Lett. 93 (2004) 014104, Phys. Rev. E 72 (2005) 056215.

Z. Pluhar, H. A. Weidenmüller, Phys. Rev. Lett. 110 (2013) 034101, Phys. Rev. E 88 (2013) 022902,
Phys. Rev. Lett. 112 (2014) 144102, J. Math. Phys.: Math. Theor. 48 (2015) 275102.

In chaotic quantum graphs supersymmetry leads to variables defined in coset space. The problem is known but all treatments so far separate universal mode and massive modes as though they were defined in ordinary vector space.

A. Altland, S. Gnutzmann, F. Haake, T. Micklitz, Rep. Prog. Phys. 78 (2015) 086001.

Present treatment takes full account of coset space structure for the case of the two-point function. Can we prove the conjecture?

# 2. Approach

Define two-point function as derivative of a generating function. Use supersymmetry to average that function over phases. Yields effective action in coset space. That is used to identify universal mode and massive modes. Express effective action in terms of these variables. Gaussian approximation for massive modes is starting point for perturbative expansion.

Every term in the expansion so generated, combined with source terms for massive modes, has form of Gaussian superintegral. Must show that every such term vanishes in limit of large graph size.

Can be shown on average over all graphs. For a proof use strict upper bounds. These cannot be shown to vanish for infinite graph size. Discuss reasons and consequences.

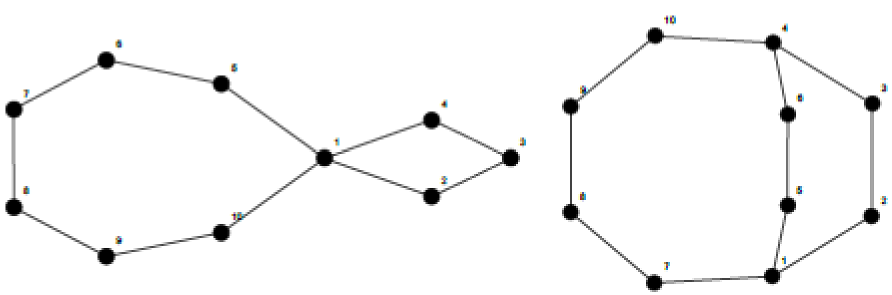
# 3. Chaotic Quantum Graphs. Supersymmetry

T. Kottos and U. Smilansky, Ann. Phys. 274 (1999) 76.

Quantum Graph: V vertices connected by B bonds. Connected and simple. Directed bonds with direction d labeled (b d). Schrödinger wave carries same wave number k on all bonds and a phase $\phi_{bd}$ that breaks T-invariance. Hermitean boundary conditions on all vertices. Incoming and outgoing waves on bonds connected to same vertex α related by unitary matrix $\sigma^{\alpha}$. Totality of all these defines unitary bond scattering matrix $\Sigma^{(B)}_{bd,b'd'}$ . Amplitude propagation on graph defined by matrix

$$\mathcal{B}_{bd,b'd'} = (\sigma_1^d \Sigma^{(B)})_{bd,b'd'}$$

where $\sigma_1^d$ is first Pauli spin matrix in directional space. All bond lengths incommensurate.



Perron-Frobenius operator is

$$\mathcal{F}_{bd,b'd'} = |\mathcal{B}_{bd,b'd'}|^2$$

That operator governs relaxation of classical system towards equilibrium (equal occupation probability for all bonds). Matrix $\mathcal{F}$ is bistochastic, one eigenvalue is +1. All remaining eigenvalues obey $|\lambda_i| \leq 1$. We assume that $|\lambda_i| \leq 1 - a < 1$, even in the limit $B \to \infty$ : Spectrum has a finite gap of size $a$. Classical relaxation is exponentially fast. Proof of universality for weaker condition as used by some authors seemingly not applicable to all orders of perturbation expansion. To keep gap from closing as B increases, connectivity of graph must increase.

Unitary symmetry realized by averaging separately and independently over phases $\phi_{bd}$. Consider only two-point function: Product of retarded and advanced Green functions. Using supersymmetry this is written as derivative of generating function. Average calculated using color-flavor transformation (exact). Yields supermatrices $Z_{bd;ss'}$ and $\tilde{Z}_{bd;ss'}$, both of dimension 2 where s = (B, F). Related by symmetry. M. R. Zirnbauer, J. Math. Phys. 38 (1997) 2007

Averaged two-point function is integral over all $Z_{bd;ss'}$ and $\tilde{Z}_{bd;ss'}$. Integrand carries in exponent minus the effective action (supertrace implies summation over (b d))

$$\mathcal{A} = -\mathrm{STr}\ln(1 - Z\tilde{Z}) + \mathrm{STr}\ln(1 - w_+\mathcal{B}Z\mathcal{B}^\dagger w_-\tilde{Z})$$

The factors $w_\pm$ carry the difference in wave numbers in the advanced and the retarded Green functions and are irrelevant for what follows. Will be suppressed. So action is

$$\mathcal{A}(Z,\tilde{Z}) = -\mathrm{STr}\ln(1 - Z\tilde{Z}) + \mathrm{STr}\ln(1 - \mathcal{B}Z\mathcal{B}^\dagger\tilde{Z})$$

Exponential is multiplied by the "source terms"

$$\frac{\pi^2}{B^2}\Big(\mathrm{STr}[\sigma_3^s(1 - Z\tilde{Z}))^{-1}Z\tilde{Z}]\ \mathrm{STr}[\sigma_3^s(1 - \tilde{Z}Z)^{-1}\tilde{Z}Z] \\ +\mathrm{STr}[\sigma_3^s\tilde{Z}(1 - Z\tilde{Z}))^{-1}\sigma_3^s Z(1 - \tilde{Z}Z)^{-1}]\Big)$$

Here $\sigma_3^s$ is the third Pauli spin matrix in superspace and breaks supersymmetry. Entire information on graph dynamics located in matrix $\mathcal{B}$ .

# 4. Coset Space

Suppress indices (b, d) and rewrite action identically as

$$\mathcal{A} = -\mathrm{STr}\ln\frac{2}{1+Q\Lambda} + \mathrm{STr}\ln\left(1 - M\frac{Q\Lambda-1}{Q\Lambda+1}\right)$$

where

$$Q = g(Z)\Lambda g^{-1}(Z)$$

is Efetov's Q-matrix and where in retarded-advanced notation

$$\Lambda = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad M = \begin{pmatrix} \mathcal{B} & 0 \\ 0 & \mathcal{B}^\dagger \end{pmatrix},$$

$$g(Z) = \begin{pmatrix} (1 - Z\tilde{Z})^{-1/2} & 0 \\ 0 & (1 - \tilde{Z}Z)^{-1/2} \end{pmatrix} \begin{pmatrix} 1 & Z \\ \tilde{Z} & 1 \end{pmatrix}.$$

The matrix Q remains unchanged if we replace $g \to gk$ provided that $[k, \Lambda] = 0$. Therefore, Q and $\mathcal{A}$ are defined in a coset space G/K with fundamental form $Q = g\Lambda g^{-1} = gk\Lambda k^{-1}g^{-1}$. We read $k$ as gauge transformation. With

$g = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ we have $Z = B(g)D^{-1}(g) = B(gk)D^{-1}(gk)$

$$\tilde{Z} = C(g)A^{-1}(g) = C(gk)A^{-1}(gk)$$

as gauge-invariant coordinates of Q.

# 5. Universal Mode and Massive Modes

Universal Mode: Consider group element $g_0$ that in directed-bond space is multiple of unit matrix. Associated Q-matrix is $Q = g_0 \Lambda g_0^{-1}$. The gauge-invariant coordinates

$$Y = B_0 D_0^{-1} \ , \ \tilde{Y} = C_0 A_0^{-1}$$

define the universal mode. Define massive modes $(\zeta_{bd}, \tilde{\zeta}_{bd})$ by expanding $(Z_{bd}, \tilde{Z}_{bd})$ around $(Y, \tilde{Y})$, respecting coset structure. Write $(Z_{bd}, \tilde{Z}_{bd})$ as coordinates of $g_0 g(\zeta_{bd})$, replace $(\zeta_{bd}, \tilde{\zeta}_{bd})$ by gauge-invariant variables $(\xi_{bd}, \tilde{\xi}_{bd})$ , find $Z_{bd} = (Y + \xi_{bd})(1 + \tilde{Y}\xi_{bd})^{-1}$, $\tilde{Z}_{bd} = (\tilde{Y} + \tilde{\xi}_{bd})(1 + Y\tilde{\xi}_{bd})^{-1}$ . Expand in powers of $(\xi_{bd}, \tilde{\xi}_{bd})$.

Mathematically, linearization in $(\zeta_{bd}, \tilde{\zeta}_{bd})$ means that we consider the vector bundle of tangent vector spaces over $G/K$. For the 2 B variables $(\zeta_{bd}, \tilde{\zeta}_{bd})$ the approximation is that all 2 B tangent vector spaces together form a linear space. Justified if massive modes provide small corrections. Requirements: Size of gap, the variables $(Z, \tilde{Z})$ must cluster closely about the universal mode.

To retain the correct number of independent variables we impose the constraints $\sum_{bd} \xi_{bd} = 0 = \sum_{bd} \tilde{\xi}_{bd}$.

# 6. Effective Action

An invariance property of the action allows us to show that under the transformation $Z_{bd} \to (Y, \xi_{bd})$ the action takes the form

$$\mathcal{A}(Z,\tilde{Z}) \approx \mathcal{A}_{\text{bare}} - \frac{2i\pi\kappa}{\Delta}\mathrm{STr}_s \frac{1}{1-Y\tilde{Y}}$$

where last term has standard form and where

$$\mathcal{A}_{\text{bare}} = -\mathrm{STr}\ln(1-\xi\tilde{\xi}) + \mathrm{STr}\ln(1-\mathcal{B}\xi\mathcal{B}^\dagger\tilde{\xi})$$

For the source terms define $Q(\xi,\tilde{\xi}) = g(\xi)\Lambda g^{-1}(\xi)$ . The contribution due to the massive modes is

$$\frac{\pi^2}{B^2}\sum_{bd}\mathrm{STr}_s\Big(\Sigma(Y,\tilde{Y})[Q(\xi_{bd},\tilde{\xi}_{bd})-1]\Sigma'(Y,\tilde{Y})[Q(\xi_{bd},\tilde{\xi}_{bd})-1]\Big)$$
$$+\frac{\pi^2}{B^2}\Big\{\sum_{bd}\mathrm{STr}_s\Big(\Sigma(Y,\tilde{Y})[Q(\xi_{bd},\tilde{\xi}_{bd})-1]\Big)$$
$$\times\sum_{b'd'}\mathrm{STr}_s\Big(\Sigma'(Y,\tilde{Y})[Q(\xi_{b'd'},\tilde{\xi}_{b'd'})-1]\Big)\Big\}$$

Clear separation of contributions due to universal mode and due to massive modes. To show that all integrals vanish for $B \to \infty$ .

# 7. Gaussian Approximation

Expand $\mathcal{A}_{\rm bare}$ in powers of $(\xi,\tilde{\xi})$ and keep only terms of second order. Gives

$$\mathcal{A}_0 = \sum_{\mu\nu} {\rm STr}_s[\xi_\mu(\delta_{\mu\nu} - \mathcal{F}_{\mu\nu})\tilde{\xi}_\nu]$$

Expand Perron-Frobenius operator $\mathcal{F}$ in terms of its eigenvalues $\lambda_i$ and left and right eigenfunctions $\langle w_i|$ and $|u_i\rangle$ with $\langle w_i|u_j\rangle = \delta_{ij}$ . Define new variables

$$\phi_k = \sum_\mu \xi_\mu u_{k\mu} \ , \ \tilde{\phi}_k = \sum_\nu w_{k\nu}\tilde{\xi}_\nu \ .$$

Then

$$\mathcal{A}_0 = \sum_{k\geq 2} {\rm STr}_s[\phi_k(1-\lambda_k)\tilde{\phi}_k]$$

defines Gaussian superintegrals. Leading eigenvalue $\lambda_1 = 1$ does not contribute. Expand $\exp\{-\mathcal{A}_{\rm bare} + \mathcal{A}_0\}$ in Taylor series. Resulting Gaussian integrals exist because of cutoff in spectrum of $\mathcal{F}$ . General integral is

$$\int {\rm d}(\xi,\tilde{\xi}) \prod_{i=1}^n \xi_{\mu_i;s_i t_i}\tilde{\xi}_{\nu_i;t'_i s'_i} \exp\{-\mathcal{A}_0\}$$
$$= \prod_{i=1}^n \sum_{\rm perm} \prod_{j=1}^n \delta_{s_i s'_j}\delta_{t_i t'_j}(-)^{t_i} W_{\mu_i\nu_j}$$

where $W_{\mu\nu} = \langle\mu|\mathcal{P}(1-\mathcal{F})^{-1}\mathcal{P}|\nu\rangle$ and where $\mathcal{P}$ procects onto subspace spanned by eigenvectors with index i > 1. Matrix elements $W_{\mu\nu}$ measure the size of the fluctuations of massive modes $(\xi,\tilde{\xi})$ . Must be sufficiently small for perturbative approach to work.

Expansion of $\exp\{-\mathcal{A}_{\rm bare} + \mathcal{A}_0\}$ in Taylor series and multiplication with source terms for massive modes yields the general term (without numerical factors)

$$\frac{1}{B^2}\Big\langle \mathrm{STr}[(1-Y\tilde{Y})^{-1}\sigma_3^s(\xi\tilde{\xi})^{s_1}]\ \mathrm{STr}[(1-Y\tilde{Y})^{-1}\sigma_3^s(\tilde{\xi}\xi)^{s_2}] \\ \times \prod_{i=0}^{m}\mathrm{STr}(\xi\tilde{\xi})^{n_i}\prod_{j=0}^{k}\mathrm{STr}\left(\mathcal{B}\xi\mathcal{B}^\dagger\tilde{\xi}\right)^{l_j}\Big\rangle$$

Evaluated with integral formula on previous page.

Constraints due to supersymmetry: A nonzero result for the supertraces is obtained only if supersymmetry is broken by the factors $\sigma_3^s$ in both the retarded and the advanced sector for every factor $\xi$ and for every factor $\tilde{\xi}$ in every supertrace. Develop algorithm to identify surviving terms.

Have to show that surviving terms vanish for $B \to \infty$ .

# 8. Order-of-Magnitude Estimates

We need to estimate the dependence of the general term on the dimension (2 B) of directed bond space for large B and to show that it vanishes for $B \to \infty$ . Do that first using mean values based on completeness:

$$\langle bd|\mathcal{P}(1-\mathcal{F})^{-1}\mathcal{P}|bd\rangle \approx \frac{1}{2B}\sum_{bd}\langle bd|\mathcal{P}(1-\mathcal{F})^{-1}\mathcal{P}|bd\rangle = \frac{1}{2B}\sum_{i\geq 2}\frac{1}{1-\lambda_i} \leq \frac{1}{a} \; .$$

$$\prod_{i=1}^{n}\langle b_i d_i|\mathcal{P}(1-\mathcal{F})^{-1}\mathcal{P}|b_{i+1}d_{i+1}\rangle \approx \frac{1}{a^n(2B)^{n-1}}\left(\delta_{b_{i+1}b_1}\delta_{d_{i+1}d_1} - \frac{1}{2B}\right) \; .$$

Unitarity of $\mathcal{B}$ implies $|\mathcal{B}_{bd,b'd'}| \approx \frac{1}{\sqrt{2B}}$ . Every unrestricted summation over directed bond space is of order (2 B).

In that way we show that all terms due to integration over massive modes vanish on average for $B \to \infty$ . But that captures only qualitative aspects of the problem.

Question: How big are the fluctuations?

# 9. Bounds

Strict upper bounds for matrix elements are

$$|W_{\mu\nu}| \leq \frac{1}{a}\ , \quad |W_{\mu\nu}| \leq W_{\mu\nu} + \frac{N}{B}.$$

Here $a$ is the size of the gap and $N$ is independent of $B$ for $B \to \infty$ . Take account of structure of matrix $\mathcal{B}$ . For completely connected graph

$$|\mathcal{B}_{\mu\nu}| \leq \frac{z}{(2B)^{1/4}}$$

where $z$ is independent of $B$ for sufficiently smooth boundary conditions at the vertices. Range of summation indices $(\mu, \nu)$ is $(2B)^{1/2}$ .

Cannot show that general term vanishes for $B \to \infty$ . Reason: In supertraces containing matrices $\mathcal{B}$ , fluctuations of matrix elements $W_{\mu\nu}$ about their mean values are too large.
Decomposition of variables $(Z, \tilde{Z})$ into universal mode and (weakly fluctuating) massive modes is questionable.

# 10. More Stringent Bounds

Focus attention on supertraces that contain matrices $\mathcal{B}$ and that cause the difficulty. Use Cauchy-Schwarz inequality

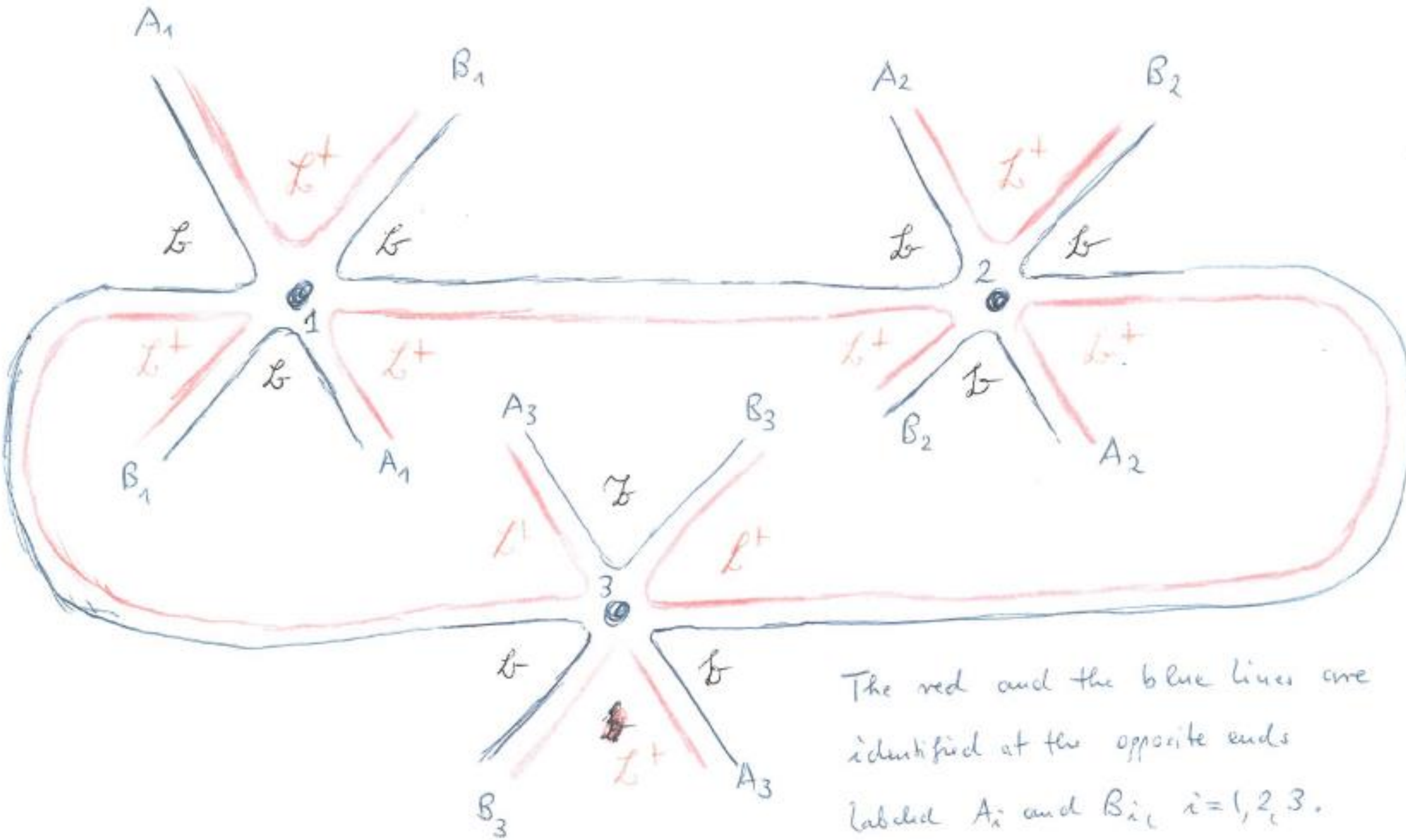
$$\left| \sum_l a_l b_l \right| \leq \left( \sum_l |a_l|^2 \right)^{1/2} \left( \sum_l |b_l|^2 \right)^{1/2}$$

The difficulty persists: Cannot show that some of the terms permitted by supersymmetry vanish for $B \to \infty$ . Example:

$$[\mathrm{STr}(\xi \mathcal{B} \tilde{\xi} \mathcal{B}^\dagger)^3]^n$$

Graphical representation for n = 3 on next slide. As n increases, upper bound approaches unity from below. Useless.

Cannot think of more stringent bounds.




The red and the blue lines are identified at the opposite ends labelled $A_i$ and $B_i$, $i=1,2,3$.

# 11. Discussion and Conclusions

Study of two-point function of chaotic connected simple quantum graphs.

Unitary symmetry, incommensurate bond lengths, spectrum of Frobenius-Perron operator has finite gap.

Phase average of generating function done using supersymmetry and color-flavor transformation.

Effective action defined in coset space. Separate universal mode and massive modes. Linearize the latter.

Expand effective action up to second order to generate Gaussian superintegrals over massive modes. Taylor-expand remaining terms.

Averages based on mean values show that every term in the series so generated vanishes for $B \to \infty$. But proof of universality requires strict upper bounds.

Bounds on matrix elements $W_{\mu\nu}$ fail to yield expected result.

Same difficulty using Cauchy-Schwarz inequality.

Possibly have failed to find sufficiently strict upper bounds.

But analysis of general term suggests that fluctuations of massive modes (measured in terms of fluctuations of matrix elements $W_{\mu\nu}$) are too large.

Hence our evidence suggests the following conclusion:
For the terms relevant for the perturbation expansion, the variables $(Z, \tilde{Z})$ do not cluster sufficiently closely together. It is not possible to introduce the universal mode and the massive modes in such a way that the latter possess sufficiently small fluctuations.

We do not believe that the BGS conjecture for quantum graphs can be proved perturbatively.