An approximation to δ' couplings on graphs

T. Cheon[a] and P. Exner[b,c]

a) Laboratory of Physics, Kochi University of Technology, Tosa Yamada, Kochi 782-8502, Japan
b) Department of Theoretical Physics, Nuclear Physics Institute, Academy of Sciences, 25068, Řež, Czech Republic
c) Doppler Institute, Czech Technical University, Břehová 7, 11519 Prague, Czech Republic
taksu.cheon@kochi-tex.ac.jp, exner@ujf.cas.cz

We discuss a general parametrization for vertices of quantum graphs and show, in particular, how the δ'_s and δ' coupling at an n edge vertex can be approximated by means of $n+1$ couplings of the δ type provided the latter are properly scaled.

Quantum graphs became in the last decade a useful and versatile tool to describe several classes of physical systems, in particular, various combinations of quantum wires. There are numerous papers devoted to the subject and we restrict ourselves to mentioning the bibliography given in [KS99, Ku04], where also basic concepts of theory are discussed.

The purpose of this letter is twofold. First of all we want to draw attention to useful parametrization of a general coupling at graph vertices whose advantages in the present context remained so far unnoticed. Second and more important, we address the question of physical meaning of such a coupling and suggest an answer illustrating it on a pair of simple nontrivial examples of the so-called δ'_s and δ' couplings [Ex95, Ex96a].

We consider a free spinless particle on a graph, with the Hamiltonian which acts as $H\psi_j = -\psi''_j$, where ψ_j denotes the wave function at the jth edge. Since early times it has been known that a vertex joining n graph edges can be characterized by n^2 real parameters [EŠ89] characterizing the boundary condition at the vertex. We use the symbol $\Psi(0)$ for the column vector of the boundary values at the vertex (identified conventionally with the origin of the coordinates), and analogously $\Psi'(0)$ for the vector of the derivatives, taken all in the outgoing direction.

The boundary conditions have to be chosen to make the Hamiltonian self-adjoint, or in physical terms, to ensure conservation of the probability current at the vertex. A general form of such a coupling was found in [KS99]. It is described by a pair of $n \times n$ matrices A, B such that $\mathrm{rank}\,(A,B) = n$ and AB^* is self-adjoint; the boundary values have to satisfy the conditions

$$A\Psi(0) + B\Psi'(0) = 0\,. \tag{1}$$

They have an advantage in comparison to earlier parameterizations relating $\Psi(0)$ and $\Psi'(0)$ by a single matrix, because the latter is typically singular for a subset of parameters, albeit a zero-measure one.

On the other hand, the matrix pair in (1) is non-unique; one would prefer to have a condition analogous to $\psi(0)\cos\theta + \psi'(0)\sin\theta = 0$ is case of a single edge end. Such conditions exist, they were obtained independently in [FT00, CFT01] for a generalized point interaction, $n = 2$, and in [Ha00] for any $n \geq 1$. It is easy to derive them: the self-adjointness requires vanishing of the boundary form, $\sum_{j=1}^n (\bar\psi_j \psi'_j - \bar\psi'_j \psi_j)(0) = 0$, which occurs iff the norms $\|\Psi(0) \pm i\ell\Psi'(0)\|_{\mathbb{C}^n}$ with a fixed nonzero ℓ coincide, so the two vectors must be related by an $n\times n$ unitary matrix. The length parameter is not important because matrices corresponding to two different values are related by

$$U' = \frac{(\ell+\ell')U + \ell - \ell'}{(\ell-\ell')U + \ell + \ell'}\,. \tag{2}$$

Thus we set $\ell = 1$, which means a choice of the length scale, and put

$$A = U - I\,, \quad B = i(U+I)\,; \tag{3}$$

the edges are obviously fully decoupled at the vertex iff U is diagonal. It is easy to check that any such pair satisfies the above quoted requirements from [KS99]. Conversely, to any A, B with these properties there is a $U \in U(n)$ and an invertible C such that $U = C(A+iB)$. Indeed, such a U must satisfy $UU^* = C(BB^* + AA^*)C^*$ since $AB^* = BA^*$ by assumption. The matrix $BB^* + AA^*$ is strictly positive because its null space is

$$\ker A^* \cap \ker B^* = (\mathrm{ran}\, A)^\perp \cap (\mathrm{ran}\, B)^\perp = (\mathrm{ran}\, A \cup\, \mathrm{ran}\, B)^\perp = \{0\}\,. \tag{4}$$

In particular, it is Hermitean so $C := (BB^* + AA^*)^{-1/2}$ makes sense, it is Hermitean and invertible.

The parametrization (3) simplifies various previous results. For instance, the eigenspace of U with eigenvalue -1 gives the projection $P = P_1$ in [Ku04] which makes Lemma 4 and the following claims of this paper rather transparent. Likewise, the on-shell scattering matrix for a star graph of n halflines with the considered coupling equals

$$S_U(k) = \frac{(k-1)I + (k+1)U}{(k+1)I + (k-1)U}\,, \tag{5}$$

which makes a discussion of its properties simpler than in Sec. 2 of [KS99].

To give an example of the parametrization (3), denote by $\mathcal{J}$ the $n \times n$ matrix whose all entries are equal to one. It is a straightforward exercise to check that $U = \frac{2}{n+i\alpha}\mathcal{J} - I$ describes the standard δ *coupling*,

$$\psi_j(0) = \psi_k(0) =: \psi(0)\,,\ j,k = 1,\dots,n\,, \quad \sum_{j=1}^n \psi_j'(0) = \alpha\psi(0) \tag{6}$$

with $\alpha \in \mathbb{R}$; the case $\alpha = 0$ corresponds to the "free motion" at the vertex, so-called Kirchhoff boundary conditions, while $\alpha = \infty$ gives $U = -I$, the full Dirichlet decoupling. In a similar way, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the singular counterpart, so-called δ_s' *coupling* [Ex95, Ex96a],

$$\psi_j'(0) = \psi_k'(0) =: \psi'(0)\,,\ j,k = 1,\dots,n\,, \quad \sum_{j=1}^n \psi_j(0) = \beta\psi'(0) \tag{7}$$

with $\beta \in \mathbb{R}$; for $\beta = \infty$ we get $U = I$, the full Neumann decoupling.

Let us mention another "dual" pair of vertex couplings in which the wave functions exhibit permutation symmetry. The more regular one of these is the "permuted" δ, or δ_p *coupling*, given by the boundary conditions

$$\sum_{j=1}^n \psi_j(0) = 0\,, \quad \psi_j'(0) - \psi_k'(0) = \frac{\alpha}{n}(\psi_j(0) - \psi_k(0))\,,\ j,k = 1,\dots,n\,, \tag{8}$$

with $\alpha \in \mathbb{R}$. It generalizes the δ_s interaction of [TFC01] and one can check easily that the corresponding matrix equals $U = \frac{n-i\alpha}{n+i\alpha}I - \frac{2}{n+i\alpha}\mathcal{J}$. Its counterpart is the so-called δ' *coupling* [Ex95, Ex96a],

$$\sum_{j=1}^n \psi_j'(0) = 0\,, \quad \psi_j(0) - \psi_k(0) = \frac{\beta}{n}(\psi_j'(0) - \psi_k'(0))\,,\ j,k = 1,\dots,n\,, \tag{9}$$

with $\beta \in \mathbb{R}$, which corresponds to $U = -\frac{n+i\beta}{n-i\beta} I + \frac{2}{n-i\beta} \mathcal{J}$. The infinite values of the parameters refer again to the Dirichlet and Neumann decoupling of the graph edges, respectively.

Note that in these four examples, the connection condition at the origin is totally symmetric with respect to the interchange of edge indices. Consequently, their U are constructed from symmetric matrices I and $\mathcal{J}$.

If one wants to continue analysis of such graphs, the first question to be answered is about the physical meaning and possible use of the whole family of such general couplings. What concerns the second part, a recent inspiration comes from the domain of quantum computing, where the generalized point interactions parameterized by elements of the group $U(2)$ have been proposed as an alternative realization of a qubit [CFT04]; an extension to higher degree vertices opens, of course, interesting possibilities. To make use of them, however, one has to understand whether there is a meaningful way to "construct" vertices with different couplings.

The currently available results suggest that this goal cannot be achieved in a purely geometrical way, by squeezing a system of branching tubes with the same topology as the graph. Several such approximations was analyzed recently [KZ01, RS01, Sa01, EP03]; they all lead either to trivial (Kirchhoff) boundary conditions, or to graphs having an extended state Hilbert space with extra dimensions due to the vertices. Their common feature was that the transverse ground state was a constant function. Hence a nontrivial results might be obtained through tubes with Dirichlet boundaries, but this problem is open for a long time and notoriously difficult.

Approximations using potentials scaled in the usual way, i.e. preserving their integrals, do yield nontrivial results [Ex96b] but only for couplings with wave functions continuous at the junction, which is just the family (6). This is not sufficient and more singular coupling need other means. Our main aim here is to explore a natural alternative with approximating interactions scaled in a *nonlinear* way as a generalization of the procedure proposed in [CS98a, CS98b] and analyzed from the viewpoint of the convergence topology in [AN00, ENZ01]. To keep things simple we will analyze here the δ'_s and δ' couplings leaving the general case to a subsequent paper.

Consider first the Hamiltonian H_β on the graph Γ consisting on n halflines coupled at a single vertex by the conditions (7). Consider further the same graph with additional vertices of degree two at each arm, all at the same distance $a > 0$ from the common junction. The approximating family will be constructed as follows. The operators act, of course, as $\psi_j \mapsto -\psi''_j$ at each arm; the wave functions satisfy the δ *conditions* (6) at the central vertex with a coupling parameter $\alpha = b$, to be specified later, and another δ *coupling* (6), this time with the parameter c, at each of the additional vertices. We call such an operator $H^{b,c}(a)$.

The crucial feature that allows us to simplify the treatment in the present situation is a symmetry. Each of the Hamiltonians H_β and $H^{b,c}(a)$ decomposes into a nontrivial part which acts on the one-dimensional subspace of $\mathcal{H} = \bigoplus_{j=1}^n L^2(\mathbb{R}_+)$ consisting of functions symmetric with respect to permutations, $\psi_j(x) = \psi_k(x)$ for all j,k, and the $(n-1)$-dimensional part corresponding to Dirichlet and Neumann condition at the central vertex for the δ and δ'_s coupling, respectively. Notice that the matrices U corresponding to these coupling have each one simple eigenvalue and another one equal to ∓ 1, respectively, of multiplicity $n-1$.

To see what the choice of the effective coupling constants b, c should be, let us first modify to our problem the argument of [CS98a]. As we have said, in the nontrivial sector all the functions are the same, so we may drop the arm index. The boundary values at $x = 0$ and $x = a$ are related by

$$\psi(a) = \psi(0) + a\psi'(0) + \mathcal{O}(a^2)\,, \quad \psi'(a-) = \psi'(0+) + \mathcal{O}(a)\,, \tag{10}$$

$$\psi'(a+) = \psi'(a-) + c\psi(a)\,, \quad \psi'(0+) = b\psi(0)\,. \tag{11}$$

Eliminating $\psi(0)$ and $\psi'(0+)$ from here, we get in the leading order the relation $B(a)\psi(a) = \psi'(a+)$, where

$$B(a) := c + \frac{b}{1+ab}\,; \tag{12}$$

hence the needed limit, $\beta\psi'(0+) = n\psi(0)$, is achieved as $a \to 0+$ if we choose

$$b(a) := -\frac{\beta}{na^2}\,, \quad c(a) := -\frac{1}{a}\,. \tag{13}$$

In the orthogonal complement to the permutation-symmetric subspace one we can again drop the index, because the operators act in the same way on all the linear combinations of $\sum_{j=1}^n d_j\psi_j(x)$ which we can choose as the basis here, i.e. those satisfying $\sum_{j=1}^n d_j = 0$. The second one of the conditions (11) is now replaced by $\psi(0) = 0$. Eliminating then the boundary values at $x = 0$ we get in the leading order the relation $\psi'(a+) = (c + a^{-1})\psi(a) + \mathcal{O}(a)$. The right-hand side vanishes with the parameter choice (13), giving Neumann condition, $\psi'(0+) = 0$, in the limit.

Now we can state and prove our main result.

Theorem 1 *$H^{b,c}(a) \to H_\beta$ as $a \to 0+$ in the norm-resolvent sense provided the coupling constants b, c are chosen in correspondence with (13).*

Proof: By the same symmetry argument as above we can again reduce the problem to investigation of a pair of halfline problems. Let us start with the one having Dirichlet condition at the origin, so the free Green's function at energy k^2 is

$$G_k(x,y) = \frac{\sin kx_<}{k}\, \mathrm{e}^{ikx_>}\,, \tag{14}$$

where as usual $x_<$ is the smaller one of the values x, y and vice versa. The Green's function of the operator with the δ interaction at $x = a$ is obtained easily by Krein's formula [AGHH, Appendix A]

$$G_k^c(x,y) = G_k(x,y) + \frac{G_k(x,a)G_k(a,y)}{-c^{-1} - G_k(a,a)}\,. \tag{15}$$

On the other hand, the Green's function referring to Neumann boundary is

$$G_k^N(x,y) = \frac{\cos kx_<}{k}\, \mathrm{e}^{ikx_>}\,; \tag{16}$$

our aim is to show that the last two converge to each other for some $k^2 \in \mathbb{C}$. It is convenient to choose $k = i\kappa$ with $\kappa > 0$; we will see below that the denominator of the last term at the right-hand side of (15) is then nonzero for a small enough. Since the functions involved are uniformly bounded around zero, it is sufficient to compute the difference in the case when neither of the arguments is smaller than a. For the sake of definiteness suppose that $a \le x \le y$; then (15) and (16) give

$$G_{i\kappa}^c(x,y) - G_{i\kappa}^N(x,y) = \frac{\mathrm{e}^{-\kappa x}\mathrm{e}^{-\kappa y}}{\kappa} \left[-1 + \frac{\sinh^2 \kappa a}{-\kappa c^{-1} - \mathrm{e}^{-\kappa x} \sinh^2 \kappa a} \right]. \tag{17}$$

If $c = -a^{-1}$ the last term behaves as $1 + \mathcal{O}(a)$ for $a \to 0+$, so

$$\lim_{a \to 0+} G_{i\kappa}^c(x,y) = G_{i\kappa}^N(x,y) \tag{18}$$

holds for all $x, y > 0$.

Consider next the case with the δ coupling at the origin using the same parameter values, namely $k = i\kappa$ and $a \le x \le y$. We are interested in the following two Green's functions,

$$G^b_{i\kappa}(x,y) = \frac{\mathrm{e}^{-\kappa y}}{\kappa(b+\kappa)}\,(b\sinh\kappa x + \kappa\cosh\kappa x)\,, \tag{19}$$

$$G^\beta_{i\kappa}(x,y) = \frac{\mathrm{e}^{-\kappa y}}{\kappa(n+\beta\kappa)}\,(n\sinh\kappa x + \beta\kappa\cosh\kappa x)\,, \tag{20}$$

which replace (14) and (16), respectively, in the present case. The first of them determines the full approximating Green's function by Krein's formula,

$$G^{b,c}_k(x,y) = G^b_k(x,y) + \frac{G^b_k(x,a)G^b_k(a,y}{-c^{-1} - G^b_k(a,a)}\,. \tag{21}$$

Using the relations (13) we express the difference

$$G^{b,c}_{i\kappa}(x,y) - G^\beta_{i\kappa}(x,y) = \frac{\mathrm{e}^{-\kappa y}}{\kappa}\left[\frac{b\sinh\kappa x + \kappa\cosh\kappa x}{b+\kappa}\right.$$
$$\left. + \frac{\frac{\mathrm{e}^{-\kappa x}}{(b+\kappa)^2}(b\sinh\kappa x + \kappa\cosh\kappa x)^2}{\kappa a - \frac{\mathrm{e}^{-\kappa a}}{b+\kappa}(b\sinh\kappa x + \kappa\cosh\kappa x)} - \frac{n\sinh\kappa x + \beta\kappa\cosh\kappa x}{n+\beta\kappa}\right] \tag{22}$$

The first term in the bracket tends to $\sinh\kappa x$ as $a \to 0+$, while the third one is independent of a, so their sum in the limit gives

$$-\frac{\beta\kappa\,\mathrm{e}^{-\kappa x}}{n+\beta\kappa}\,. \tag{23}$$

Next we take the middle term without the factor $\mathrm{e}^{-\kappa x}$ and expand the numerator and denominator to the second power in a; this gives its limit which differs just by the sign from (23), in other words

$$\lim_{a\to 0+} G^{b,c}_{i\kappa}(x,y) = G^\beta_{i\kappa}(x,y) \tag{24}$$

holds again for all $x, y > 0$. To conclude the proof we have just to realize that as functions of x, y the differences (17) and (22) decay exponentially, so the corresponding resolvent differences converge to zero even in the Hilbert-Schmidt norm. □

Let us add that the proven result opens way to approximation of H_β by Hamiltonians with more regular interactions. We have mentioned that the central δ in $H^{b,c}(a)$ can be approximated by a family of potentials scaled in the usual way, the same is true for the δ interactions at the points $x_j = a$. As in the related problem discussed in [ENZ01], the question then is how fast have these approximating potentials to shrink with respect to a.

Consider finally the case of δ' *coupling*, i.e. the Hamiltonian $\tilde{H}_\beta$ on our star graph with the boundary conditions (9) at the vertex. The approximating family will be constructed in a similar way as above; the difference is that now the wave functions will satisfy the δ_p *conditions* (8) at the central vertex with a coupling parameter $\alpha = b$, to be specified. The rest is the same, there is another δ *coupling* (6) with the parameter called again c at each of the additional vertices; we denote such an operator $\tilde{H}^{b,c}(a)$.

To realize that this problem can be again reduced to a one-dimensional analysis, denote $\varepsilon := \mathrm{e}^{2\pi i/n}$ and introduce

$$\mathcal{G}_r := \left\{ (\psi(x), \varepsilon^r \psi(x), \dots, \varepsilon^{r(n-1)}\psi(x)) \,:\, \psi \in L^2(\mathbb{R}_+) \right\} . \tag{25}$$

The graph state Hilbert space can be written as $\mathcal{H} = \bigoplus_{r=0}^{n-1} \mathcal{G}_r$. Indeed, any vector of $\mathcal{H}$ is a unique linear combination of the vectors from $\mathcal{G}_r$, because the determinant of the corresponding linear system is the Vandermond determinant of $1, \varepsilon, \dots, \varepsilon^{n-1}$, which is nonzero because the latter are mutually different. It is straightforward to see that the subspaces $\mathcal{G}_r$ are invariant under the Hamiltonians in question; the δ_p and δ' couplings acts "trivially" at the origin corresponding to Dirichlet and Neumann condition, respectively, while on each of the subspaces $\mathcal{G}_r$, $r = 1, \dots, n$, these boundary conditions are replaced by $\psi'(0) = \frac{\alpha}{n}\psi(0)$ and $\psi(0) = \frac{\beta}{n}\psi'(0)$. Thus we can choose

$$b(a) := -\frac{\beta}{a^2}\,, \quad c(a) := -\frac{1}{a}\,, \tag{26}$$

and repeat the above considerations, arriving at the following conclusion.

Theorem 2 *$\tilde{H}^{b,c}(a) \to \tilde{H}_\beta$ holds in the norm-resolvent sense as $a \to 0+$ if the coupling constant families b, c are given by (26).*

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