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# Discrete Schrödinger equation on graphs: An effective model for branched quantum lattice

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**Abstract** – We propose an approach to quantize discrete networks (graphs with discrete edges). We introduce a new exact solution of the discrete Schrödinger equation that is used to write the solution for quantum graphs. The formulation of the problem and derivation of secular equation for arbitrary quantum graphs is presented. The application of the approach for the star graph is demonstrated by obtaining eigenfunctions and eigenvalues explicitely. The practical application of the model in conducting polymers and branched molecular chains is discussed.



**Introduction.** – Modeling of quantum particle motion in low-dimensional branched structures is of importance for many practical applications, especially for the designing and optimization of functional properties of quantum materials. A powerful tool for such purpose is to use quantum graph theory. The advantage of quantum graphs in modeling quantum transport in low-dimensional branched structures and networks comes from the fact that the description can be effectively reduced to a one-dimensional Schrödinger (Dirac) equation on metric graphs. In most of the cases, quantum-graphs–based approach allows one to obtain an exact solution to the problem for arbitrary graph topologies.

Quantum graphs are determined as the branched quantum wires, which are connected to each other at the nodes (vertices) according to a certain rule called the topology of a graph. Initially, the quantum graphs were introduced for modeling of electron motion in low-dimensional molecular structures in the quantum chemistry of organic molecules. In particular, refs. [1–3], where the electron motion in branched aromatic molecules was studied, can be considered as a pioneering attempt. However, the strict formulation of the quantum graph concept, where the latter was defined as branched quantum wire, has been presented a few decades later by Exner and Seba in [4]. The next step in the systematic study was done by Kostrykin and Schrader, who proposed general vertex boundary conditions ensuring self-adjointness of the Schrödinger operator on graphs [5]. Later the quantum graph concept was used in different contexts (see refs. [6–9]) and an experimental realization in microwave networks was done [8]. For an overview of different mathematical aspects of the quantum graph theory, we refer to the books [7,10,11]. Some physically important problems of the quantum graphs theory are studied in refs. [12–20]. Different issues of evolution and spectral equations on fractal and discrete systems, including graphs, are considered in [21–29].

In this paper, we consider a version of a quantum graph with discrete edges, *i.e.*, each branch represents a discrete chain of finite length. Such a system models branched lattices, where particle motion occurs in the quantum regime.

Using the solution of the discrete Schrödinger equation on a finite 1D lattice, we construct a solution of the problem for the discrete quantum graph, which satisfies vertex boundary conditions. Finally, the eigenvalues are determined in terms of a secular equation.

**Exact solution and spectrum of the discrete Schrödinger equation on a finite chain.** – The discrete Schrödinger equation has attracted attention in the context of mathematical physics, exactly solvable models and spectral theory [30–33]. The one-dimensional

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time-independent Schrödinger equation for a free particle is written as

$$\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} + k^2\Psi(x) = 0, \tag{1}$$

on the infinite line $x \in (-\infty, +\infty)$, where $\hbar = 2m = 1$ and $\Psi(x)$ is the wave function. The discrete version of the Schrödinger equation can be obtained by using the standard finite-difference scheme with the step size $a > 0$ for the second-order derivative as

$$\frac{1}{a^2}\left[\Psi^{(a)}(x_n^{(a)} - a) - 2\Psi^{(a)}(x_n^{(a)}) + \Psi^{(a)}(x_n^{(a)} + a)\right] + k^2\Psi^{(a)}(x_n^{(a)}) = 0, \tag{2}$$

where $x_n^{(a)} = na$ and $n$ is an integer number.

Here we propose an exact solution of eq. (2) which can be written as

$$\Psi^{(a)}(x_n^{(a)}) = Ag_+(a)^{x_n^{(a)}/a} + Bg_-(a)^{x_n^{(a)}/a}, \tag{3}$$

where $A$ and $B$ are constants and

$$g_\pm(a) = 1 + \frac{-k^2a^2 \pm ka\sqrt{k^2a^2 - 4}}{2}.$$

The consistency of this solution with the solution of the continuous case can be shown by considering its limit for $a \to 0$ for a fixed point $x_n^{(a)}$. For brevity we set

$$z_\pm := \frac{-k^2a^2 \pm ka\sqrt{k^2a^2 - 4}}{2} \quad \text{and} \quad \alpha := x_n^{(a)}.$$

As $z_\pm$ tends to zero for $a \to 0$, we obtain

$$\begin{aligned}\lim_{a\to 0}\left(g_\pm(a)\right)^{\alpha/a} &= \lim_{a\to 0}\left(1 + z_\pm\right)^{\alpha/a} \\ &= \lim_{a\to 0}\left[\left(1 + z_\pm\right)^{1/z_\pm}\right]^{\alpha z_\pm/a} \\ &= \exp\left(\lim_{a\to 0}\alpha z_\pm/a\right) = e^{\pm ik\alpha}.\end{aligned} \tag{4}$$

One can easily show that

$$\begin{aligned}\lim_{a\to 0}\Psi^{(a)}(\alpha) &= \lim_{a\to 0}\left(A[g_+(a)]^{\alpha/a} + B[g_-(a)]^{\alpha/a}\right) \\ &= Ae^{ik\alpha} + Be^{-ik\alpha}.\end{aligned} \tag{5}$$

A graphical representation of the convergence of the solution (3) to the solution of the continuous case with a decrease of the step size $a$ is shown in fig. 1.

Now let us consider the problem on the finite discrete interval $[0, L]$ with step size $a = L/N$ for some $N \in \mathbb{N}$ and $x_n^{(a)} = na$ for $n = 0, \ldots, N$. Imposing the Dirichlet boundary condition as

$$\Psi^{(a)}(0) = 0, \quad \Psi^{(a)}(Na) = 0 \tag{6}$$

leads to the following homogeneous system of linear equations for $A$ and $B$:

$$\begin{aligned}&A + B = 0, \\ &Ag_+(a)^N + Bg_-(a)^N = 0.\end{aligned} \tag{7}$$

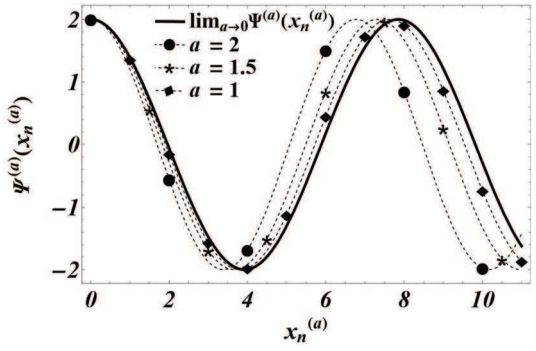


Fig. 1: Analytic solution of the discrete Schrödinger equation in eq. (3) for different values of the step size $a$ and limit of the solution in eq. (5) for parameters $k = 0.8$, $A = B = 1$.

The existence of non-trivial solutions of the above algebraic system leads to the following secular equation with respect to $k$:

$$g_+(a)^N = g_-(a)^N. \tag{8}$$

First, we consider the case $k^2a^2 > 4$ and $k > 0$. Then

$$g_+(a) - g_-(a) = 2ka\sqrt{k^2a^2 - 4} > 0$$

and $g_+(a) > g_-(a)$ follows. Hence (8) does not hold. A similar arguments shows the same for the case $k^2a^2 > 4$ and $k < 0$.

It remains to consider the case $k^2a^2 \le 4$. Then

$$g_\pm(a) = 1 + \frac{-k^2a^2 \pm ika\sqrt{4 - k^2a^2}}{2}. \tag{9}$$

We write $g_\pm(a)$ as

$$g_\pm(a) = |g_\pm(a)|e^{i\varphi_\pm(a)}, \tag{10}$$

and we have

$$\begin{aligned}\mathrm{Re}(g_\pm(a)) &= 1 - \frac{k^2a^2}{2}, \\ \mathrm{Im}(g_\pm(a)) &= \pm\frac{1}{2}ka\sqrt{4 - k^2a^2}.\end{aligned}$$

As $|g_\pm(a)| = 1$, we obtain

$$\begin{aligned}\varphi_+(a) &= \begin{cases}\arccos\left(1 - k^2a^2/2\right), & \text{if } k > 0, \\ 2\pi - \arccos\left(1 - k^2a^2/2\right), & \text{if } k < 0,\end{cases} \\ \varphi_-(a) &= \begin{cases}2\pi - \arccos\left(1 - k^2a^2/2\right), & \text{if } k > 0, \\ \arccos\left(1 - k^2a^2/2\right), & \text{if } k < 0.\end{cases}\end{aligned} \tag{11}$$

By substitution of these equations into the secular equation (8) we see that $N\varphi_+(a) - N\varphi_-(a)$ equals a multiple of $2\pi$, which gives by (11)

$$\arccos\left(1 - k^2a^2/2\right) = \frac{\pi m}{N},$$

where $m$ is an integer. Hence for every integer $m$ we obtain a solution $k_m$,

$$k_m = \pm\frac{1}{a}\sqrt{2 - 2\cos\left(\frac{\pi m}{N}\right)}. \tag{12}$$

Table 1: The first five nonzero eigenvalues $k$ for Dirichlet (left) and Neumann (right) boundary condition compared with the continuous case.

| Continuous case | $a = 0.1$ $N = 10$ | $a = 0.01$ $N = 100$ | $a = 0.002$ $N = 500$ |
|---|---|---|---|
| $\pi$ | 3.1286893 | 3.1414634 | 3.1415874 |
| $2\pi$ | 6.1803398 | 6.2821518 | 6.2831439 |
| $3\pi$ | 9.0798099 | 9.4212901 | 9.4246384 |
| $4\pi$ | 11.7557050 | 12.5581039 | 12.5660398 |
| $5\pi$ | 14.1421356 | 15.6918191 | 15.7073173 |

| Continuous case | $a = 0.1$ $N = 10$ | $a = 0.01$ $N = 100$ | $a = 0.002$ $N = 500$ |
|---|---|---|---|
| $\pi$ | 3.4729635 | 3.1731927 | 3.1478832 |
| $2\pi$ | 6.8404028 | 6.3455866 | 6.2957352 |
| $3\pi$ | 9.9999999 | 9.5163831 | 9.4435249 |
| $4\pi$ | 12.8557521 | 12.6847839 | 12.5912209 |
| $5\pi$ | 15.3208888 | 15.8499913 | 15.7387923 |

That is, eq. (2) equipped with Dirichlet boundary conditions has solutions only if $k \in \{k_m : m \in \mathbb{Z}\}$. Obviously, the $k_m$ depend also on the step size $a$. If the step size $a$ tends to zero, then $k_m$ converges to the eigenvalues of the continuous case on the interval $[0, L]$, as the following calculation shows:

$$\begin{aligned}\lim_{a\to 0} k_m &= \pm\sqrt{\lim_{a\to 0}\frac{2-2\cos\left(\frac{\pi m a}{L}\right)}{a^2}} \\ &= \pm\frac{\pi m}{L}\sqrt{\lim_{a\to 0}\frac{\sin\left(\frac{\pi m a}{L}\right)}{\frac{\pi m a}{L}}} = \pm\frac{\pi m}{L}.\end{aligned} \tag{13}$$

Analogously one can impose Neumann boundary condition as

$$\Psi^{(a)}(a) - \Psi^{(a)}(0) = 0, \quad \Psi^{(a)}(Na) - \Psi^{(a)}(Na - a) = 0, \tag{14}$$

which leads to the following homogeneous system of linear equations:

$$\begin{aligned}&A(g_+(a) - 1) + B(g_-(a) - 1) = 0,\\ &A(g_+(a)^N - g_+(a)^{N-1})\\ &+B(g_-(a)^N - g_-(a)^{N-1}) = 0.\end{aligned} \tag{15}$$

The secular equation in this case is written as

$$\det\begin{pmatrix} g_+(a) - 1 & g_-(a) - 1 \\ g_+(a)^N - g_+(a)^{N-1} & g_-(a)^N - g_-(a)^{N-1}\end{pmatrix} = 0. \tag{16}$$

Substitution of the above definition of $g_\pm(a)$ to the determinant equation (16) yields the following expression:

$$\begin{aligned}&(e^{i\varphi_+(a)} - 1)(e^{i\varphi_-(a)} - 1)(e^{i\varphi_+(a)(N-1)}\\ &- e^{i\varphi_-(a)(N-1)}) = 0,\end{aligned}$$

or

$$\varphi_\pm(a) = 2\pi p, \quad \varphi_+(a) - \varphi_-(a) = \frac{2\pi m}{N-1},$$

where $p$ and $m$ are integer numbers. Using the expression of $\varphi_\pm(a)$, one can derive the eigenvalues as

$$k_m = \pm\frac{1}{a}\sqrt{2 - 2\cos\left(\frac{\pi m}{N-1}\right)}. \tag{17}$$

Similarly, it is easy to show that the convergence of the eigenvalues to the continuous case as shown for the Dirichlet boundary condition is

$$\lim_{a\to 0} k_m = \pm\frac{\pi m}{L}. \tag{18}$$

We collect the first five nonzero eigenvalues of continuous Schrödinger equation (1) with Dirichlet and Neumann boundary conditions defined on the interval $[0, 1]$ which are given by $k_m = \pi m$, $m = 1, \ldots, 5$ and compare them in table 1 with the first five nonzero eigenvalues of the discrete Schrödinger equation (2) with Dirichlet (6) and Neumann (14) boundary conditions on the interval $[0, 1]$, respectively, for different values of step size $a$.

**Basic theory of quantum graphs.** – In this section, we will briefly recall the introduction of the quantum graphs and their spectrum by following ref. [6]. A graph consists of $V$ vertices, where $V$ is a natural number, and it is connected by $E$ edges, $E \in \mathbb{N}$. If vertices $i$ and $j$ are connected we call it the $(i, j)$ edge. Here we always assume that at most one edge connects the same two vertices and moreover, that there are no loops, *i.e.*, there is no edge of the form $(i, i)$.

The topology of graph is defined by its $V \times V$ adjacency matrix as

$$C_{i,j} = C_{j,i} = \begin{cases}1, & \text{if } i \text{ and } j \text{ are connected,}\\ 0, & \text{otherwise,}\end{cases} \tag{19}$$

where $i, j = 1, 2, 3, \ldots, V$. The number of edges can be found in terms of the adjacency matrix by $E = \frac{1}{2}\sum_{i,j=1}^{V} C_{i,j}$.

The coordinate $x_{i,j}$ on the edge $(i, j)$ is assigned as $[0, L_{i,j}]$ for all $C_{i,j} = 1$ and $i < j$, where $L_{i,j}$ is the length of the edge $(i, j)$. The wave function $\Psi$ is a vector function with $E$ components, where each component is defined as $\Psi_{i,j}(x_{i,j})$ for $C_{i,j} = 1$. The Schrödinger equation on each edge of the graph is written as (in units $\hbar = 2\,\mathrm{m} = 1$)

$$\frac{\mathrm{d}^2\Psi_{i,j}(x_{i,j})}{\mathrm{d}x^2} + k^2\Psi_{i,j}(x_{i,j}) = 0. \tag{20}$$

As usual, the Schrödinger operator $H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ on the graph is defined componentwise on each edge of

the graph

$$\Psi_{i,j}(x_{i,j}) \mapsto -\frac{\mathrm{d}^2\Psi_{i,j}(x_{i,j})}{\mathrm{d}x^2}.$$

Usually, one associates boundary conditions to the operator $H$. Without any boundary conditions, the Schrödinger operator $H$ satisfies

$$\langle H\Psi, \Phi\rangle - \langle \Psi, H\Phi\rangle = \sum_{\substack{i,j=1\\ i<j}}^{V} C_{i,j}\left[\Psi_{i,j}(x_{i,j})\frac{\mathrm{d}\Phi^*_{i,j}(x_{i,j})}{\mathrm{d}x} - \Phi^*_{i,j}(x_{i,j})\frac{\mathrm{d}\Psi_{i,j}(x_{i,j})}{\mathrm{d}x}\right]\Bigg|_{x_{i,j}=0}^{x_{i,j}=L_{i,j}}. \quad (21)$$

Obviously, whenever the Schrödinger operator $H$ is self-adjoint, the expression in (21) is zero. *E.g.*, this is the case when the functions from the domain satisfy continuity on the graph. That is, for each vertex there exists a complex number $\phi_i$, $i \in \{1, \ldots, V\}$, such that

$$\Psi_{i,j}(x_{i,j})\big|_{x_{i,j}=0} = \phi_i, \quad \Psi_{i,j}(x_{i,j})\big|_{x_{i,j}=L_{i,j}} = \phi_j, \quad (22)$$

for $i, j$ such that $C_{i,j} = 1$, $i < j$, and some current conservation rule [6],

$$-\sum_{j<i} C_{i,j}\frac{\mathrm{d}\Psi_{j,i}(x_{j,i})}{\mathrm{d}x}\bigg|_{x_{j,i}=L_{j,i}} + \sum_{j>i} C_{i,j}\frac{\mathrm{d}\Psi_{i,j}(x_{i,j})}{\mathrm{d}x}\bigg|_{x_{i,j}=0} = \lambda_i\phi_i, \quad (23)$$

for some real parameters $\lambda_i$ for $i$ in $\{1, \ldots, V\}$. Note that the case $\lambda_i = 0$ for all $i$ in $\{1, \ldots, V\}$ is called Kirchhoff rule.

The solution of the Schrödinger equation on the graph in (20) can be written as

$$\Psi_{i,j}(x_{i,j}) = C_{i,j}\left[A_{i,j}\sin[k(L_{i,j} - x_{i,j})] + B_{i,j}\sin(kx_{i,j})\right], \quad (24)$$

for all $i < j$. Substituting the solution (24) into the vertex boundary conditions (22) and (23) leads to the secular equations as

$$\begin{aligned} C_{i,j}A_{i,j}\sin(kL_{i,j}) &= C_{i,j}\phi_i,\\ C_{i,j}B_{i,j}\sin(kL_{i,j}) &= C_{i,j}\phi_j, \end{aligned} \quad (25)$$

for $i, j$ such that $C_{i,j} = 1$ and $i < j$, and

$$\sum_{j<i} C_{i,j}k\left[A_{j,i} - B_{j,i}\cos(kL_{j,i})\right] + \sum_{j>i} C_{i,j}k\left[-A_{i,j}\cos(kL_{i,j}) + B_{i,j}\right] = \lambda_i\phi_i, \quad (26)$$

for all $i$ in $\{1, \ldots, V\}$.

This is a system of linear homogeneous equations for the unknowns $A_{i,j}$, $B_{i,j}$ and $\phi_i$ and has a non-trivial solution only when

$$\det(M(k)) = 0, \quad (27)$$

where $M(k)$ is a matrix where all the coefficients of the linear equations (25) and (26) are collected. It depends on the eigenvalue parameter $k$ and its size is

$$(2E + V) \times (2E + V).$$

**Branched lattices.** –

*Arbitrary branching topology.* Adhering to the formulation of the quantum graph problem proposed in [6], in this subsection, we present a prescription for solving the problem for discrete quantum graphs.

The discrete graph is a set of $V$ vertices connected by $E$ discrete edges. We denote the edge which connects the vertices $i$ and $j$ as $(i, j)$ for $i < j$.

For $(i, j)$ such that $C_{i,j} = 1$ (*i.e.*, vertex $i$ and vertex $j$ are connected) we assign discrete coordinates of the edge $x_0^{(a_{i,j})}, \ldots, x_{N_{i,j}}^{(a_{i,j})}$, which has step size $a_{i,j}$. Here $x_0^{(a_{i,j})} = 0$ and $x_{N_{i,j}}^{a_{i,j}}$ is the right endpoint. In other words, each edge of the graph is an interval with discrete points starting at zero and ending at $x_{N_{i,j}}^{(a_{i,j})} = L_{i,j} = N_{i,j}a_{i,j}$.

The wave function $\Psi$ is a vector with $E$ components and each of its components is a vector in $\mathbb{C}^{N_{i,j}+1}$ defined on each edge $(i, j)$ as

$$\left(\Psi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})})\right)_{n_{i,j}=0}^{N_{i,j}},$$

with $C_{i,j} = 1$, where $i < j$.

The discrete Schrödinger equation on each edge is given by

$$\frac{1}{a_{i,j}^2}[\Psi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})} - a_{i,j}) - 2\Psi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})}) + \Psi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})} + a_{i,j})] + k^2\Psi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})}) = 0, \quad (28)$$

where $1 \le n_{i.j} \le N_{i,j} - 1$ and $C_{i,j} = 1$, $i < j$.

We use the standard Euclidean inner product on the discrete graph

$$\langle \Psi, \Phi\rangle = \sum_{\substack{i,j=1\\ i<j}}^{V}\sum_{n_{i,j}=0}^{N_{i,j}} C_{i,j}\Psi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})})\Phi_{i,j}^{(a_{i,j})*}(x_{n_{i,j}}^{(a_{i,j})}). \quad (29)$$

where elements of $E$ component wave function vector $\Phi$ on the discrete graph are defined as

$$\left(\Phi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})})\right)_{n_{i,j}=0}^{N_{i,j}},$$

for $(i, j)$ such that $C_{i,j} = 1$, where $i < j$.

As usual, the discrete Schrödinger operator $H_d$ on the graph corresponds to the negative second discrete derivative. It is defined componentwise on each edge of the graph via

$$\Psi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})}) \mapsto -\frac{1}{a_{i,j}^2}[\Psi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})} - a_{i,j}) - 2\Psi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})}) + \Psi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})} + a_{i,j})].$$

It satisfies

$$\langle H_d\Psi,\Phi\rangle-\langle\Psi,H_d\Phi\rangle=\sum_{\substack{i,j=1\\ i<j}}^{V}C_{i,j}[\Psi_{i,j}^{(a_{i,j})}(0)\Phi_{i,j}^{(a_{i,j})*}(a_{i,j})$$
$$-\Psi_{i,j}^{(a_{i,j})}(a_{i,j})\Phi_{i,j}^{(a_{i,j})*}(0)$$
$$+\Psi_{i,j}^{(a_{i,j})}(L_{i,j})\Phi_{i,j}^{(a_{i,j})*}(L_{i,j}-a_{i,j})$$
$$-\Psi_{i,j}^{(a_{i,j})}(L_{i,j}-a_{i,j})\Phi_{i,j}^{(a_{i,j})*}(L_{i,j})]. \tag{30}$$

In fact, $H_d$ is a matrix, and, hence, it is self-adjoint if and only if (30) is zero. Similarly to the previous section, we impose a continuity condition and some current conservation rule. The continuity condition reads as

$$\Psi_{i,j}^{(a_{i,j})}(0)=\phi_i,\quad \Psi_{i,j}^{(a_{i,j})}(L_{i,j})=\phi_j, \tag{31}$$

for some complex numbers $\phi_i$ for all $i<j$ and $C_{i,j}=1$. The discrete version of the current conservation

$$-\sum_{j<i}C_{i,j}[\Psi_{j,i}^{(a_{j,i})}(L_{j,i})-\Psi_{j,i}^{(a_{j,i})}(L_{j,i}-a_{j,i})]$$
$$+\sum_{j>i}C_{i,j}[\Psi_{i,j}^{(a_{i,j})}(a_{i,j})-\Psi_{i,j}^{(a_{i,j})}(0)]=\lambda_i\phi_i, \tag{32}$$

for some real parameters $\lambda_i$ for $i$ in $\{1,\dots,V\}$.

Inspired from eq. (3) we use a somehow different linear combination of the fundamental solution in (3) which is adapted to the above continuity and current conservation law similar to (24) as

$$\Psi_{i,j}^{(a_{i,j})}(x_{n_{i,j}}^{(a_{i,j})})=$$
$$C_{i,j}B_{i,j}\left[g_+(a_{i,j})^{\frac{x_{n_{i,j}}^{(a_{i,j})}}{a_{i,j}}}-g_-(a_{i,j})^{\frac{x_{n_{i,j}}^{(a_{i,j})}}{a_{i,j}}}\right]$$
$$+C_{i,j}A_{i,j}\left[g_+(a_{i,j})^{\frac{L_{i,j}-x_{n_{i,j}}^{(a_{i,j})}}{a_{i,j}}}-g_-(a_{i,j})^{\frac{L_{i,j}-x_{n_{i,j}}^{(a_{i,j})}}{a_{i,j}}}\right], \tag{33}$$

for $i<j$, where

$$g_\pm(a_{i,j})=1+\frac{-k^2a_{i,j}^2\pm ka_{i,j}\sqrt{k^2a_{i,j}^2-4}}{2}.$$

These functions are the exact solution of the discrete Schrödinger equation (28). Continuous limit of the solution can be obtained by considering the limit at $a_{i,j}\to 0$ for fixed point $x_{i,j}^{(a_{i,j})}=\alpha_{i,j}$. Similarly, as is shown in the section, one obtains

$$\lim_{a_{i,j}\to 0}\Psi_{i,j}^{(a_{i,j})}(\alpha_{i,j})=C_{i,j}B_{i,j}\left[e^{ik\alpha_{i,j}}-e^{-ik\alpha_{i,j}}\right]$$
$$+C_{i,j}A_{i,j}[e^{ik(L_{i,j}-\alpha_{i,j})}-e^{-ik(L_{i,j}-\alpha_{i,j})}]. \tag{34}$$

The right-hand side of eq. (34) is analogue of the solution of the continuous Schrödinger equation on a continuous graph in eq. (24).

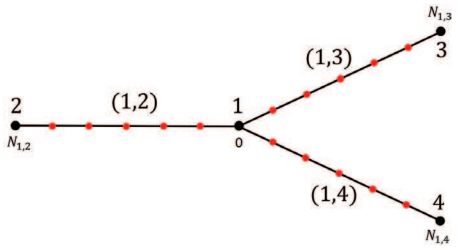


Fig. 2: Discrete star graph.

The vertex boundary conditions in eqs. (31) and (32) lead to the following homogeneous system of linear equations:

$$A_{i,j}f_{i,j}(N_{i,j})=\phi_i,\quad B_{i,j}f_{i,j}(N_{i,j})=\phi_j, \tag{35}$$
$$\sum_{j<i}C_{i,j}\big\{A_{i,j}f_{i,j}(1)+B_{i,j}\big[f_{i,j}(N_{i,j}-1)-f_{i,j}(N_{i,j})\big]\big\}$$
$$+\sum_{j>i}C_{i,j}\big\{A_{i,j}\left[f_{i,j}(N_{i,j}-1)-f_{i,j}(N_{i,j})\right]+B_{i,j}f_{i,j}(1)\big\}=$$
$$\lambda_i\phi_i, \tag{36}$$

where $f_{i,j}(n_{i,j})=g_+(a_{i,j})^{n_{i,j}}-g_-(a_{i,j})^{n_{i,j}}$. This is a system of homogeneous equations for $A_{i,j}$, $B_{i,j}$ and $\phi_i$, which has a non-trivial solution when

$$\det(M(k))=0, \tag{37}$$

where $M(k)$ matrix has the same size and structure as in the third section.

*Star branched lattice.* In this subsection, we consider a quantum star graph with three discrete edges (see fig. 2). For such a graph, $N_{1,j}a_{1,j}=L_{1,j}$ is the length of the edge $(1,j)$ for $j=2,3,4$.

We choose $\lambda_1=\lambda_2=\lambda_3=\lambda_4=0$. Then the continuity conditions (31) and the current conservation (32) are for $j=2,3,4$

$$\begin{aligned}&\Psi_{1,j}^{(a_{1,j})}(0)=\phi_1,\quad \Psi_{1,j}^{(a_{1,j})}(L_{1,j})=\phi_j,\\ &\Psi_{1,j}^{(a_{1,j})}(L_{1,j})-\Psi_{1,j}^{(a_{1,j})}(L_{1,j}-a_{1,j})=0,\\ &\sum_{j=2}^{4}[\Psi_{1,j}^{(a_{1,j})}(a_{1,j})-\Psi_{1,j}^{(a_{1,j})}(0)]=0.\end{aligned} \tag{38}$$

Substitution of the solution in eq. (33) into (38) yields the secular equations

$$\begin{aligned}&A_{1,j}f_{1,j}(N_{1,j})=\phi_1,\quad B_{1,j}f_{1,j}(N_{1,j})=\phi_j,\\ &A_{1,j}f_{1,j}(1)+B_{1,j}\left[f_{1,j}(N_{1,j}-1)-f_{1,j}(N_{1,j})\right]=0,\\ &\sum_{j=2}^{4}\left\{A_{1,j}\left[f_{1,j}(N_{1,j}-1)-f_{1,j}(N_{1,j})\right]+B_{1,j}f_{1,j}(1)\right\}=0.\end{aligned} \tag{39}$$

The above system of equations has a non-trivial solution when

$$\det\left(M(k)\right)=0, \tag{40}$$

Table 2: The first five nonzero eigenvalues $k$ compared with the continuous case on the star graph.

| | Continuous | $a = 0.1$ | $a = 0.01$ | $a = 0.005$ |
|---|---|---|---|---|
| 1 | 1.1799688 | 1.2293914 | 1.1847666 | 1.1823638 |
| 2 | 1.6768750 | 1.7771792 | 1.6865131 | 1.6816835 |
| 3 | 2.0943951 | 2.0905692 | 2.0943568 | 2.0943855 |
| 4 | 2.7486684 | 2.8462967 | 2.7654332 | 2.7570666 |
| 5 | 2.8559933 | 2.9088003 | 2.8558962 | 2.8559690 |

where the $M(k)$ matrix is the same as the continuous version of the star graph

$$M(k) = \begin{pmatrix} \Lambda^{(1)} & W(k) & 0 \\ \Lambda^{(2)} & 0 & W(k) \\ 0 & U^{(1)}(k) & U^{(2)}(k) \end{pmatrix}. \tag{41}$$

The elements of the above matrices are

$$\Lambda^{(1)} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \quad \Lambda^{(2)} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

$$W(k) = \begin{pmatrix} f_{1,2}(N_{1,2}) & 0 & 0 \\ 0 & f_{1,3}(N_{1,3}) & 0 \\ 0 & 0 & f_{1,4}(N_{1,4}) \end{pmatrix},$$

$$U^{(1)}(k) = \begin{pmatrix} r_{1,2}(N_{1,2}) & r_{1,3}(N_{1,3}) & r_{1,4}(N_{1,4}) \\ f_{1,2}(1) & 0 & 0 \\ 0 & f_{1,3}(1) & 0 \\ 0 & 0 & f_{1,4}(1) \end{pmatrix},$$

$$U^{(2)}(k) = \begin{pmatrix} f_{1,2}(1) & f_{1,3}(1) & f_{1,4}(1) \\ r_{1,2}(N_{1,2}) & 0 & 0 \\ 0 & r_{1,3}(N_{1,3}) & 0 \\ 0 & 0 & r_{1,4}(N_{1,4}) \end{pmatrix},$$

where $r_{1,j}(N_{1,j}) = f_{1,j}(N_{1,j}-1) - f_{1,j}(N_{1,j})$. This secular equation can be solved numerically to provide eigenvalues of discrete quantum star graph. Here one should note that if the lengths of the edges are equal the eigenvalue spectrum becomes degenerate, *i.e.*, has multiple eigenvalues. To avoid such situation, when we solve the secular equation, we choose lengths of the edges as rationally independent. The first five nonzero eigenvalues are calculated for the considered star graph (see table 2), where the step size for each edge of the graph is chosen to be equal, $a_{1,j} = a$ and lengths of edges of the graph are chosen as $L_{1,2} = 0.8$, $L_{1,3} = 1.1$, $L_{1,4} = 1.5$. In each column (3–5 columns) in table 2 we present nonzero eigenvalues by choosing the different values of step size $a$ for the star graph. The results show the convergence of solutions to the solutions of the continuous case calculated using eq. (27) for the continuous star graph for the same lengths of edges.

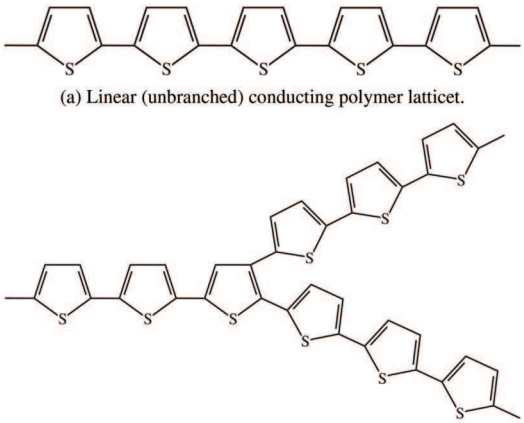


Fig. 3: Conducting polymer chains.

*Possible experimental realization of the model.* Here we briefly discuss the possible practical application of our model to so-called conducting polymers. These latter are the pol-conjugated (polymer) molecular chains exhibiting semiconducting electronic properties and therefore are called organic semiconductors. Conducting polymers are the basic functional materials for organic electronics and so-called polymer-based film organic photovoltaics (see *e.g.*, refs. [34–39], for a review of conducting polymers and their applications). The structure of conducting polymers presents a discrete lattice (chain) with the hexagonal basic cell (see fig. 3(a)). Charge carrier dynamics in such structure can be described in terms of the discrete Schrödinger equation given by eq. (2). An important problem arising in the context of charge dynamics in conducting polymers is modeling electron or exciton (in some cases polarons and solitons) transport with account of its discrete structure. The solution of such a problem allows us to compute the electronic band structure of the material and tuning of its electronic properties. The latter is important for functional optimization of conducting polymers and improving of device performance in organic photovoltaics. Recently, the structures consisting of branched conducting polymer chains attracted much attention in the context of polymer-based photovoltaics and organic electronics (see, *e.g.*, refs. [34,39,40] for a review). In the simplest case, such polymer can have a star-branched structure (see fig. 3(b)). Our model for branched quantum lattice based on the use of discrete Schrödinger equation on the metric graph can be effectively used for the description of charge carrier dynamics and computation of the electronic band spectrum in branched conducting polymers [34,40]. Also, charge current, and current-voltage characteristics in the AC-driven case can be computed. Another possible application can be using DSE for modeling of so-called coherent Ising machines, which can be realized using the network states [41]. Also the model we proposed can be used for description of chip-based photonic graph states [42] and holonomic quantum gates [43].

**Conclusion.** – In this paper, we considered the problem of the discrete Schrödinger equation on a metric graph, by focusing on its analytical solution and continuum limit. An exact solution of DSE on a finite interval is obtained. Consistency of the result with their continuum counterpart is shown by explicit calculation of the continuum limit of the solution. The result is extended to the case of quantum graph of arbitrary topology. The application of the obtained result to the special case of quantum star graph is demonstrated by imposing the vertex matching conditions given in the form of continuity and Kirchhoff rule. It is shown that the secular equation derived for star graph reproduces its well-know continuum counterpart. The practical application of the proposed model to branched conducting polymers is discussed.

* * *

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