Dirac particles on periodic quantum graphs

J. R. Yusupov ,[1] K. K. Sabirov,[2,3] and D. U. Matrasulov[1,4]
[1]*Yeoju Technical Institute in Tashkent, 156 Usman Nasyr Street, 100121 Tashkent, Uzbekistan*
[2]*Tashkent University of Information Technologies, 108 Amir Temur Street, 100200 Tashkent, Uzbekistan*
[3]*Tashkent State Technical University named after Islam Karimov, 2 Universitet Street, 100095 Tashkent, Uzbekistan*
[4]*Turin Polytechnic University in Tashkent, 17 Niyazov Street, 100095 Tashkent, Uzbekistan*

(Received 29 November 2020; revised 17 April 2021; accepted 7 July 2021; published 28 July 2021)

We consider the Dirac equation on periodic networks (quantum graphs). The self-adjoint quasiperiodic boundary conditions are derived. The secular equation allowing us to find the energy spectrum of the Dirac particles on periodic quantum graphs is obtained. Band spectra of the periodic quantum graphs of different topologies are calculated. Universality of the probability to be in the spectrum for certain graph topologies is observed.

DOI: 10.1103/PhysRevE.104.014219

I. INTRODUCTION

Quantum graphs have attracted much attention as an effective tool for modeling particle and wave dynamics in branched quantum structures. 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 into a one-dimensional Schrödinger (Dirac) equation on metric graphs, which can be exactly solved in most of the cases. Quantum graphs are determined as the branched quantum wires, which are connected to each other at the nodes (vertices). Wave and particle dynamics in such systems are described in terms of quantum mechanical wave equations on metric graphs. Initially, quantum mechanical treatment of a particle motion in branched structures was considered in quantum chemistry of organic molecules. References [1–3], where the electron motion in branched aromatic molecules was studied, can be considered as a pioneering attempt for the study of particle motion in quantum graphs. However, the strict formulation of the quantum graph concept, where the latter was defined as a branched quantum wire, has been presented a few decades later by Exner and Seba in [4]. Further progress was made by Kostrykin and Schrader, who proposed general vertex boundary conditions providing self-adjointness of the Schrödinger equation on quantum graphs [5]. Later the quantum graph concept has been used in different contexts (see Refs. [6–19]) and an experimental realization in microwave networks was done [17]. Despite considerable progress made on the study of different aspects of quantum graph theory, most of the studies are limited by considering the nonrelativistic case, i.e., unlike its nonrelativistic counterpart, the study of relativistic quantum dynamics on graphs is still remaining out of focus in quantum graphs theory. Bulla and Trenkler treated Dirac equation on graphs in [20]. Later this problem was considered in [21,22], where strict formulation of the problem with the self-adjoint vertex boundary conditions were presented and spectral and scattering properties were studied. However, the research in this topic did not get further development. In [23], the problem of reflectionless quasiparticle transport in quantum graphs was studied. In [24], the Bogoliubov–de Gennes equation on graphs modeling Majorana fermions in branched quantum wires was considered. Physical systems, which can be modeled in terms of the Dirac equation on periodic quantum graphs appear, e.g., in polymer physics. The well known Su-Schriefer-Heeger (SSH) model [25–27] describing polaron dynamics in conducting polymers, such as, e.g., polyacethylene in its continuum version leads to the Dirac type equation [28,29]. When one considers so-called (periodically) branched conducting polymers, polaron transport in such structures can be described in terms of the Dirac equation on periodic quantum graphs [30,56]. Synthesis and study of electrophysical properties of such branched polymers have been reported recently in the literature [31–34]. Another system where the Dirac equation on periodic quantum graphs can be applied comes from optics, where the optical emulation of one-dimensional (1D) Dirac fermions is possible [35,36].

In this paper, we address the problem of the Dirac equation on periodic quantum graphs. In particular, we present a model for Dirac quasiparticles in branched lattices, which can be mapped on to the periodic quantum graphs. We note that different aspects of the Schrödinger equation on periodic quantum graphs have been studied in detail in Refs. [37–50]. Some mathematical properties of the continuum and discrete Schrödinger operator on graphs are studied in [42–44,48]. An effective numerical method for the determination of the spectra of the Schrödinger operator on periodic metric graphs is presented in [45]. Physically acceptable models of quantum graphs and a very effective approach for the treatment of their band spectra and dispersion relations have been proposed in [11]. Quantum transport in periodic quantum graphs is considered in a very recent paper [50]. It is important to note that during the past decade, the problem of wave dynamics in networks has been successfully extended to the case of the nonlinear wave equation (see, e.g., Refs. [51–57] and references therein). The tight binding approach for studying band spectra of periodic quantum graphs is developed in [49]. Bethe-Sommerfeld conjecture $\mathbb{Z}^2$-periodic graphs are studied in [39].

The paper is organized as follows. In the next section we briefly recall the Dirac equation on quantum graphs. Section III presents the boundary conditions and general secular equation for the Dirac equation on periodic quantum graphs. In Sec. IV we compute and study the band spectra of the periodic graphs of different topologies. In Sec. V the probability that a randomly chosen momentum belongs to the spectrum of the periodic graph is investigated. Finally, Sec. VI presents some concluding remarks.

II. DIRAC EQUATION ON QUANTUM GRAPHS

As mentioned above, quantum graphs are determined as one- or quasi-one-dimensional branched quantum wires, where the wave dynamics can be described in terms of quantum mechanical wave equations on metric graphs, for which the boundary conditions at the branching points (vertices) and bond ends are imposed. The metric graph itself is determined as a set of bonds with assigned length and which are connected to each other at the vertices according to a rule called the topology of a graph, which is given in terms of the adjacency matrix [6,8]:

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

for $i, j = 1, 2, \dots, N$.

Here, following Ref. [21], we briefly give the general description of the Dirac equation on quantum graphs. For the sake of simplicity we will do this for a star graph. However, extension to an arbitrary graph is rather trivial. Let's consider the Dirac equation (in the units $\hbar = m = c = 1$) on the star graph with N bonds with finite lengths, $b_j \sim [0, L_j]$, $j = 1, 2, ..., N$, given by

$$\mathcal{D}\psi_j = E\psi_j, \tag{1}$$

where $\psi_j = (\phi_j, \chi_j)^\top$, and the Dirac operator is given as

$$\mathcal{D} := -i\sigma_y\partial_x + \sigma_z, \tag{2}$$

with σ_y and σ_z being the Pauli matrices:

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

To solve Eq. (1), one needs to impose the boundary conditions at the vertices. Such boundary conditions should keep the Dirac operator on a graph as self-adjoint. In the case of the Schrödinger equation on graphs general boundary conditions providing the self-adjointness have been derived in [5]. We introduce the following skew-Hermitian bilinear quadratic form for the above star graph:

$$\begin{aligned} \Omega(\psi, \varphi) &= \langle \mathcal{D}\psi, \varphi\rangle - \langle \psi, \mathcal{D}\varphi\rangle \\ &= \sum_{j=1}^{N}[\phi_j(0)v_j^*(0) - \phi_j(L_j)v_j^*(L_j) \\ &\quad - \chi_j(0)u_j^*(0) + \chi_j(L_j)u_j^*(L_j)], \end{aligned} \tag{3}$$

where $\psi = (\psi_1, \psi_2, ..., \psi_N)$, $\varphi = (\varphi_1, \varphi_2, ..., \varphi_N)$, and $\psi_j = (\phi_j, \chi_j)^\top$, $\varphi_j = (u_j, v_j)^\top$.

Then one can prove (see [21]) that the self-adjointness of the Dirac operator on graph is provided by the following requirement:

$$\Omega(\psi, \varphi) = 0. \tag{4}$$

A set of vertex boundary conditions fulfilling this requirement can be written as

$$\begin{aligned} &\phi_1(0) = \phi_2(0) = ... = \phi_N(0), \\ &\chi_1(0) + \chi_2(0) + ... + \chi_N(0) = 0, \\ &\phi_1(L_1) = \phi_2(L_2) = ... = \phi_N(L_N) = 0. \end{aligned} \tag{5}$$

The choice of the vertex coupling comes from the physical motivation, i.e., from their relevance to real physical systems appearing in condensed matter physics.

The general secular equation for finding the eigenvalues k_n which are derived from the boundary conditions (5), can be written as [22]

$$\det \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ e^{ik\mathbf{L}} & e^{-ik\mathbf{L}} \end{pmatrix} = 0, \tag{6}$$

where

$$\mathbf{A} = \begin{pmatrix} \mathbf{1}_{N-1}^T & -\mathbf{I}_{N-1} \\ 1 & \mathbf{1}_{N-1} \end{pmatrix},$$

$$\mathbf{B} = \begin{pmatrix} \mathbf{1}_{N-1}^T & -\mathbf{I}_{N-1} \\ -1 & -\mathbf{1}_{N-1} \end{pmatrix},$$

with $\mathbf{1}_{N-1} = \underbrace{(1, 1, ..., 1)}_{N-1}$, $\mathbf{I}_{N-1}$ is $(N-1)\times(N-1)$ the identity matrix, and $e^{ik\mathbf{L}} = \mathrm{diag}(e^{ikL_1}, e^{ikL_2}, ..., e^{ikL_N})$.

For positive energies E the general solution of Eq. (1) can be written in the form of plane waves as

$$\psi_j(x,k) = \mu_j(k)\begin{pmatrix} 1 \\ i\gamma(k) \end{pmatrix}e^{ikx} + \hat{\mu}_j(k)\begin{pmatrix} 1 \\ -i\gamma(k) \end{pmatrix}e^{-ikx} \tag{7}$$

with $k > 0$ and

$$\gamma(k) := \frac{E-1}{k},\ E = \sqrt{k^2+1}. \tag{8}$$

The coefficients $\mu_j(k)$ and $\hat{\mu}_j(k)$ are determined by imposed boundary conditions that provide self-adjointness of $\mathcal{D}$.

Similarly to that in [6], one can define also the bond scattering matrix, $\mathbf{S} = S_{(ij)(lm)}$, which describes scattering of the Dirac particle on bond (ij) to that on bond (lm) [(ij) and (lm) must be connect at m [21]]. The secular equation in terms of the scattering matrix can be written as [21]

$$\det(\mathbf{I} - \mathbf{S}) = 0.$$

Spectral (with the focus on quantum chaos) and scattering properties of Dirac particles on graphs have been studied in [21] using the above secular equations and properties of the S matrix. Also, the analysis of the time-reversal symmetry in the transmission matrix and the properties of the trace formula

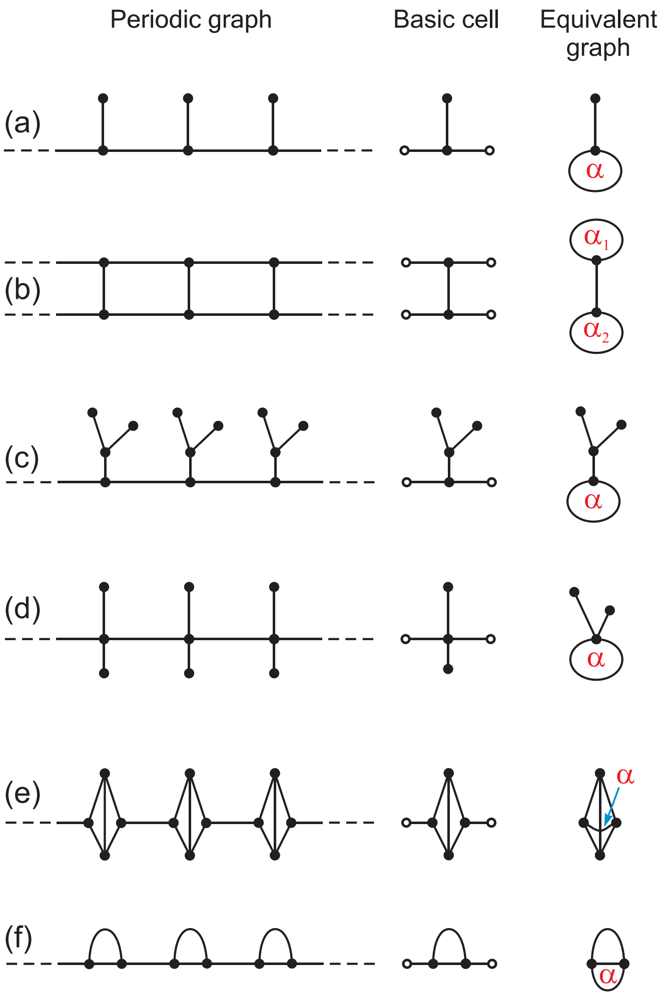

FIG. 1. Some types of periodic graphs with their basic cells and corresponding equivalent graphs.

have been considered in [21]. A zeta function based study of the Dirac operator on graphs was presented in [22].

III. DIRAC PARTICLES ON PERIODIC QUANTUM GRAPHS

Here, using an extension of the approach, developed in [37], we consider a Dirac equation on a periodic graph by computing band spectra of different topologies. Within such an approach, one can treat a wide variety of periodic graphs. Although one can construct different types of periodic graphs using simple graphs as "unit cells," we will focus on the types presented in Fig. 1. In our approach, a periodic graph is considered as a repeating structure of basic graphs, which can be called unit cells, i.e., the "graph lattice" is a periodic or quasiperiodic structure of basic graphs. We assume that in all cases, a periodic or quasiperiodic graph can be "mapped" onto the simple graphs, which (for each graph) are shown in the last column in Fig. 1. We note that there is a well developed and powerful approach for the treatment of spatially periodic quantum systems, which is known under different names, such as the Bloch method, the Floquet method, and the Gelfand transformation. Within such an approach, the prescription for

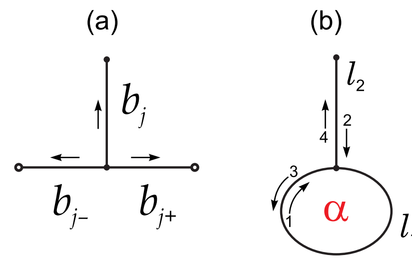

FIG. 2. (a) Mapping of the jth basic cell of the comb graph on to its equivalent, (b) a loop vested with a magnetic flux. Arrows show directions of the assigned coordinates.

solving the Dirac equation on a periodic graph can be formulated as follows:

(i) Write Dirac equation on each bond of the basic cell.

(ii) Impose the vertex boundary conditions for each node of the basic cell.

(iii) Impose the "intercell" boundary conditions for the whole periodic graph.

(iv) Derive the secular equation in terms of the scattering matrix from the vertex and intercell boundary conditions.

(v) Construct the scattering matrix and find eigenvalues from the secular equation.

Below we demonstrate the application of this prescription for the periodic comb graph presented in Fig. 1(a). We define the bonds of the graph as $b_{j\pm} \sim (0, l_1/2)$, $b_j \sim (0, l_2)$, $j = ..., -1, 0, 1, ...$ (see Fig. 2). Directions of assigned coordinates on each bond are shown by arrows in Fig. 2(a). To each bond b_j of the graph we assign a coordinate x_j, which indicates the position along the bond: for bond b_1 it is $x_j \in [0, l_1/2]$. One can use the shorthand notation $\Psi_j(x)$ for $\Psi_j(x_j)$ and it is understood that x is the coordinate on the bond j to which the component Ψ_j refers.

On each bond of this graph we have the following one-dimensional Dirac equation (in the units $\hbar = m = c = 1$):

$$-\partial_x \chi_b + \phi_b = E\phi_b, \quad \partial_x \phi_b - \chi_b = E\chi_b, \tag{9}$$

for $b \in \{b_{j-}, b_{j+}, b_j\}$.

The vertex boundary conditions for each basic cell are imposed as

$$\phi_{b_{j-}}(0) = \phi_{b_{j+}}(0) = \phi_{b_j}(0), \tag{10}$$

$$\chi_{b_{j-}}(0) + \chi_{b_{j+}}(0) + \chi_{b_j}(0) = 0, \tag{11}$$

$$\chi_{b_j}(l_2) = 0. \tag{12}$$

For the periodic graph presented in Fig. 1(a), one can impose the following quasiperiodic (intercell) conditions:

$$\phi_{b_{j+}}(l_1/2) = e^{i\alpha}\phi_{b_{j-}}(l_1/2), \tag{13}$$

$$\chi_{b_{j+}}(l_1/2) = -e^{i\alpha}\chi_{b_{j-}}(l_1/2). \tag{14}$$

Vertices with these boundary conditions are denoted by the empty circles in Figs. 1 and 2. It can be shown that the boundary conditions (13) and (14) do not break the self-adjointness of the Dirac operator on graph, since they are consistent with Eq. (4)

A general solution of the system of Eq. (9) can be written as

$$\begin{pmatrix} \phi_b(x) \\ \chi_b(x) \end{pmatrix} = \mu_b \begin{pmatrix} 1 \\ i\gamma \end{pmatrix} e^{ikx} + \hat{\mu}_b \begin{pmatrix} 1 \\ -i\gamma \end{pmatrix} e^{-ikx}. \tag{15}$$

For the whole periodic graph in Fig. 1(a), for the direction 1 [see Fig. 2(b)]the general solution can be written in terms of the following outgoing and incoming waves at the vertex:

$$\begin{aligned} \begin{pmatrix} \phi_1(l_1 - x) \\ \chi_1(l_1 - x) \end{pmatrix} &= e^{i\alpha} \begin{pmatrix} \phi_{b_{j-}}(x) \\ -\chi_{b_{j-}}(x) \end{pmatrix}, \\ \begin{pmatrix} \phi_1(x) \\ \chi_1(x) \end{pmatrix} &= \begin{pmatrix} \phi_{b_{j+}}(x) \\ \chi_{b_{j+}}(x) \end{pmatrix}. \end{aligned} \tag{16}$$

From the periodic boundary conditions given by Eqs. (13)–(14) and Eq. (15) we have

$$\begin{pmatrix} \phi_1(y) \\ \chi_1(y) \end{pmatrix} = \mu_1^{(1)} e^{i\alpha + ikl_1} \begin{pmatrix} 1 \\ -i\gamma \end{pmatrix} e^{-iky} + \hat{\mu}_1^{(1)} e^{i\alpha - ikl_1} \begin{pmatrix} 1 \\ i\gamma \end{pmatrix} e^{iky}, \quad \frac{l_1}{2} \leqslant y \leqslant l_1, \tag{17}$$

$$\begin{pmatrix} \phi_1(y) \\ \chi_1(y) \end{pmatrix} = \mu_1^{(2)} \begin{pmatrix} 1 \\ i\gamma \end{pmatrix} e^{iky} + \hat{\mu}_1^{(2)} \begin{pmatrix} 1 \\ -i\gamma \end{pmatrix} e^{-iky}, \quad 0 \leqslant y \leqslant \frac{l_1}{2}, \tag{18}$$

where

$$\hat{\mu}_1^{(1)} = \mu_1^{(2)} e^{-i\alpha + ikl_1}, \; \hat{\mu}_1^{(2)} = \mu_1^{(1)} e^{i\alpha + ikl_1}. \tag{19}$$

For the direction 4 we have

$$\begin{pmatrix} \phi_4(x) \\ \chi_4(x) \end{pmatrix} = \mu_4 \begin{pmatrix} 1 \\ i\gamma \end{pmatrix} e^{ikx} + \hat{\mu}_4 \begin{pmatrix} 1 \\ -i\gamma \end{pmatrix} e^{-ikx}. \tag{20}$$

From the boundary conditions (10)–(12) we have

$$\begin{aligned} &\mu_1^{(1)} + \hat{\mu}_1^{(1)} = \mu_1^{(2)} + \hat{\mu}_1^{(2)} = \mu_4 + \hat{\mu}_4, \\ &\mu_1^{(1)} - \hat{\mu}_1^{(1)} + \mu_1^{(2)} - \hat{\mu}_1^{(2)} + \mu_4 - \hat{\mu}_4 = 0, \\ &\mu_4 e^{ikl_2} = \hat{\mu}_4 e^{-ikl_2}. \end{aligned} \tag{21}$$

From Eqs. (19) and (21) we obtain the following secular equation for finding the eigenvalues of the relativistic spin-half quasiparticle on periodic quantum graph:

$$F(k;\alpha) := \det(\mathbf{I} - \mathbf{S}) = 0, \tag{22}$$

where $\mathbf{I}$ is the four-dimensional identity matrix and $\mathbf{S}$ is the scattering matrix, which depends on the graph topology. For the comb graph in Fig. 1(a), the explicit form of $\mathbf{S}$ can be written as

$$\mathbf{S} = \begin{pmatrix} e^{-i\alpha + ikl_1} & 0 & e^{-i\alpha} - e^{ikl_1} & 0 \\ -1 + e^{-i\alpha + ikl_1} & 0 & e^{ikl_1} - e^{-i\alpha} & e^{ikl_2} \\ -e^{ikl_1} & e^{i\alpha} & 0 & e^{i\alpha + ikl_2} \\ 0 & e^{ikl_2} & 0 & 0 \end{pmatrix}.$$

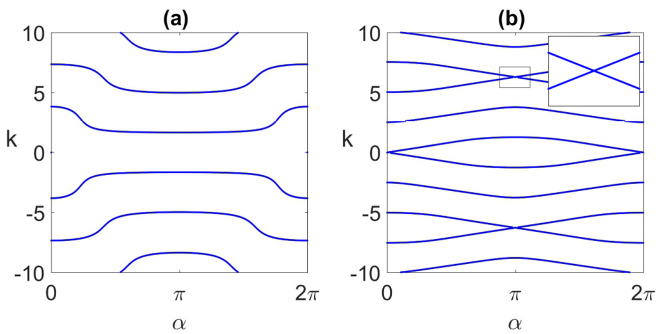

FIG. 3. Band spectra of a Dirac particle on the periodic comb graph (presented in Fig. 2). Lengths are fixed by the relation $l_1 = \beta l_2$, where l_2 is unit length ($l_2 = 1$) for the values $\beta = 0.2$ (a) and $\beta = 2.5$ (b).

IV. BAND SPECTRA OF THE DIRAC PARTICLES ON PERIODIC QUANTUM GRAPHS

An important characteristic of the periodic quantum structure is its band spectrum, which is the eigenenergy spectrum as a function of a system parameter. It characterizes most of the electronic properties, including electric conductance. Usually, for spatially periodic systems the band structure is symmetric with respect to the gap lying between the conductance and valence bands. This concerns also periodic branched structures described in terms of periodic quantum graphs. The periodicity of the graph is considered here with respect to basic cells. From the practical viewpoint, it is important to study dependence of the band spectra on the topology of a periodic graph and from different metric parameters of the basic cell. The latter implies the question how does the band spectrum change by changing the length of bonds connecting basic cells (l_1 in Fig. 2)?

Thus, using the secular equation (22) that holds true for an arbitrary periodic quantum graph, we calculate the band spectrum of a Dirac particle on the comb graph. We study the behavior of the band spectrum by fixing the length of l_2 as a unit and changing the length of l_1 given via the relation $l_1 = \beta l_2$.

Figure 3 presents the band spectra of the comb graph [see Fig. 1(a)] plotted for two values of β: $\beta = 0.2$ and $\beta = 2.5$. One can observe that the gap between the levels decreases when β increases, which means increasing the distance between ridges. Moreover, one can see level crossing (see insets).

Similarly, one can calculate the band spectra for periodic ladder and loop graphs, presented in Figs. 1(b) and 1(f), respectively. For the sake of simplicity, for the ladder graph we choose $\alpha_1 = \alpha_2 = \alpha$, and for the loop graph we choose the equal lengths of the loop and the bond connecting the loop ends. The scattering matrices for these graphs can be written as

$$\mathbf{S}_{\text{ladder}} = \begin{pmatrix} e^{-i\alpha+ikl_1} & 0 & 0 & e^{-i\alpha} - e^{ikl_1} & 0 & 0 \\ 0 & e^{-i\alpha+ikl_1} & 0 & 0 & e^{-i\alpha} - e^{ikl_1} & 0 \\ 1 & 0 & 0 & e^{ikl_1} & 0 & -e^{ikl_2} \\ -e^{i\alpha} + e^{ikl_1} & 0 & e^{i\alpha} & e^{i\alpha+ikl_1} & 0 & e^{i\alpha+ikl_2} \\ 0 & -e^{i\alpha} + e^{ikl_1} & e^{i\alpha+ikl_2} & 0 & e^{i\alpha+ikl_1} & -e^{i\alpha} \\ 0 & 1 & -e^{ikl_2} & 0 & e^{ikl_1} & 0 \end{pmatrix},$$

$$\mathbf{S}_{\text{loop}} = \begin{pmatrix} 0 & 1 & 0 & -e^{ikl_1} & e^{ikl_2} & 0 \\ 0 & 0 & e^{-i\alpha+ikl_3} & 0 & -e^{ikl_2} & e^{-i\alpha} \\ e^{ikl_1} & 0 & 0 & 1 & 0 & -e^{ikl_3} \\ -e^{ikl_1} & e^{ikl_2} & 0 & 0 & 1 & 0 \\ e^{-ikl_2} & e^{-ikl_2} & -e^{-i\alpha+ikl_3-ikl_2} & -e^{ikl_1-ikl_2} & 0 & e^{-i\alpha-ikl_2} \\ -e^{ikl_1-ikl_3} & -e^{ikl_2-ikl_3} & e^{-ikl_3} & e^{-ikl_3} & e^{-ikl_3} & 0 \end{pmatrix},$$

where $l_2 = l_3$ according to our assumption above.

Figure 4 presents band spectra for the periodic ladder graph for the same values of β and l_2 (the length of ladder steps). The spectral picture is the same as that for the comb graph; the gap between the levels decreases when β increases. But the band spectrum manifests avoided crossing of the levels (see inset).

In Fig. 5 plots of the band spectra for periodic loop graph are presented for the same values of parameters as those for the comb and ladder graphs. For both values of β a crossing of levels can be observed.

This study shows that the electronic properties of the periodic quantum structure strongly depend on the system parameter β, which in our case is the distance between basic cells.

V. PROBABILITY TO BE IN THE SPECTRUM

A remarkable result of the Ref. [37], where a nonrelativistic counterpart of our problem is considered, is revealing the universal behavior of the probability that a randomly chosen momentum belongs to the spectrum of the periodic graph. Namely, the probability to be in the spectrum does not depend on the edge lengths and is also invariant within some classes of graph topologies. The basic cell classes, which manifest such a behavior, are the decorations that attach to the base line by means of a single edge, e.g., as in Figs. 2(a)–2(c). Such behavior cannot be observed, for instance, in cases of decorations presented in Figs. 2(d)–2(f). Investigating such a probability and existence of universality properties for a relativistic case should be interesting both from fundamental as well as practical viewpoints.

The same trick used in [37] (but originally belonging to Barra and Gaspard [12]) can be directly applied to our case. To calculate the band spectrum of the considered periodic quantum graph: we introduce a new function

$$\Phi(\kappa_1 = kl_1, \kappa_2 = kl_2; \alpha) := F(k; \alpha), \tag{23}$$

where κ_1 and κ_2 need only be known modulo 2π. In this way, for a fixed α we found solutions of

$$\Phi(\vec{\kappa}; \alpha) = 0, \tag{24}$$

where $\vec{\kappa}(k) = (kl_1, kl_2) \mod 2\pi$ and k belongs to the spectrum of the periodic graph.

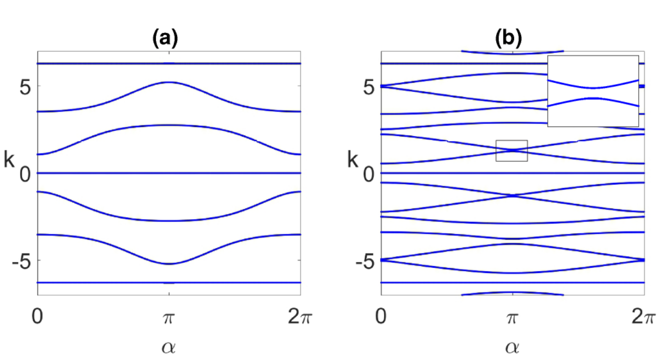

FIG. 4. Band spectra of a Dirac particle on the periodic ladder graph. Lengths are fixed by the relation $l_1 = \beta l_2$, where l_2 is unit length ($l_2 = 1$) for the values $\beta = 0.2$ (a) and $\beta = 2.5$ (b).

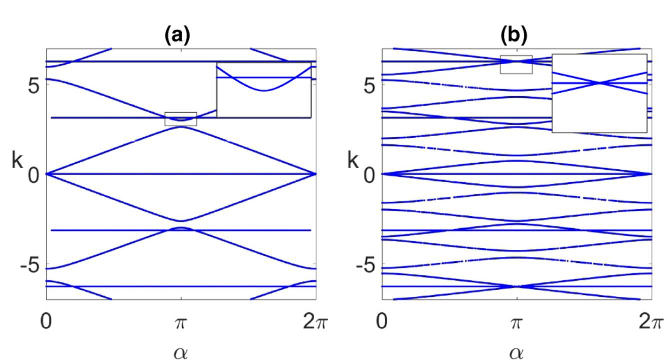

FIG. 5. Band spectra of a Dirac particle on the periodic loop graph. Lengths are fixed by the relation $l_1 = \beta l_2$, where l_2 is unit length ($l_2 = 1$) for the values $\beta = 0.2$ (a) and $\beta = 2.5$ (b).

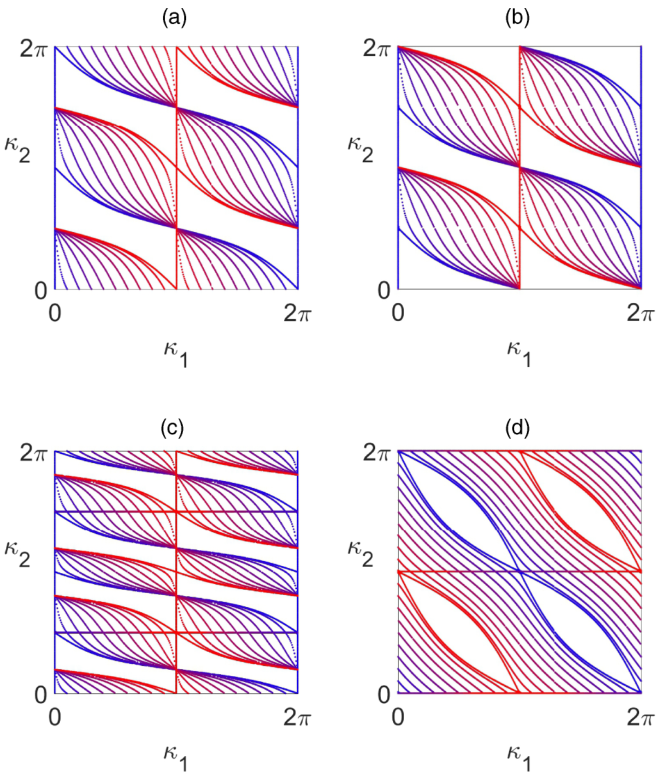

FIG. 6. The zero sets of $\Phi(k_1, k_2; \alpha)$ for a range of values of $\alpha \in [0, \pi]$ for (a) the periodic comb, (b) ladder, (c) periodic graph shown in Fig. 2(c), and (d) loop graphs using color scale from blue ($\alpha = 0$) to red ($\alpha = \pi$).

Figure 6 presents dependence of k_2 on k_1 at different values of α calculated using Eq. (24) for the four periodic graph topologies depicted in Figs. 2(a)–2(c) and 2(f).

Using the same approach used in [37], we calculate the probability p_σ for a random k to be in the spectrum σ. However, unlike the nonrelativistic counterpart where probability can be estimated analytically [37], in the relativistic case the secular equation has very complicated form. Therefore one should compute the probability numerically. Using the symmetry properties of the spectrum plotted in Fig. 6 one can calculate the probability by finding the area of 1/8-th of the zero sets, which is the part in the lower left corner, bounded by the coordinate axes and the function $\kappa_2 = \varphi(\kappa_1; \pi)$. The numerical calculations of the probability to be in the spectrum show that for (a) comb and (b) ladder graphs and (c) the graph shown in Fig. 2(c) it takes the (same) value $p_\sigma \approx 0.64$, while for (d) the loop graph the probability is different, $p_\sigma \approx 0.73$. A similar situation was observed for the nonrelativistic counterpart considered in [37]. Thus, for the relativistic case described by the Dirac equation on periodic graphs we observed similar universality for the decorations that attach to the base line by means of a single edge (at least for the topologies presented in Fig. 2).

VI. CONCLUSIONS

We studied the Dirac equation on periodic quantum graphs with a focus on the eigenvalue problem. The secular equation allowing us to find a band spectrum of Dirac quasiparticles in networks is derived from quasiperiodic boundary conditions. It is shown that these latter do not break the self-adjointness of the Dirac operator on graphs. Band spectra of different periodic graphs are computed. Universality of the probability to be in the spectrum for certain graph topologies is shown by numerical calculations. The above model can find applications in the study of electronic properties of different quasi-one-dimensional branched (periodic) structures, such as, e.g., periodically branched conducting polymers, where transport of polarons can be described in terms of the Dirac equation on graphs.

[1] L. Pauling, J. Chem. Phys. **4**, 673 (1936).
[2] K. Ruedenberg and C. W. Scherr, J. Chem. Phys. **21**, 1565 (1953).
[3] S. Alexander, Phys. Rev. B **27**, 1541 (1983).
[4] P. Exner, P. Seba, and P. Stovicek, J. Phys. A: Math. Gen. **21**, 4009 (1988).
[5] V. Kostrykin and R. Schrader, J. Phys. A: Math. Gen. **32**, 595 (1999)
[6] T. Kottos and U. Smilansky, Ann. Phys. **274**, 76 (1999).
[7] P. Kuchment, Waves Random Media **14**, S107 (2004).
[8] S. Gnutzmann and U. Smilansky, Adv. Phys. **55**, 527 (2006).
[9] N. Goldman and P. Gaspard, Phys. Rev. B **77**, 024302 (2008).
[10] P. Exner and H. Kovarik, *Quantum Waveguides* (Springer, Cham, 2015).
[11] G. Berkolaiko and P. Kuchment, *Introduction to Quantum Graphs, Mathematical Surveys and Monographs* (AMS, 2013).
[12] F. Barra and P. Gaspard, J. Stat. Phys. **101**, 283 (2000).
[13] S. Gnutzmann, J. P. Keating, and F. Piotet, Ann. Phys. **325**, 2595 (2010).
[14] D. Mugnolo, *Semigroup Methods for Evolution Equations on Networks* (Springer-Verlag, Berlin, 2014).
[15] S. Gnutzmann, H. Schanz, and U. Smilansky, Phys. Rev. Lett. **110**, 094101 (2013).
[16] J. Bolte and G. Garforth, J. Phys. A: Math. Theor. **50**, 105101 (2017).
[17] O. Hul, S. Bauch, P. Pakonski, N. Savytskyy, K. Zyczkowski, and L. Sirko, Phys. Rev. E **69**, 056205 (2004).
[18] J. R. Yusupov, K. K. Sabirov, M. Ehrhardt, and D. U. Matrasulov, Phys. Lett. A **383**, 2382 (2019).
[19] D. U. Matrasulov, J. R. Yusupov, and K. K. Sabirov, J. Phys. A **52**, 155302 (2019).
[20] W. Bulla and T. Trenkler, J. Math. Phys. **31**, 1157 (1990).
[21] J. Bolte and J. Harrison, J. Phys. A: Math. Gen. **36**, L433 (2003).
[22] J. Harrison, T. Weyand, and K. Kirsten, J. Math. Phys. **57**, 102301 (2016).
[23] J. R. Yusupov, K. K. Sabirov, Q. U. Asadov, M. Ehrhardt, and D. U. Matrasulov, Phys. Rev. E **101**, 062208 (2020).

[24] K. K. Sabirov, J. Yusupov, D. Jumanazarov, and D. Matrasulov, Phys. Lett. A **382**, 2856 (2018).
[25] W. P. Su, J. R. Schrieffer, A. J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979).
[26] A. J. Heeger, Rev. Mod. Phys. **73**, 681 (2001).
[27] A. J. Heeger, S. Kivelson, J. R. Schrieffer, and W.-P. Su, Rev. Mod. Phys. **60**, 781 (1988).
[28] D. K. Campbell and A. R. Bishop, Phys. Rev. B **24**, 4859(R) (1981).
[29] D. K. Campbell and A. R. Bishop, Nucl. Phys. B **200**, 297 (1982).
[30] K. K. Sabirov, J. R. Yusupov, Kh. Sh. Matyokubov, NANOSYSTEMS: Phys., Chem., Math. **11**, 183 (2020).
[31] M. Goll, A. Ruff, E. Muks, F. Goerigk, B. Omiecienski, I. Ruff, R. C. Gonzalez-Cano, J. T. L. Navarrete, M. C. R. Delgado, and S. Ludwigs, Beilstein J. Org. Chem. **11**, 335 (2015).
[32] H. Higginbotham, K. Karon, P. Ledwon, and P. Data, Display and Imaging **2**, 207 (2017).
[33] T. Soganci, O. Gumusay, H. C. Soyleyici, and M. Ak, Polymer **134**, 187 (2018)
[34] H. Li, M. J. Catanzaro, S. Tretiak, and V. Y. Chernyak, J. Phys. Chem. Lett. **5**, 641 (2014).
[35] F. Dreisow, M. Heinrich, R. Keil, A. Tunnermann, S. Nolte, S. Longhi, and A. Szameit, Phys. Rev. Lett. **105**, 143902 (2010).
[36] J. M. Zeuner, N. K. Efremidis, R. Keil, F. Dreisow, D.N. Christodoulides, A. Tunnermann, S. Nolte, and A. Szameit, Phys. Rev. Lett. **109**, 023602 (2012).
[37] R. Band, G. Berkolaiko, Phys. Rev. Lett. **111**, 130404 (2013).
[38] Yu.-Ch. Luo, E. O. Jatulan, Ch.-K. Law, J. Phys. A **52**, 165201 (2019).
[39] P. Exner and O. Turek, J. Phys. A: Math. Theor. **50**, 455201 (2017).
[40] D. Barseghyan and A. Khrabustovskyi, J. Phys. A: Math. Theor. **48**, 255201 (2015).
[41] G. Berkolaiko and M. Kha, Lett. Math. Phys. **32**, 2965 (2020).
[42] E. Korotyaev and N. Saburova, J. Math. Anal. Appl. **420**, 576 (2014).
[43] E. Korotyaev and N. Saburova, J. Math. Anal. Appl. **436**, 104 (2016).
[44] E. Korotyaev and N. Saburova, J. Funct. Anal. **272**, 1625 (2017).
[45] V. Barrera-Figueroa and V. S. Rabinovich, J. Phys. A: Math. Theor. **50**, 215207 (2017).
[46] L. Alon, R. Band, and G. Berkolaiko, Commun. Math. Phys. **362**, 909 (2018).
[47] G. Berkolaiko, Y. Latushkin, and S. Sukhtaiev, Adv. Math. **352**, 632 (2019).
[48] E. Korotyaev and N. Saburova, Math. Annal. **377**, 723 (2020).
[49] G. Berkolaiko, Y. Canzani, G. Cox, and J. L. Marzuola,arXiv:2004.12931 v2.
[50] P. Exner and J. Lipovský, Phys. Lett. A **384**, 126390 (2020)
[51] Z. Sobirov, D. Babajanov, D. Matrasulov, K. Nakamura, and H. Uecker, Europhys. Lett. **115**, 50002 (2016).
[52] R. Adami, E. Serra, and P. Tilli, Commun. Math. Phys. **352**, 387 (2017).
[53] A. Kairzhan and D. E. Pelinovsky, J. Phys. A: Math. Theor. **51**, 095203 (2018).
[54] K. K. Sabirov, S. Rakhmanov, D. Matrasulov, and H. Susanto, Phys. Lett. A **382**, 1092 (2018).
[55] D. Babajanov, H. Matyoqubov, and D. Matrasulov, J. Chem. Phys. **149**, 164908 (2018).
[56] J. R. Yusupov, Kh. Sh. Matyokubov, K. K. Sabirov and D. U. Matrasulov, Chem. Phys. **537**, 110861 (2020).
[57] D. Matrasulov, K. Sabirov, D. Babajanov, and H. Susanto, Europhys. Lett. **130**, 67002 (2020).