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Quantum graphs with vertices of a preferred orientation

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ABSTRACT

Motivated by a recent application of quantum graphs to model the anomalous Hall effect we discuss quantum graphs the vertices of which exhibit a preferred orientation. We describe an example of such a vertex coupling and analyze the corresponding band spectra of lattices with square and hexagonal elementary cells showing that they depend heavily on the network topology, in particular, on the degrees of the vertices involved.

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1. Introduction

Quantum graphs represent an exceptionally fruitful concept both from the theoretical point of view as well as a tool for numerous applications – for a review and a rich bibliography we refer to the monograph [1]. The present letter is motivated by a recent application of the quantum graph technique to the anomalous Hall effect [6]. The idea of this work is to model the motion of electrons in atomic orbitals by a network of rings with a δ coupling in their junctions; the one considered in [6] is topologically equivalent to a square lattice giving rise to the Kronig–Penney-type spectrum [2].

The model is simple and elegant but it has a drawback. In the real situation only atomic orbitals with particular angular momentum values are involved; to model such a situation in the quantum-graph setting one has to break the time-reversal invariance by assuming that electrons move on the rings in one direction only. Since this cannot be justified from the first principles, one is inspired to think how quantum graphs with a preferred orientation may look like. It is clear that restriction cannot be imposed on the edges on which the particle moves as on one-dimensional line segments. On the other hand, the vertex coupling offers such a possibility. While the couplings used typically in various models, the Kirchhoff one and more generally the δ coupling, as well as various versions of the δ' coupling and others, are time-reversal invariant, the general self-adjoint conditions given by (1) below lose this property if the matrices A, B are nonreal. The question is whether some couplings in this broad class can be associated with a rotational motion in lattice models of the mentioned type. Our goal is to introduce and analyze the simplest example of that type. We focus here on its properties rather to an application to particular physical effects; this would require to employ a more general class of such couplings with parameters that will allow, in particular, to tune the 'rotation'.

The coupling we are going to discuss will be introduced in the next section where we will derive the appropriate spectral and scattering properties of a star-graph system. Then, in Sections 3 and 4, we will analyze spectra of periodic lattices with the square and hexagon basic cells, respectively. Our main observation is that the transport properties of these systems depend heavily on the lattice topology, in particular, on the vertex degree of its junctions.

2. Vertex coupling with a preferred orientation

Consider a star graph with N semi-infinite edges which meet at a single vertex. The state Hilbert space associated with it is $\bigoplus_{j=1}^{N} L^2(\mathbb{R}_+)$, the elements of which are $\Psi = \{\psi_j\}$, and the Hamiltonian of the system in the absence of external fields is negative Laplacian, $H\{\psi_j\} = \{-\psi_j''\}$, where as usual we employ the units in which $\hbar = 2m = 1$. To make H self-adjoint, one has to specify its domain by imposing suitable matching conditions to the boundary

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values of the functions $\{\psi_j\} \in \bigoplus_{j=1}^N H^2(\mathbb{R}_+)$. It is well known [5] that in general such conditions can be written as

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

where the $N \times N$ matrices A, B are such that the $N \times 2N$ matrix $(A|B)$ has the full rank and A^*B is Hermitean; alternatively one writes $A = U - I$, $B = i(U + I)$ where U is an $N \times N$ unitary matrix [3,4].

Consider the reversion operator, $R\{\psi_j\} = \{\psi_{N+1-j}\}$. In contrast to the commonly used vertex couplings we are interested in those giving rise to Hamiltonians that *do not* commute with R. In this paper we are going to consider the simplest example of this type in which the coupling exhibits 'maximum rotation' at a fixed energy, here conventionally set to occur at the momentum $k = 1$ (this fixes the momentum scale, of course, to change it one can put $k = p/p_0$ for a suitable p_0). This is achieved by choosing

$$U = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}$$

which is obviously unitary. In the component form, writing for simplicity $\psi_j = \psi_j(0+)$ and $\psi'_j = \psi'_j(0+)$, $j = 1, \cdots, N$, the matching conditions are

$$(\psi_{j+1} - \psi_j) + i(\psi'_{j+1} + \psi'_j) = 0\,, \quad j \in \mathbb{Z}\,(\mathrm{mod}\, N)\,; \tag{2}$$

note that they are non-trivial only for $N \geq 3$. The non-invariance under R is obvious, the first bracket changes sign under the reversion.

Let us look how the spectrum of the operator H determined by the conditions (2) looks like. It not difficult to check that its essential component is absolutely continuous and coincides with the positive half of the real axis. As for discrete spectrum in the negative part, it follows from general principles that its dimension cannot exceed N. In fact the eigenvalues are easy to find: if we write the supposed solution as $\psi_j(x) = c_j e^{-\kappa x}$ and plug this Ansatz into (2) we get a system of equations for the coefficients c_i. The requirement of its solvability yields the spectral condition

$$(\kappa - i)^N + (-1)^{N-1}(\kappa + i)^N = 0\,,$$

which has solutions for any $N \geq 3$. Specifically, the star graph Hamiltonian H has eigenvalues $-\kappa^2$, where

$$\kappa = \tan\frac{\pi m}{N} \tag{3}$$

with m running through $1, \cdots, [\frac{N}{2}]$ for N odd and $1, \cdots, [\frac{N-1}{2}]$ for N even. Thus the discrete spectrum is always nonempty, in particular, H has a single negative eigenvalue for $N = 3, 4$ which is equal to -1 and -3, respectively.

The quantity of interest in the continuous spectrum is the scattering matrix. It is straightforward to show [1] that the on-shell S-matrix at the momentum k is

$$S(k) = \frac{k - 1 + (k+1)U}{k + 1 + (k-1)U}\,. \tag{4}$$

In particular, in accord with the construction the rotation is maximal for $k = 1$ because then $S = U$ and one sees that a wave arriving at the vertex on the jth edge is diverted to the $(j-1)$th one, cyclically. It might seem that relation (4) implies that the transport becomes trivial at small and high energies, since $\lim_{k\to 0} S(k) = -I$ and $\lim_{k\to\infty} S(k) = I$.

However, more caution is needed; the formal limits may lead to a false result if the $+1$ or -1 are eigenvalues of the matrix U. A counterexample can be found in vertices with Kirchhoff coupling. In that case U has only ± 1 as its eigenvalues and it is well known that the corresponding on-shell S-matrix is independent of k and it is *not* a multiple of the identity.

Let us thus look at the right-hand side of (4) more closely. A straightforward, even if a bit tedious computation yields the explicit form of $S(k)$: denoting

$$\eta := \frac{1-k}{1+k}$$

we have

$$S_{ij}(k) = \frac{1-\eta^2}{1-\eta^N}\left\{-\eta\,\frac{1-\eta^{N-2}}{1-\eta^2}\,\delta_{ij} + (1-\delta_{ij})\,\eta^{(j-i-1)(\mathrm{mod}\,N)}\right\}. \tag{5}$$

In the lowest vertex degree cases formula (5) yields

$$S(k) = \frac{1+\eta}{1+\eta+\eta^2}\begin{pmatrix} -\frac{\eta}{1+\eta} & 1 & \eta \\ \eta & -\frac{\eta}{1+\eta} & 1 \\ 1 & \eta & -\frac{\eta}{1+\eta} \end{pmatrix} \tag{6}$$

and

$$S(k) = \frac{1}{1+\eta^2}\begin{pmatrix} -\eta & 1 & \eta & \eta^2 \\ \eta^2 & -\eta & 1 & \eta \\ \eta & \eta^2 & -\eta & 1 \\ 1 & \eta & \eta^2 & -\eta \end{pmatrix} \tag{7}$$

for $N = 3, 4$, respectively. We see that $\lim_{k\to\infty} S(k) = I$ holds for $N = 3$ and more generally for all odd N, while for the even ones the limit is not a multiple of identity. This is obviously related to the fact that in the latter case U has both ± 1 as its eigenvalues, while for N odd -1 is missing.

3. Square lattices

As indicated, our main topic in this letter are properties of periodic lattice graphs with the described reversion non-invariant coupling (2) at the vertices. Our first example is the square lattice of the edge length $\ell > 0$. The system is periodic, hence its energy bands are obtained through investigation on the elementary-cell component of the Hamiltonian at a fixed value of the quasimomentum [1, Chap. 4]. We choose edge coordinates increasing in the direction up and right and use the abbreviation $\omega_j = e^{i\theta_j}$, $j = 1, 2$, for the Bloch phase factors. To match the four wave functions at a fixed vertex, conventionally labeled as $x = 0$, we write the Ansatz

$$\begin{aligned} \psi_1(x) &= a_1 e^{ikx} + b_1 e^{-ikx}\,, \\ \psi_2(x) &= a_2 e^{ikx} + b_2 e^{-ikx}\,, \\ \psi_3(x) &= \omega_1\left(a_1 e^{ik(x+\ell)} + b_1 e^{-ik(x+\ell)}\right), \\ \psi_4(x) &= \omega_2\left(a_2 e^{ik(x+\ell)} + b_2 e^{-ik(x+\ell)}\right). \end{aligned} \tag{8}$$

Plugging the corresponding boundary values $\psi_j(0)$, $\psi'_j(0)$, $j = 1, 2, 3, 4$, into the conditions (2) taking into account that the derivatives there are taken in the direction away from the vertex, we get a system of linear equations for the coefficients a_j, b_j which is solvable provided the determinant

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