Reducible Fermi Surfaces for Non-symmetric Bilayer Quantum-Graph Operators

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Abstract. This work constructs a class of non-symmetric periodic Schrödinger operators on metric graphs (quantum graphs) whose Fermi, or Floquet, surface is reducible. The Floquet surface at an energy level is an algebraic set that describes all complex wave vectors admissible by the periodic operator at the given energy. The graphs in this study are obtained by coupling two identical copies of a periodic quantum graph by edges to form a bilayer graph. Reducibility of the Floquet surface for all energies ensues when the coupling edges have potentials belonging to the same asymmetry class. Two potentials are said to be in the same asymmetry class if their spectral A-functions $a(\lambda)$, defined in the article, are identical. Symmetric potentials have $a(\lambda) \equiv 0$. If the potentials of the connecting edges belong to different asymmetry classes, then typically the Floquet surface is not reducible. Bilayer graphene is a notable exception. Its Floquet surface is the zero set of a single composite variable and therefore is always reducible.

Key words: quantum graph, graph operator, periodic operator, bound state, embedded eigenvalue, reducible Fermi surface, local perturbation, defect state, coupled graphs, Floquet transform

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1 Introduction

The Fermi surface for a periodic Schrödinger operator $-\nabla^2 + q(x)$ ($x \in \mathbb{R}^n$) is the analytic set of complex wavevectors $(k_1, \ldots, k_n)$ for which the operator admits a (non-square-integrable) state at a fixed energy $\lambda$. For periodic Schrödinger operators on metric graphs, known as quantum graphs, the Fermi surface is an algebraic set in the variables $(z_1, \ldots, z_n) = (e^{ik_1}, \ldots, e^{ik_n})$—that is, the zero set of a polynomial in several variables. The reducibility of the Fermi surface into the union of two algebraic sets is important because it is intimately related to the existence of embedded eigenvalues induced by a local perturbation of the operator. It is proved in [17] that reducibility is required for a local perturbation to engender a square-integrable eigenfunction with unbounded support at an energy that is embedded in the continuous spectrum.

That a polynomial in several variables generically cannot be factored nontrivially indicates that a quantum graph must possess special features in order that a local defect be able to support an embedded eigenvalue with eigenfunction having unbounded support. The typical feature is symmetry. For a class of operators possessing reflectional symmetry, it is proved in [22] §3 that such eigenfunctions are possible due to the decomposition of the operator on even and odd states, which, in turn, effects a canonical reduction of the Fermi surface. The present work addresses the reducibility of the Fermi surface for a certain class of quantum graphs that are not decomposable by symmetry. Although the underlying metric graphs are reflectionally symmetric, the Schrödinger operators on them are not. The construction of embedded eigenvalues is not investigated here.

Reducibility or irreducibility of the Fermi surface has been established for precious few periodic operators. It is irreducible for all but finitely many energies for the discrete two-dimensional Laplacian plus a periodic potential [14] and for the continuous Laplacian plus a separable potential in two and three dimensions [4, 16]. And as mentioned already, it is reducible for quantum graphs that admit a reflectional symmetry. This work adds to that list a large class of non-reflectionally-symmetric operators with reducible Fermi surface.
The fundamental object of study is the “bilayer graph” obtained by coupling two identical copies of a quantum graph by edges connecting corresponding vertices, as shown in Fig. 1. The potential \( q_e(x) \) of the action of the Schrödinger operator on a connecting edge \( e \), namely \(-d^2/dx^2 + q_e(x)\), imparts asymmetry to the graph. An entire spectral function \( a(\lambda) \), called the A-function, associated to any potential \( q(x) \), is introduced (equation 2.17, §2.1). Its significance is that it decides whether two different potentials are compatible with regard to their asymmetry. One of the main results of this work, Theorem 6 in section 6, is that reducibility of the Floquet surface occurs when the coupling edges have potentials belonging to the same asymmetry class, two potentials being in the same class if their spectral A-functions \( a(\lambda) \) are identical. Symmetric potentials have \( a(\lambda) \equiv 0 \). Exceptionally, bilayer quantum-graph graphene turns out to have a reducible Fermi surface regardless of the two asymmetry classes of the connecting edges, as reported in Theorem 6 in section 6. These two main theorems in this work can be paraphrased as follows.

**Theorem 0.**
(a) The Fermi surface of a periodic bilayer quantum graph is reducible if the potentials \( q_e(x) \) of all the connecting edges \( e \) possess the same spectral asymmetry function (A-function) \( a(\lambda) \).
(b) The Fermi surface of bilayer graphene is reducible regardless of the two A-functions of the connecting edges.

To construct a bilayer graph, one starts with a given periodic quantum graph \((\tilde{\Gamma}, \tilde{A})\), where \( \tilde{\Gamma} \) is a metric graph and \( \tilde{A} \) is a Schrödinger operator defined on it (section 3). The periodicity means that there is a faithful \( \mathbb{Z}^n \) action on \( \tilde{\Gamma} \) that commutes with \( \tilde{A} \). The action of \( g = (g_1, \ldots, g_n) \in \mathbb{Z}^n \) is viewed as a shift along along the vector \( g_1 v_1 + \cdots + g_n v_n \), with \( \{v_j\}_{j=1}^n \) being independent generating period vectors. This quantum graph is declared to be a single layer. A bilayer periodic quantum graph \((\Gamma, A)\) is then built by taking two copies of the single layer and coupling them by edges that connect corresponding vertices, as in Fig. 1. Although the bare bilayer metric graph possesses reflectional symmetry about the centers of the connecting edges, the potentials associated to the connecting edges are allowed to be asymmetric.

![Figure 1: An example of a bilayer quantum graph based on the single-layer hexagonal graphene structure.](image)

Floquet modes \( u(x) \) of \((\Gamma, A)\) are simultaneous eigenfunctions of \( A \) and the \( \mathbb{Z}^n \) action,

\[
Au = \lambda u, \quad u(g \cdot) = z^g u \tag{1.1}
\]

for \( g = (g_1, \ldots, g_n) \in \mathbb{Z}^n \). Here, \( \lambda \in \mathbb{C} \) is called the energy and \( z = (z_1, \ldots, z_n) \in (\mathbb{C}^*)^n \) is called the vector of Floquet multipliers associated with each of the \( n \) fundamental shifts, and \( z^g = z_1^{g_1} \cdots z_n^{g_n} \). The wavevector \( k = (k_1, \ldots, k_n) \in \mathbb{C}^n \) is such that \( z = e^{ik} \), that is \( z_\ell = e^{ik_\ell} \) for \( \ell = 1, \ldots, n \), and its components are defined up to the addition of an integer multiple of \( 2\pi i \). Floquet modes are never square integrable.

The dispersion relation \( D(\lambda, z) = 0 \) describes the pairs \((\lambda, z)\) for which \((\Gamma, A)\) admits a Floquet mode. The function \( D(\lambda, z) \) is called the dispersion function; it is analytic in \( \lambda \) and a Laurent polynomial in \( z \). As a subset of \( \mathbb{C} \times (\mathbb{C}^*)^n \), the dispersion relation is known as the Bloch variety or dispersion surface of \((\Gamma, A)\).

The present study concerns this relation for fixed energy \( \lambda \) considered as an algebraic curve in \((\mathbb{C}^*)^n \). This set \( \Phi_\lambda = \Phi_{A,\lambda} \) is called the Floquet surface or Floquet variety for \( A \) at energy \( \lambda \),

\[
\Phi_\lambda := \{ z \in (\mathbb{C}^*)^n : D(\lambda, z) = 0 \} \tag{1.2}
\]
When considered as a function of the wavevector $k$, it is the Fermi surface we have been discussing. The reducibility of $\Phi_\lambda$ is equivalent to the factorization of $D(\lambda, z)$ as a Laurent polynomial in the several variables $z = (z_1, \ldots, z_n)$ into two distinct factors. This reveals a deep connection between factorability of polynomials in several variables and embedded eigenvalues. The connection transpires through the Floquet transform (the Fourier transform with respect to the $\mathbb{Z}^n$ symmetry group) as demonstrated in \cite{17} in the proof of Theorem 6 (p. 679).

This article establishes the following hierarchy of symmetry properties of periodic bilayer quantum graphs and the corresponding reducibility properties of the Floquet surface.

1. Symmetric connecting edges: vanishing A-function $a(\lambda) = 0$. Reducibility of the Floquet surface $\Phi_\lambda$ is obtained by a canonical decomposition of the bilayer graph operator onto the even and odd states with respect to the reflectional symmetry about the connecting edges. This was shown in \cite{22} and is reviewed in section 4.

2. Asymmetric connecting edges with identical A-functions $a(\lambda)$. Reducibility of the Floquet surface $\Phi_\lambda$ is obtained by an energy-dependent decomposition of the operator reduced to the generalized (not square integrable) eigenspace of Floquet modes for each given energy $\lambda$. The proof is in section 5.

3. Asymmetric connecting edges with different A-functions $a(\lambda)$: bilayer graphene. Reducibility of the Floquet surface $\Phi_\lambda$ is obtained due to a special reduction of the dispersion function $D(\lambda, z)$ to a function of a single composite variable $\zeta = (1 + z_1 + z_2)(1 + z_1^{-1} + z_2^{-1})$. The analysis is carried out in section 6.

4. Asymmetric connecting edges with different A-functions $a(\lambda)$: general case. Irreducibility of the Floquet surface $\Phi_\lambda$ is generic. It is proved for a simple example in section 7.

The following natural questions deserve particular attention.

- When the connecting edges are symmetric (case 1), the components of the bilayer quantum graph $(\Gamma, A)$ acting in the even and odd spaces of states can be realized as operators on “decorated” copies of the single-layer graph $\hat{\Gamma}$. These decorations are obtained by attaching a dangling edge to each vertex of the single layer and imposing a self-adjoint condition on the terminal, or free, vertex of that edge. It turns out that, when the connecting edges are not symmetric, such a realization is not possible (Theorem 5).

- The graphene structure is known to possess remarkable properties; most notably, the hexagonal structure is responsible for conical singularities in the dispersion surface \cite{2, 12}. Its bilayer form emerges again as special in this work. The calculation in section 6 reveals that the bipartite property of bilayer graphene is responsible for the reducibility of its Floquet surface, independently of the asymmetry classes of the connecting edges. The implication is that spectrally embedded bound states should be more common in bilayer graphene than in other bilayer models. Interesting aspects of locally defective bilayer graphene can be found in the literature, for example \cite{9, 19}.

- It is noteworthy that not only does bilayer graphene possess a reducible Floquet surface, but, importantly, that the Floquet modes of the two components the Floquet surface lie in independent two-dimensional subspaces of the four-dimensional parameter space of Floquet modes at any given energy. (This property is automatic in the first two cases in the hierarchy because of the decomposition of the reduced operator.) More precisely, single-layer graph graphene has two vertices in one period (fundamental domain of the $\mathbb{Z}^n$ action), and thus bilayer graphene has four. The values of a Floquet mode at these four vertices determines its values on the entire graph, as long as the energy is not a Dirichlet eigenvalue of any edge of the graph. As $z = (z_1, z_2)$ traverses one component of the algebraic curve $D(\lambda, z) = 0$ with $\lambda$ fixed, the corresponding Floquet mode, considered as an element of the four-dimensional complex vector space $\mathbb{C}^4$ with components equal to the values of the mode at the four vertices of the fundamental domain, remains within a two-dimensional subspace of $\mathbb{C}^4$. The Floquet modes of the other component remain within a complementary two-dimensional subspace. This is part of Theorem 6.
The separation of the Floquet modes corresponding to the two components of the Floquet surface into two complementary linear spaces enters the construction of embedded eigenvalues supported by a local defect. The question therefore arises as to whether there are periodic bilayer quantum graphs for which the Floquet surface is reducible but for which the spaces of Floquet modes of the two components are not independent. This case is intermediate between cases 3 and 4. One also wonders whether reducibility when connecting edges have different asymmetry classes is always due to the reduction of the dispersion function to a function of a single composite variable.

Section 2 introduces the spectral A-function and defines the notion of an asymmetry class of connecting edges. Section 3 lays down the precise construction of periodic bilayer quantum graphs. Section 4 reviews the case of symmetric coupling potentials, and Section 5 proves the main Theorem 4 on reducibility for coupling potentials with compatible asymmetries. Section 6 presents the special case of bilayer graphene, and Section 7 addresses generic periodic bilayer quantum graphs.

2 Analysis of a single edge and asymmetry

Let the edge \( e \) connecting the vertices \( v \) and \( w \) be parameterized by identifying it with the interval \([0, 1]\), directed from \( v \) to \( w \). This allows one to define a Schrödinger operator \(-d^2/dx^2 + q(x)\) on \( e \), with \( q \in L^2([0, 1], \mathbb{R}) \cong L^2(e, \mathbb{R})\). When the same edge \( e \) is considered as directed from \( w \) to \( v \), it is identified with \([0, 1]\) by replacing \( x \) with \( 1-x \), and the Schrödinger operator now takes the form \(-d^2/dx^2 + \tilde{q}(x)\), in which \( \tilde{q}(x) \) denotes the reflection of \( q \) about the center of the interval \([0, 1]\),

\[
\tilde{q}(x) = q(1-x).
\]  

(2.3)

In order to avoid burdensome technicalities, it is convenient to identify a function \( u : e \to \mathbb{C} \) with the corresponding function of the parameter \( x \) by writing \( u : [0, 1] \to \mathbb{C} \). Let a function \( u \) in the Sobolev space \( H^2(0, 1) \cong H^2(e) \) of square-integrable functions with square-integral derivatives satisfy the eigenvalue condition

\[
(-d^2/dx^2 + q(x) - \lambda)u = 0
\]

(2.4)
on \((0, 1)\). Since the vertices \( v \) and \( w \) are identified with the points 0 and 1, one can write

\[
\begin{align*}
  u(v) &= u(0), & u(w) &= u(1) \\
  u'(v) &= du/dx(0), & u'(w) &= -du/dx(1).
\end{align*}
\]

(2.5)

The reason for the minus sign is that it is appropriate to treat the two vertices symmetrically, taking the derivative at each vertex in the direction pointing out of the vertex and into the edge.

2.1 Spectral functions for an edge: The A-function

Given an edge \( e \) directed from \( v \) to \( w \) with parameter \( x \in [0, 1] \), let \( c_q(x, \lambda) \) and \( s_q(x, \lambda) \) be a fundamental pair of solutions to \((-d^2/dx^2 + q(x) - \lambda)u = 0\) satisfying the initial conditions

\[
\begin{align*}
  c_q(0, \lambda) &= 1, & s_q(0, \lambda) &= 0 \\
  c_q'(0, \lambda) &= 0, & s_q'(0, \lambda) &= 1,
\end{align*}
\]

(2.6)
in which the prime denotes the derivative with respect to the first argument \( x \). Define

\[
\begin{align*}
  c_{(v,w)}(\lambda) &= c(\lambda) := c_q(1, \lambda), & s_{(v,w)}(\lambda) &= s(\lambda) := s_q(1, \lambda), \\
  c'_{(v,w)}(\lambda) &= c'(\lambda) := c_q'(1, \lambda), & s'_{(v,w)}(\lambda) &= s'(\lambda) := s_q'(1, \lambda),
\end{align*}
\]

(2.7)
in which the dependence on \( q \) is suppressed. When the edge \( e \) is directed from \( w \) to \( v \), the corresponding quantities have \( \tilde{q} \) in place of \( q \); they will also be abbreviated by use of a tilde. For example,

\[
c_{(w,v)}(\lambda) = \tilde{c}(\lambda) := c_{\tilde{q}}(1, \lambda).
\]

(2.8)
These four functions are entire and of exponential order $1/2$ and have their roots on the real line [13 §1.1].

An important observation is that $s(\lambda)$ is a function of the undirected edge $\{v, w\}$, whereas $c(\lambda)$ is a function of the directed edge $(v, w)$. Using the $x$-invariance of the Wronskian $c(x, \lambda)s'(x, \lambda) - c'(x, \lambda)s(x, \lambda)$, it is straightforward to show that $\tilde{c} = s'$, $s = \tilde{s}$, and $c' = c''$. One obtains therefrom the following relations among these entire functions.

\begin{align}
    s\{v, w\} &:= s_{(v, w)} = s = \tilde{s} = s_{(w, v)}, \\
    c'\{v, w\} &:= c'_{(v, w)} = c' = \tilde{c'} = c'_{(w, v)}, \\
    c_{(v, w)} &:= c = \tilde{s}' = s'_{(w, v)}, \\
    s'_{(v, w)} &:= s' = \tilde{c} = c_{(w, v)}. 
\end{align}

Define the transfer matrix $T_q(\lambda)$ for the edge $e$ directed from $v$ to $w$, for the potential $q$ and spectral value $\lambda$, to be the matrix that takes Cauchy data $(u(v), u'(v))$ at $v$ to Cauchy data $(u(w), u'(w))$ at $w$. Define the Dirichlet-to-Neumann, or DtN, map $G_q(\lambda)$ as that which takes Dirichlet data $(u(v), u(w))$ to Neumann data $(u'(v), u'(w))$. Using the identity $s'(\lambda) = \tilde{c}(\lambda)$, one obtains

\begin{align}
    \begin{bmatrix}
    c(\lambda) & s(\lambda) \\
    -c'(\lambda) & -\tilde{c}(\lambda)
    \end{bmatrix}
    T_{e(\lambda)}
    \begin{bmatrix}
    u(v) \\
    u'(v)
    \end{bmatrix}
    &=
    \begin{bmatrix}
    u(w) \\
    u'(w)
    \end{bmatrix}, \\
    \frac{1}{s(\lambda)}
    \begin{bmatrix}
    -c(\lambda) & 1 \\
    1 & -\tilde{c}(\lambda)
    \end{bmatrix}
    G_{e(\lambda)}
    \begin{bmatrix}
    u(v) \\
    u(w)
    \end{bmatrix}
    &=
    \begin{bmatrix}
    u'(v) \\
    u'(w)
    \end{bmatrix}.
\end{align}

$G_q(\lambda)$ is a meromorphic function with simple poles at the roots of $s(\lambda)$, which are the Dirichlet eigenvalues of $-d^2/dx^2 + q(x)$ on $e$ [13 Lemma 1.1.1]. It is akin to the Weyl-Titchmarsh M-function for an interval [13 §1.4.4].

The potential $q$ is uniquely decomposed into symmetric and anti-symmetric parts with respect to reflection about the center of $e$,

\begin{align}
    q(x) &= q_+(x) + q_-(x), \\
    \tilde{q}(x) &= q_+(x) - q_-(x). 
\end{align}

Define two entire spectral functions associated with the potential $q$,

\begin{align}
    a(\lambda) &= \frac{1}{2} \{c(\lambda) - \tilde{c}(\lambda)\}, \quad \text{(spectral A-function)} \\
    b(\lambda) &= \frac{1}{2} \{c(\lambda) + \tilde{c}(\lambda)\}.
\end{align}

The first of these shall be known as the spectral asymmetry function, or “A-function” associated with $q(x)$.

**Definition 1.** Two potentials $q_1$ and $q_2$ in $L^2([0, 1], \mathbb{R})$ are said to be in the same asymmetry class if their associated A-functions are identical. Such potentials are said to have compatible asymmetries.

Observe that the A-function is a function of a directed edge; it is additively inverted under a change of direction. Thus, if $q$ is considered to be a function defined on an edge $e$ rather than a function of $x \in [0, 1]$, a direction must be specified in order to determine the A-function; precisely,

\begin{align}
    a_{(v, w), q} &= -a_{(w, v), q}.
\end{align}

That this is a good definition is manifest by the following theorem, which relies on a uniqueness theorem by G. Borg for an inverse spectral problem.
\textbf{Theorem 2.} The A-function \( a(\lambda) \) associated with the potential \( q \in L^2([0,1], \mathbb{R}) \) satisfies
\[
c'(\lambda) a(\lambda) = -\int_0^1 q_-(x) c(x,\lambda) \tilde{c}(x,\lambda) \, dx, \tag{2.20}\]
and \( q \) is symmetric if and only if \( a \) vanishes identically, that is,
\[
q(x) = q(1-x) \iff a(\lambda) = 0. \tag{2.21}
\]
The first equality is in the sense of \( L^2 \) (almost every \( x \)), and the second means for all \( \lambda \in \mathbb{C} \).

\textbf{Proof.} Let \( q(x) = q_+(x) + q_-(x) \) be such that \( q_+(x) = q_+(1-x) \) and \( q_-(x) = -q_-(1-x) \). The functions \( c = c(x,\lambda) \) and \( \tilde{c} = \tilde{c}(x,\lambda) \) satisfy
\[
-c'' + (q_+(x) + q_-(x))c + \lambda c = 0 \tag{2.22}
\]
\[
-c'' + (q_+(x) - q_-(x))\tilde{c} + \lambda \tilde{c} = 0, \tag{2.23}
\]
in which the prime denotes differentiation with respect to the first argument \( x \), with
\[
c(0,\lambda) = \tilde{c}(0,\lambda) = 1, \quad c'(0,\lambda) = \tilde{c}'(0,\lambda) = 0. \tag{2.24}
\]
Multiplying the first differential equation by \( \tilde{c} \) and the second by \( c \) and then subtracting yields
\[
(c\tilde{c}' - c\tilde{c}')' + 2q_-c\tilde{c} = 0. \tag{2.25}
\]
Using the initial conditions for \( c \) and \( \tilde{c} \) and the fact that \( c'(1,\lambda) = \tilde{c}'(1,\lambda) \), one obtains the formula in the proposition.

The second part of the theorem is a consequence of Borg’s theorem on the determination of \( q \) from the spectra for two different boundary conditions (\cite[Theorem 1.4.4]{7}). The zero set of \( c(\lambda) \) is equal to the spectrum for the potential \( q \) with boundary conditions \( u'(0) = 0 \) and \( u(1) = 0 \) (N-D spectrum), and the zero set of \( c'(\lambda) \) is the spectrum for \( q \) with conditions \( u'(0) = 0 \) and \( u'(1) = 0 \) (N-N spectrum). Given that \( a(\lambda) = 0 \), one has both \( c(\lambda) = \tilde{c}(\lambda) \) and \( c'(\lambda) = \tilde{c}'(\lambda) \), which implies that the N-D spectra for both potentials \( q \) and \( \tilde{q} \) are identical and the N-N spectra for both potentials are identical. This is sufficient, by Borg’s Theorem, to guarantee the (almost-everywhere) equality of \( q \) and \( \tilde{q} \). The author is indebted to his colleagues \cite{8} for pointing out the applicability of Borg’s theorem to this situation. \( \square \)

Theorem 2 implies that the symmetric functions \( q_c(x) \) form a single asymmetry class associated with \( a(\lambda) = 0 \).

\subsection{Riemann surface for an edge}

Analysis of the decomposition of coupled quantum-graph operators and the reduction of the Floquet surface in subsequent sections is based on the spectral resolution of the the DtN map \( G(\lambda) \) for each directed connecting edge \( e = (v,w) \). This spectral resolution is naturally defined on the Riemann surface associated with the characteristic polynomial of \( G(\lambda) \). A complete theory of the spectral resolution of meromorphic operators in finite dimensions on Riemann surfaces is available in \cite[Ch.3 §4]{5}.

It is convenient to deal with the entire matrix function
\[
s(\lambda)G(\lambda) = -\begin{bmatrix} b(\lambda) & 0 \\ 0 & b(\lambda) \end{bmatrix} + \begin{bmatrix} -a(\lambda) & 1 \\ 1 & a(\lambda) \end{bmatrix}, \tag{2.26}
\]
and treat the spectral theory of the trace-free part of \( s(\lambda)G(\lambda) \),
\[
N(\lambda) = \begin{bmatrix} -a(\lambda) & 1 \\ 1 & a(\lambda) \end{bmatrix}, \tag{2.27}
\]

\[6\]
which involves only the A-function of the edge. The characteristic polynomial in $\mu$ of $N(\lambda)$ is
\begin{equation}
 p(\lambda, \mu) = \mu^2 - (a(\lambda)^2 + 1). \tag{2.28}
\end{equation}

One computes that the projection associated to an eigenvalue $\mu$ is
\begin{equation}
 P_\mu = \frac{1}{2\mu} \begin{bmatrix}
 (a(\lambda) + \mu)^{-1} & 1 \\
 1 & a(\lambda) + \mu
\end{bmatrix}. \tag{2.29}
\end{equation}

This is a meromorphic matrix function on a Riemann surface, described next.

$N(\lambda)$ has an analytic eigenvalue $\mu$ on the Riemann surface defined by the zero-set of $p(\lambda, \mu)$,
\begin{equation}
 S = \{ (\lambda, \mu) \in \mathbb{C}^2 : \mu^2 = a(\lambda)^2 + 1 \} . \tag{2.30}
\end{equation}

The corresponding eigenvalue of $s(\lambda)G(\lambda)$ is $-b(\lambda) + \mu$, and the other eigenvalue is $-b(\lambda) - \mu$. The projection $S \rightarrow \mathbb{C} :: (\lambda, \mu) \mapsto \lambda$ is regularized over the set of points
\begin{equation}
 \{ \lambda \in \mathbb{C} : a(\lambda) \in \{ i, -i \} \} \quad \text{(ramification points).} \quad \tag{2.31}
\end{equation}

About a point $(\lambda_0, \mu)$ with $\mu \neq 0$, that is, where $\lambda_0$ is not a ramification point, the variable $\lambda$ serves locally as a complex coordinate for $S$. At a point $(\lambda_0, 0)$ on $S$ above a ramification point $\lambda_0$, the relation $p(\lambda, \mu) = 0$ can be written as
\begin{equation}
 \mu^2 = (\lambda - \lambda_0)^n f(\lambda), \quad f(\lambda_0) \neq 0, \quad n \geq 1. \tag{2.32}
\end{equation}

If $n = 1$, then $\mu$ serves as a local analytic coordinate for $S$ about $(\lambda_0, 0)$. When $n \geq 2$, the point $(\lambda_0, 0) \in S$ is singular but can be regularized as follows. Let $\tilde{f}(\lambda)$ be analytic and non-vanishing in a neighborhood of $\lambda = \lambda_0$ with the property that $\tilde{f}(\lambda)^2 = f(\lambda)$. In the case that $n = 2m$ is even, there are two sheets above a neighborhood of $(\lambda_0, 0)$,
\begin{equation}
 \{ (\lambda, \mu) : \mu = (\lambda - \lambda_0)^m \tilde{f}(\lambda) \} \quad \text{and} \quad \{ (\lambda, \mu) : \mu = -(\lambda - \lambda_0)^m \tilde{f}(\lambda) \} . \tag{2.33}
\end{equation}

In a neighborhood of $\lambda_0$, each sheet has $\lambda$ as an analytic coordinate and the two sheets intersect only in $(\lambda_0, 0)$. By a mild abuse of notation, one can replace the two local sheets by their disjoint union so that $S$ becomes regular at $(\lambda_0, 0)$. In the case that $n = 2m + 1$ is odd, a neighborhood of $(\lambda_0, 0)$ in $S$ can be realized as a connected complex surface by taking $w = \sqrt{\lambda - \lambda_0}$ as an analytic coordinate. More precisely, a neighborhood of $0$ in the $w$-plane maps onto a neighborhood of $(\lambda_0, 0)$ in $S$ by means of the map
\begin{equation}
 w \mapsto \left( w^2 + \lambda_0, w^{2m+1} \tilde{f}(w^2 + \lambda_0) \right) . \tag{2.34}
\end{equation}

The projections $P_\mu$ are meromorphic functions on $S$, regularized as described. The principal part at a point where $a(\lambda_0) = \pm i$ is
\begin{equation}
 \frac{\pm 1}{2f(\lambda_0)(\lambda - \lambda_0)^m} \begin{bmatrix}
 \mp i & 1 \\
 1 & \pm i
\end{bmatrix} \quad \text{for } n = 2m \tag{2.35}
\end{equation}
and
\begin{equation}
 \frac{1}{2f(\lambda_0)w^{2m+1}} \begin{bmatrix}
 \mp i & 1 \\
 1 & \pm i
\end{bmatrix} \quad \text{for } n = 2m + 1. \tag{2.36}
\end{equation}

### 3 Bilayer quantum graphs: Coupling by edges

This section defines a periodic quantum graph and the procedure of coupling two identical graphs with auxiliary edges to form a new periodic quantum graph called a bilayer quantum graph, formalized in Definition 3.4. Some background and notation is needed for providing a precise construction to support this definition.

This section also describes the energy-dependent reduction to a combinatorial graph and the Floquet transform and the Floquet surface (or Fermi surface) for these periodic graphs. The description of quantum graphs essentially follows [6], but the notation is developed to suit periodic bilayer quantum graphs.
### 3.1 Periodic quantum graphs

A periodic quantum graph $\Gamma$ consists of the following structure. Some of the notation may seem technical, but it is all very natural.

1. An underlying graph with vertex set $V = V(\Gamma)$ and edge set $E = E(\Gamma)$ is endowed with an action by the group $\mathbb{Z}^n$ that preserves the vertex-edge incidence and such that $\Gamma/\mathbb{Z}^n$ is a finite graph. The action of $g \in \mathbb{Z}^n$ on a vertex or edge of $\Gamma$ is denoted by $v \mapsto gv$ or $e \mapsto ge$. A fundamental domain of the $\mathbb{Z}^n$ action is denoted by $W$.

An edge in $e \in E$ is an unordered set $e = \{v, w\}$ of vertices. It will be necessary to allow any edge $\{v, w\}$ to assume either of the two directions associated with the ordered pairs $(v, w)$ and $(w, v)$. For each vertex $v \in V$, let $E(v)$ denote the set of directed edges incident to $v$, directed away from $v$,

$$E(v) := \{(v, w) : \{v, w\} \in E\}. \quad (3.37)$$

Thus, if $e = (v, w) \in E(v)$, then $\tilde{e} = (w, v) \in E(w)$. The symbol $e$ may denote either an edge or a directed edge; a directed edge may also be denoted with an arrow $\vec{e}$ when the distinction between undirected and directed is necessary.

2. $\Gamma$ becomes a metric graph by associating each edge $e = \{v, w\} \in E$ with an interval $[0, L_e]$. The directed edge $\vec{e} = (v, w)$ is referred to coordinate $x_\vec{e} \in [0, L_e]$ with $x_\vec{e} = 0$ corresponding to $v$ and $x_\vec{e} = L_e$ corresponding to $w$. The oppositely directed edge $\tilde{e} = (w, v)$ is referred to coordinate $x_{\tilde{e}} \in [0, L_e]$, with $x_{\tilde{e}} + x_\vec{e} = L_e$. Assume that this metric structure is invariant under the action of $\mathbb{Z}^n$, and let the action of $g \in \mathbb{Z}^n$ on a point $x$ in $\Gamma$ be denoted by $x \mapsto gx$ ($x$ may be in the interior of an edge or at an endpoint corresponding to a vertex). This “metrization” allows one to define standard function spaces on any edge $e$, such as the Sobolev spaces $H^s(e)$.

3. One renders $\Gamma$ a periodic quantum graph by pairing it with a Schrödinger operator $A$ that commutes with the $\mathbb{Z}^n$ action. On each edge $e$, $A$ acts by $-D^2 + q_e(x)$. Here, $D^2 = d^2/dx^2$, with $\vec{e}$ referring to either direction; and $x$ is any point along $e$. $A$ acts on functions $f = \{f_e\}_{e \in E}$ defined on all of $\Gamma$ and that satisfy a Robin condition at each vertex

$$\sum_{e \in E(v)} f'_e(v) = \alpha_v f(v). \quad (R)$$

Here, $f_e$ is the restriction of a function $f$ on $\Gamma$ to $e$, and if $e = (v, w)$, $f'_e(v)$ is the derivative of $f_e$ at the vertex $v$ directed away from $v$ toward $w$, that is, the derivative from the right of $f_e$ with respect to the coordinate $x_e$ at $x_e = 0$. The vertex condition $[R]$ is also known as a $\delta$-type coupling or matching condition $[\Pi]$.

To define $A$ precisely, first set

$$H^2(\Gamma) = \{ f = \{f_e\}_{e \in E} : f \text{ is continuous}; f_e \in H^2(e) \forall e \in E; f, f', f'' \in L^2(\Gamma) \}, \quad (3.38)$$

in which derivatives $f'$ and $f'' = D^2f$ are taken on each edge with respect to the coordinates introduced above; and let $q = \{q_e\}_{e \in E}$, with $q_e \in L^2(e)$ for each $e \in E(\Gamma)$ be a real-valued potential function. Then the domain of $A$ and its action thereon are given by

$$\mathcal{D}(A) = \{ f \in H^2(\Gamma) : f \text{ satisfies } [R] \forall v \in V(\Gamma) \}, \quad (3.39)$$

$$(Af)(x) = -f''(x) + q(x)f(x). \quad (3.40)$$

The Robin condition $[R]$ makes sense because $f \in H^2(\Gamma)$ has well defined derivatives at the endpoints of each edge. That $A$ is self-adjoint in $L^2(\Gamma)$ is subsumed by [6, Theorem 1.4.4].

The periodicity of $A$ means that $\alpha_{gv} = \alpha_v$ and $q_{ge}(gx) = q_e(x)$ for all $v \in V(\Gamma)$ and $x \in e \in E(\Gamma)$ and for all $g \in \mathbb{Z}^n$.

The Floquet modes of $A$ (simultaneous eigenfunctions of $A$ and $\mathbb{Z}^n$) do not lie in $\mathcal{D}(A)$, but in a larger space of functions that are locally like those in $\mathcal{D}(A)$,

$$H^{2R}_{\text{loc}}(\Gamma) = \{ f = \{f_e\}_{e \in E} : f \text{ is continuous}; f_e \in H^2(e) \forall e \in E; f \text{ satisfies } [R] \forall v \in V \}. \quad (3.41)$$
Reduction to a combinatorial graph. It is common to investigate the eigenvalue problem \((A - \lambda)u = 0\) for \(u \in H^2_\text{loc}(\Gamma)\) by reducing it to an equivalent nonlinear-in-\(\lambda\) eigenvalue problem \(\mathfrak{A}(\lambda)\bar{u} = 0\) for a combinatorial graph, as long as \(\lambda\) is not a Dirichlet eigenvalue for any edge, that is, \(s_e(\lambda) := s_q(\lambda) = 0\) for all \(e \in \mathcal{E}(\Gamma)\). This means that the equation \((A - \lambda)u = 0\) is equivalent to \(\mathfrak{A}(\lambda)\bar{u} = 0\), where \(\bar{u}\) is the restriction of \(u\) to \(\mathcal{V}(\Gamma)\) and \(\mathfrak{A}(\lambda)\) is a periodic (i.e., \(\mathbb{Z}^n\)-invariant) operator that acts on functions defined on \(\mathcal{V}(\Gamma)\). This reduction is accomplished by invoking the Dirichlet-to-Neumann map \(G_{q_e}(\lambda)\) for each edge \(e\) to rewrite the Robin condition solely in terms of the values of the function \(u\) at \(v\) and all of its adjacent vertices. One obtains

\[
H_{\text{loc}}(\Gamma) \ni \mathfrak{A}(\lambda)\bar{u}(v) := \sum_{e = (v, w) \in \mathcal{E}(v)} \frac{1}{s_e(\lambda)} \bar{u}(w) - \bar{u}(v) \left( \alpha_v + \sum_{e \in \mathcal{E}(v)} \frac{c_e(\lambda)}{s_e(\lambda)} \right) = 0. \tag{R'}
\]

As a definition of the operator \(\mathfrak{A}(\lambda)\), it is understood that \(\bar{u} : \mathcal{V}(\Gamma) \rightarrow \mathbb{C}\) is arbitrary. In conclusion, one has

\[
(A - \lambda)u = 0 \iff \mathfrak{A}(\lambda)\bar{u} = 0. \tag{3.42}
\]

\(\mathfrak{A}(\lambda)\) is called the reduced \(\lambda\)-dependent combinatorial operator associated with the quantum-graph operator \(A - \lambda I\), or, more simply, associated with \(A\).

The Dirichlet spectrum of a quantum graph \((\Gamma, A)\) is the set \(\sigma_D(A)\) consisting of all the eigenvalues of all the edges. For a periodic quantum graph for which a fundamental domain consists of a finite number of vertices and edges (that is, the set of orbits of the \(\mathbb{Z}^n\) action is a finite graph), this set is discrete,

\[
\sigma_D(A) = \{ \lambda \in \mathbb{C} : \exists \bar{e} \in \mathcal{V}(\Gamma), s_e(\lambda) = 0 \}. \tag{3.43}
\]

3.2 Floquet transform and Floquet surface

The Floquet transform is the Fourier transform with respect to the \(\mathbb{Z}^n\) action on the graph \(\Gamma\). Given a function \(f\), whose domain \(\Gamma\) includes points on the edges in the case of a metric graph, or just the vertex set of the graph in the case of a combinatorial one, define its Floquet transform by

\[
\hat{f}(z, x) := \sum_{g \in \mathbb{Z}^n} f(gx) z^{-g} \quad \text{for} \quad z = (z_1, \ldots, z_n) \in (\mathbb{C}^*)^n, \tag{3.44}
\]

in which \(z^h = z_1^{h_1} \cdots z_n^{h_n}\) for \(h \in \mathbb{Z}^n\). This is a formal Laurent series in the symbol \(z\) whose coefficients are shifts of \(f\). The essential property of \(\hat{f}\) is its quasi-periodicity in \(x\),

\[
\hat{f}(z, gx) = \hat{f}(z, x) z^g, \tag{3.45}
\]

which makes \(\hat{f}(z, \cdot)\) an eigenfunction for the \(\mathbb{Z}^n\) action with eigenvalue \(z^g\) for \(g \in \mathbb{Z}^n\).

If \(f \in L^2\), then one has the Fourier inversion theorem

\[
f(x) = \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \hat{f}(z, x) dV(z), \tag{3.46}
\]

in which \(dV\) is the \(n\)-dimensional volume measure on the \(n\)-torus

\[
\mathbb{T}^n := \{ z \in \mathbb{C}^n : |z_1| = \cdots = |z_n| = 1 \}. \tag{3.47}
\]

Property 3.45 shows that \(\hat{f}(z, \cdot)\) is determined by its restriction to a fundamental domain \(W\) of \(\Gamma\). When \(\hat{f}\) is considered as a function of variables \(z \in \mathbb{T}^n\) and \(x \in W\), the Floquet transform is a unitary transformation of Hilbert spaces,

\[
\hat{\cdot} : L^2(\Gamma) \rightarrow L^2(\mathbb{T}^n; L^2(W)). \tag{3.48}
\]

When \(x\) is restricted to \(W\), \(\hat{f}(z, x)\) reduces to a Laurent polynomial if \(f\) is supported in a finite number of translations \(gW\) of \(W\).
If an operator $A$ commutes with the $\mathbb{Z}^n$ action, the Floquet transform converts $A$ into a multiplication operator in the variable $z$ in the sense that
\[
(Af)(z, \cdot) = \hat{A}(z)f(z, \cdot),
\]
(3.49)
in which $\hat{A}(z)$ is a linear operator in $L^2(W)$. If $A$ is a periodic quantum-graph operator, as described in the previous section, then the operator $\hat{A}(z)$ has the form $-D^2 + q(x)$ as a differential operator, and it depends on $z$ only through its domain, which consists restrictions to $W$ of functions in the space $H^2_z(\Gamma)$ of eigenfunctions for $\mathbb{Z}^n$,
\[
H^2_z(\Gamma) := \{ f \in H^{2,R}_0(\Gamma) : f(g \cdot) = z^g f \ \forall g \in \mathbb{Z}^n \}.
\]
(3.50)
Under the Floquet transform, the combinatorial graph operator $\mathfrak{A}(\lambda)$ becomes an operator $\hat{\mathfrak{A}}(\lambda, z)$. This operator acts in the finite-dimensional complex vector space $L^2(\mathcal{V}(W)) = \mathbb{C}^{\mathcal{V}(W)}$, which consists of functions defined on the vertex set of a fundamental domain $W$ (so $\mathcal{V}(W)$ acts like a basis). A typical element of $\mathbb{C}^{\mathcal{V}(W)}$ is denoted by $u = \{u(v)\}_{v \in \mathcal{V}(W)}$ (or $\bar{u}$ for the restriction of a function on a metric graph to its vertex set). Thus
\[
\hat{\mathfrak{A}}(\lambda, z) : \mathbb{C}^{\mathcal{V}(W)} \to \mathbb{C}^{\mathcal{V}(W)}.
\]
(3.51)
The operator $\hat{\mathfrak{A}}(\lambda, z)$ is a Laurent polynomial in $z$ with matrix-valued coefficients that are meromorphic in $\lambda$ with poles at the Dirichlet eigenvalues of the edges.

For any fixed value of the spectral variable $\lambda \in \mathbb{C}$, the Floquet surface for $\lambda$ is defined to be the set
\[
\Phi_\lambda := \left\{ z \in (\mathbb{C}^*)^n : \exists \text{nontrivial solution of } \hat{\mathfrak{A}}(\lambda, z)\bar{u} = 0 \right\}.
\]
(3.52)
If $\lambda \not\in \sigma_D(A)$, then the nontrivial solvability of $(\hat{A}(z) - \lambda)u = 0$ is equivalent to the nontrivial solvability of $\hat{\mathfrak{A}}(\lambda, z)\bar{u} = 0$. This is in turn equivalent to the vanishing of the Laurent polynomial
\[
D(\lambda, z) := \det \hat{\mathfrak{A}}(\lambda, z),
\]
(3.53)
that is,
\[
\Phi_\lambda = \left\{ z \in (\mathbb{C}^*)^n : D(\lambda, z) = 0 \right\} \quad \text{for } \lambda \not\in \sigma_D(A).
\]
(3.54)

### 3.3 Constructing a bilayer periodic graph

Let $(\tilde{\Gamma}, \hat{\mathfrak{A}})$ be a periodic quantum graph, as described in the previous section, with vertex set $\tilde{\mathcal{V}}$, edge set $\hat{\mathcal{E}}$ and potential functions $\{q_e\}_{e \in \hat{\mathcal{E}}}$. Let a new periodic quantum graph $(\Gamma, A)$ be constructed by connecting pairs of respective vertices of two disjoint copies of $(\tilde{\Gamma}, \hat{\mathfrak{A}})$ with unit-length edges endowed with potentials that preserve the periodicity. Precisely, the vertex set $\mathcal{V} = \mathcal{V}(\Gamma)$ is the disjoint union
\[
\mathcal{V} := \tilde{\mathcal{V}} \sqcup \hat{\mathcal{V}} = \mathcal{V} \times \{1, 2\},
\]
(3.55)
so an element of $\mathcal{V}$ is of the form $(v, 1)$ or $(v, 2)$, with $v \in \mathcal{V}$. The edge set is
\[
\mathcal{E} := \hat{\mathcal{E}} \sqcup \hat{\mathcal{E}} \cup \mathcal{E}_c,
\]
(3.56)
in which the set of connecting edges is
\[
\mathcal{E}_c := \left\{ e_v := \{(v, 1), (v, 2)\} : v \in \mathcal{V} \right\}
\]
(3.57)
and one identifies an element $\{(v, w), i\} \in \hat{\mathcal{E}} \sqcup \hat{\mathcal{E}}$ with the element $\{(v, i), (w, i)\}$ of pairs of vertices in $\mathcal{V}$. The graph $\Gamma$ inherits the group action of $\mathbb{Z}^n$, so it is $n$-fold periodic.

Of course, the edges of $\Gamma$ in the two copies of $\tilde{\Gamma}$ inherit the coordinates and potentials from $\tilde{\Gamma}$, that is, for $e = \{(v, i), (w, i)\}$, one has $q_e = q_{\{(v, w)\}}$, which naturally allows one to use the coordinate $x_{(v, w)}$ for the directed edge $((v, i), (w, i))$. Each connecting edge $e \in \mathcal{E}_c$ is endowed with a coordinate in $[0, 1]$ (so
Let \( L_e = 1 \) and a potential function \( q_e \). These potentials are assumed to be periodic, that is \( q_{ge}(gx) = q_e(x) \) for all \( g \in Z^n \) and all \( e \in E \). For the connecting edge \( \{(v, 1), (v, 2)\} \) associated with the vertex \( v \in \Gamma \), it is convenient to denote the potential by \( q_v \),

\[
q_{\{(v, 1), (v, 2)\}} = q_v.
\]

(3.58)

The spectral functions \( s_v(\lambda) \) for undirected connecting edges and the functions \( c_v(\lambda) \) for directed connecting edges are denoted by

\[
\begin{align*}
\{s_{\{(v, i), (v, \bar{i})\}} &= s_v(\lambda) & i, \bar{i} & \in \{1, 2\}, & i \neq \bar{i}.
\end{align*}
\]

(3.59)

The \( a \) and \( b \) functions for the directed connecting edge \( \{(v, 1), (v, 2)\} \) are

\[
\begin{align*}
a_v(\lambda) &= \frac{1}{2} (c_{v,1}(\lambda) - c_{v,2}(\lambda)) \\
b_v(\lambda) &= \frac{1}{2} (c_{v,1}(\lambda) + c_{v,2}(\lambda)).
\end{align*}
\]

(3.60)

The Dirichlet-to-Neumann matrix for \( \{(v, 1), (v, 2)\} \) is

\[
s_v(\lambda) G_v(\lambda) = \begin{bmatrix} -c_{v,1}(\lambda) & 1 \\ 1 & -c_{v,2}(\lambda) \end{bmatrix} = - \begin{bmatrix} b_v(\lambda) & 0 \\ 0 & b_v(\lambda) \end{bmatrix} + \begin{bmatrix} -a_v(\lambda) & 1 \\ 1 & a_v(\lambda) \end{bmatrix}.
\]

(3.61)

Having the metric graph \( \Gamma \) together with the potentials on its edges, section 3.1 defines a self-adjoint operator \( A \) in \( L^2(\Gamma) \), with the same Robin condition \((\mathbb{R})\). This operator commutes with the \( Z^n \) action because of the periodicity of the potentials \( q_v \).

**Definition 3** (bilateral graphs). Let be given a quantum graph \((\hat{\Gamma}, \hat{A})\) with a \( Z^n \) symmetry group and potentials \( \{q_v : v \in \mathcal{V}(\hat{\Gamma})\} \) defined on edges \( \{(v, 1), (v, 2)\} \), identified with the interval \([0,1] \), of the the disjoint union \( \mathcal{V}(\hat{\Gamma}) \sqcup \mathcal{V}(\hat{\Gamma}) \). Let the potentials \( q_v \) be invariant under \( Z^n \). The periodic quantum graph \((\Gamma, A)\) obtained by connecting two copies of \((\hat{\Gamma}, \hat{A})\) by edges with the potentials \( q_v \), as described in this section, is called the bilateral quantum graph associated to \((\hat{\Gamma}, \hat{A})\) and the potentials \( \{q_v : v \in \mathcal{V}(\hat{\Gamma})\} \).

**Reduction to a combinatorial graph.** In the formulation of the eigenvalue problem \((A - \lambda)u = 0\) in terms of the restriction \( \tilde{u} \) of \( u \) to the vertex set \( \mathcal{V} \), the operator \( \mathfrak{A}(\lambda) \) in \([\mathbb{R}]\) has to be augmented, for the \( i \)th copy of \( \mathcal{V} \) \( (i \in \{1, 2\}) \), by adding to it the following terms coming from the connecting edges:

\[
- \frac{c_{v,i}(\lambda)}{s_v(\lambda)} \tilde{u}((v, i)) + \frac{1}{s_v(\lambda)} \tilde{u}((v, \bar{i})) \quad i, \bar{i} \in \{1, 2\}, & i \neq \bar{i}.
\]

(3.62)

This is valid whenever \( \lambda \notin \sigma_D(A) \). Define operators that are diagonal with respect to \( \hat{\mathcal{V}} \), for \( i = 1, 2 \),

\[
\mathbf{C}(\lambda) := \text{diag} \left( \frac{1}{s_v(\lambda)} \right), \quad \mathbf{C}_i(\lambda) := \text{diag} \left( \frac{c_{v,i}(\lambda)}{s_v(\lambda)} \right),
\]

(3.63)

that is, \( [\mathbf{C}(\lambda)\tilde{u}] (v) = s_v(\lambda)^{-1} \tilde{u}(v) \), and similarly for \( \mathbf{C}_i(\lambda) \). Then the operator \( \mathfrak{A}(\lambda) \) has the following block form with respect to the decomposition \( \mathcal{V} = \hat{\mathcal{V}} \sqcup \hat{\mathcal{V}} \):

\[
\mathfrak{A}(\lambda) \equiv \begin{bmatrix} \hat{\mathfrak{A}}(\lambda) & 0 \\ 0 & \hat{\mathfrak{A}}(\lambda) \end{bmatrix} + \begin{bmatrix} -\mathbf{C}_1(\lambda) & \mathbf{C}(\lambda) \\ \mathbf{C}(\lambda) & -\mathbf{C}_2(\lambda) \end{bmatrix}.
\]

(3.64)

Under the Floquet transform, this operator becomes

\[
\hat{\mathfrak{A}}(\lambda, z) \equiv \begin{bmatrix} \hat{\mathfrak{A}}(\lambda, z) & 0 \\ 0 & \hat{\mathfrak{A}}(\lambda, z) \end{bmatrix} + \begin{bmatrix} -\mathbf{C}_1(\lambda) & \mathbf{C}(\lambda) \\ \mathbf{C}(\lambda) & -\mathbf{C}_2(\lambda) \end{bmatrix}.
\]

(3.65)
The operator $\mathcal{G}(\lambda)$ is the “energy-dependent coupling operator”. It does not depend on $z$ because the connecting edges do not connect vertices in two different $\mathbb{Z}^n$-translates of a fundamental domain $W$. When considered as being applied to functions $u|_{V(W)}$ restricted to the vertices in $W$, they become finite diagonal matrices with respect to the natural basis of complex functions on the finite set $V(W) = V(W') \sqcup V(W)$.

As described in section $3.2$, $\mathcal{A}(\lambda, z)$ acts in the space $\mathbb{C}^{V(W)}$. The block form (3.65) is with respect to the decomposition

$$\mathbb{C}^{V(W)} = \mathbb{C}^{V(W')} \times \mathbb{C}^{V(W')} \cong \mathbb{C}^2 \otimes \mathbb{C}^{V(W')}.$$  

(3.66)

This identification with the tensor product $\mathbb{C}^2 \otimes \mathbb{C}^{V(W')}$ provides a convenient way to express the operator $\mathcal{A}(\lambda, z)$. The block operator $\mathcal{G}(\lambda)$ defined in (3.65) has diagonal blocks, so it is a simple sum of tensor products. Let $E_v$ denote the projection in $\mathbb{C}^{V(W)}$ to the $v$-component (that is, $[E_v(u)](w) = v(u)\delta_{vw}$, where $\delta_{vw}$ is the Kronecker symbol); then

$$\mathcal{G}(\lambda) = \sum_{v \in V(W)} G_v(\lambda) \otimes E_v. \tag{3.67}$$

The operators $\mathcal{A}(\lambda)$ and $\mathcal{A}(\lambda, z)$ can now be written

$$\mathcal{A}(\lambda) = \mathcal{A}(\lambda) + \sum_{v \in V(W)} G_v(\lambda) \otimes E_v, \tag{3.68}$$

$$\mathcal{A}(\lambda, z) = \mathcal{A}(\lambda, z) + \sum_{v \in V(W)} G_v(\lambda) \otimes E_v, \tag{3.69}$$

in which $I_2$ is the identity $2 \times 2$ matrix.

4 Coupling by symmetric edges

When the potentials $q_v$ on the connecting edges of the bilayer graph $\Gamma$ are symmetric about their midpoints, $A$ has reflectional symmetry. This means that $A$ commutes with the reflection in $\Gamma$ which maps each copy of $\Gamma$ to the other and reflects each connecting edge about its center. Thus $A$ is invariant on the eigenspaces $\mathcal{H}_+$ and $\mathcal{H}_-$ of this reflection; the former consists of functions that are even with respect to the reflection (eigenvalue $1$), and the latter consists of odd functions (eigenvalue $-1$). With respect to the orthogonal decomposition $L^2(\Gamma) = \mathcal{H}_+ \oplus \mathcal{H}_-$, the operator $A$ has a decomposition

$$A = A_+ + A_-.$$  

(4.70)

This kind of symmetric periodic quantum graph is studied in $[22, \S 3.2]$. Both $A_+$ and $A_-$ are unitarily equivalent to quantum-graph operators $\hat{A}_+$ and $\hat{A}_-$ defined on the metric graph $\Gamma_d$ that is “half” of $\Gamma$, consisting of $\Gamma$ plus a dangling edge attached to each vertex. For $v \in \mathcal{V}(\Gamma)$, this dangling edge is half of the connecting edge $e_v$. By restricting functions in $\mathcal{D}(A_+) = \mathcal{D}(A) \cap \mathcal{H}_+$ to $\Gamma_d$, one obtains the domain of $\hat{A}_+$, which possesses the Neumann boundary condition $du/dx = 0$ at the free vertices of the dangling edges. And the restriction of functions in $\mathcal{D}(A_-) = \mathcal{D}(A) \cap \mathcal{H}_-$ to $\Gamma_d$ is the domain of $\hat{A}_-; \mathcal{H}_-$; it possesses the Dirichlet condition $u = 0$ at the free vertices.

This decomposition of $A$ renders its Floquet surface canonically reducible. Let $\mathfrak{A}_+(\lambda)$ and $\mathfrak{A}_-(\lambda)$ be the reduced $\lambda$-dependent combinatorial operators for $A_+$ and $A_-$ and $\mathfrak{A}_+(\lambda, z)$ and $\mathfrak{A}_-(\lambda, z)$ their Floquet transforms. The Floquet surface for $A$ at energy $\lambda$ is just

$$\Phi_{\lambda} = \{ z \in (\mathbb{C}^n)^* : (\det \mathfrak{A}_+(\lambda, z))(\det \mathfrak{A}_-(\lambda, z)) = 0 \}, \tag{4.71}$$

which is reducible into the union of the Floquet surfaces of the two quantum-graph operators $\hat{A}_+$ and $\hat{A}_-$.
5 Coupling within an asymmetry class

If the potentials connecting two copies of the periodic quantum graph $\hat{\Gamma}$ are not symmetric, it is no longer possible to decompose the bilayer-graph Schrödinger operator $A$ into two components unitarily equivalent to decorated quantum graphs, as described in the previous section. But if the potentials belong to same asymmetry class, it turns out that the reduced $\lambda$-dependent combinatorial operator $\mathfrak{A}(\lambda)$ can be reduced. Its invariant subspaces depend on $\lambda$, so this reduction does not proceed from a reduction of $A$. Nevertheless, the energy-dependent reduction does lead to a factorization of the determinant $D(\lambda, z)$ as a Laurent polynomial in $z = (z_1, \ldots, z_n)$ and therefore reducibility of the Floquet surface for all energies $\lambda$.

Let the potentials of all of the connecting edges of a bilayer graph $\Gamma$ possess the same A-function, $a_\nu(\lambda) = a(\lambda) \quad \forall \nu \in \mathcal{V}(\hat{W})$. (5.72)

Then the DtN map has a trace-free part that is independent of the vertex,

$$s_v(\lambda)G_v(\lambda) = - \left[ \begin{array}{cc} b_v(\lambda) & 0 \\ 0 & b_v(\lambda) \end{array} \right] + \left[ \begin{array}{cc} -a(\lambda) & 1 \\ 1 & a(\lambda) \end{array} \right],$$

which can be decomposed by means of the spectral resolution of the second matrix

$$s_v(\lambda)G_v(\lambda) = -b_v(\lambda)I_2 + \mu P_\mu - \mu P_{-\mu}$$

with $\mu^2 = a(\lambda)^2 + 1$.

When the potentials on the connecting edges are symmetric and therefore $a(\lambda) = 0$, one has $\mu^2 = 1$ and the eigenvalues become constant. The Riemann surface $\hat{S}$ separates into two copies of the $\lambda$-plane, one with $\mu = 1$ and one with $\mu = -1$. Since the eigen-projections $P_1$ and $P_{-1}$ are now constant, they provide a decomposition of the full quantum-graph operator $A$. This is evidenced in the $\mu$-dependence of the diagonal matrices $\mathfrak{D}(\lambda)$ in the following theorem.

**Theorem 4.** Let $(\hat{\Gamma}, \hat{\mathcal{A}})$ be a periodic quantum graph and $(\Gamma, A)$ a bilayer quantum graph obtained by joining two copies of $(\hat{\Gamma}, \hat{\mathcal{A}})$ by edges whose potentials lie in the asymmetry class associated with the A-function $a(\lambda)$.

*The Floquet surface $\Phi_\lambda$ of $(\Gamma, A)$ is reducible for all $\lambda \notin \sigma_D(A)$ to the union of two surfaces,*

$$\Phi_\lambda = \Phi_\lambda^+ \cup \Phi_\lambda^-,$$  

(5.75)

*in which

$$\Phi_\lambda^\pm = \left\{ z \in (\mathbb{C}^*)^n : \det (\hat{\mathfrak{A}}(\lambda, z) + \mathfrak{D}(\lambda)) = 0 \right\},$$

(5.76)

*the diagonal matrices $\mathfrak{D}(\lambda)$ are defined by

$$\mathfrak{D}(\lambda) := \text{diag}_{v \in W} \left( \frac{-b_v(\lambda) \pm \mu}{s_v(\lambda)} \right),$$

(5.77)

*and $\hat{\mathfrak{A}}(\lambda, z)$ is the Floquet transform of the combinatorial reduction of $\hat{\mathcal{A}} - \lambda I$.*

**Proof.** Because of the $\nu$-independence of $P_\mu$, the coupling operator

$$\mathfrak{G}(\lambda) = \sum_{v \in \mathcal{V}(\hat{W})} G_v(\lambda) \otimes E_v$$

(5.78)

in (3.65,3.67) can be resolved as

$$\mathfrak{G}(\lambda) = \sum_{v \in \mathcal{V}(\hat{W})} \frac{1}{s_v(\lambda)} \left( -b_v(\lambda)I_2 + \mu (P_\mu(\lambda) - P_{-\mu}(\lambda)) \right) \otimes E_v \quad = P_\mu \otimes \sum_{v \in \mathcal{V}(\hat{W})} \frac{-b_v(\lambda) + \mu}{s_v(\lambda)} E_v + P_{-\mu} \otimes \sum_{v \in \mathcal{V}(\hat{W})} \frac{-b_v(\lambda) - \mu}{s_v(\lambda)} E_v.$$  

(5.79)
To write $\mathfrak{A}(\lambda)$ in block form with respect to the projections $P_{\pm \mu}$ and $E_v$, set

$$
\mathcal{D}^+(\lambda) := \text{diag} \left( \frac{-b_v(\lambda) + \mu}{s_v(\lambda)} \right), \quad \mathcal{D}^-(\lambda) := \text{diag} \left( \frac{-b_v(\lambda) - \mu}{s_v(\lambda)} \right),
$$

and the block form is

$$
\mathfrak{A}(\lambda) = \begin{bmatrix}
\hat{\mathfrak{A}}(\lambda) + \mathcal{D}^+(\lambda) & 0 \\
0 & \hat{\mathfrak{A}}(\lambda) + \mathcal{D}^-(\lambda)
\end{bmatrix}.
$$

Since the connecting edges do not connect vertices in two distinct $\mathbb{Z}^n$-translates of a fundamental domain $W$ of $\Gamma$, $\mathcal{D}(\lambda, z) = \mathcal{D}(\lambda)$ as an operator in $\mathbb{C}^{\mathcal{V}(W)}$, and thus

$$
\hat{\mathcal{A}}(\lambda, z) \equiv \begin{bmatrix}
\hat{\mathfrak{A}}(\lambda, z) + \mathcal{D}^+(\lambda) & 0 \\
0 & \hat{\mathfrak{A}}(\lambda, z) + \mathcal{D}^-(\lambda)
\end{bmatrix}.
$$

Since the Floquet surface for $A$ at energy $\lambda$ is

$$
\Phi_\lambda = \left\{ z \in (\mathbb{C}^*)^n : \det \hat{\mathfrak{A}}(\lambda, z) = 0 \right\},
$$

the factorization stated in the theorem follows from the block-diagonal form of $\hat{\mathfrak{A}}(\lambda, z)$.

One can ask whether the operators $\hat{\mathfrak{A}}(\lambda) + \mathcal{D}^+(\lambda)$ can be realized as the $\lambda$-dependent combinatorial reduction on $\mathcal{V}(\hat{\Gamma})$ of a quantum graph obtained as a “decoration” of $\hat{\Gamma}$, that is, by attaching a dangling edge to each vertex $v$, where the edge dangling from vertex $v$ has potential $q^A(x)$, and these potentials commute with the $\mathbb{Z}^n$ action (they are periodic).

$\hat{\mathfrak{A}}(\lambda) + \mathcal{D}^+(\lambda)$ acts on functions $f : \mathcal{V}(\hat{\Gamma}) \to \mathbb{C}$ whose restriction to the vertices of the edge $e_v = \{(v, 1), (v, 2)\}$ lies in the one-dimensional image of the eigen-projection $P_{\mu}$. In other words, its domain consists of functions of the form $\psi_{\mu} \otimes g$, where $\psi_{\mu} \in \mathbb{C}^2$ spans the image of $P_{\mu}$ and $g : \mathcal{V}(\hat{\Gamma}) \to \mathbb{C}$ is in the domain of $\hat{\mathfrak{A}}(\lambda)$. This means that $f$ is completely determined by its restriction to one of the copies of $\hat{\Gamma}$. Its restriction to one copy is just a scalar multiple of its restriction to the other, that multiple being equal to the ratio of the components of the eigenvector $\psi_{\mu}$ of $N(\lambda)$.

The terminal vertex of the edge dangling from vertex $v \in \mathcal{V}(\hat{\Gamma})$ is subject to a Robin boundary condition relating value to derivative. This imposes a $\lambda$-dependent Dirichlet-to-Neumann condition at the vertex $v$,

$$
u'(v) = -m_v(\lambda) u(v),
$$

in which the function $m_v(\lambda)$ is the Weyl-Titchmarsh M-function for the half interval. This has the effect of adding the term $m_v(\lambda) \tilde{u}(v)$ to the expression defining $\mathfrak{A}(\lambda)$ in $[R]$. The combinatorial reduction for the decorated graph, defined on $\mathcal{V}(\hat{\Gamma})$ is therefore

$$
\hat{\mathfrak{A}}(\lambda) + \mathfrak{M}(\lambda),
$$

in which

$$
\mathfrak{M}(\lambda) = \text{diag} \left( m_v(\lambda) \right).
$$

The functions $m_v(\lambda)$ are meromorphic functions of $\lambda$ having all of their poles on the real axis.

By comparing $\mathfrak{M}(\lambda)$ to $\mathcal{D}^+(\lambda)$ as given in (5.80), one sees that the requirement that

$$
\hat{\mathfrak{A}}(\lambda) + \mathcal{D}^+(\lambda) = \hat{\mathfrak{A}}(\lambda) + \mathfrak{M}(\lambda)
$$

implies that the functions $(-b_v(\lambda) + \mu)/s_v(\lambda)$ must be meromorphic in $\mathbb{C}$. But this is possible only when $\mu$ has no branch cuts, which requires that $a(\lambda)^2 + 1 \neq 0$ for all $\lambda$. This occurs when $a_v(\lambda) = 0$ for all $v \in \mathcal{V}(\hat{\Gamma})$, and the eigenvalues of $N(\lambda)$ reduce to constants $\mu = \pm 1$. This is the case for symmetric edges, as discussed above. The following theorem summarizes this discussion.
Theorem 5 (realizability of components). Let \((\Gamma, A)\) be a periodic bilayer quantum graph associated to the periodic quantum graph \((\bar{\Gamma}, \bar{A})\) and coupling potentials \(\{q_v : v \in \mathcal{V}(\bar{\Gamma})\}\), such that each potential \(q_v\) possesses the same spectral \(A\)-function \(a(\lambda)\). If the set \(\{\lambda \in \mathbb{C} : a(\lambda) \in \{\pm i\}\}\) is nonempty, then the components \(\Phi^+_\lambda\) and \(\Phi^-_\lambda\) of the Floquet surface \(\Phi_\lambda\) of \((\Gamma, A)\) cannot be realized as the Floquet surface of any decoration of \((\bar{\Gamma}, \bar{A})\) obtained by attaching a dangling edge to each vertex with a self-adjoint condition at each terminal vertex.

It appears that, for any fixed value of the energy \(\lambda\), the Floquet surface offers no insight into realizability of its components. The obstruction to realizability is the branch points in the \(\lambda\) variable. This question is related to that of the determination of the graph operator from its dispersion function, which is understood for discrete graph Laplacians \([14]\). There is substantial literature on how the properties of metric graphs and Schrödinger operators on them are determined by various spectral data \([1, 3, 10, 15, 18, 20, 21]\).

6 Coupling with different asymmetry classes: reducible case of bilayer graphene

When the connecting edges of a periodic bilayer quantum graph do not belong to the same asymmetry class, one can no longer expect to obtain reducibility of the Floquet surface. Remarkably, however, it turns out that the quantum-graph model of bilayer graphene has a reducible Floquet surface regardless of the potentials placed on the two connecting edges of a fundamental domain. This is because the determinant of \(\hat{\mathcal{A}}(\lambda, z)\) is a function of a single composite variable of \(z = (z_1, z_2)\). This seems to be due to the bipartite nature of the hexagonal structure—vertices translationally equivalent to any one of the two vertices of a fundamental domain are connected only to translates of the other vertex. Not only is the Floquet surface reducible, but the the Floquet modes corresponding to the two components (considered as elements of \(\mathbb{C}^4\) when restricted to the vertices of a fundamental domain) lie in two independent two-dimensional subspaces. These findings are stated in Theorem 6

When the \(A\)-functions \(a_v(\lambda)\) are not identical over all the vertices in a fundamental domain \(W\), the form (5.79) of \(\Phi(\lambda)\) cannot be split into two tensor products with complementary eigen-projections. These projections depend in general on the vertex, and when there are only two vertices \(v_1\) and \(v_2\), one has

\[
\Phi(\lambda) = s_1(\lambda)^{-1} \left[ -b_1(\lambda) + \mu_1 (P_{\mu_1} - P_{-\mu_1}) \right] \otimes E_1 + s_2(\lambda)^{-1} \left[ -b_2(\lambda) + \mu_2 (P_{\mu_2} - P_{-\mu_2}) \right] \otimes E_2 ,
\]

in which \(\mu_j\) for \(j = 1, 2\) are functions on the Riemann surfaces \(\{(\lambda, \mu_j) : \mu_j^2 = a_j(\lambda)^2 + 1\}\).

Let \((\bar{\Gamma}, \bar{A})\) be the quantum graph model of graphene with the same potential \(q(x)\) on each of the three edges emanating from a vertex; see Fig. 1. Let \((\Gamma, A)\) be the bilayer quantum graph associated with \((\bar{\Gamma}, \bar{A})\) and any choice of potentials \(q_1(x) = q_{v_1}(x)\) and \(q_2(x) = q_{v_2}(x)\) on the connecting edges in a fundamental domain \(W\). The Floquet transform of the combinatorial reduction \(\hat{\mathcal{A}}(\lambda)\) of \(A\) is

\[
\hat{\mathcal{A}}(\lambda, z) = \frac{1}{s(\lambda)} \begin{pmatrix} -3\tilde{c}(\lambda) - \alpha\hat{s}(\lambda) & w' \\ w & -3\tilde{c}(\lambda) - \alpha\hat{s}(\lambda) \end{pmatrix},
\]

in which \(w\) and \(w'\) are composite variables in \(\mathbb{C}^+ \times \mathbb{C}^+\),

\[
w = 1 + z_1 + z_2, \quad w' = 1 + z_1^{-1} + z_2^{-1}.
\]

The Floquet transform of the operator \(\hat{\mathcal{A}}(\lambda, z)\) for bilayer graphene, where the two sheets are coupled by edges with potentials in two different asymmetry classes, is

\[
\hat{\mathcal{A}}(\lambda, z) = I \otimes \hat{\mathcal{A}}(\lambda, z) + \Phi(\lambda).
\]
Its block form with respect to the resolution $I = P_{+\mu_1} + P_{-\mu_1}$ by the eigen-projections for vertex $v_1$ is

$$
\hat{s}(\lambda) \hat{A}(\lambda, z) \cong \begin{bmatrix}
\Omega_1^+(\lambda) & w' & 0 & 0 \\
\Omega_2^+(\lambda) & 0 & 0 & w \\
0 & 0 & \Omega_1^- (\lambda) & 0 \\
0 & r(\lambda) & w & \Omega_2^- (\lambda)
\end{bmatrix},
$$

(6.92)

in which the $\lambda$-dependent functions are meromorphic, with

$$
\Omega_j^+(\lambda) = -3\hat{c}(\lambda) - \alpha \hat{s}(\lambda) + \hat{s}(\lambda) s_j(\lambda)^{-1} (-b_j(\lambda) \pm \nu_j), \quad \text{for } j = 1, 2
$$

(6.93)

$$
r(\lambda) = 0 \quad \text{if and only if } \ a_1(\lambda) = a_2(\lambda),
$$

and $\nu_1 = \mu_1$ is the eigenvalue of the matrix $N(\lambda)$ involving $a_1(\lambda)$, defined on its Riemann surface. For each $\zeta \in \mathbb{C}$, define the algebraic curves

$$
F_\zeta := \left\{(z_1, z_2) \in (\mathbb{C}^*)^2 : (1 + z_1 + z_2)(1 + z_1^{-1} + z_2^{-1}) = \zeta \right\}.
$$

(6.94)

**Theorem 6** (Floquet surface for bilayer graphene). Let $(\Gamma, A)$ be the bilayer graphene quantum graph constructed above. Given an energy $\lambda \in \mathbb{C} \setminus \sigma_D(A)$,

1. The Floquet surface $\Phi_\lambda$ is the zero set in $(\mathbb{C}^*)^2$ of a quadratic polynomial $D_\lambda(\zeta)$ of the composite variable

$$
\zeta = (1 + z_1 + z_2)(1 + z_1^{-1} + z_2^{-1}).
$$

(6.95)

$D_\lambda(\zeta)$ is the characteristic polynomial, as a function of $\zeta$, of the matrix

$$
R(\lambda) = \begin{bmatrix}
\Omega_1^+(\lambda)\Omega_2^-(\lambda) & \Omega_1^- (\lambda)r(\lambda) \\
\Omega_1^+(\lambda)r(\lambda) & \Omega_1^- (\lambda)\Omega_2^- (\lambda)
\end{bmatrix}.
$$

(6.96)

2. $\Phi_\lambda$ is reducible into components of the form $F_\zeta$, where $\zeta$ takes on the two eigenvalues of $R(\lambda)$. (The components coincide when $R(\lambda)$ has an eigenvalue of multiplicity two.)

3. Whenever $R(\lambda)$ has two distinct eigenvalues, the Floquet modes of the two components of $\Phi_\lambda$ lie in two independent two-dimensional subspaces of the four-dimensional space of non-$L^2$ $\lambda$-eigenfunctions of the quantum-graph operator $A$ for bilayer graphene restricted to one fundamental domain of the underlying metric graph $\Gamma$.

**Proof.** One computes the determinant

$$
\det (\hat{s}(\lambda) \hat{A}(\lambda, z)) = (ww' - \Omega_1^+ \Omega_2^-)(ww' - \Omega_1^- \Omega_2^+) - (\Omega_1^+ \Omega_2^-) r_2^2.
$$

(6.97)

Denote by $[\psi_1^+ \psi_2^+ \psi_1^- \psi_2^-]$ the nullspace of the matrix in (6.92) for a point $z = (z_1, z_2)$ on $F_\zeta(\lambda)$, with $\zeta = ww'$ being a root of the determinant as a function of the composite variable $ww' = (1 + z_1 + z_2)(1 + z_1^{-1} + z_2^{-1})$. The first and third rows of that matrix yield

$$
\begin{bmatrix}
\psi_1^+
\
\psi_2^+
\end{bmatrix} = u_\zeta^+ \begin{bmatrix}
-w'
\
\Omega_1^+ (\lambda)
\end{bmatrix},
\begin{bmatrix}
\psi_1^-
\
\psi_2^-
\end{bmatrix} = u_\zeta^- \begin{bmatrix}
-w'
\
\Omega_1^- (\lambda)
\end{bmatrix},
$$

(6.98)

for some scalar functions $u_\zeta^+(\lambda)$ and $u_\zeta^-(\lambda)$. The second and fourth rows yield that $[u_\zeta^+(\lambda) \ u_\zeta^-(\lambda)]^t$ is annihilated by $R(\lambda) - \zeta I$. The first and second statements of the theorem follow.

If $\zeta \neq 0$, the nullspace of the matrix in (6.92) is the span of the vector

$$
\zeta \begin{bmatrix}
u_\zeta^+(\lambda)
0
0
u_\zeta^-(\lambda)
\end{bmatrix} + (1 + z_1 + z_2) \begin{bmatrix}0
-u_\zeta^+(\lambda)\Omega_1^+(\lambda)
-u_\zeta^-(\lambda)\Omega_1^- (\lambda)
0
\end{bmatrix},
$$

(6.99)
and if $\zeta = 0$, the nullspace is spanned by

$$
\begin{bmatrix}
  u_+^{\zeta}(\lambda) \\
  0 \\
  u_-^{\zeta}(\lambda) \\
  0
\end{bmatrix}
\text{ if } 1 + z_1 + z_2 = 0 \quad \text{and } \begin{bmatrix}
  0 \\
  -u_+^{\zeta}(\lambda)\Omega_1^+(\lambda) \\
  0 \\
  -u_-^{\zeta}(\lambda)\Omega_1^-(\lambda)
\end{bmatrix}
\text{ if } 1 + z_1^{-1} + z_2^{-1} = 0.
$$

(6.100)

This completes the proof of the theorem.

A more detailed description of the curves $F_\zeta$ is given by the Proposition 8 below. Together with the expression (6.100) of the spaces in $\mathbb{C}^4$ that determine the Floquet modes, one can determine the full set of Floquet modes associated to a given component $F_\zeta$ of the Floquet surface $\Phi_\lambda$ of $(\Gamma, A)$. In particular, if the eigenvalue $\zeta$ of $R(\lambda)$ is nonzero, then the nullspaces of $\mathcal{A}(\lambda, z)$, as $z \in (\mathbb{C}^*)^2$ runs over the component $F_\zeta$, comprise the two-dimensional space

$$
\text{span}
\begin{bmatrix}
  u_+^{\zeta}(\lambda) \\
  0 \\
  u_-^{\zeta}(\lambda) \\
  0
\end{bmatrix},
\begin{bmatrix}
  0 \\
  -u_+^{\zeta}(\lambda)\Omega_1^+(\lambda) \\
  0 \\
  -u_-^{\zeta}(\lambda)\Omega_1^-(\lambda)
\end{bmatrix}
$$

(6.101)

except for at most three complex one-dimensional subspaces of this span.

The following lemma aids in the proof of the proposition. The proofs are elementary.

**Lemma 7.** Numbers $z_1, z_2 \in \mathbb{C}^*$ and $q, q' \in \mathbb{C}$ satisfy the system

$$
\begin{align*}
q &= z_1 + z_2 \\
q' &= z_1^{-1} + z_2^{-1}
\end{align*}
$$

(6.102)

if and only if

$$
\begin{align*}
\{z_1, z_2\} &= \{z \in \mathbb{C}^* : q'z + qz^{-1} = qq'\} \quad \text{if } qq' \neq 0, \\
\{z_1, z_2\} &= \{\{z, -z\} : z \in \mathbb{C}^*\} \quad \text{if } qq' = 0.
\end{align*}
$$

(6.103)

Additionally, $z_1 = z_2$ if and only if $qq' = 4$; and, in this case, $z = q/2$. If $qq' = 0$, both $q$ and $q'$ vanish.

**Proposition 8.**

$$
\begin{align*}
F_\zeta &= \bigcup_{w \in \mathbb{C} \setminus \{0, 1, \zeta\}} \{(z_1, z_2) \in (\mathbb{C}^*)^2 : (z_1, z_2) = \{z : \frac{1}{w-1}z + \frac{w}{\zeta-w}z^{-1} = 1\}\}, \quad \text{for } \zeta \notin \{0, 1\} \quad (6.104) \\
F_1 &= \bigcup_{w \in \mathbb{C} \setminus \{0, 1\}} \{(z_1, z_2) \in (\mathbb{C}^*)^2 : (z_1, z_2) = \{z : \frac{1}{w-1}z + \frac{w}{\zeta-w}z^{-1} = 1\}\} \cup \{(z, -z) : z \in \mathbb{C}^*\} \quad (6.105) \\
F_0 &= \{(z_1, z_2) : 1 + z_1 + z_2 = 0 \text{ or } 1 + z_1^{-1} + z_2^{-1} = 0\}
\end{align*}
$$

(6.106)

The intersection of the two surfaces whose union forms $F_0$ consists of the two points $(z_1, z_2)$ of the set $\{(e^{i\pi/3}, e^{-i\pi/3}), (e^{-i\pi/3}, e^{i\pi/3})\}$.

### 7 Coupling with different asymmetry classes: irreducible case

The reducibility of the Floquet surface of bilayer graphene regardless of the asymmetry classes of the connecting edges is not typical for bilayer quantum graphs. It is the bipartite property of graphene that is responsible. Although irreducibility is generically expected, proving it can be involved. This section presents a simple example in which a proof is not too long.
Consider a bilayer quantum graph \((\Gamma, A)\) associated with the square periodic graph \((\hat{\Gamma}, \hat{A})\) illustrated in Fig. 2. A fundamental domain of \(\hat{\Gamma}\) contains two adjacent fundamental domains of a perfect square lattice, and thus contains two vertices \(v_1\) and \(v_2\). In \((\Gamma, A)\), corresponding vertices on the two copies of \(\hat{\Gamma}\) are connected by potentials with A-functions \(a_1(\lambda)\) and \(a_2(\lambda)\). The analog of the block form (6.92) is in this case

\[
\begin{bmatrix}
\Omega^+_1(\lambda) + \zeta_2 & \xi' \\
\xi & \Omega^+_2(\lambda) + \zeta_2 \\
0 & 0 & 0 & r(\lambda) \\
0 & r(\lambda) & \Omega^-_1(\lambda) + \zeta_2 & \xi' \\
0 & \xi & \Omega^-_2(\lambda) + \zeta_2 & 0
\end{bmatrix},
\]

in which (assuming for simplicity that the potentials of \((\hat{\Gamma}, \hat{A})\) are symmetric so that \(\tilde{c}(\lambda) = \hat{c}(\lambda)\))

\[
\Omega^+_j(\lambda) = -4\tilde{c}(\lambda) - \alpha\hat{s}(\lambda) + \hat{s}(\lambda)s_j(\lambda)^{-1}(-b_j(\lambda) \pm \nu_j), \quad \text{for } j = 1, 2
\]

\[
r(\lambda) = 0 \quad \text{if and only if } a_1(\lambda) = a_2(\lambda),
\]

and \(\nu_1 = \mu_1\). The dependence on \(z_1\) and \(z_2\) comes through

\[
\xi = 1 + z_1, \quad \xi' = 1 + z_1^{-1}, \\
\zeta_1 = z_1 + z_1^{-1}, \quad \zeta_2 = z_2 + z_2^{-1}, \\
w_1w'_1 = 2 + \zeta_1.
\]

**Proposition 9.** The Floquet surface of the periodic bilayer quantum graph \((\Gamma, A)\) described above is reducible at energy \(\lambda\) if and only if

\[
r^2(\lambda) \left( \Omega^+_1(\lambda) - \Omega^-_1(\lambda) \right)^2 \left( r^2(\lambda) - \left( \Omega^+_2(\lambda) - \Omega^-_2(\lambda) \right) \left( \Omega^+_1(\lambda) - \Omega^-_1(\lambda) \right) \right) = 0.
\]

As expected, this meromorphic function of \(\lambda\) vanishes identically when \(r(\lambda) \equiv 0\), which occurs exactly when the A-functions \(a_1(\lambda)\) and \(a_2(\lambda)\) for the potentials of the two edges are identical.

**Proof.** The determinant of (7.107) turns out to be a function of \(\zeta_1\) and \(\zeta_2\), which means that it is invariant under \(z_1 \mapsto z_1^{-1}\) and \(z_2 \mapsto z_2^{-1}\),

\[
D(\lambda; z_1, z_2) = \zeta_1^2 + \zeta_1 \left( p^+(\lambda, \zeta_2) + p^-(\lambda, \zeta_2) \right) + p^+(\lambda, \zeta_2)p^-(\lambda, \zeta_2) - r(\lambda)^2q(\lambda, \zeta_2),
\]

in which

\[
p^+(\zeta_2) = 2 - (\Omega^+_1 + \zeta_2)(\Omega^+_2 + \zeta_2) \tag{7.112}
\]

\[
p^-(\zeta_2) = 2 - (\Omega^-_1 + \zeta_2)(\Omega^-_2 + \zeta_2) \tag{7.113}
\]

\[
q(\zeta_2) = \left( \Omega^+_1 + \zeta_2 \right) \left( \Omega^-_1 + \zeta_2 \right). \tag{7.114}
\]
Suppress the dependence on $\lambda$ and assume that $D$ has the factorization

$$D(z_1, z_2) = (z_1 + \gamma(z_2) + \beta z_1^{-1}) (z_1 + \delta(z_2) + \beta^{-1} z_1^{-1}),$$

$$= z_1^2 + z_1^{-2} + z_1(\gamma(z_2) + \delta(z_2)) + z_1^{-1}(\beta^{-1} \gamma(z_2) + \beta \delta(z_2)) + \beta + \beta^{-1} + \gamma(z_2) \delta(z_2)$$  \hspace{1cm} (7.115)

in which $\gamma(z_2)$ and $\delta(z_2)$ are Laurent polynomials and $\beta$, as well as the coefficients of $\gamma(z_2)$ and $\delta(z_2)$ depend on $\lambda$. This leads to the equations

$$\gamma(z_2) + \delta(z_2) = \beta^{-1} \gamma(z_2) + \beta \delta(z_2) = p^+(z_2) + p^-(z_2)$$

$$\beta + \beta^{-1} + \gamma(z_2) \delta(z_2) = 2 + p^+(z_2)p^-(z_2) - r^2 q(z_2).$$  \hspace{1cm} (7.116)

Because of this, $\gamma(z_2)$ and $\delta(z_2)$ must have the form

$$-\gamma(z_2) = z_2^2 + \gamma_1 z_2 + \gamma_0 + \gamma_{-1} z_2^{-1} + z_2^{-2}$$

$$-\delta(z_2) = z_2^2 + \delta_1 z_2 + \delta_0 + \delta_{-1} z_2^{-1} + z_2^{-2}.$$  \hspace{1cm} (7.117)

Now it is shown that $\gamma(z)$ and $\delta(z)$ (putting $z_2 = z$ for now) are functions of $\zeta = z + z^{-1}$, which is to say that $\gamma_1 = \gamma_{-1}$ and $\delta_1 = \delta_{-1}$. They can be written in terms of $\zeta$ and $\zeta^- = z - z^{-1}$,

$$-\gamma(z) = \zeta^2 + \gamma_1 \zeta + \gamma_0 + \gamma_{-1} \zeta^- + \gamma_{0}^-,$$

$$-\delta(z) = \zeta^2 + \delta_1 \zeta + \delta_0 + \delta_{-1} \zeta^- + \delta_{0}^-,$$  \hspace{1cm} (7.118)

in which $\gamma_{0}^- = \gamma_0 - 2$ and $\delta_{0}^- = \delta_0 - 2$. Their product is

$$\gamma(z) \delta(z) = \zeta^4 + \zeta^3 (\gamma_1 + \delta_1) + \zeta^2 (\gamma_1 \delta_1 + \gamma_{-1} \delta_{-1} + \gamma_{0}^- + \delta_{0}^-) + \zeta (\gamma_1 \delta_0 + \delta_1 \gamma_0^- + \gamma_{0}^- \delta_{0}^- - 4 \gamma_{-1} \delta_{-1}$$

$$+ \zeta^- (\gamma_{-1} \zeta^2 + \delta_{0}^- \zeta + \delta_{0}^-) + \delta_{-1} (\zeta^2 + \gamma_1 \zeta + \gamma_{0}^-)),$$  \hspace{1cm} (7.119)

and it is a function of $\zeta$. Thus the latter expression multiplying $\zeta^-$ must vanish identically. This is equivalent to the vanishing of three quantities:

$$\gamma_{-1} + \delta_{-1} = 0,$$

$$\gamma_{-1} \delta_{1} + \delta_{-1} \gamma_{1} = 0,$$

$$\gamma_{-1} \delta_{0} + \delta_{-1} \gamma_{0}^- = 0.$$  \hspace{1cm} (7.120, 7.121, 7.122)

As long as not all of $\delta_{+}$, $\gamma_{+}$, $\delta_{0}$, and $\gamma_{0}$ are zero, one obtains $\gamma_{-} = 0$ and $\delta_{-} = 0$. This makes $\gamma(z)$ and $\delta(z)$ polynomial functions of $\zeta$.

This yields the factorization

$$D(z_1, z_2) = \zeta_1^2 + \zeta_1 (p^+(\zeta_2) + p^-(\zeta_2)) + p^+(\zeta_2)p^-(\zeta_2) - r^2 q(\zeta_2)$$

$$= \left(\zeta_1 + \gamma(\zeta_2)\right) \left(\zeta_1 + \delta(\zeta_2)\right).$$  \hspace{1cm} (7.123)

So the roots of $D$ as a function of $\zeta_1$ are polynomials in $\zeta_2$. This means that the $\zeta_1$-discriminant

$$D_1(\zeta_2) = (p^+(\zeta_2) - p^-(\zeta_2))^2 + 4 r^2 q(\zeta_2)$$  \hspace{1cm} (7.124)

is the square of a polynomial. This, in turn, means that the $\zeta_2$-discriminant

$$D_2 = \left[2cd + 4r^2(\Omega_1^+ + \Omega_1^-)\right]^2 - 4 \left(c^2 - 4r^2\right) \left(d^2 - 4r^2\Omega_1^+ \Omega_1^-\right)$$  \hspace{1cm} (7.125)

vanishes. A page of calculations yields

$$D_2 = 16 r^2 \left(\Omega_1^+ - \Omega_1^-\right)^2 \left(r^2 - (\Omega_1^+ - \Omega_1^-) \left(\Omega_2^+ - \Omega_1^-\right)\right).$$  \hspace{1cm} (7.126)
Recall now that all the quantities here are meromorphic functions of $\lambda$.

The other possible factorization of $D$ is

$$D(z_1, z_2) = (1 + \beta z_1^{-1}) (z_2^2 + \gamma(z_2) z_1 + \delta(z_2) + \beta^{-1} z_1^{-1}),$$

(7.127)

which leads to the equations

$$\gamma(z_2) + \beta = \beta \delta(z_2) + \beta^{-1} = p^+(z_2) + p^-(z_2)$$
$$\delta(z_2) + \beta \gamma(z_2) = 2 + p^+(z_2) p^-(z_2) - r^2 q(z_2).$$

(7.128)

The first of these implies that $\gamma$ and $\delta$ are both of the form $-z^2 + \cdots - z^{-2}$, which is untenable in view of the second of these equations.

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