Théorie spectrale des nouveaux matériaux

CIRM

Spectrally embedded bound states for quantum graphs

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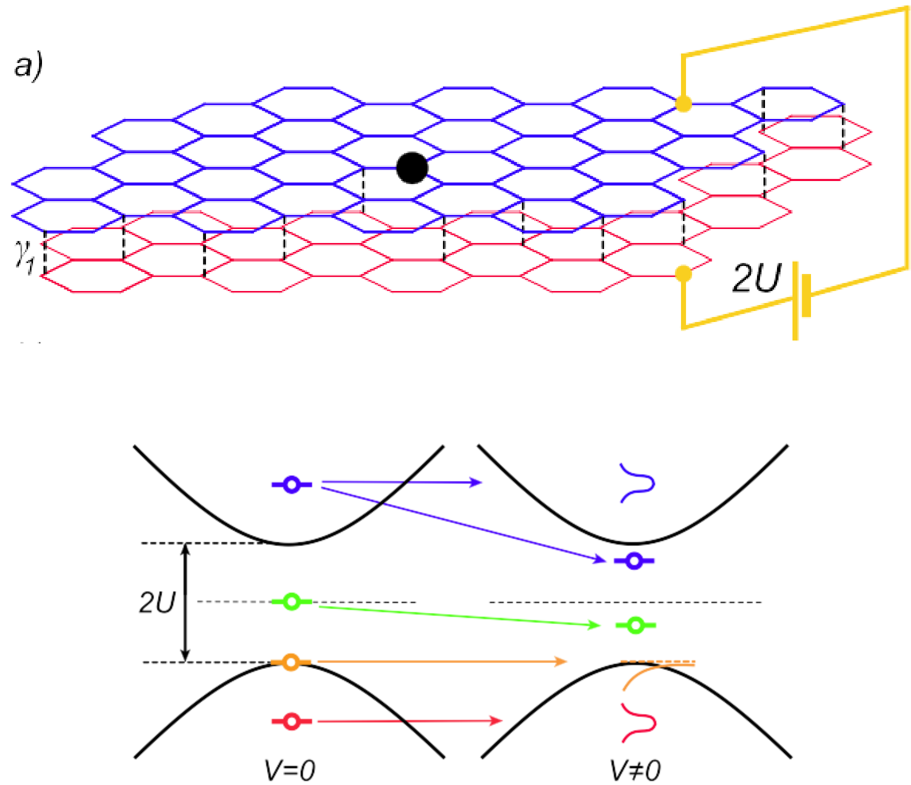
Bilayer graphene: Impurity states in the continuum



V. V. Mkhitaryan and E. G. Mishchenko, Localized states due to expulsion of resonant impurity levels from the continuum in bilayer graphene, Phys. Rev. Lett. 110, 086805 (2013)

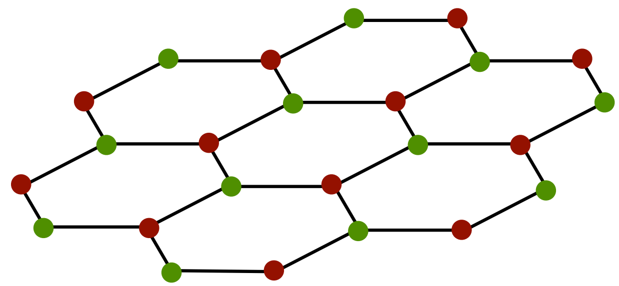
Graph models for graphene

Combinatorial graph

Edges are interactions between vertices

$\rightsquigarrow$ Self-adjoint operator

$A : \ell^2(\mathcal{V}(\Gamma)) \to \ell^2(\mathcal{V}(\Gamma))$



Metric graph

Edges have operator $-\partial_{xx} + \mathring{q}(x)$

$\rightsquigarrow$ Self-adjoint operator

$A : \mathrm{dom}(A) \to L^2(\Gamma)$

Γ has a $\mathbb{Z}^2$ symmetry generated by $\mathfrak{t}_1$ and $\mathfrak{t}_2$; A commutes with $\mathfrak{t}_1$, $\mathfrak{t}_2$.

A Floquet mode is a non-L^2 simultaneous eigenfunction of $\mathfrak{t}_1$, $\mathfrak{t}_2$, A.

$$\mathrm{dom}(A) = \left\{ f \in L^2(\Gamma) \cap \bigoplus_{e\in\mathcal{E}(\Gamma)} H^2(e) \ : \ \sum_{e\in\mathcal{E}_v(\Gamma)} f_e'(v) = 0 \ \ \forall\, v \in \mathcal{V}(\Gamma) \right\}$$

Dispersion relation: $D(z_1, z_2, \lambda) = 0 \iff \exists$ a Floquet mode for (z_1, z_2, λ)

Floquet transform of $f(x)$ on Γ: $\hat{f}(z_1, z_2, x) = \sum_{m,n\in\mathbb{Z}} f(\mathfrak{t}_1^m \mathfrak{t}_2^n x) z_1^{-m} z_2^{-n}$

$$(Af)\hat{\ }(z_1, z_2, x) = \hat{A}(z_1, z_2)\hat{f}(z_1, z_2, x)$$

Floquet surface for λ: $\{\text{singular locus of } \hat{A}(z_1, z_2) - \lambda\} = \{D(z_1, z_2, \lambda) = 0\}$

Spectrum of A: $\{\lambda \in \mathbb{R} : D(z_1, z_2, \lambda) = 0 \text{ for some } |z_1| = 1, |z_2| = 1\}$

Reducibility vs. **embedded eigenvalues**

a) Embedded defect eigenvalues:
Need separation of evanescent and propagating modes

b) Reducibility of the Floquet surface:
Algebraic point of view through Floquet transform

c) Decomposition of the graph operator:
Spectral bands can come from decoupled parts of the system

d) Invariant subgraphs:
System component isomorphic to periodic subgraph
$\rightsquigarrow$ component of the Floquet surface
... but not *vice-versa* !

e) Finite symmetry groups of the graph:
Symmetries produce invariant subgraphs

Reducibility vs. **embedded eigenvalues**

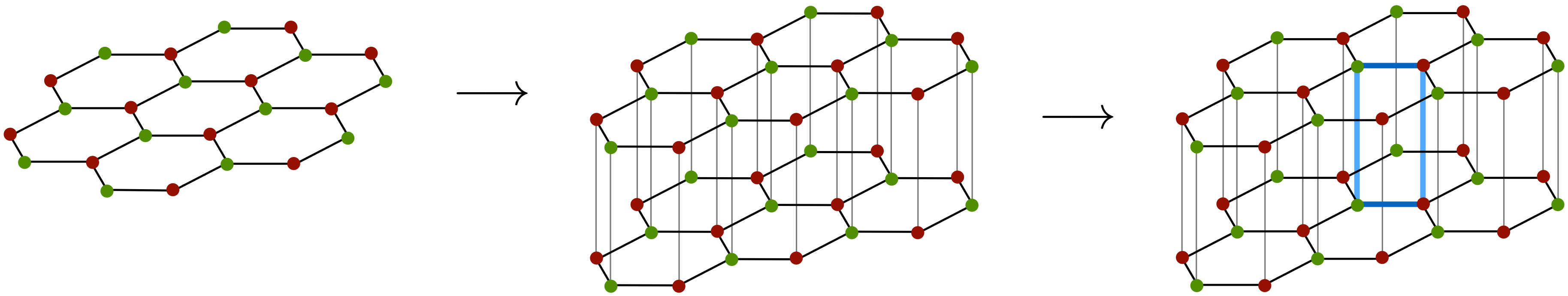
Theorem. (Kuchment and Vainberg)
Let $\lambda \in \sigma(A)$, and let the Floquet surface $\Psi_{A,\lambda}$ be irreducible.
If u is in $L^2(\Gamma)$, V is a local perturbation of A, and

$$(A + V)u = \lambda u \,,$$

then u has compact support.

P. Kuchment and B. Vainberg, On the Structure of Eigenfunctions Corresponding to Embedded Eigenvalues of Locally Perturbed Periodic Graph Operators, Commun. Math. Phys. 268 (2006)

Coupling two layers $\Longrightarrow$ embedded eigenvalues



A single layer of graphene $\longrightarrow$

Couple two layers
$\rightsquigarrow$
two decoupled function subspaces
$\rightsquigarrow$
reducible Floquet surface
$\rightsquigarrow$
splitting of spectrum

$\longrightarrow$

Local defect
$\rightsquigarrow$
non-embedded eigenvalue in one subspace
$\rightsquigarrow$
embedded in continuum of the other subspace

Combinatorial graphs with **reducible Floquet surface**

A and L : periodic self-adjoint operators on an n-periodic combinatorial graph.

$$\begin{array}{rl} \text{bias} & : \; B = \cos(\theta)\, L \\ \text{coupling} & : \; \Gamma = e^{i\phi} \sin(\theta)\, L \end{array} \quad \Longrightarrow \quad L^2 = B^2 + \Gamma\Gamma^*$$

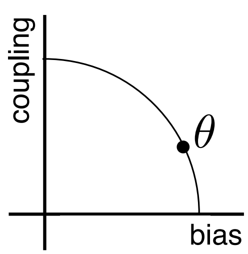
$$\mathcal{A} = \begin{bmatrix} A+B & \Gamma \\ \Gamma^* & A-B \end{bmatrix}, \quad \tilde{\mathcal{A}} = \begin{bmatrix} A+L & 0 \\ 0 & A-L \end{bmatrix}, \quad \mathcal{U} = \begin{bmatrix} e^{i\phi}\cos(\frac{\theta}{2})I & -\sin(\frac{\theta}{2})I \\ \sin(\frac{\theta}{2})I & e^{-i\phi}\cos(\frac{\theta}{2})I \end{bmatrix}$$

$\Longrightarrow$ $\quad \mathcal{A}\mathcal{U} = \mathcal{U}\tilde{\mathcal{A}}$ $\quad$ with $\mathcal{A}$ and $\tilde{\mathcal{A}}$ self-adjoint and $\mathcal{U}$ unitary.

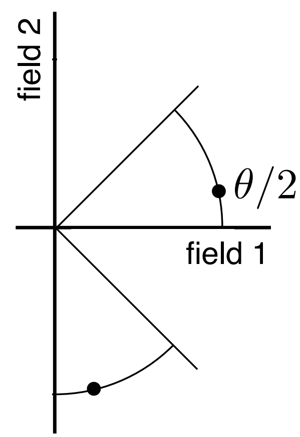
$$\det\left(\hat{\mathcal{A}}(z) - \lambda I\right) = \det\left(\hat{A}(z) + \hat{L}(z) - \lambda I\right) \det\left(\hat{A}(z) - \hat{L}(z) - \lambda I\right)$$

$\Longrightarrow$ $\quad \Psi_{\mathcal{A},\lambda}$ is reducible for all λ.

Interpretation:



$\Longrightarrow$



field components of the columns of $\mathcal{U}$

$\theta = \pi/2 \rightsquigarrow$ even and odd motions

Algebraic proofs via the Floquet transform

V a localized defect: $(A + V - \lambda I)u = 0 \iff (A - \lambda I)u = -Vu =: f$

Floquet transform:

$$\widehat{A}(z,\lambda)\hat{u} = \hat{f} \implies \hat{u}(z_1,z_2) = R(z_1,z_2,\lambda)\frac{\hat{f}(z_1,z_2)}{D(z_1,z_2,\lambda)} = R(z_1,z_2,\lambda)g(z_1,z_2)$$

$= \text{Laurent polynomial} \implies u$ compactly supported

Reducible case: $D(z_1,z_2,\lambda) = D_1(z_1,z_2,\lambda)D_2(z_1,z_2,\lambda)$

Let $\lambda \in$ spectrum of A be such that

$\{\lambda \in \mathbb{R} : D_1(z_1,z_2,\lambda) \neq 0 \quad \text{for all } |z_1| = 1,\ |z_2| = 1\}$

$\{\lambda \in \mathbb{R} : D_2(z_1,z_2,\lambda) = 0 \text{ for some } |z_1| = 1,\ |z_2| = 1\}$

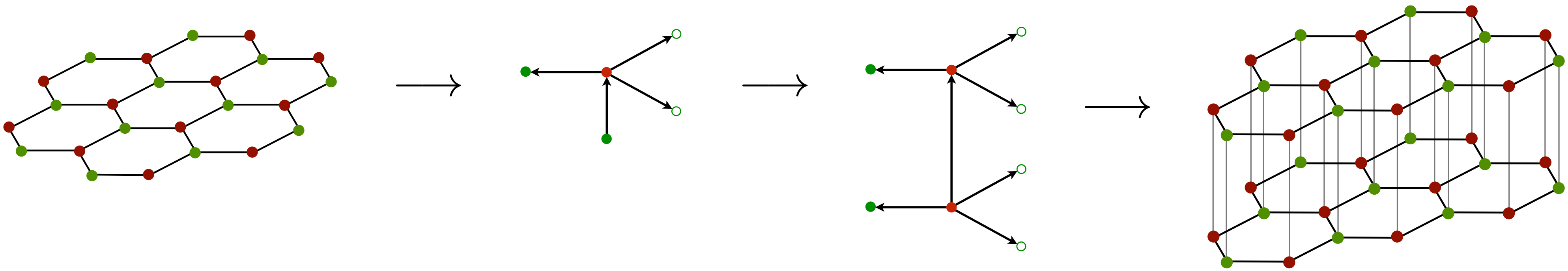
$\implies$

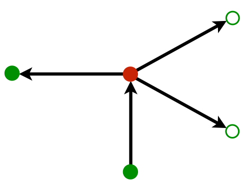
$$\hat{u}(z_1,z_2) = R(z_1,z_2,\lambda)\frac{\hat{f}(z_1,z_2)}{D_1(z_1,z_2,\lambda)D_2(z_1,z_2,\lambda)} = R(z_1,z_2,\lambda)\frac{g(z_1,z_2)}{D_1(z_1,z_2,\lambda)}$$

$\neq \text{Laurent polynomial} \implies u$ not compactly supported

Metric graphs with **reducible Floquet surface**

Symmetric case





Decorate a graph by a "dangling edge" on a vertex of each fundamental domain.

Then connect two copies at the free vertex.

(1) Dirichlet endpoint condition:
Isomorphic to the antisymmetric invariant space

(2) Neumann endpoint condition:
Isomorphic to the symmetric invariant space

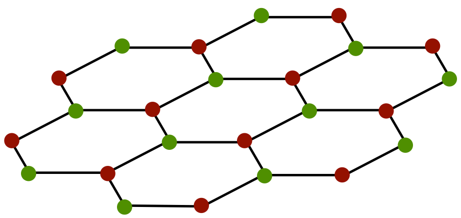
} A non-embedded eigenvalue of one space may be embedded in the continuum of the other.

Metric graphs with **reducible Floquet surface**

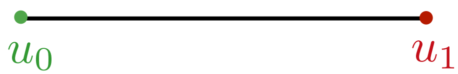
Asymmetric case

At a fixed energy λ:

Reduce metric graph to combinatorial graph. Put $\underline{u} = u|_{\mathcal{V}(\Gamma)}$



$$\big(-\partial_{xx} + \mathring{q}(x)\big)u = \lambda u$$



$$u_0' = \big(u_1 - \mathring{c}(\lambda)u_0\big)/\mathring{s}(\lambda)$$

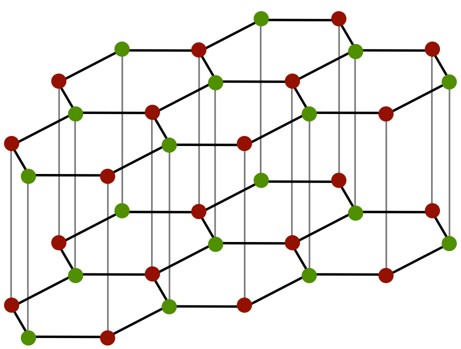
$\Longrightarrow$

$(\mathring{A} - \lambda I)u = 0$ on $\mathring{\Gamma}$

$\Longleftrightarrow$

$\mathring{\mathfrak{A}}(\lambda)\underline{u} = 0$ on $\mathcal{V}(\mathring{\Gamma})$

Couple two layers by edges with asymmetric potential $q(x)$:

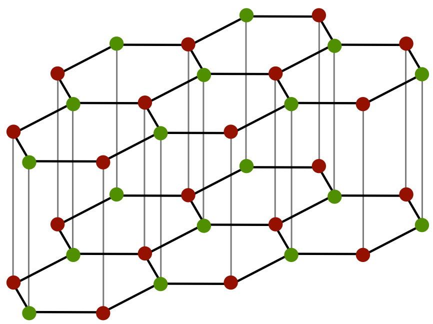


$\longrightarrow$

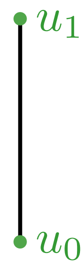
Operator A
on coupled
metric graph
Γ

Creating a metric graph with **reducible Floquet surface**

(1) Couple two layers by edges with asymmetric potential $q(x)$:



$\longrightarrow$



$$\big(-\partial_{xx} + q(x)\big)u = \lambda u$$

$$u_0' = \big(u_1 - c(\lambda)u_0\big)/s(\lambda)$$

$$u_1' = \big(u_0 - s'(\lambda)u_1\big)/s(\lambda)$$

$\Longrightarrow$ Operator A on coupled metric graph Γ

(2) Reduce metric graph to combinatorial graph at fixed energy λ:

$$\big(A - \lambda I\big)u = 0 \qquad \Longleftrightarrow \qquad \begin{bmatrix} \mathring{\mathfrak{A}}(\lambda) - \frac{c(\lambda)}{s(\lambda)}I & \frac{1}{s(\lambda)}I \\ \frac{1}{s(\lambda)}I & \mathring{\mathfrak{A}}(\lambda) - \frac{s'(\lambda)}{s(\lambda)}I \end{bmatrix} \begin{bmatrix} \underline{u}_{\text{top}} \\ \underline{u}_{\text{bot}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

(3) This matrix operator $\mathfrak{A}$ is decomposable with components A_1 and A_2.

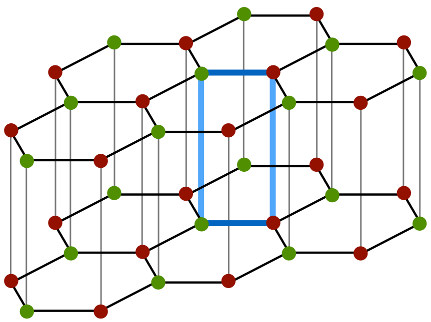
(4) Choose λ so that $0 \in \sigma_c(A_1)$ but $0 \notin \sigma_c(A_2)$.

(5) Choose a local defect for $\mathfrak{A}$ that produces an embedded eigenvalue.

(6) Locally perturb $q(x)$ in A to realize this perturbation of $\mathfrak{A}$.
This **asymmetric** metric graph operator has **embedded eigenvalue**.

Components of Floquet surface for a **metric graph**

The Floquet surface of the unperturbed graph must be reducible.
$\rightsquigarrow$ Find its components.



$$\begin{bmatrix} u_0 \\ u_0' \end{bmatrix} \xrightarrow{\;(-\partial_{xx}+q(x))u=\lambda u\;} \begin{bmatrix} u_1 \\ u_1' \end{bmatrix}, \qquad \begin{bmatrix} c(\lambda) & s(\lambda) \\ -c'(\lambda) & -s'(\lambda) \end{bmatrix}$$

Eigenvalues η of $\begin{bmatrix} c(\lambda) & s(\lambda) \\ -c'(\lambda) & -s'(\lambda) \end{bmatrix}$ satisfy $\eta - \eta^{-1} = s'(\lambda) - c(\lambda)\,.$

Solutions corresponding to η and $-\eta^{-1}$ have the same Dirichlet-to-Neumann ratio at both ends:

$$\frac{u'}{u} = \delta_+(\lambda) := \frac{\eta(\lambda) - c(\lambda)}{s(\lambda)} \quad \text{and} \quad \frac{u'}{u} = \delta_-(\lambda) := \frac{-\eta(\lambda)^{-1} - c(\lambda)}{s(\lambda)}$$

This leads to two dispersion relations for the coupled quantum graph:

$$D(z_1, z_2, \lambda) := \det \begin{bmatrix} z_1 + z_2 + 1 & \mathring{s}(\lambda)\delta_\pm(\lambda) - 3\mathring{c}(\lambda) \\ \mathring{s}(\lambda)\delta_\pm(\lambda) - 3\mathring{c}(\lambda) & z_1^{-1} + z_2^{-1} + 1 \end{bmatrix} = 0$$

Reducibility and friends revisited

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Need separation of evanescent and propagating modes

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Some literature

P. Kuchment and B. Vainberg, On the Structure of Eigenfunctions Corresponding to Embedded Eigenvalues of Locally Perturbed Periodic Graph Operators, Commun. Math. Phys. 268 (2006).

P. Kuchment and B. Vainberg, On absence of embedded eigenvalues for Schrödinger operators with perturbed periodic potentials, Commun. Part. Diff. Equat., 25(9–10) (2000) 1809–1826.

S. P. Shipman, Eigenfunctions of Unbounded Support for Embedded Eigenvalues of Locally Perturbed Periodic Graph Operators, Commun. in Math. Phys. 332 (2) (2014) 605–626.

K. Ando, H. Isozaki, H. Morioka, Spectral Properties of Schrödinger Operators on Perturbed Lattices, Annales Henri Poincaré (2015).