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Edge states of Schrödinger equations on graphene with zigzag boundaries

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http://www.maebashi-it.ac.jp/˜niikuni/slide/20210611.pdf

作用素論セミナー

1 Background

◇ トポロジカル絶縁体

⋯内部（Bulk）は絶縁体だが表面（Edge）は伝導体.

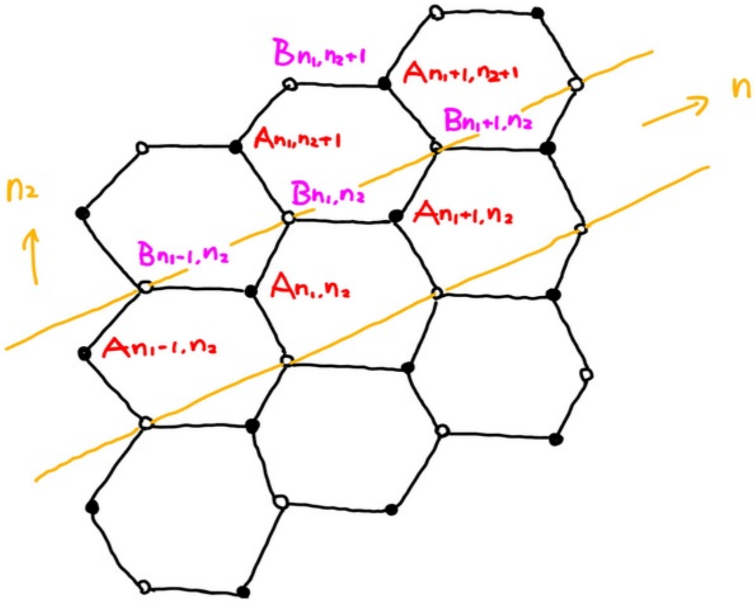
⇒全空間 (Bulk) における周期系のスペクトルのギャップ内にあるエネルギー準位が, 境界 (Edge) のある周期系の固有値になっている状態.

実際, G. M. Graf, M. Porta (2013) では, バルクハミルトニアンとエッジハミルトニアンを構成し, それぞれに対応する指数（バルク指数・エッジ指数）を定義して, 両指数間の関係（バルク・エッジ対応）を議論している.

◇ A discrete Bulk Hamiltonian on Graphene in $\ell^2(\mathbb{Z}^2, \mathbb{C}^2)$

Let $0 \neq t \in \mathbb{R}$ be a constant (hopping parameter).

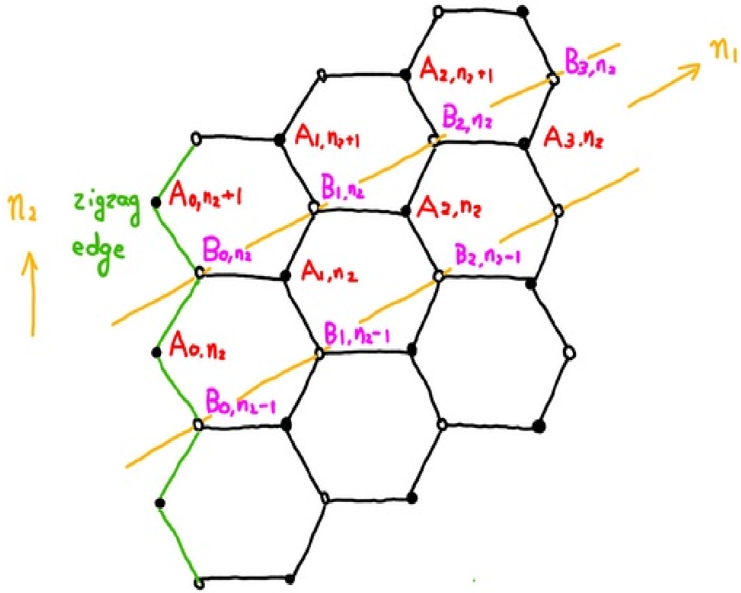
$$\begin{cases} (H_1\psi)^{\mathrm{A}}_{n_1,n_2} = -t(\psi^{\mathrm{B}}_{n_1,n_2} + \psi^{\mathrm{B}}_{n_1,n_2-1} + \psi^{\mathrm{B}}_{n_1-1,n_2}), \\ (H_1\psi)^{\mathrm{B}}_{n_1,n_2} = -t(\psi^{\mathrm{A}}_{n_1,n_2+1} + \psi^{\mathrm{A}}_{n_1+1,n_2} + \psi^{\mathrm{A}}_{n_1,n_2}), \end{cases} \qquad (n_1, n_2) \in \mathbb{Z}^2.$$



A discrete Edge Hamiltonian on Grahene in $\ell^2(\mathbb{N} \times \mathbb{Z}, \mathbb{C}^2)$

$$\begin{cases} (H_1^\sharp \psi)^{\mathrm{A}}_{n_1,n_2} = -t(\psi^{\mathrm{B}}_{n_1,n_2} + \psi^{\mathrm{B}}_{n_1,n_2-1} + \psi^{\mathrm{B}}_{n_1-1,n_2}), \\ (H_1^\sharp \psi)^{\mathrm{B}}_{n_1,n_2} = -t(\psi^{\mathrm{A}}_{n_1,n_2+1} + \psi^{\mathrm{A}}_{n_1+1,n_2} + \psi^{\mathrm{A}}_{n_1,n_2}), \end{cases} \quad (n_1, n_2) \in \mathbb{N} \times \mathbb{Z}$$

with the Dirichlet boundary condition on the zigzag edge.



A fiber operator of $H_1(k)$ and $H_1^\sharp(k)$

For a quasi-momentum $k \in S^1 = [-\pi, \pi]$, define fiber operators $\{H_1(k)\}_{k \in S^1}$ in $\ell^2(\mathbb{Z}, \mathbb{C}^2)$ as

$$\begin{cases} (H_1(k)\psi)^{\mathrm{A}}_{n_1} = -t(\psi^{\mathrm{B}}_{n_1} + e^{-ik}\psi^{\mathrm{B}}_{n_1} + \psi^{\mathrm{B}}_{n_1-1}), \\ (H_1(k)\psi)^{\mathrm{B}}_{n_1} = -t(e^{ik}\psi^{\mathrm{A}}_{n_1} + \psi^{\mathrm{A}}_{n_1+1} + \psi^{\mathrm{A}}_{n_1}), \end{cases} \qquad n_1 \in \mathbb{Z}$$

and $\{H_1^\sharp(k)\}_{k \in S^1}$ in $\ell^2(\mathbb{N}, \mathbb{C}^2)$ as

$$\begin{cases} (H_1^\sharp(k)\psi)^{\mathrm{A}}_{n_1} = -t(\psi^{\mathrm{B}}_{n_1} + e^{-ik}\psi^{\mathrm{B}}_{n_1} + \psi^{\mathrm{B}}_{n_1-1}), \\ (H_1^\sharp(k)\psi)^{\mathrm{B}}_{n_1} = -t(e^{ik}\psi^{\mathrm{A}}_{n_1} + \psi^{\mathrm{A}}_{n_1+1} + \psi^{\mathrm{A}}_{n_1}), \end{cases} \qquad n_1 \in \mathbb{N}$$

with the Dirichlet boundary condition $\psi^A_0 = \psi^B_0 = 0$.

Then,

$$\tilde{H}_1 := \int_{S^1}^{\oplus} H_1(k) \frac{dk}{2\pi}$$

in the Hilbert space $\mathcal{H} := L^2(S^1, \ell^2(\mathbb{Z}, \mathbb{C}^2), \frac{dk}{2\pi})$ is defined as

$$(\tilde{H}_1\psi)(k) = H_1(k)\psi(k), \quad k \in S^1, \quad \psi \in \mathrm{dom}(\tilde{H}_1).$$

The domain of $\tilde{H}_1$ is defined by the set of $\psi \in \mathcal{H}$ such that

- $\psi(k) \in \mathrm{dom}(H_1(k))$,
- $\displaystyle\int_{S^1} \|H_1(k)\psi(k)\|^2_{\ell^2(\mathbb{Z},\mathbb{C}^2)} \frac{dk}{2\pi} < \infty$.

In a similar way, $\tilde{H}_1^\sharp := \displaystyle\int_{S^1}^{\oplus} H_1^\sharp(k) \frac{dk}{2\pi}$ is defined.

The periodicity of H_1 and $H_1^\sharp$ on n_2 yields

$$H_1 \simeq \int_{S^1}^{\oplus} H_1(k) \frac{dk}{2\pi} \quad \text{and} \quad H_1^\sharp \simeq \int_{S^1}^{\oplus} H_1^\sharp(k) \frac{dk}{2\pi}.$$

Let $(T, T(k)) = (H_1, H_1(k)), (H_1^\sharp, H_1^\sharp(k))$. According to [Reed-Simon IV, Section XIII], we have

- $\lambda \in \sigma(T)$
  $\iff$ For any $\epsilon > 0$, the following is valid:

$$m(\{k \in S^1 | \quad \sigma(T(k)) \cap (\lambda - \epsilon, \lambda + \epsilon) \neq \emptyset\}) > 0.$$

- $\lambda \in \sigma_p(T) \iff m(\{k \in S^1 | \quad \lambda \in \sigma_p(T(k))\}) > 0.$

Proposition 1.1. (*[Graf-Porta, 2013], [Fujita at el, 1996]*) *For* $k \in (-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi)$, $0 \in \sigma_p(H_1^\sharp(k))$. *Thus,* $0 \in \sigma_p(H_1^\sharp)$.

Proof. Note that $H_1^\sharp(k)\psi = 0$ ($\psi = (\psi_n^A, \psi_n^B)^\top$) is equivalent to

$$\begin{cases} \psi_{n-1}^B + (1 + e^{-ik})\psi_n^B = 0, \\ \psi_{n+1}^A + (1 + e^{ik})\psi_n^A = 0, \end{cases} \qquad n \in \mathbb{N}.$$

Since $1 + e^{-ik} = 0 \Leftrightarrow k = \pm\pi$ and the Dirichlet b.c. $\psi_0^B = 0$,

$$\psi_n^B \equiv 0, \qquad n \in \mathbb{N}_0.$$

For $k \in (-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi)$, we have

$$\cos k < -\frac{1}{2} \Longleftrightarrow (1 + \cos k)^2 + \sin^2 k < 1 \Longleftrightarrow |1 + e^{ik}| < 1.$$

Thus, we have

$$\psi_{n+1}^A = -(1+e^{ik})\psi_n^A, \quad n \in \mathbb{N}.$$

Hence, we have

$$\|\psi\|_{\ell^2(\mathbb{N},\mathbb{C}^2)}^2 = \sum_{n=0}^{\infty} |\psi_n^A|^2 = \frac{1}{1-|1+e^{ik}|^2}|\psi_1^A|^2 < +\infty$$

for any $\psi_1^A \in \mathbb{C}$. Thus, $0 \in \sigma_p(H_1^\sharp(k))$.

Since $m((-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi))$ is positive, we have

$$0 \in \sigma_p(H_1^\sharp).$$

□

2　Aim and Known Results

Aim of this talk

　グラフェン上の Bulk Hamiltonian H と Edge Hamiltonian $H^\sharp$ のスペクトルを比較して, Bulk Hamitonian の固有値ではないが, Edge Hamiltonian の固有値であるようなエネルギー順位が存在することを調べる.

- ハミルトニアンは, 量子グラフとして記述されるものを扱う.
- バルクハミルトニアンに対応する量子グラフは, 2007年に, P. Kuchment–O. Post が調査済.
- エッジハミルトニアン特有の固有値を探すカギは, ベクトル

$$\mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

◇ An Edge Hamiltonian $H^\sharp$ in $L^2(\Gamma_{\mathrm{Edge}})$ on Graphene

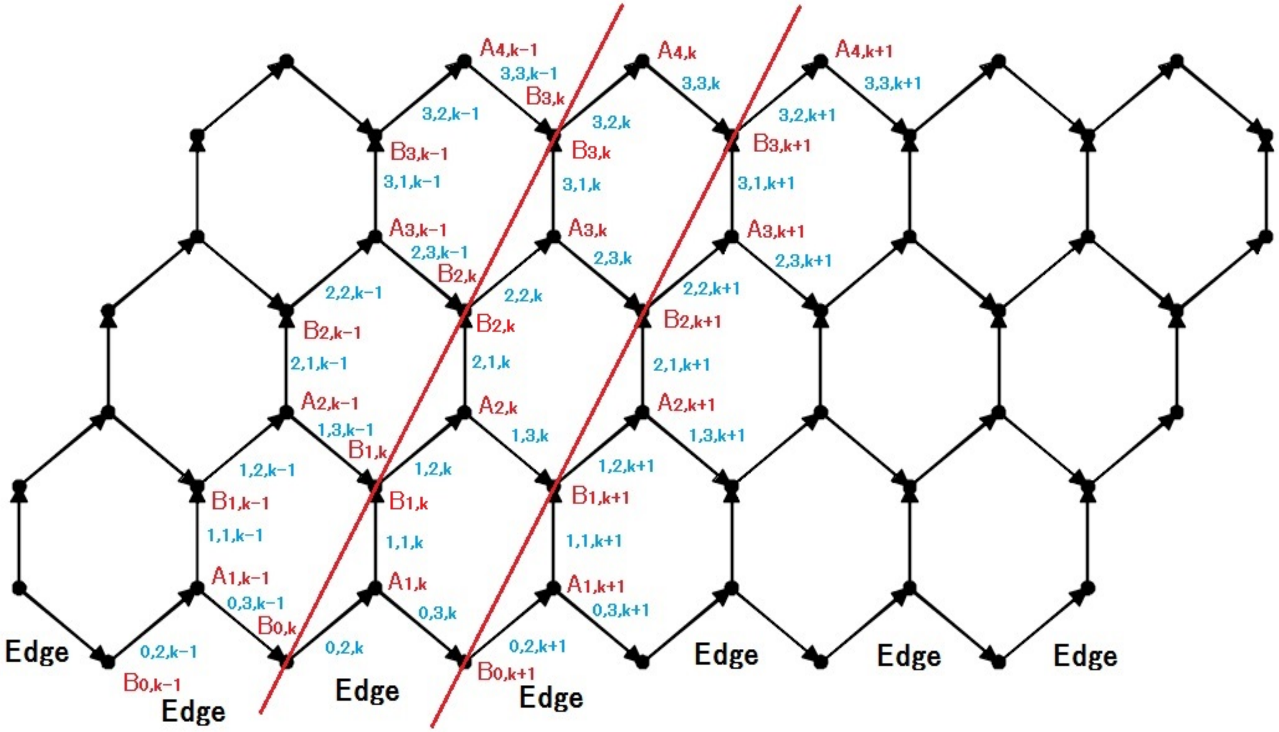


Fig. 1 Γ_{Edge}; Graphene with zigzag boundaries.

(1) $\Gamma_{\mathrm{Edge}} = (E_{\mathrm{Edge}}, V_{\mathrm{Edge}})$.

(2) $q \in L^2(0,1)$; real-valued.

(3) For $\forall e \in E_{\mathrm{Edge}}$, the Edge Hamiltonian $H^\sharp$ in $L^2(\Gamma_{\mathrm{Edge}})$ acts as

$$(H^\sharp y)_e(x) = -y_e''(x) + q(x)y_e(x), \quad x \in (0,1) \simeq e,$$

where $y \in \mathrm{Dom}(H^\sharp)$ satisfies

(a) the Kirchhoff vertex condition at $\forall v \in V_{\mathrm{Edge}} \setminus \partial\Gamma_{\mathrm{Edge}}$,

(b) the Dirichlet boundary condition on (zigzag) edges.

◇ A Bulk Hamiltonian H in $L^2(\Gamma_{\mathrm{Bulk}})$ on Graphene

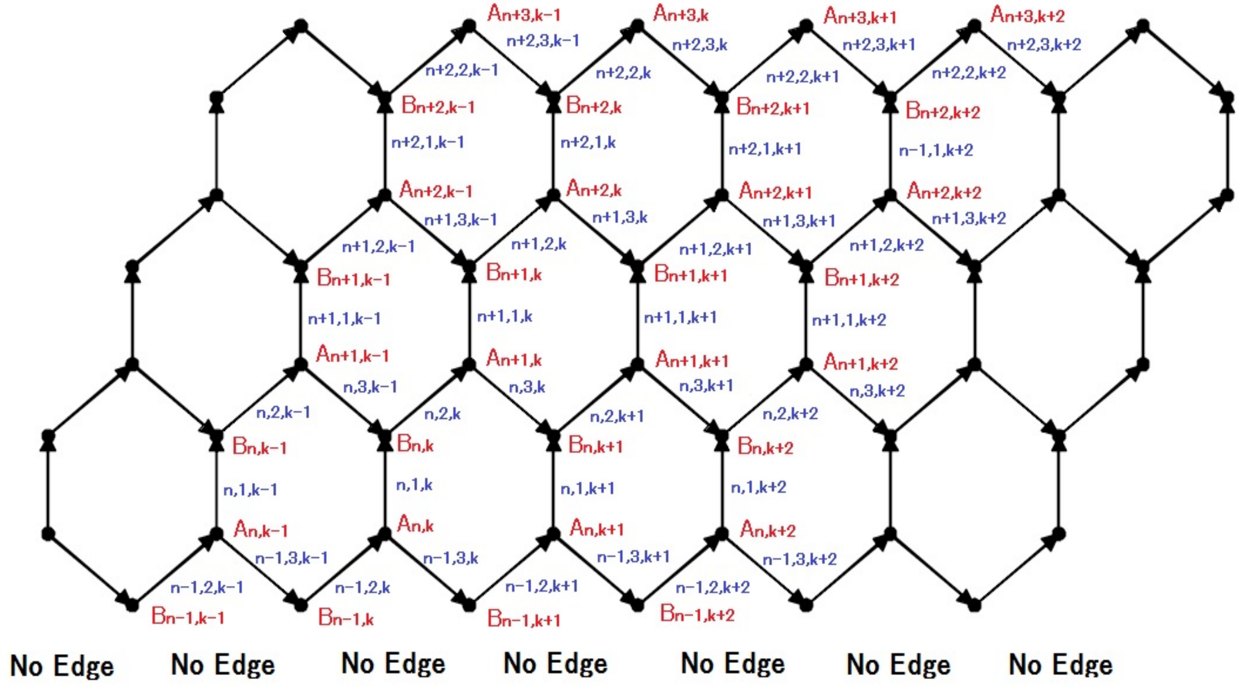


Fig. 2 Γ_{Bulk}; Graphene without any boundary.

(1) $\Gamma_{\mathrm{Bulk}} = (E_{\mathrm{Bulk}}, V_{\mathrm{Bulk}})$.
(2) $q \in L^2(0,1)$; real-valued.
(3) For $\forall e \in E_{\mathrm{Bulk}}$, the Bulk Hamiltonian H in $L^2(\Gamma_{\mathrm{Bulk}})$ acts as

$$(Hy)_e(x) = -y_e''(x) + q(x)y_e(x), \quad x \in (0,1) \simeq e,$$

where $y \in \mathrm{Dom}(H)$ satisfies the Kirchhoff vertex condition at $\forall v \in V_{\mathrm{Bulk}}$:

$$\begin{cases} y_{n,1,k}(0) = y_{n-1,2,k}(1) = y_{n-1,3,k}(0), \\ y'_{n,1,k}(0) - y'_{n-1,2,k}(1) + y'_{n-1,3,k}(0) = 0 \end{cases} \quad \text{at } A_{n,k},$$

$$\begin{cases} y_{n,1,k}(1) = y_{n,2,k}(0) = y_{n,3,k-1}(1), \\ -y'_{n,1,k}(1) + y'_{n,2,k}(0) - y'_{n,3,k-1}(1) = 0 \end{cases} \quad \text{at } B_{n,k}.$$

$\diamond$ Known Results

Notations

(1) Let σ_D be the set of eigenvalues of the spectral problem

$$-y'' + qy = \lambda y \quad \text{on} \quad (0,1) \quad \text{and} \quad y(0) = y(1) = 0.$$

(2) Expand q to the 1-periodic function. Let $\theta(x,\lambda)$ and $\varphi(x,\lambda)$ be the solutions to $-y'' + qy = \lambda y$ in $\mathbb{R}$ satisfying

$$(\theta(0,\lambda), \theta'(0,\lambda)) = (1,0) \quad \text{and} \quad (\varphi(0,\lambda), \varphi'(0,\lambda)) = (0,1).$$

(3) We put

$$\Delta(\lambda) = \frac{\theta(1,\lambda) + \varphi'(1,\lambda)}{2} \quad \text{and} \quad \Delta_-(\lambda) = \frac{\theta(1,\lambda) - \varphi'(1,\lambda)}{2}.$$

Theorem 2.1. *(P. Kuchment–O. Post, 2007)*
(i) (Basic spectral structure) There exists some sequence

$$\lambda_0^+ < \lambda_1^- \le \lambda_1^+ < \lambda_2^- \le \lambda_2^+ < \cdots < \lambda_j^- \le \lambda_j^+ < \cdots \to +\infty$$

such that

$$\sigma(H) = \sigma_{ac}(H) \cup \sigma_p(H),$$

where

$$\sigma_p(H) = \sigma_D, \quad \sigma_{ac}(H) = \bigcup_{j=1}^{\infty} B_j$$

and $B_j = [\lambda_{j-1}^+, \lambda_j^-]$ *for each* $j \in \mathbb{N}$.

(ii) (Dispersion Relation) There exists a family of fiber operators $\{H(\mu_1, \mu_2)\}$ such that

$$H \simeq \int_{S^2}^{\oplus} H(\mu_1, \mu_2) \frac{d\mu_1 d\mu_2}{(2\pi)^2}.$$

For each quasi-momentum $(\mu_1, \mu_2) \in S^2 := [-\pi, \pi]^2$, the dispersion relation is consisting of $S^2 \times \sigma_D$ and the variety

$$9\Delta^2(\lambda) - \Delta_-^2(\lambda) = 1 + 8 \cos \frac{\mu_1 - \mu_2}{2} \cos \frac{\mu_1}{2} \cos \frac{\mu_2}{2}.$$

※ Kuchment and Post proved these results for even potentials. Evenness can be removed as stated above.

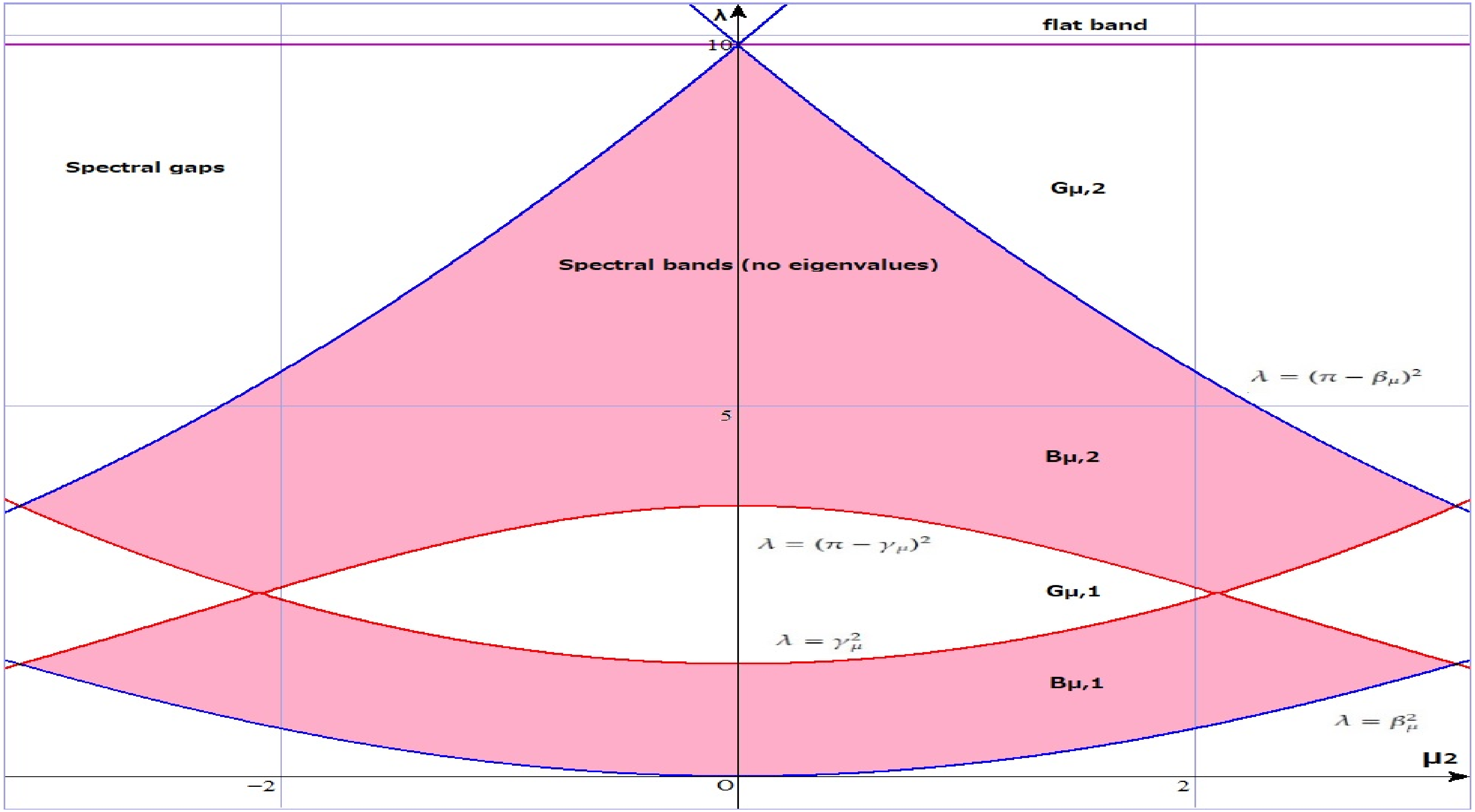


Fig. 3 The dispersion relation for H in the unperturbed case.

Put

$$F(\mu_1, \mu_2) = 1 + 8\cos\frac{\mu_1 - \mu_2}{2}\cos\frac{\mu_1}{2}\cos\frac{\mu_2}{2}.$$

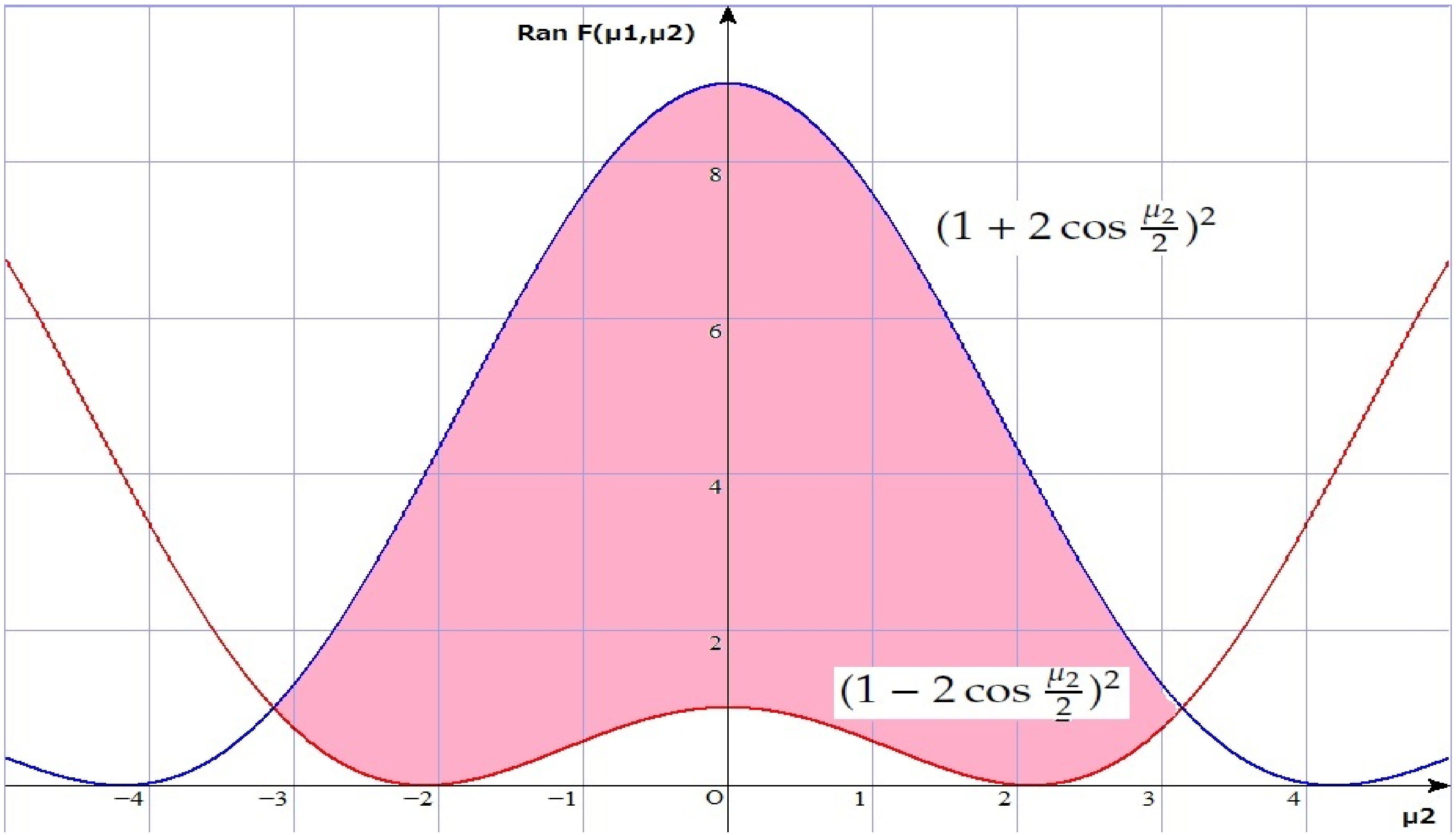
For a fixed μ_2, we use $F_{\mu_2}(\mu_1) := F(\mu_1, \mu_2)$. Its derivative check is explicitly written:

(i) If $\mu_2 = \pi$, then we have $\frac{dF_{\mu_2}}{d\mu_1}(\mu_1) = 0$ and $F(\mu_1, \pi) = 1$.

(ii) If $\mu_2 = 0$, then we have $F(\mu_1, 0) = 1 + 8\cos^2\frac{\mu_1}{2} \in [1, 9]$.

(iii) If $\mu_2 \in (0, \pi)$, we have the followings:

μ_1	$-\pi$		$\frac{\mu_2}{2} - \pi$		$\frac{\mu_2}{2}$		π
$\frac{dF_{\mu_2}}{d\mu_1}$		$-$	0	$+$	0	$-$	
F_{μ_2}	1	$\searrow$	$(1 - 2\cos\frac{\mu_2}{2})^2$	$\nearrow$	$(1 + 2\cos\frac{\mu_2}{2})^2$	$\searrow$	1


Ran F(μ1,μ2)
8
6
4
2
$(1+2\cos\frac{\mu_2}{2})^2$
$(1-2\cos\frac{\mu_2}{2})^2$
−4
−3
−2
−1
O
1
2
3
4
μ2

Thus, the following conditions are equivalent when $q \equiv 0$:

- $\exists(\mu_1, \mu_2) \in S^2$ s.t. $9\cos^2\sqrt{\lambda} = F(\mu_1, \mu_2)$
- $\exists\mu_2 \in S^1$ s.t. $(1 - 2\cos\frac{\mu_2}{2})^2 \le 9\cos^2\sqrt{\lambda} \le (1 + 2\cos\frac{\mu_2}{2})^2$.
- $\exists\mu_2 \in S^1$ s.t.

$$\lambda \in \bigcup_{n=1}^{\infty} B_{\mu_2,n},$$

where

$$\begin{cases} \beta_\mu = \arccos\left\{\frac{1}{3}\left(1 + 2\cos\frac{\mu}{2}\right)\right\}, \quad \gamma_\mu = \arccos\left\{\frac{1}{3}\left|2\cos\frac{\mu}{2} - 1\right|\right\}, \\ \xi^+_{\mu,2n-2} = \{(n-1)\pi + \beta_\mu\}^2, \quad \xi^-_{\mu,2n-1} = \{(n-1)\pi + \gamma_\mu\}^2, \\ \xi^+_{\mu,2n-1} = (n\pi - \gamma_\mu)^2, \quad \xi^-_{\mu,2n} = (n\pi - \beta_\mu)^2, \\ B_{\mu,2n-1} = [\xi^+_{\mu,2n-2}, \xi^-_{\mu,2n-1}], \quad B_{\mu,2n} = [\xi^+_{\mu,2n-1}, \xi^-_{\mu,2n}]. \end{cases}$$

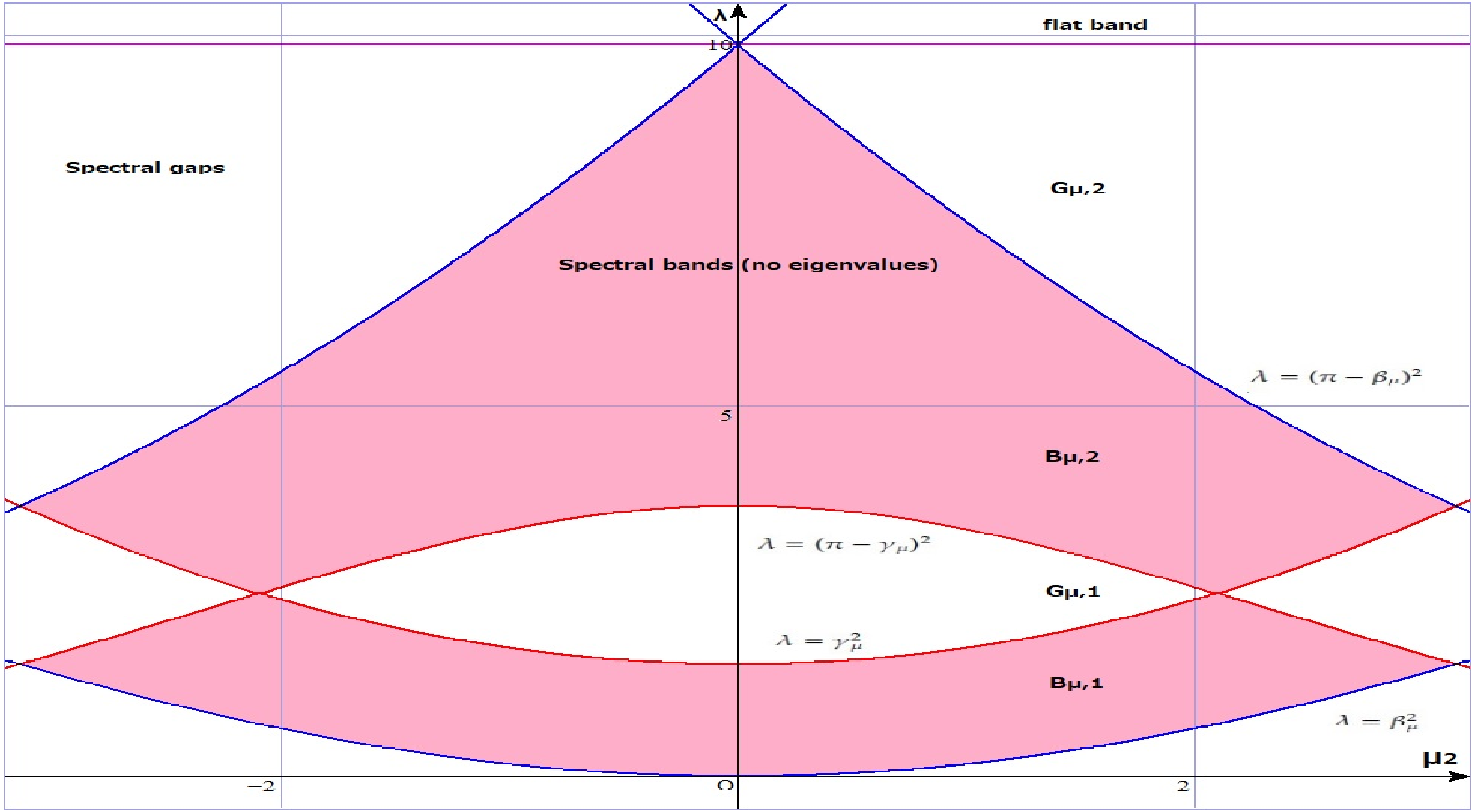


Fig. 4 The dispersion relation for H in the unperturbed case.

3 Main Results for $H^\sharp$

We put $\sigma_p^\sharp = \sigma_p(H^\sharp) \setminus \sigma_p(H)$. For a $\lambda \in \sigma_p^\sharp$, the corresponding eigenfunction is called an edge state.

Theorem 3.1. *(N, 2021, "Results in Mathematics")*
(i) (Basic spectral structure) We have

$$\sigma(H^\sharp) = \sigma(H) \cup \sigma_p^\sharp = \left(\bigcup_{j=1}^{\infty} B_j\right) \cup \sigma_D \cup \sigma_p^\sharp.$$

(ii) (Existence of edge states) The energies for edge states can be characterized as the infinite set

$$\sigma_p^\sharp = \{\lambda \in \mathbb{R} | \quad \theta(1,\lambda) + 2\varphi'(1,\lambda) = 0\} \neq \emptyset.$$

(iii) (Location of the eigenvalues) Let us recall

$$\lambda_0^+ < \lambda_1^- \le \lambda_1^+ < \lambda_2^- \le \lambda_2^+ < \cdots < \lambda_j^- \le \lambda_j^+ < \cdots \to +\infty$$

and $B_j = [\lambda_{j-1}^+, \lambda_j^-]$ *for each* $j \in \mathbb{N}$.
Putting

$$G_j = (\lambda_j^-, \lambda_j^+) \quad \text{and} \quad \overline{G_j} = [\lambda_j^-, \lambda_j^+]$$

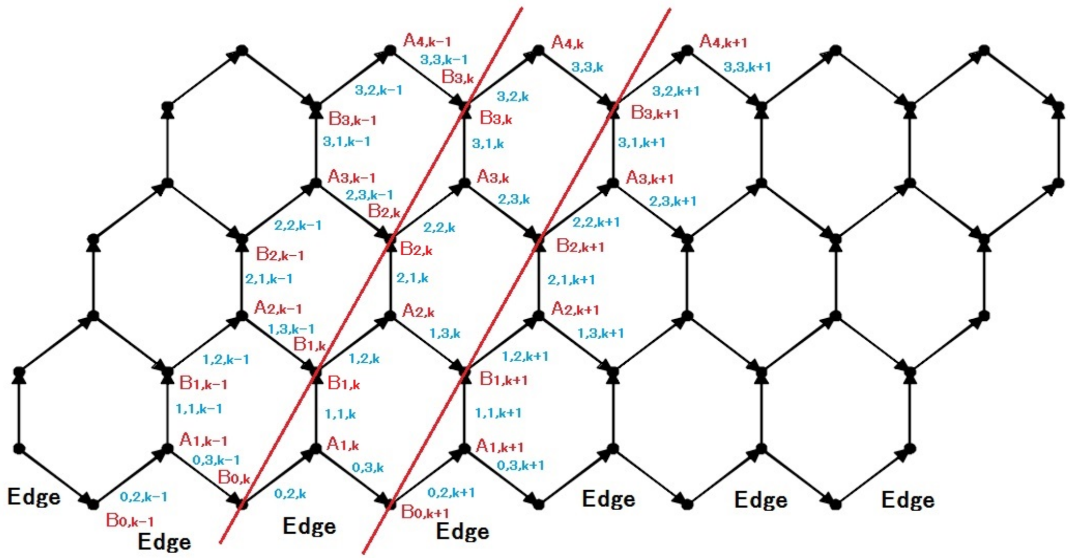
for each $j \in \mathbb{N}$, *we have*

$$\sigma_D \subset \bigcup_{n=1}^{\infty} \overline{G_{2n}} \quad \text{and} \quad \sigma_p^\sharp \subset \bigcup_{n=1}^{\infty} \overline{G_{2n-1}}.$$

4 Main Results for fiber operators of $H^\sharp$

Since $H^\sharp$ is periodic in $\mathbf{a}_2 = \overrightarrow{A_{1,0}A_{1,1}}$, we construct

$$H^\sharp \simeq \int_{S^1}^{\oplus} H^\sharp(\mu)\frac{d\mu}{2\pi}.$$



For each quasi-momentum $\mu \in S^1 = [-\pi, \pi]$, the fiber operator $H^\sharp(\mu)$ in $L^2(\Gamma_{\text{Edge},0})$ (see Fig. 5) acts as

$$(H^\sharp(\mu)y)_{n,j}(x) = -y''_{n,j}(x) + q(x)y_{n,j}(x), \quad x \in (0,1) \simeq \Gamma_{n,j}$$

for a pair (n, j) of indices of an edge $\Gamma_{n,j}$.

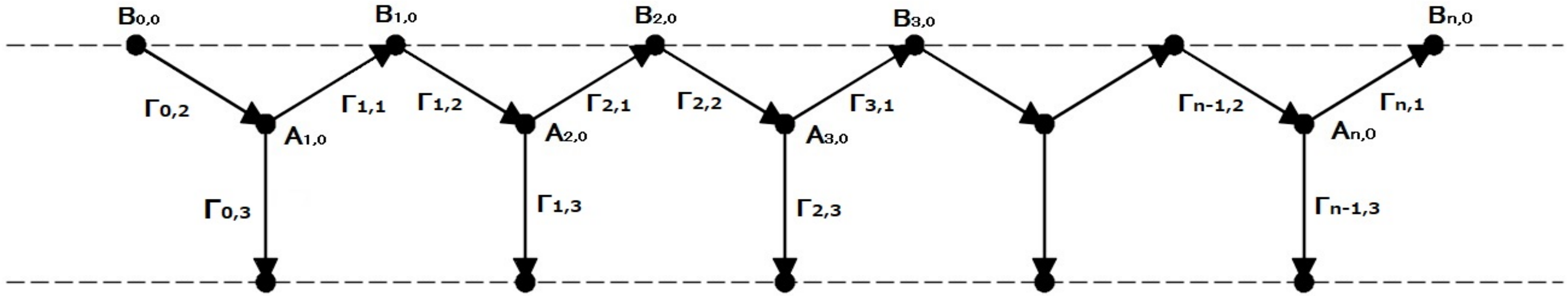
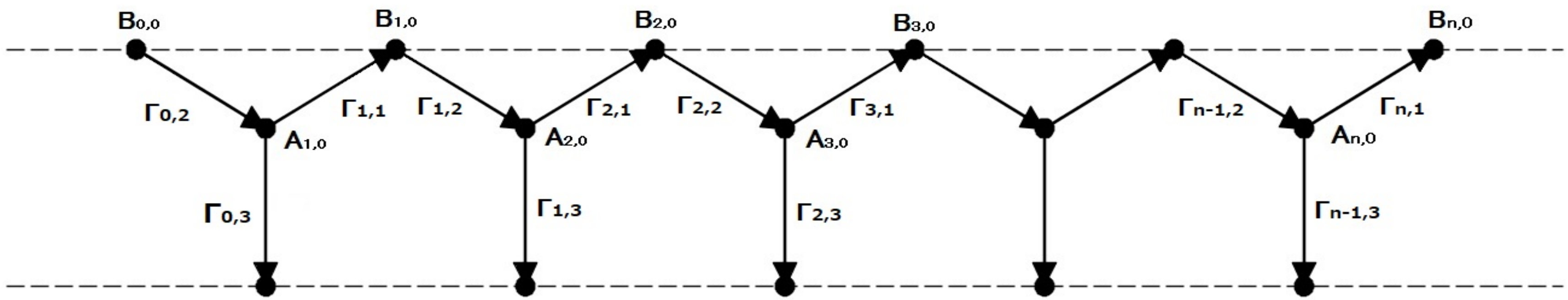


Fig. 5 The metric graph $\Gamma_{\text{Edge},0}$

Here, $y \in \mathrm{Dom}(H^\sharp(\mu))$ satisfies the vertex conditions

$$y_{n,1}(0) = y_{n-1,2}(1) = y_{n-1,3}(0), \quad y'_{n,1}(0) - y'_{n-1,2}(1) + y'_{n-1,3}(0) = 0,$$
$$y_{n,1}(1) = y_{n,2}(0) = e^{-i\mu} y_{n,3}(1), \quad -y'_{n,1}(1) + y'_{n,2}(0) - e^{-i\mu} y'_{n,3}(1) = 0$$

at vertices $\{A_{n,0}\}_{n\geq 2}$ and $\{B_{n,0}\}_{n\in\mathbb{N}_0}$ as well as the Dirichlet boundary condition: $y_{0,j}(x) \equiv 0$ ($j = 2, 3$) and $y_{1,1}(0) = 0$.



4.1 $\sigma(H^\sharp(\mu))$ in the unperturbed case

For the simplicity, we here state

the results on $\sigma(H^\sharp(\mu))$ in the case of $q \equiv 0$.

For $\mu \in [-\pi, \pi]$ and $n \in \mathbb{N}$, we recall

$$B_{\mu,2n-1} = [\xi^+_{\mu,2n-2}, \xi^-_{\mu,2n-1}], \quad B_{\mu,2n} = [\xi^+_{\mu,2n-1}, \xi^-_{\mu,2n}]$$

and define their gap

$$G_{\mu,n} = (\xi^-_{\mu,n}, \xi^+_{\mu,n}).$$

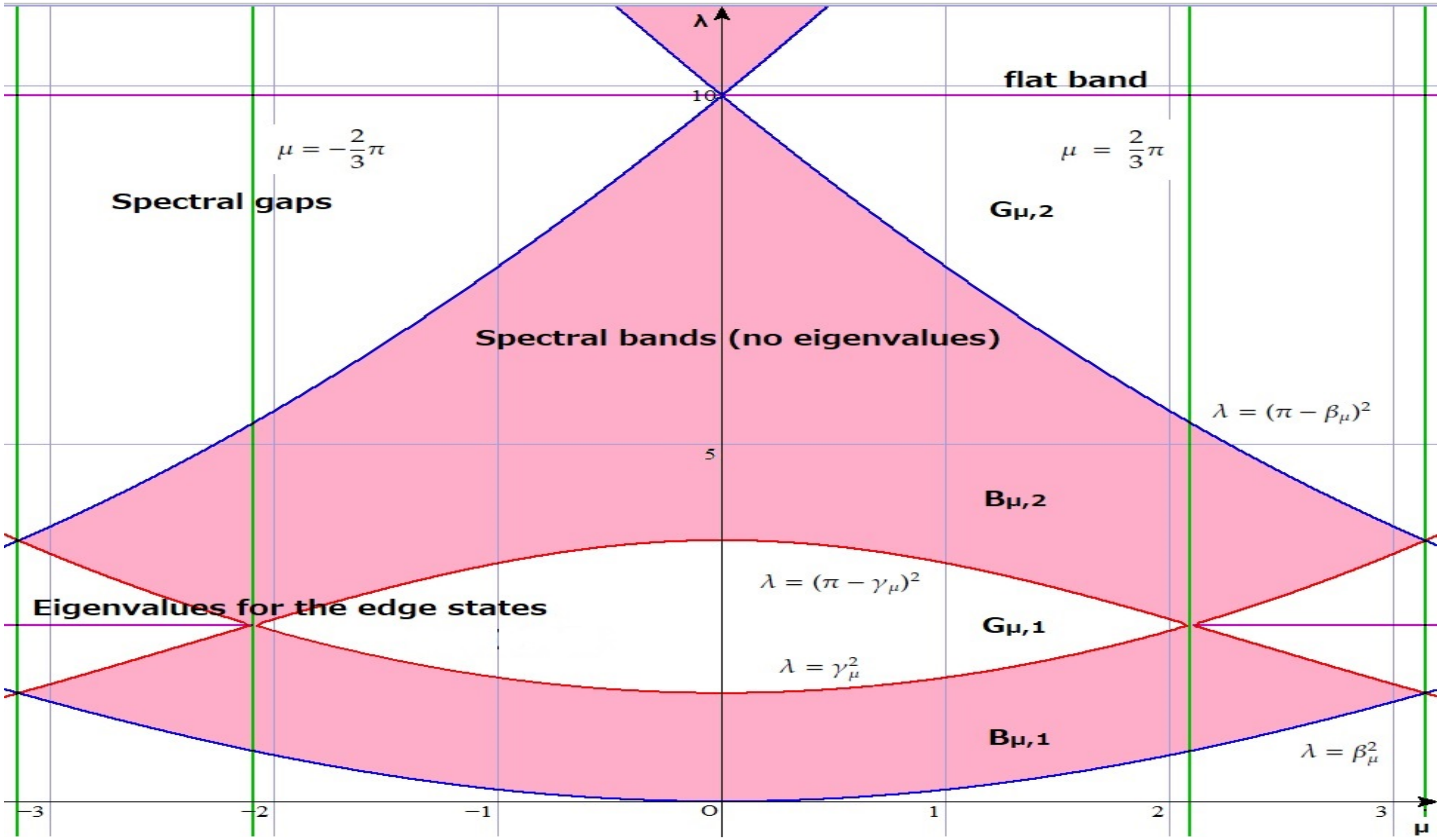


Fig. 6 The dispersion relation for $H^\sharp$ in the unperturbed case.

Theorem 4.1. *Assume that* $q \equiv 0$ *and fix* $\mu \in (-\pi, \pi)$.

(1) *If* $\lambda \in \sigma_D := \{n^2\pi^2 | \quad n \in \mathbb{N}\}$, *then we have* $\lambda \in \bigcup_{j=1}^{\infty} \overline{G_{\mu,2j}}$ *and* $\lambda \in \sigma_p(H^\sharp(\mu))$.

(2) *Let* $\lambda \notin \sigma_D$ *and* $\lambda \in \bigcup_{j=1}^{\infty} B_{\mu,j}$. *Then,* $\lambda \in \sigma(H^\sharp(\mu))$.
If $\lambda \in \bigcup_{j=1}^{\infty} B^\circ_{\mu,j}$, *then* $\lambda \notin \sigma_p(H^\sharp(\mu))$
If $\lambda \in \bigcup_{j=1}^{\infty} \partial B_{\mu,j}$ *and* $\mu \neq \pm\frac{2}{3}\pi$, *then* $\lambda \notin \sigma_p(H^\sharp(\mu))$.

(3) *Let* $\lambda \notin \sigma_D$ *and* $\lambda \in \bigcup_{j=0}^{\infty} G_{\mu,j}$.

(A) *If* $\cos\sqrt{\lambda} \neq 0$, *then* $\lambda \in \rho(H^\sharp(\mu))$.

(B) *If* $\cos\sqrt{\lambda} = 0$ *and* $\mu \neq \pm\frac{2}{3}\pi$, *then* $\lambda \in \bigcup_{j=1}^{\infty} G_{\mu,2j-1}$ *and the following three conditions are equivalent:*
(i) $\mu \in (-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi)$, *(ii)* $\lambda \in \sigma_p(H^\sharp(\mu))$,
(iii) $\lambda \in \sigma(H^\sharp(\mu))$.

For each $n \in \mathbb{N}$, we put

$$B_n = \bigcup_{\mu \in (-\pi,\pi)} B_{\mu,n} = [\left\{\frac{\pi}{2}(n-1)\right\}^2, \left(\frac{\pi}{2}n\right)^2].$$

Theoerm 4.1 yields Theorem 3.1 in the unperturbed case:

Theorem 4.2. *Assume that* $q \equiv 0$. *Then, we have*

$$\sigma(H^\sharp) = [0,\infty) = \left(\bigcup_{n=1}^{\infty} B_n\right) \cup \sigma_D \cup \sigma_p^\sharp,$$

where $\sigma_D = \{n^2\pi^2 |\ n \in \mathbb{N}\}$ *and* $\sigma_p^\sharp = \{\lambda \in \mathbb{R} |\ \cos\sqrt{\lambda} = 0\}$.

4.2 $\sigma(H^\sharp(\mu))$ in the perturbed case

For $\mu \in S^1 \setminus \{\pm\pi\} = (-\pi, \pi)$, we put

$$F(\mu, \lambda) = \frac{1}{4\cos\frac{\mu}{2}} \left(9\Delta^2(\lambda) - \Delta_-^2(\lambda) - 1 - 4\cos^2\frac{\mu}{2} \right). \qquad (1)$$

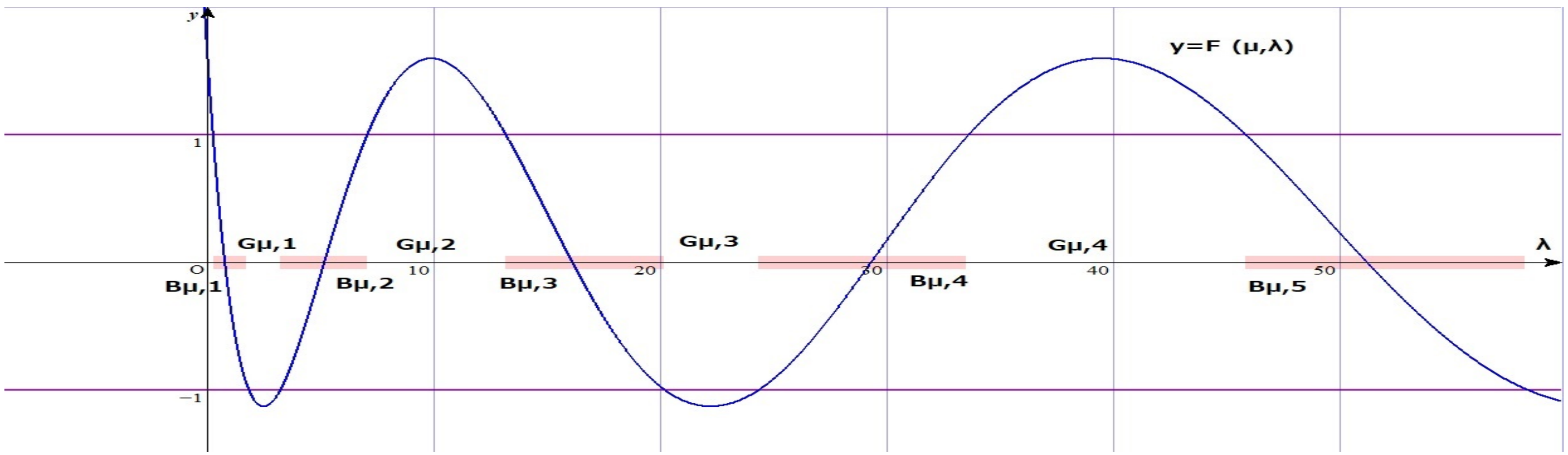
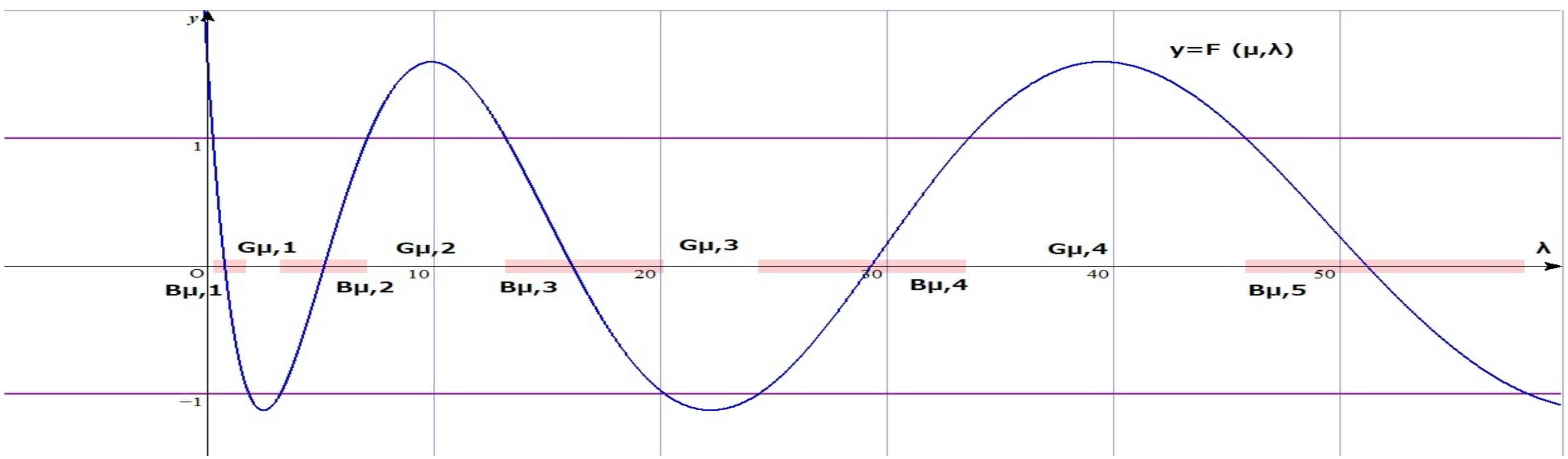


Fig. 7 A graph of the discriminant $F(\mu, \lambda)$.

The jth band $B_{\mu,j}$ and gap $G_{\mu,j}$ for $j \in \mathbb{N}$ are characterized by $F(\mu,\lambda)$ as

$$|F(\mu,\lambda)| \leq 1 \quad \text{on} \quad \bigcup_{j=1}^{\infty} B_{\mu,j} \quad \text{and} \quad |F(\mu,\lambda)| > 1 \quad \text{on} \quad \bigcup_{j=0}^{\infty} G_{\mu,j}.$$

Moreover, we put $G_{\mu,0} := (-\infty, \inf B_{\mu,1})$.



Theorem 4.3. *Fix* $\mu \in (-\pi, \pi)$.

(1) *If* $\lambda \in \sigma_D$*, then we have* $\lambda \in \bigcup_{j=1}^{\infty} \overline{G_{\mu,2j}}$ *and* $\lambda \in \sigma_p(H^\sharp(\mu))$.

(2) *Let* $\lambda \notin \sigma_D$ *and* $\lambda \in \bigcup_{j=1}^{\infty} B_{\mu,j}$*. Then,* $\lambda \in \sigma(H^\sharp(\mu))$.

If $\lambda \in \bigcup_{j=1}^{\infty} B^{\circ}_{\mu,j}$*, then* $\lambda \notin \sigma_p(H^\sharp(\mu))$.

If $\lambda \in \bigcup_{j=1}^{\infty} \partial B_{\mu,j}$ *and* $\mu \neq \pm\frac{2}{3}\pi$*, then* $\lambda \notin \sigma_p(H^\sharp(\mu))$.

(3) *Let* $\lambda \notin \sigma_D$ *and* $\lambda \in \bigcup_{j=0}^{\infty} G_{\mu,j}$.

(A) *If* $\theta(1,\lambda) + 2\varphi'(1,\lambda) \neq 0$*, then we have* $\lambda \in \rho(H^\sharp(\mu))$.

(B) *If* $\theta(1,\lambda) + 2\varphi'(1,\lambda) = 0$ *and* $\mu \neq \pm\frac{2}{3}\pi$*, then* $\lambda \in \bigcup_{j=1}^{\infty} G_{\mu,2j-1}$ *and the followings are equivalent:*

(i) $\mu \in (-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi)$, *(ii)* $\lambda \in \sigma_p(H^\sharp(\mu))$,

(iii) $\lambda \in \sigma(H^\sharp(\mu))$.

For each $n \in \mathbb{N}$, we put

$$B_n = \bigcup_{\mu \in (-\pi,\pi)} B_{\mu,n}, \quad G_n = \bigcap_{\mu \in (-\pi,\pi)} G_{\mu,n}.$$

Then, we have the statements of Theorem 3.1;

For any $q \in L^2(0,1)$, we have

$$\sigma(H^\sharp) = \left(\bigcup_{n=1}^{\infty} B_n \right) \cup \sigma_D \cup \sigma_p^\sharp,$$

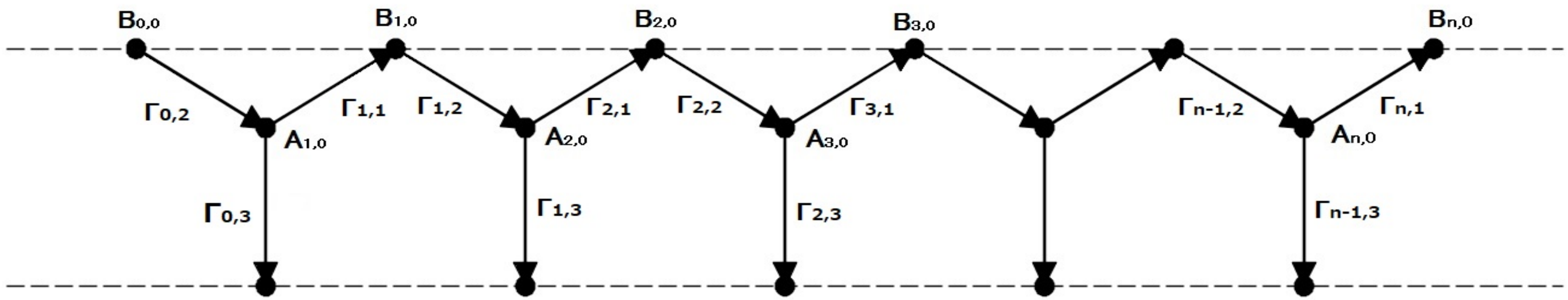
$$\sigma_D \subset \bigcup_{n=1}^{\infty} \overline{G_{2n}},$$

$$\sigma_p^\sharp = \{\lambda \in \mathbb{R} | \quad \theta(1,\lambda) + 2\varphi'(1,\lambda) = 0\} \subset \bigcup_{n=1}^{\infty} \overline{G_{2n-1}}.$$

5 Idea of the proof of Theorem 4.3 (3).

Define the transfer matrix $M(\lambda) := (m_{ij}(\lambda))_{i,j=1,2}$ by

$$\begin{pmatrix} y_{n+1,1}(0,\lambda) \\ y'_{n+1,1}(0,\lambda) \end{pmatrix} = M(\lambda) \begin{pmatrix} y_{n,1}(0,\lambda) \\ y'_{n,1}(0,\lambda) \end{pmatrix} \quad \text{for } n \in \mathbb{N}.$$



Straightforward calculations yield the following 2 lemmas:

Lemma 5.1. *Assume that* $\lambda \notin \sigma_D$ *and* $\mu \in S^1 \setminus \{\pm\pi\}$. *Preparing* $\tilde{M}(\lambda) := (1 + e^{-i\mu})M(\lambda)$, *we have*

$$\tilde{M}(\lambda) = \begin{pmatrix} 2\Delta\theta_1 + \theta_1'\varphi_1 & \varphi_1(\theta_1 + 2\varphi_1') \\ \frac{1}{\varphi_1}\left\{-4\theta_1\cos^2\frac{\mu}{2} + 2\Delta(2\Delta\theta_1 + \theta_1'\varphi_1)\right\} & -4\cos^2\frac{\mu}{2} + 2\Delta(2\Delta + \varphi_1') \end{pmatrix}.$$

Note that

- $\varphi_1 \neq 0$ for $\lambda \notin \sigma_D$,
- $1 + e^{-i\mu} \neq 0$ for $\mu \in S^1 \setminus \{\pm\pi\}$.
- We used the abbrviation

$$(\theta_1, \theta_1', \varphi_1, \varphi_1') = (\theta(1,\lambda), \theta'(1,\lambda), \varphi(1,\lambda), \varphi'(1,\lambda)).$$

Lemma 5.2. *Assume that* $\lambda \notin \sigma_D$ *and* $\mu \in S^1 \setminus \{\pm\pi\}$. *Then, the eigenvalues of* $M(\lambda)$ *are given by the formulae*

$$\rho_{\pm} = \frac{1}{2(1 + e^{-i\mu})}(d(\mu, \lambda) \pm \sqrt{D(\mu, \lambda)}),$$

where

- $d(\mu, \lambda) = 9\Delta^2(\lambda) - \Delta_-^2(\lambda) - 1 - 4\cos^2\frac{\mu}{2}$,
- $D(\mu, \lambda) = d^2(\mu, \lambda) - 16\cos^2\frac{\mu}{2}$.

Notation

- $V(\rho_\pm)$; the eigenspaces for the eigenvalues $\rho_\pm$.
- $\mathbf{e}_2 = \begin{pmatrix} 0 & 1 \end{pmatrix}^{\mathsf{T}}$.

Theorem 5.3. *Assume that* $\lambda \notin \sigma_D$ *and* $\mu \in S^1 \setminus \{\pm\pi\}$.

(I) *If* $D(\mu, \lambda) < 0$, *then* $|\rho_\pm| = 1$, $\lambda \in \sigma(H^\sharp(\mu))$, $\lambda \notin \sigma_p(H^\sharp(\mu))$.

(II) *If* $D(\mu, \lambda) > 0$, *then* $\rho_+ \overline{\rho_-} = 1$, $|\rho_\pm| \neq 1$ *and the followings:*

- *(i)* *If* $\mathbf{e}_2 \notin V(\rho_+)$ *and* $\mathbf{e}_2 \notin V(\rho_-)$, *then* $\lambda \in \rho(H^\sharp(\mu))$.
- *(ii)* *Assume that* $\mathbf{e}_2 \in V(\rho_+)$. *If* $|\rho_+| < 1$, *then* $\lambda \in \sigma_p(H^\sharp(\mu))$. *Otherwise, namely, if* $|\rho_+| > 1$, *then* $\lambda \in \rho(H^\sharp(\mu))$.
- *(iii)* *Assume that* $\mathbf{e}_2 \in V(\rho_-)$. *If* $|\rho_+| > 1$, *then* $\lambda \in \sigma_p(H^\sharp(\mu))$. *Otherwise, namely, if* $|\rho_+| < 1$, *then* $\lambda \in \rho(H^\sharp(\mu))$.

(III) *Assume that* $D(\mu, \lambda) = 0$.

- *(i)* *If* $m_{12}(\lambda) \neq 0$, *then we have* $\lambda \notin \sigma_p(H^\sharp(\mu))$.
- *(ii)* *If* $\mu \neq \pm\frac{2}{3}\pi$, *then we have* $m_{12}(\lambda) \neq 0$.

Lemma 5.4. *Let* $f : \mathbb{R}^2 \to \mathbb{R}^2$ *defined by*

$$f(\mathbf{x}) = A\mathbf{x},$$

where $A = (a_{ij})$ *with* $\operatorname{rank} A = 1$.

(I) If $a_{12} \neq 0$, *then* $\operatorname{Ker} f = \left\langle \begin{pmatrix} a_{12} \\ -a_{11} \end{pmatrix} \right\rangle$.

(II) If $a_{12} = 0$ *and* $a_{22} = 0$, *then* $\operatorname{Ker} f = \left\langle \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\rangle$.

(III) If $a_{12} = 0$ *and* $a_{22} \neq 0$, *then* $\operatorname{Ker} f = \left\langle \begin{pmatrix} a_{22} \\ -a_{21} \end{pmatrix} \right\rangle$.

Proof. Utilize the linear algebra. □

Utilizing these, we shall show Theorem 4.3 (3).

Proof of Theorem 4.3 (3). Assume that $\lambda \notin \sigma_D$, $\mu \in S^1 \setminus \{\pm\pi\}$ and $D(\mu,\lambda) > 0$. Taking

- $d(\mu,\lambda) = 9\Delta^2(\lambda) - \Delta_-^2(\lambda) - 1 - 4\cos^2\frac{\mu}{2}$,
- $D(\mu,\lambda) = d^2(\mu,\lambda) - 16\cos^2\frac{\mu}{2}$,
- $F(\mu,\lambda) = \frac{1}{4\cos\frac{\mu}{2}}(9\Delta^2(\lambda) - \Delta_-^2(\lambda) - 1 - 4\cos^2\frac{\mu}{2})$

into account, we notice that

$$D(\mu,\lambda) > 0 \iff |d(\mu,\lambda)| > 4\cos\frac{\mu}{2} \iff |F(\mu,\lambda)| > 1 \iff \lambda \in \bigcup_{j=0}^{\infty} G_{\mu,j}.$$

Proof of Theorem 4.3 (3)(A) Consider the case of $m_{12}(\lambda) \neq 0$. Then, Lemma 5.4 (I) yields

$$V(\rho_+) = \langle \begin{pmatrix} -m_{12}(\lambda) \\ -(\rho_+ - m_{11}(\lambda)) \end{pmatrix} \rangle, \quad V(\rho_-) = \langle \begin{pmatrix} -m_{12}(\lambda) \\ -(\rho_- - m_{11}(\lambda)) \end{pmatrix} \rangle.$$

This implies that $\mathbf{e}_2 \notin V(\rho_+)$ and $\mathbf{e}_2 \notin V(\rho_-)$. Theorem 5.3 (II)(i) yields $\lambda \in \rho(H^\sharp(\mu))$. Recall

- $m_{12}(\lambda) = \varphi_1(\theta_1 + 2\varphi_1')$.
- $\varphi_1 \neq 0$ for $\lambda \notin \sigma_D$.

Thus, we have Theorem 4.3 (3)(A):

$$\theta_1 + 2\varphi_1' \neq 0 \Longrightarrow \lambda \in \rho(H^\sharp(\mu)).$$

Proof of Theorem 4.3 (3)(B) Consider the case of $m_{12}(\lambda) = 0$ and $\mu \neq \pm\frac{2}{3}\pi$. Then, we have

$$
\begin{aligned}
&\theta_1 + 2\varphi_1' = 0 \\
\Rightarrow & 9\Delta^2 - \Delta_-^2 = 9\left(\frac{\theta_1 + \varphi_1'}{2}\right)^2 - \left(\frac{\theta_1 - \varphi_1'}{2}\right)^2 = \frac{1}{4}\left\{9(-\varphi_1')^2 - (-3\varphi_1')^2\right\} = 0 \\
\Rightarrow & d(\mu, \lambda) = -1 - 4\cos^2\frac{\mu}{2} < -4\cos\frac{\mu}{2} \quad (\because \mu \neq \pm\frac{2}{3}\pi) \\
\Rightarrow & |\rho_-| = \left|\frac{d(\mu, \lambda) - \sqrt{D(\mu, \lambda)}}{4\cos\frac{\mu}{2}}\right| > \frac{4\cos\frac{\mu}{2}}{4\cos\frac{\mu}{2}} = 1, \quad F(\mu, \lambda) < -1 \ (\because p.33) \\
\Rightarrow & |\rho_+| < 1, \quad \lambda \in \bigcup_{j=1}^{\infty} G_{\mu, 2j-1}.
\end{aligned}
$$

Using $9\Delta^2 - \Delta_-^2 = 0$, we derive

$$\rho_+ - m_{22}(\lambda) = \frac{1}{2(1+e^{-i\mu})}\left(-1 + 4\cos^2\frac{\mu}{2} + \left|-1 + 4\cos^2\frac{\mu}{2}\right|\right),$$

$$\rho_- - m_{22}(\lambda) = \frac{1}{2(1+e^{-i\mu})}\left(-1 + 4\cos^2\frac{\mu}{2} - \left|-1 + 4\cos^2\frac{\mu}{2}\right|\right).$$

Thus, we have

- $\rho_+ - m_{22}(\lambda) = 0 \iff \mu \in (-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi)$,
- $\rho_- - m_{22}(\lambda) = 0 \iff \mu \in (-\frac{2}{3}\pi, \frac{2}{3}\pi)$.

This combined with Lemma 5.4 (II) and (III) yields the following.

- If $\mu \in (-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi)$, then

$$V(\rho_+) = \left\langle \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\rangle \quad V(\rho_-) = \left\langle \begin{pmatrix} \rho_- - m_{22}(\lambda) \\ m_{21}(\lambda) \end{pmatrix} \right\rangle \neq \left\langle \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\rangle.$$

- If $\mu \in (-\frac{2}{3}\pi, \frac{2}{3}\pi)$, then

$$V(\rho_+) = \left\langle \begin{pmatrix} \rho_+ - m_{22}(\lambda) \\ m_{21}(\lambda) \end{pmatrix} \right\rangle \neq \left\langle \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\rangle \quad V(\rho_-) = \left\langle \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\rangle.$$

These together with $|\rho_+| < 1$ and Theorem 5.3 (II)(ii) yield the following equivalence:

$$\mu \in (-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi) \iff \mathbf{e}_2 \in V(\rho_+) \iff \lambda \in \sigma_p(H^\sharp(\mu))$$

and

$$\mu \in (-\frac{2}{3}\pi, \frac{2}{3}\pi) \iff \mathbf{e}_2 \in V(\rho_-) \iff \lambda \in \rho(H^\sharp(\mu)).$$

Thus, we derive the eigenvalue lines

$$\{\lambda \in \mathbb{R} | \quad \theta_1 + 2\varphi_1' = 0\} \subset \bigcup_{n=1}^{\infty} \overline{G_{2n-1}}.$$

□

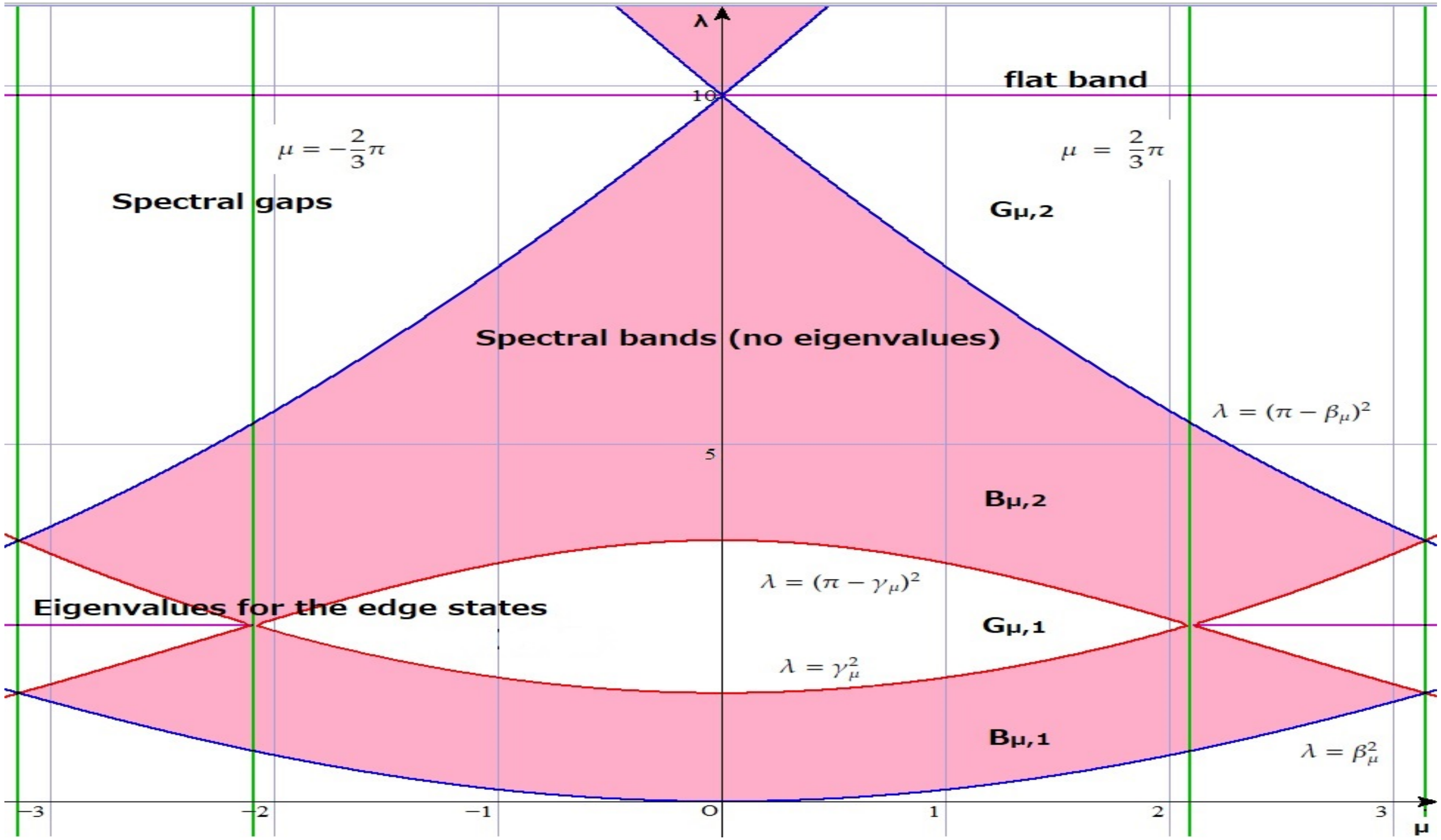


Fig. 8 The dispersion relation for $H^\sharp$ in the unperturbed case.

6 An example

Let us take a step potential

$$q(x) = \begin{cases} c & \text{if } x \in (\frac{1}{2}, 1), \\ 0 & \text{if } x \in (0, \frac{1}{2}), \end{cases} \tag{2}$$

where $c \in \mathbb{R}$. Then, we have

$$\theta(1,\lambda) = \cos\frac{\sqrt{\lambda}}{2}\cos\frac{\sqrt{\lambda - c}}{2} - \frac{\sqrt{\lambda}}{\sqrt{\lambda - c}}\sin\frac{\sqrt{\lambda - c}}{2}\sin\frac{\sqrt{\lambda}}{2},$$

$$\varphi'(1,\lambda) = \cos\frac{\sqrt{\lambda}}{2}\cos\frac{\sqrt{\lambda - c}}{2} - \frac{\sqrt{\lambda - c}}{\sqrt{\lambda}}\sin\frac{\sqrt{\lambda - c}}{2}\sin\frac{\sqrt{\lambda}}{2}.$$

For $c = 20$, we numerically draw a picture of the dispersion relation for $H^\sharp$:

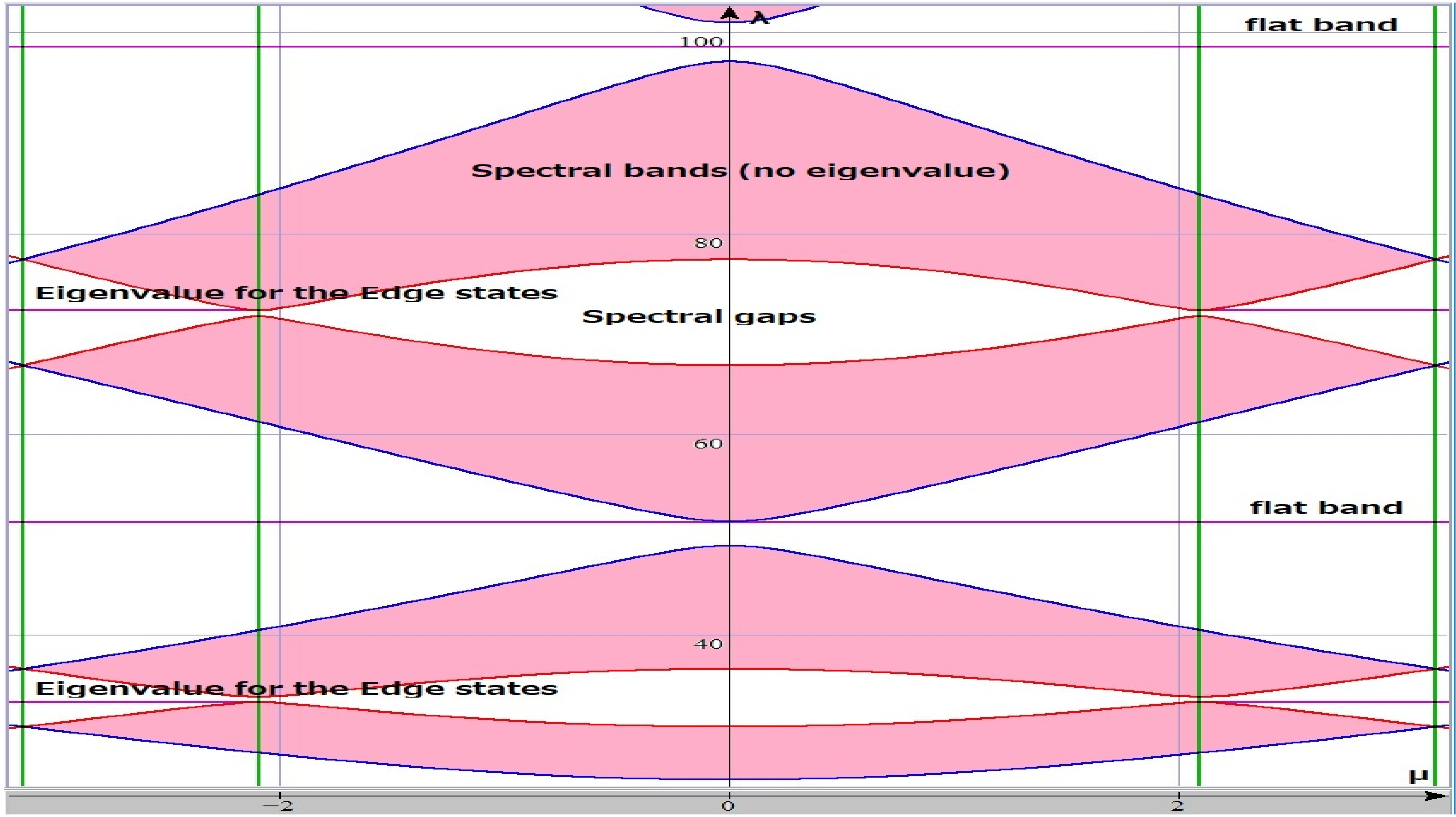


Fig. 9 The dispersion relation for $H^\sharp$ with a step potential.

Thank you for your attention.

- This talk is based on
  ”*Edge states of Schrödinger equations on graphene with zigzag boundaries*, Results in Mathematics, 76 (2021), no. 2, 55.”
- You can get this slide at the following page:
  http://www.maebashi-it.ac.jp/˜niikuni/slide/20210611.pdf

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