

23, April, 2021

Edge states of Schrödinger equations on graphene with zigzag boundaries

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1 Background

◇ トポロジカル絶縁体

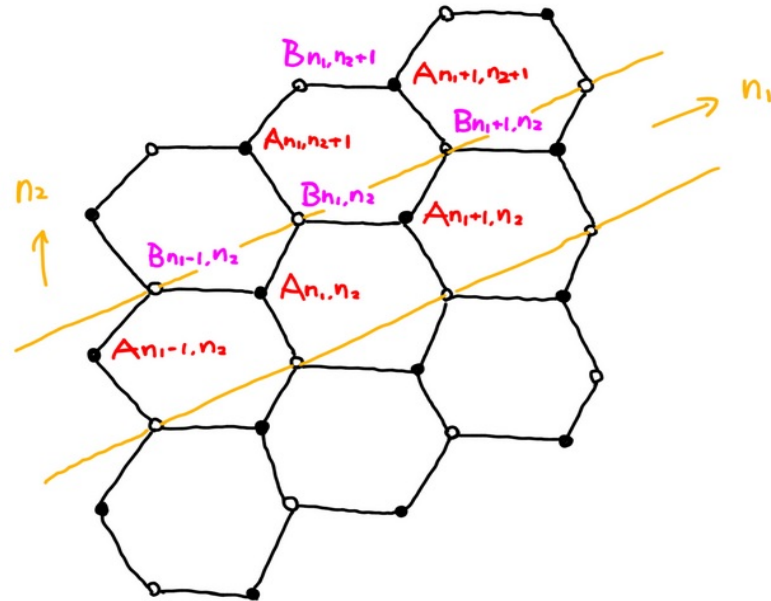
…内部 (Bulk) は絶縁体だが表面 (Edge) は伝導体.

⇒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).

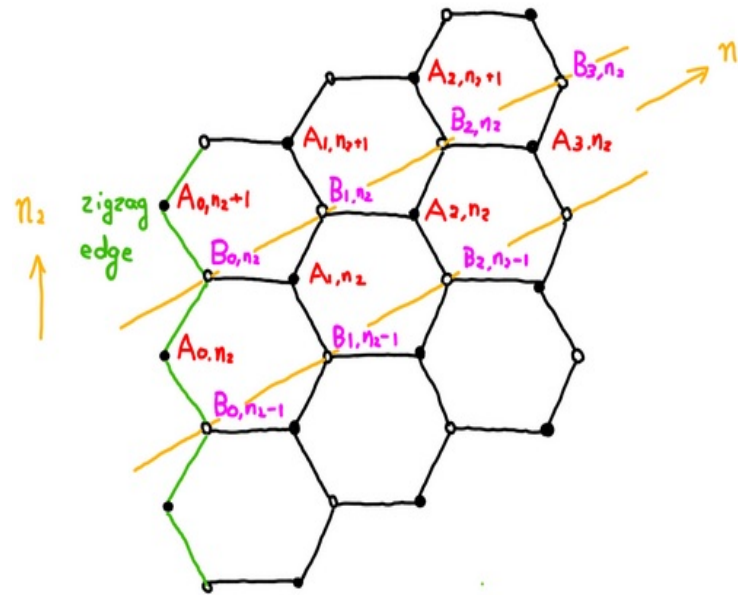
$$\begin{cases} (H_1 \psi)_{n_1, n_2}^A = -t(\psi_{n_1, n_2}^B + \psi_{n_1, n_2-1}^B + \psi_{n_1-1, n_2}^B), \\ (H_1 \psi)_{n_1, n_2}^B = -t(\psi_{n_1, n_2+1}^A + \psi_{n_1+1, n_2}^A + \psi_{n_1, n_2}^A), \end{cases} \quad (n_1, n_2) \in \mathbb{Z}^2.$$



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

$$\begin{cases} (H_1^\# \psi)_A^{n_1, n_2} = -t(\psi_B^{n_1, n_2} + \psi_B^{n_1, n_2-1} + \psi_B^{n_1-1, n_2}), \\ (H_1^\# \psi)_B^{n_1, n_2} = -t(\psi_A^{n_1, n_2+1} + \psi_A^{n_1+1, n_2} + \psi_A^{n_1, n_2}), \end{cases} \quad (n_1, n_2) \in \mathbb{N} \times \mathbb{Z}$$

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

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

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

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

with the Dirichlet boundary condition $\psi_0^A = \psi_0^B = 0$.

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

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

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

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

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

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

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

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

- $\lambda \in \sigma(T)$

$\iff$ For any $\epsilon > 0$, the following is valid:

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

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

Proposition 1.1. (*[Graf-Porta, 2013], [Fujita et al, 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

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

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

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

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

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

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, $0 \in \sigma_p(H_1^\#(k))$.

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

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

□

2 Aim and Known Results

Aim of this talk

グラフエン上の **Bulk Hamiltonian** H と **Edge Hamiltonian** $H^\#$ のスペクトルを比較して, **Bulk Hamiltonian** 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 $L^2(\Gamma_{\text{Edge}})$ on Graphene

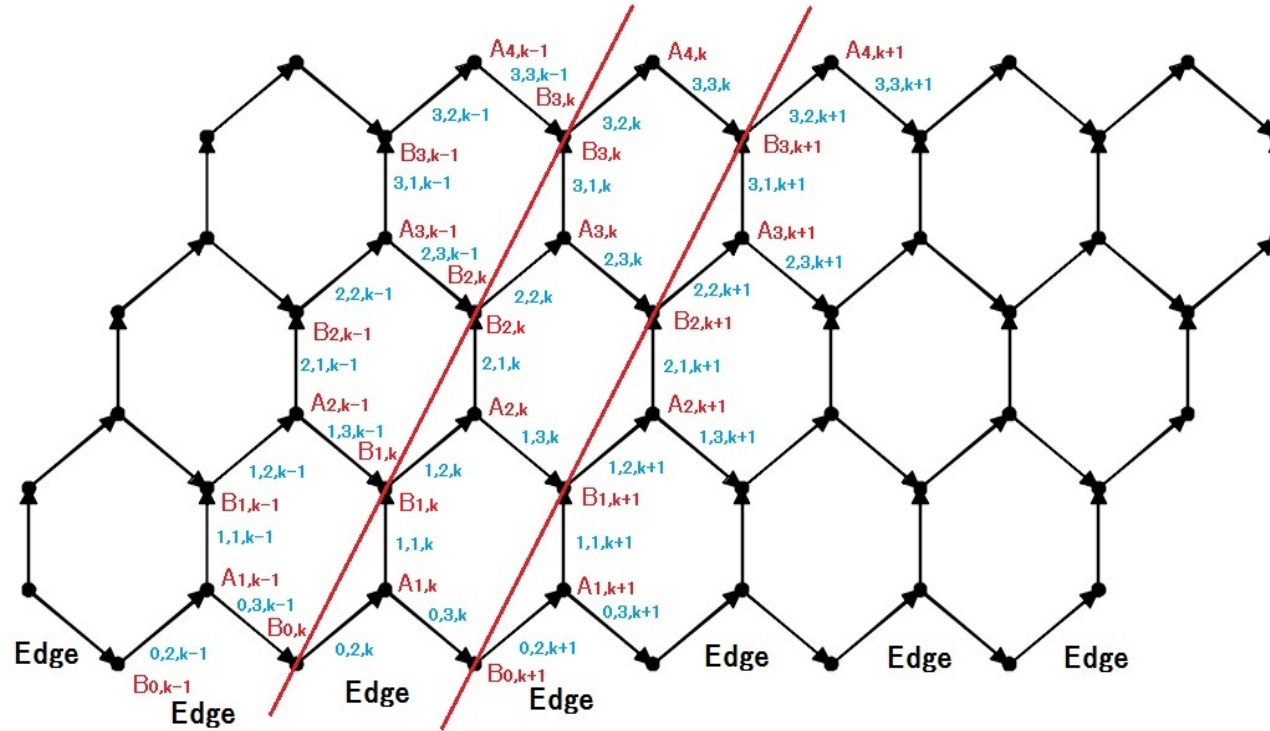


Fig. 1 Γ_{Edge} ; Graphene with zigzag boundaries.

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

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

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

- (a) the Kirchhoff vertex condition at $\forall v \in V_{\text{Edge}} \setminus \partial\Gamma_{\text{Edge}}$,
- (b) the Dirichlet boundary condition on (zigzag) edges.

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

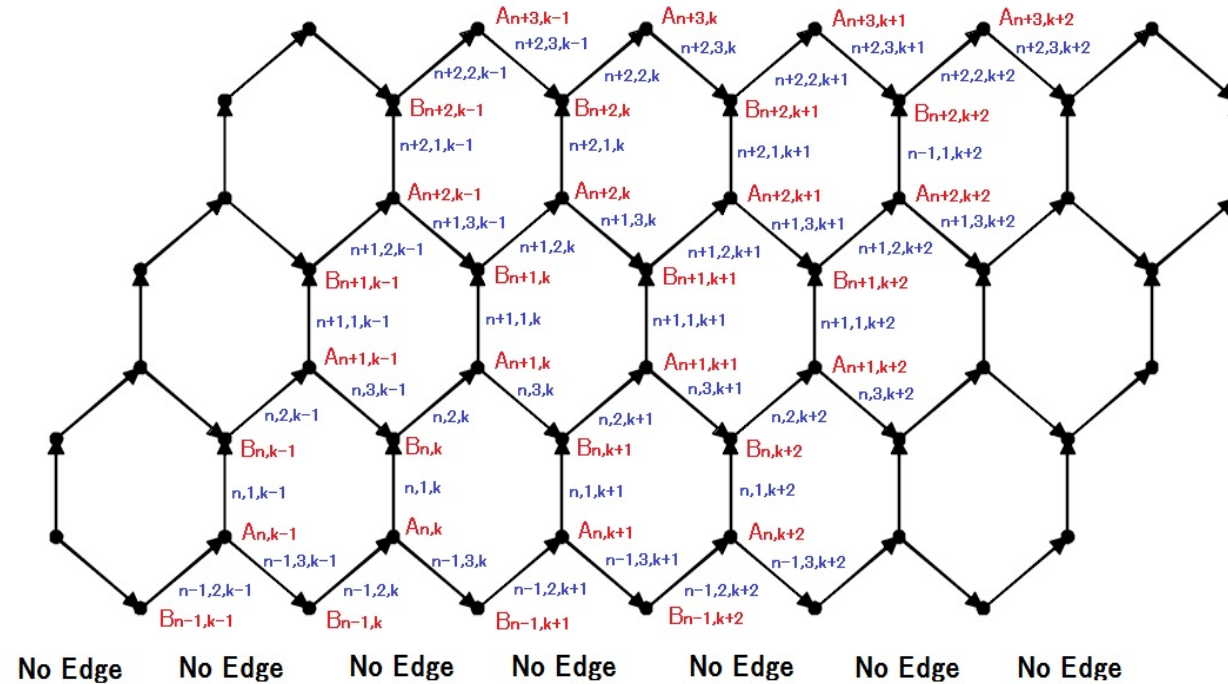


Fig. 2 Γ_{Bulk} ; Graphene without any boundary.

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

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

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

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

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

◇ 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*

$$\lambda_0^+ < \lambda_1^- \leq \lambda_1^+ < \lambda_2^- \leq \lambda_2^+ < \cdots < \lambda_j^- \leq \lambda_j^+ < \cdots \rightarrow +\infty$$

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.

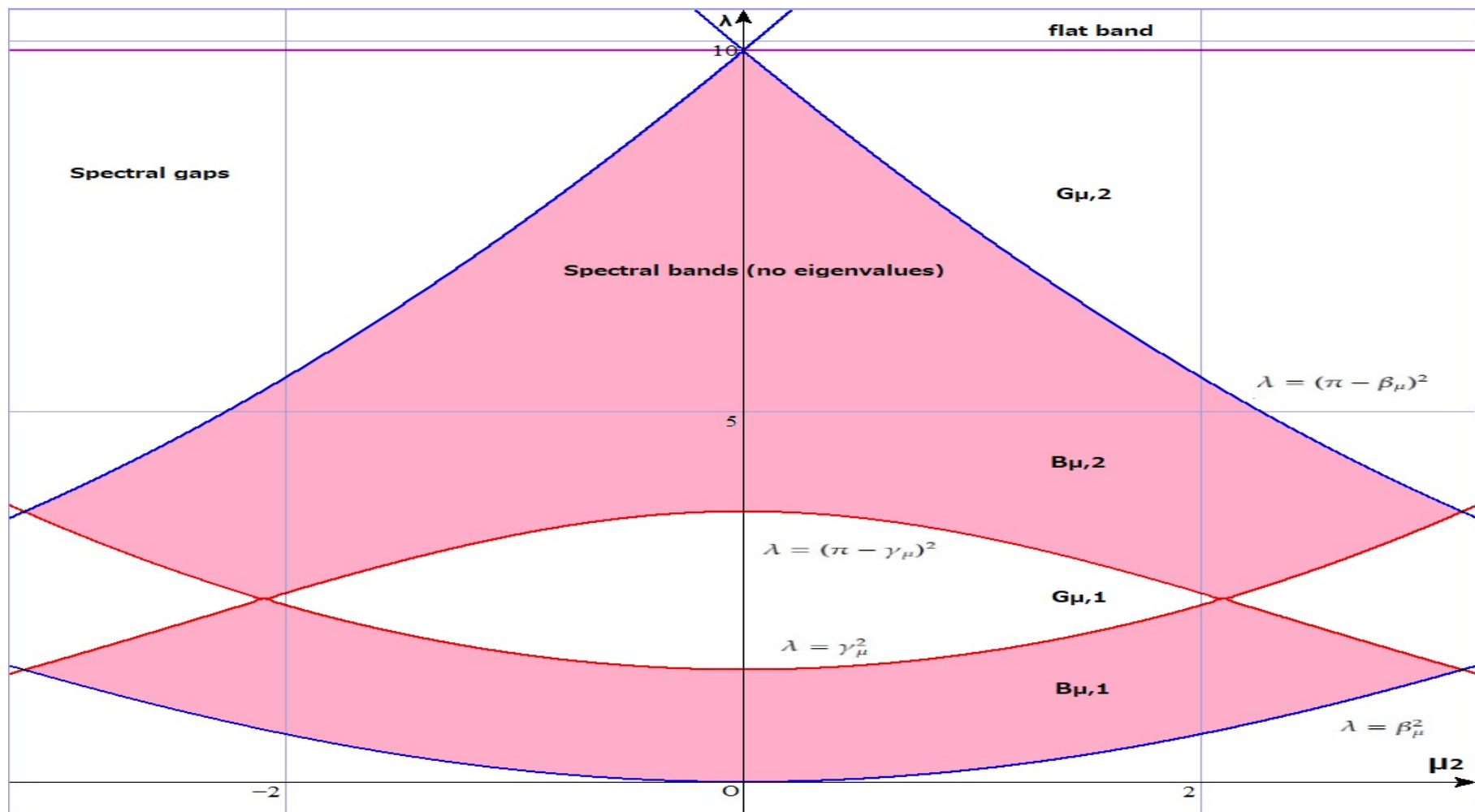


Fig. 3 The dispersion relation for H in the unperturbed case.

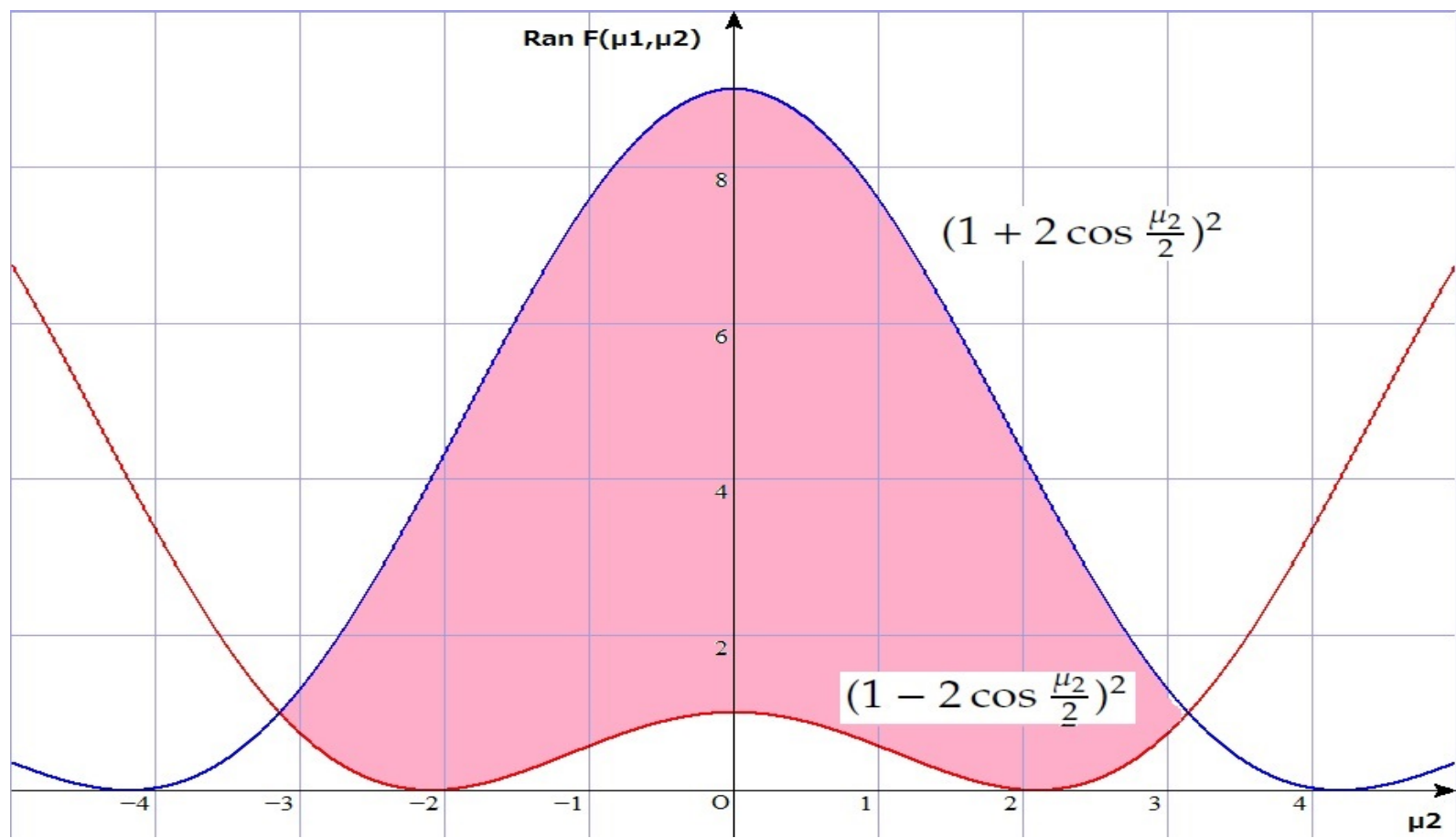
Put

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

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



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. $(1 - 2 \cos \frac{\mu_2}{2})^2 \leq 9 \cos^2 \sqrt{\lambda} \leq (1 + 2 \cos \frac{\mu_2}{2})^2$.
- $\exists \mu_2 \in S^1$ s.t.

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

where

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

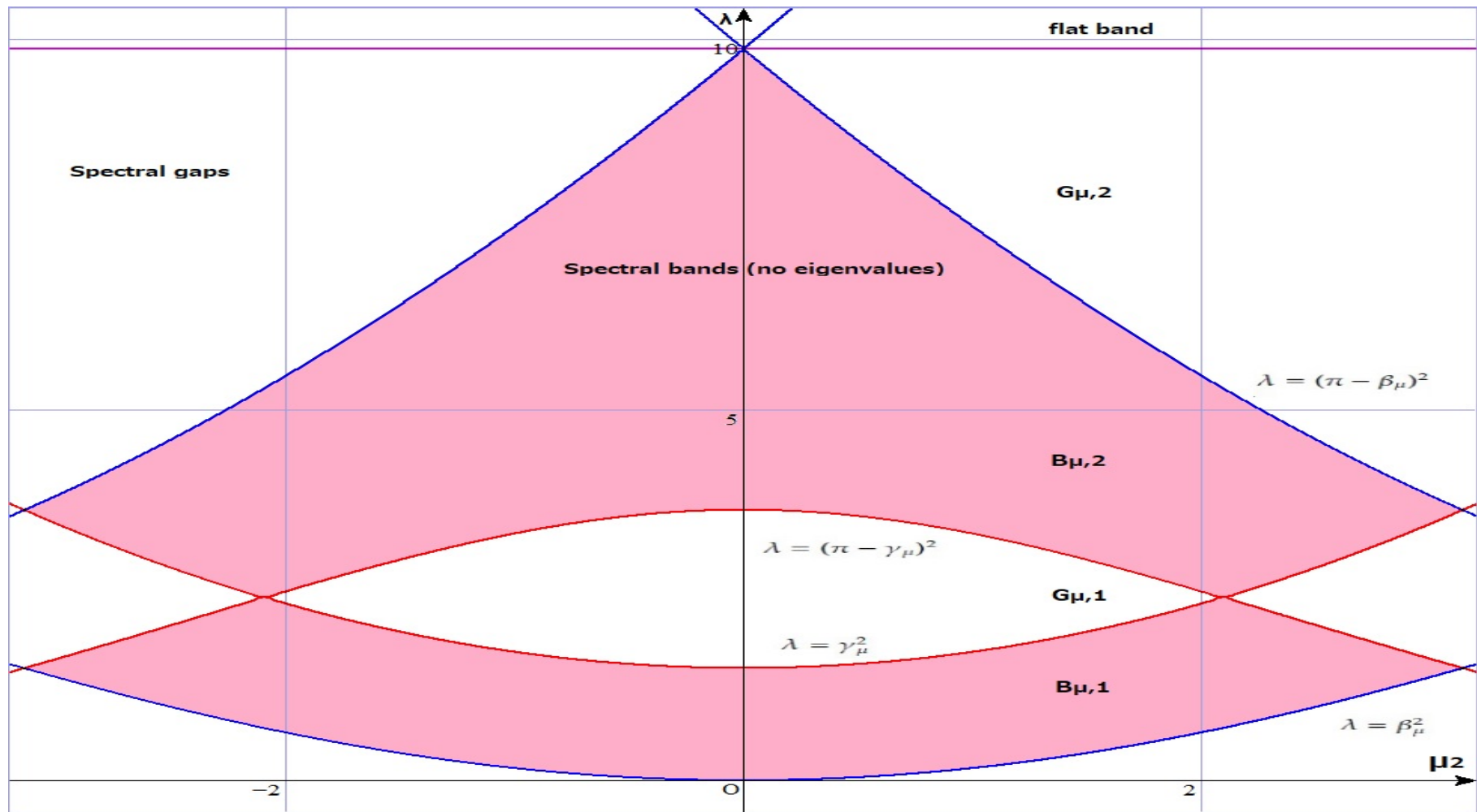


Fig. 4 The dispersion relation for H in the unperturbed case.

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

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

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

$$\lambda_0^+ < \lambda_1^- \leq \lambda_1^+ < \lambda_2^- \leq \lambda_2^+ < \cdots < \lambda_j^- \leq \lambda_j^+ < \cdots \rightarrow +\infty$$

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

Putting

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

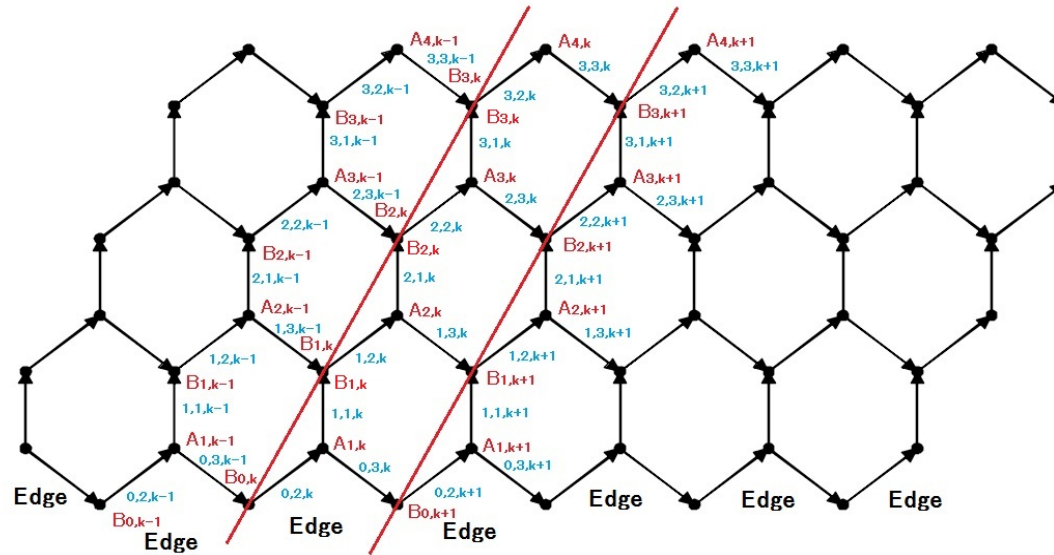
for each $j \in \mathbb{N}$, we have

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

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 $\Gamma_{n,j}$.

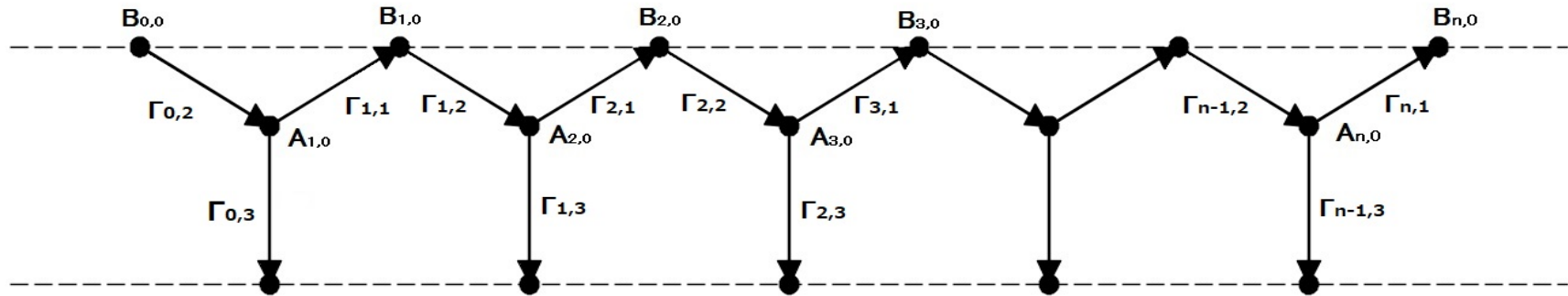


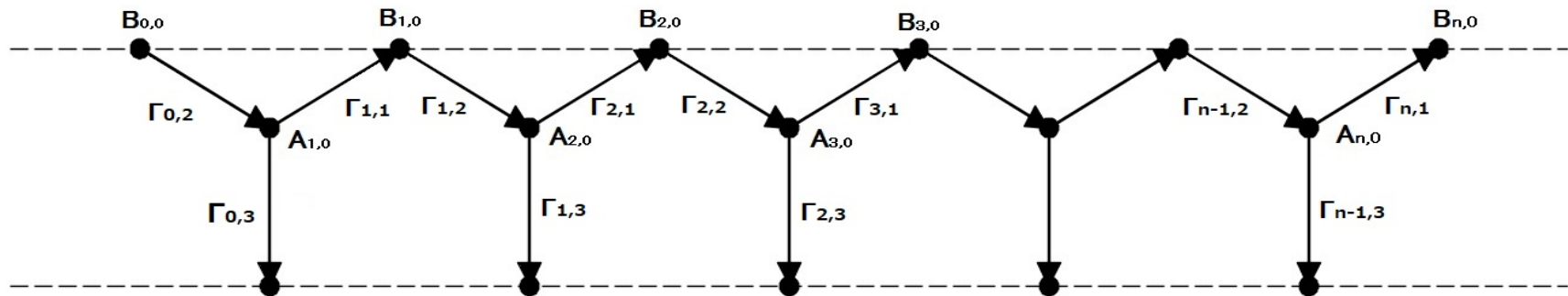
Fig. 5 The metric graph $\Gamma_{\text{Edge},0}$

Here, $y \in \text{Dom}(H^\sharp(\mu))$ 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

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

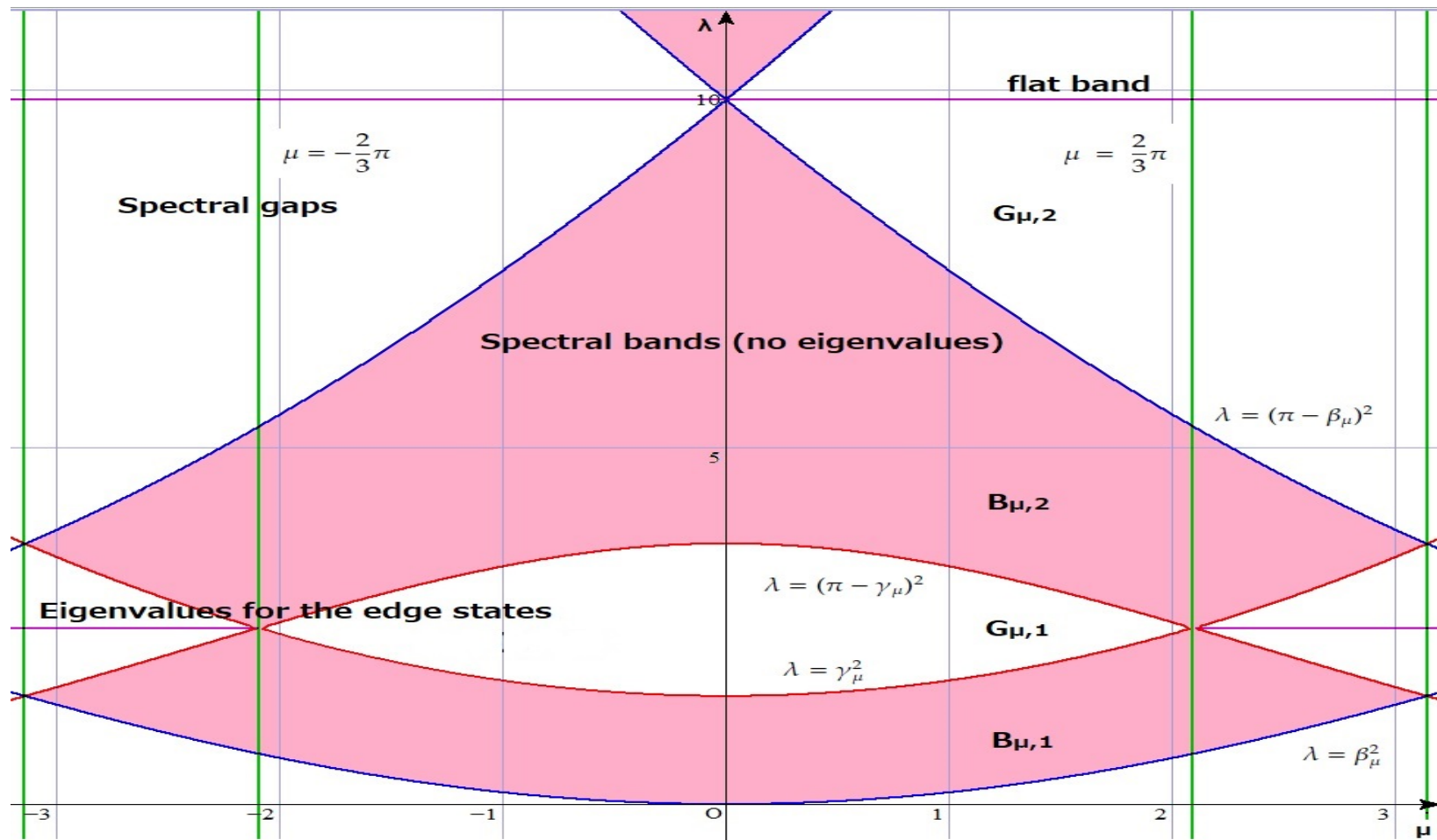


Fig. 6 The dispersion relation for $H^\sharp$ in the unperturbed case.

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

- (1) If $\lambda \in \sigma_D := \{n^2\pi^2 \mid n \in \mathbb{N}\}$, 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 $\lambda \in \bigcup_{j=1}^{\infty} B_{\mu,j}^\circ$, 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

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

Theorem 4.1 yields Theorem 3.1 in the unperturbed case:

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

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

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

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

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

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

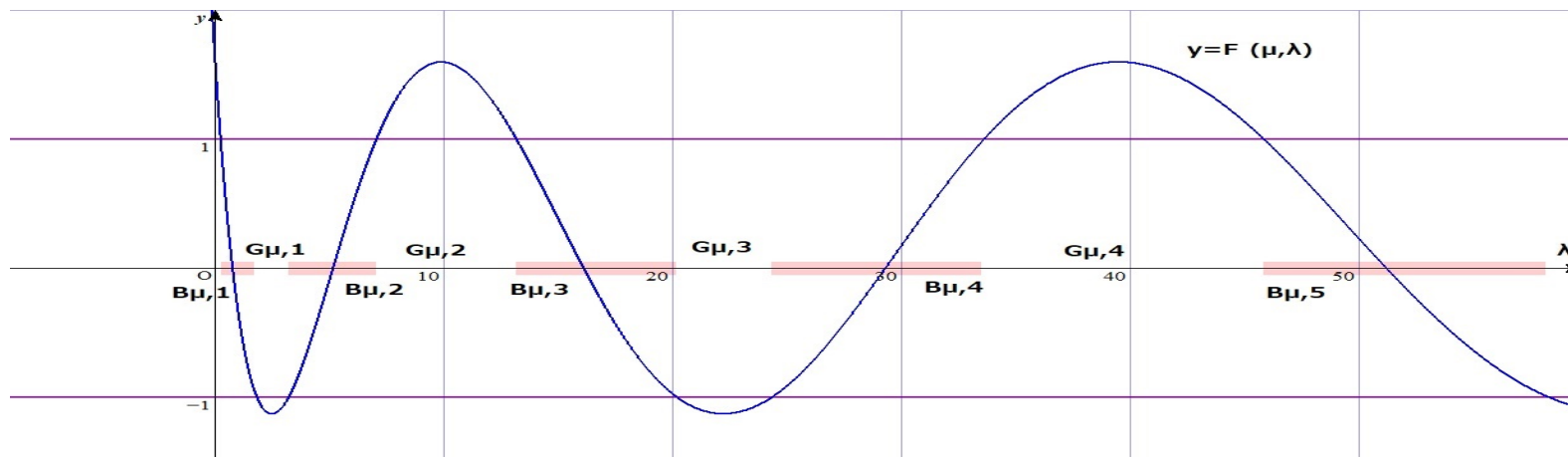
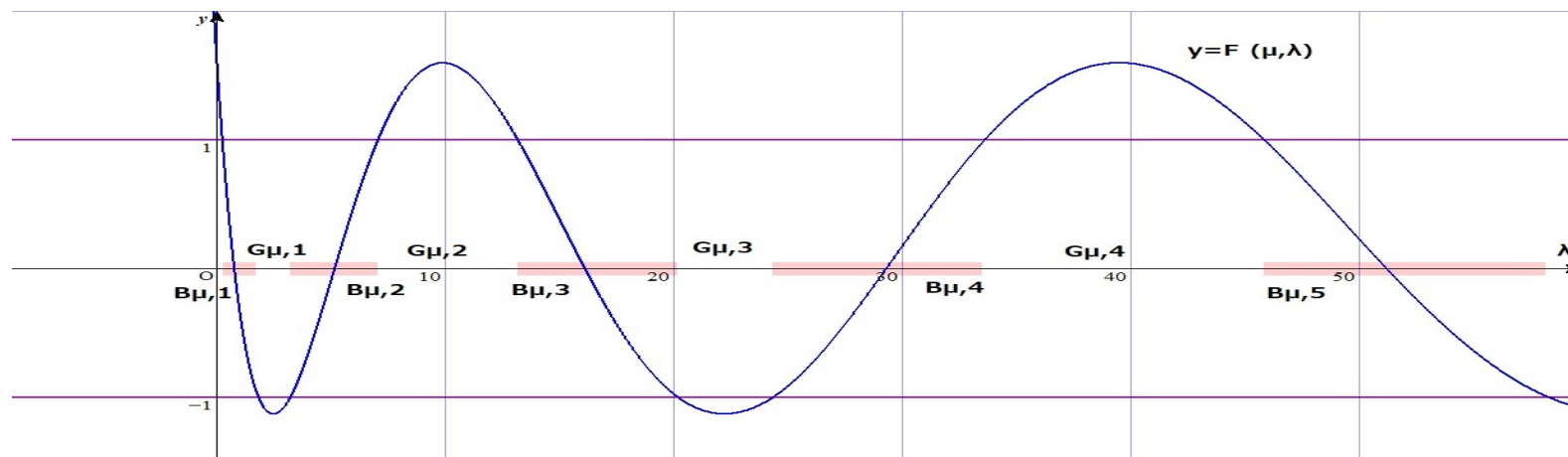


Fig. 7 A graph of the discriminant $F(\mu, \lambda)$.

The j th 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 $\lambda \in \bigcup_{j=1}^{\infty} B_{\mu,j}^\circ$, 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

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

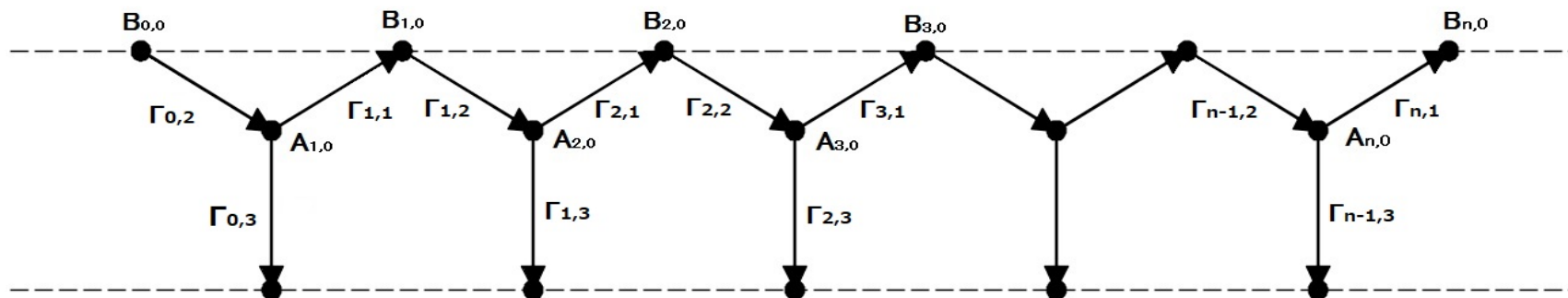
$$\sigma_D \subset \bigcup_{n=1}^{\infty} \overline{G_{2n}},$$

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

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

$$\begin{aligned} & \tilde{M}(\lambda) \\ &= \begin{pmatrix} 2\Delta\theta_1 + \theta'_1\varphi_1 & \varphi_1(\theta_1 + 2\varphi'_1) \\ \frac{1}{\varphi_1} \left\{ -4\theta_1 \cos^2 \frac{\mu}{2} + 2\Delta(2\Delta\theta_1 + \theta'_1\varphi_1) \right\} & -4 \cos^2 \frac{\mu}{2} + 2\Delta(2\Delta + \varphi'_1) \end{pmatrix}. \end{aligned}$$

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 abbreviation

$$(\theta_1, \theta'_1, \varphi_1, \varphi'_1) = (\theta(1, \lambda), \theta'(1, \lambda), \varphi(1, \lambda), \varphi'(1, \lambda)).$$

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 $\rho_{\pm}$.
- $\mathbf{e}_2 = \begin{pmatrix} 0 & 1 \end{pmatrix}^{\top}.$

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 $f : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ defined by*

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

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

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

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

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

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

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

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):

$$\theta_1 + 2\varphi'_1 \neq 0 \implies \lambda \in \rho(H^\sharp(\mu)).$$

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

$$\theta_1 + 2\varphi'_1 = 0$$

$$\Rightarrow 9\Delta^2 - \Delta_-^2 = 9\left(\frac{\theta_1 + \varphi'_1}{2}\right)^2 - \left(\frac{\theta_1 - \varphi'_1}{2}\right)^2 = \frac{1}{4} \{9(-\varphi'_1)^2 - (-3\varphi'_1)^2\} = 0$$

$$\Rightarrow d(\mu, \lambda) = -1 - 4\cos^2 \frac{\mu}{2} < -4\cos \frac{\mu}{2} \quad (\because \mu \neq \pm \frac{2}{3}\pi)$$

$$\Rightarrow |\rho_-| = \left| \frac{d(\mu, \lambda) - \sqrt{D(\mu, \lambda)}}{4\cos \frac{\mu}{2}} \right| > \frac{4\cos \frac{\mu}{2}}{4\cos \frac{\mu}{2}} = 1, \quad F(\mu, \lambda) < -1 \quad (\because p.33)$$

$$\Rightarrow |\rho_+| < 1, \quad \lambda \in \bigcup_{j=1}^{\infty} G_{\mu, 2j-1}.$$

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

$$\{\lambda \in \mathbb{R} \mid \theta_1 + 2\varphi'_1 = 0\} \subset \bigcup_{n=1}^{\infty} \overline{G_{2n-1}}.$$

□

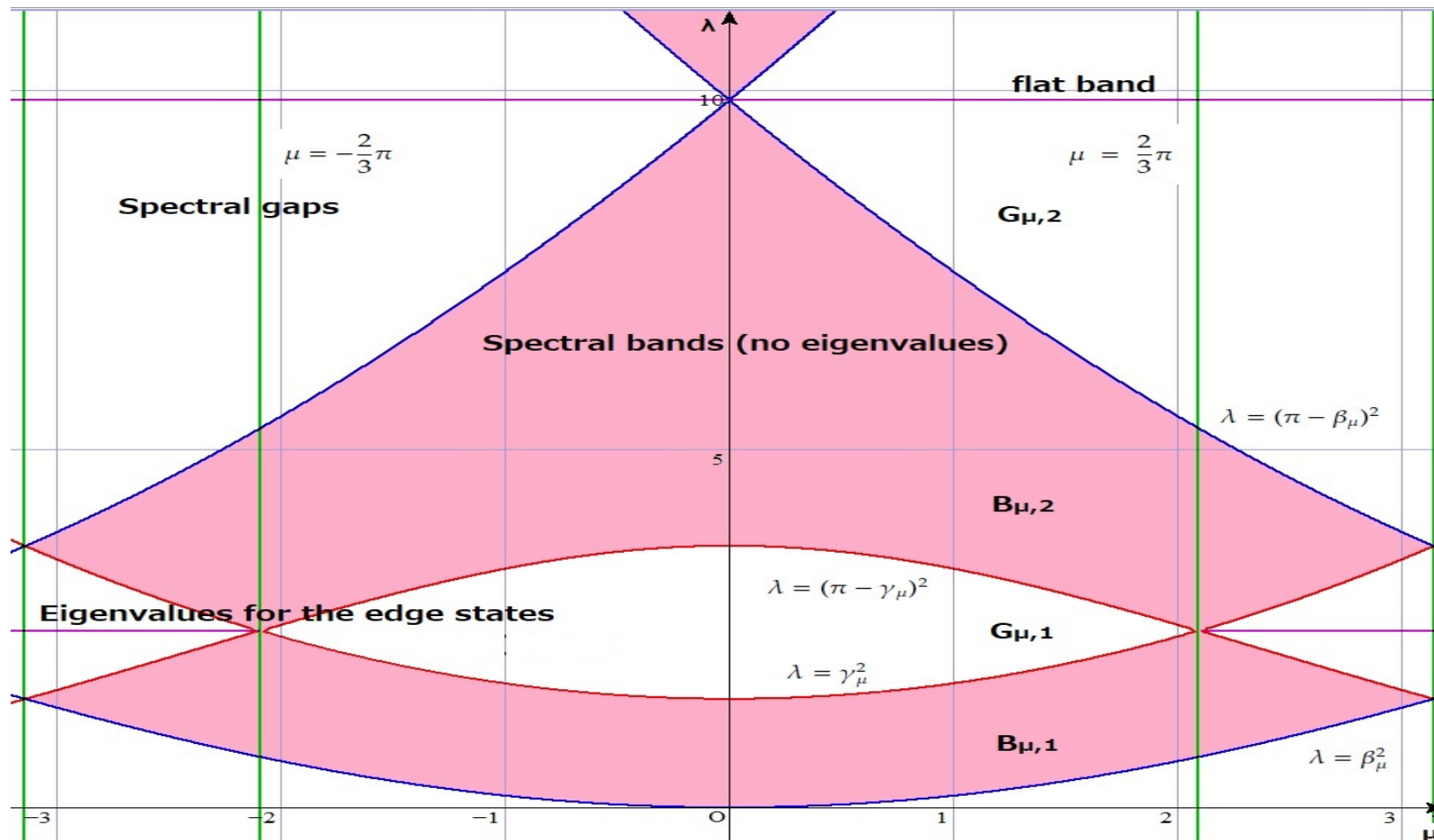


Fig. 8 The dispersion relation for $H^\sharp$ in the unperturbed case.

6 An example

Let us take a step potential

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

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

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

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

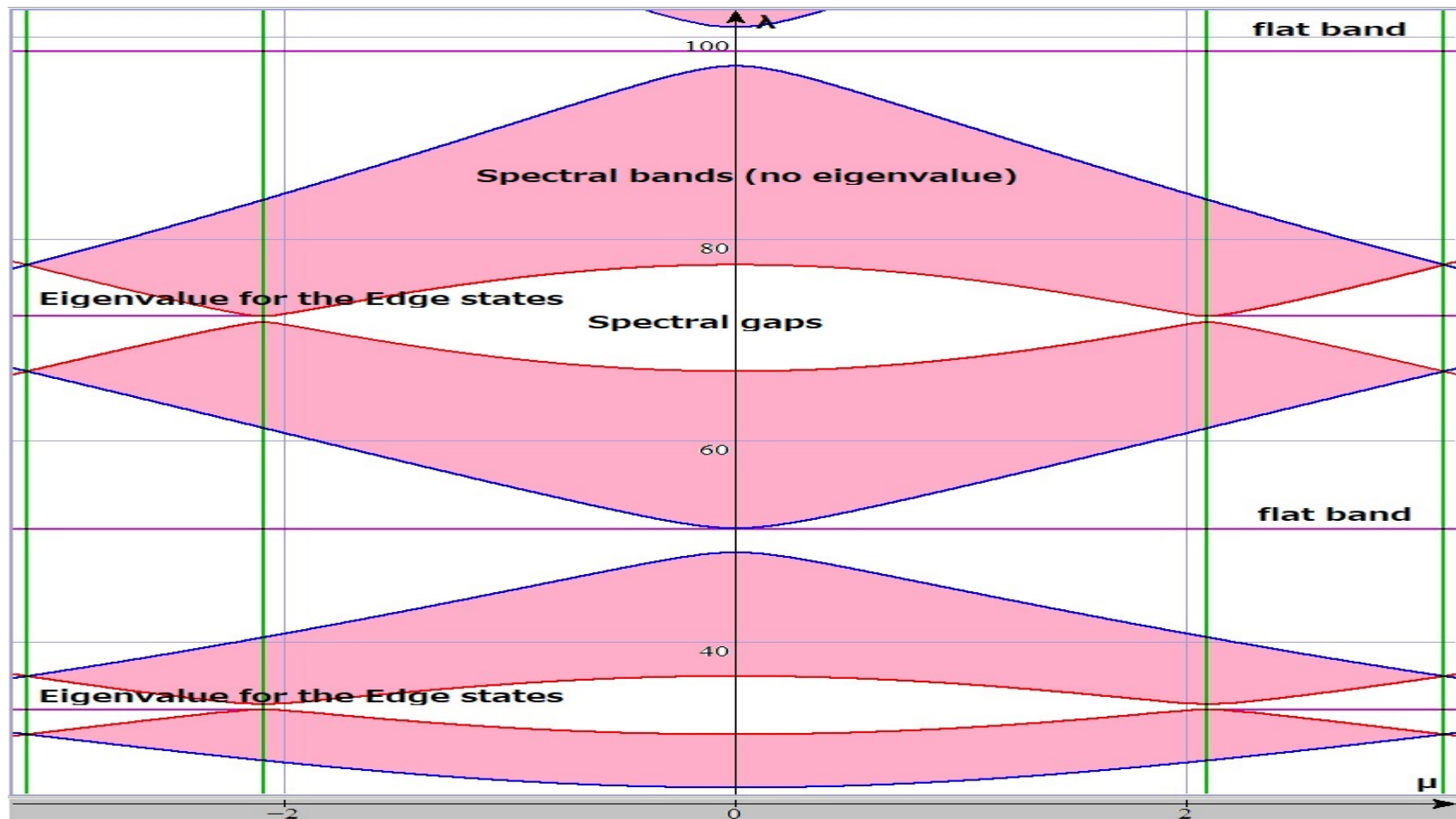


Fig. 9 The dispersion relation for $H^\#$ with a step potential.

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/20210423.pdf>

This work is supported by

JSPS KAKENHI Grant number 17K14221 and 21KO3273.