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Edge states of Schrödinger equations on graphene with zigzag boundaries

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1 Introduction

◇ Topological Insulators

⋯ They behave as an insulator in its interior (Bulk), but their surfaces (Egdes) contain conducting states.

⇒ An energy is located in the spectral gaps of a periodic media in the whole space (Bulk), but it is an eigenvalue of the periodic media with boundaries (Edges).

◇ 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.

Aim in English

Comparing the spectrum of the Bulk Hamiltonian H with the spectrum of the Edge Hamiltonian $H^\sharp$ on Graphene, we find an energy which is an eigenvalue of $H^\sharp$ but is not an eigenvalue of H.

Aim in Japanese

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が存在することを調べる.

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

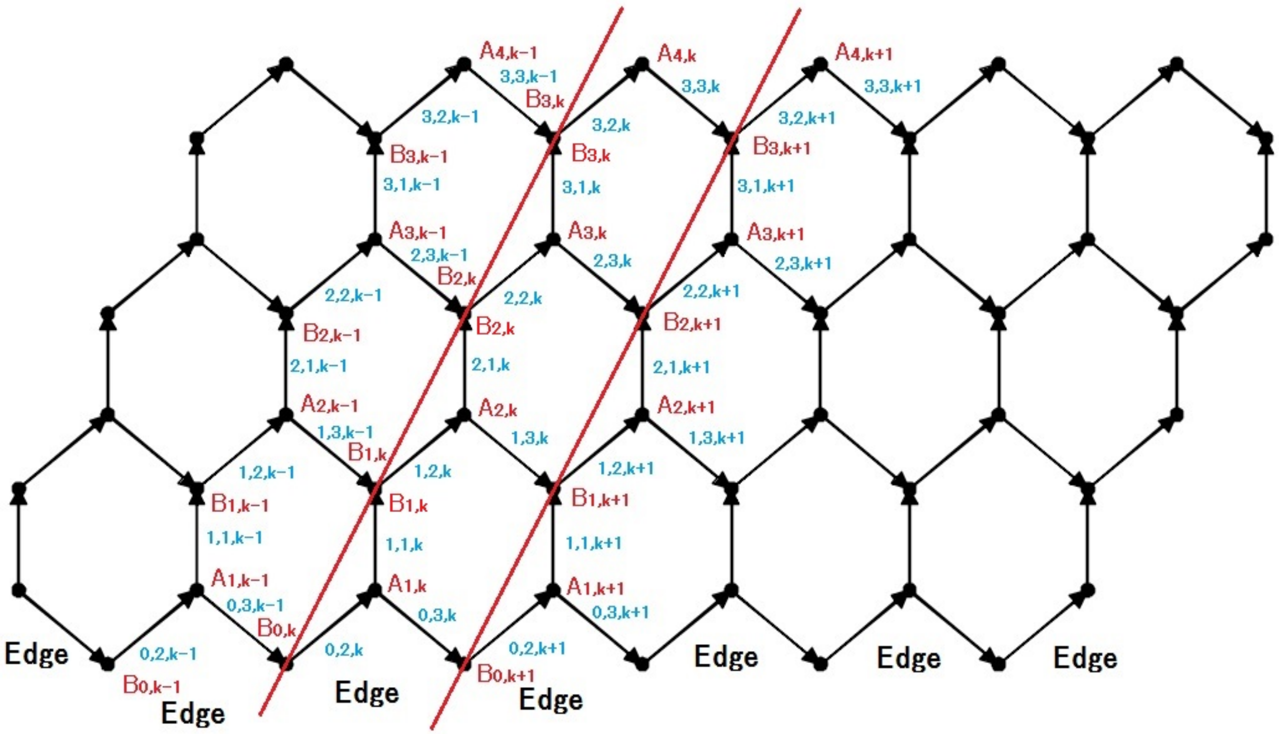


Fig. 1 Graphene with zigzag boundaries.

(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–Neumann vertex condition at $\forall v \in V_{\mathrm{Edge}}$ except (zigzag) edges,

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

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

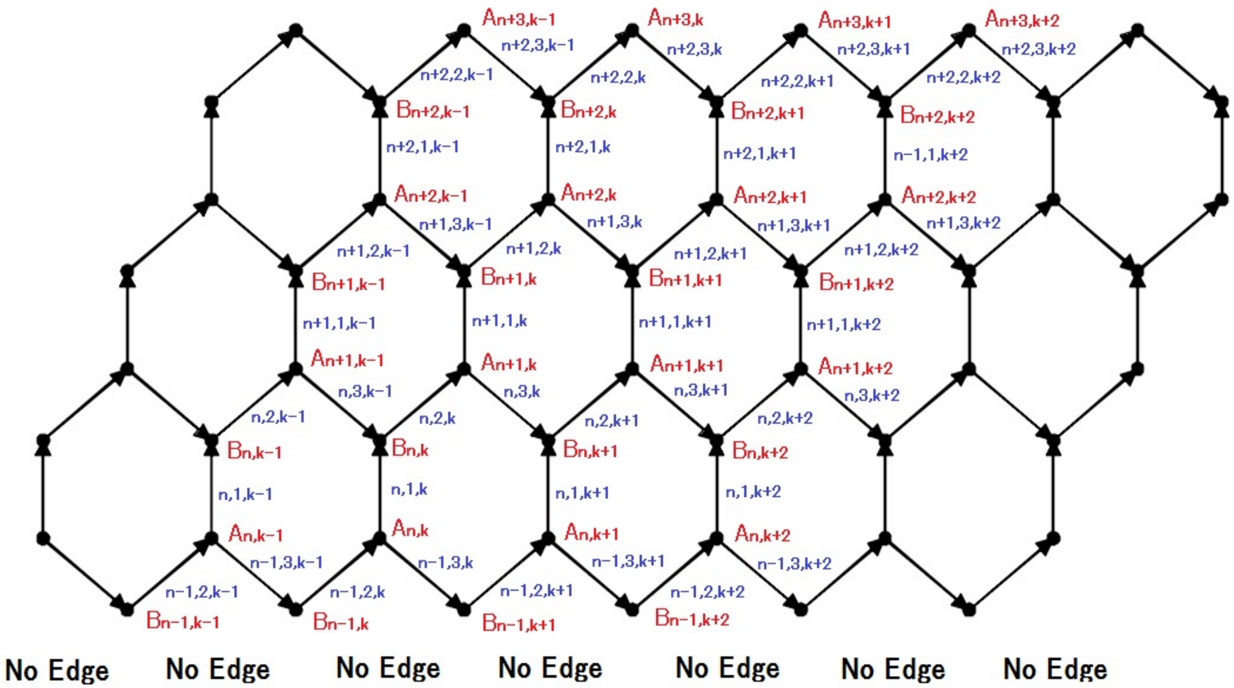


Fig. 2 Graphene without any boundary.

(1) $\Gamma_{\rm Bulk} = (E_{\rm Bulk}, V_{\rm Bulk})$.

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

(3) For $\forall e \in E_{\rm Bulk}$, the Bulk Hamiltonian H in $L^2(\Gamma_{\rm Bulk})$ 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

(a) the Kirchhoff–Neumann vertex condition at $\forall v \in V_{\rm Bulk}$.

◇ 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 1.1. *(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 for H 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.

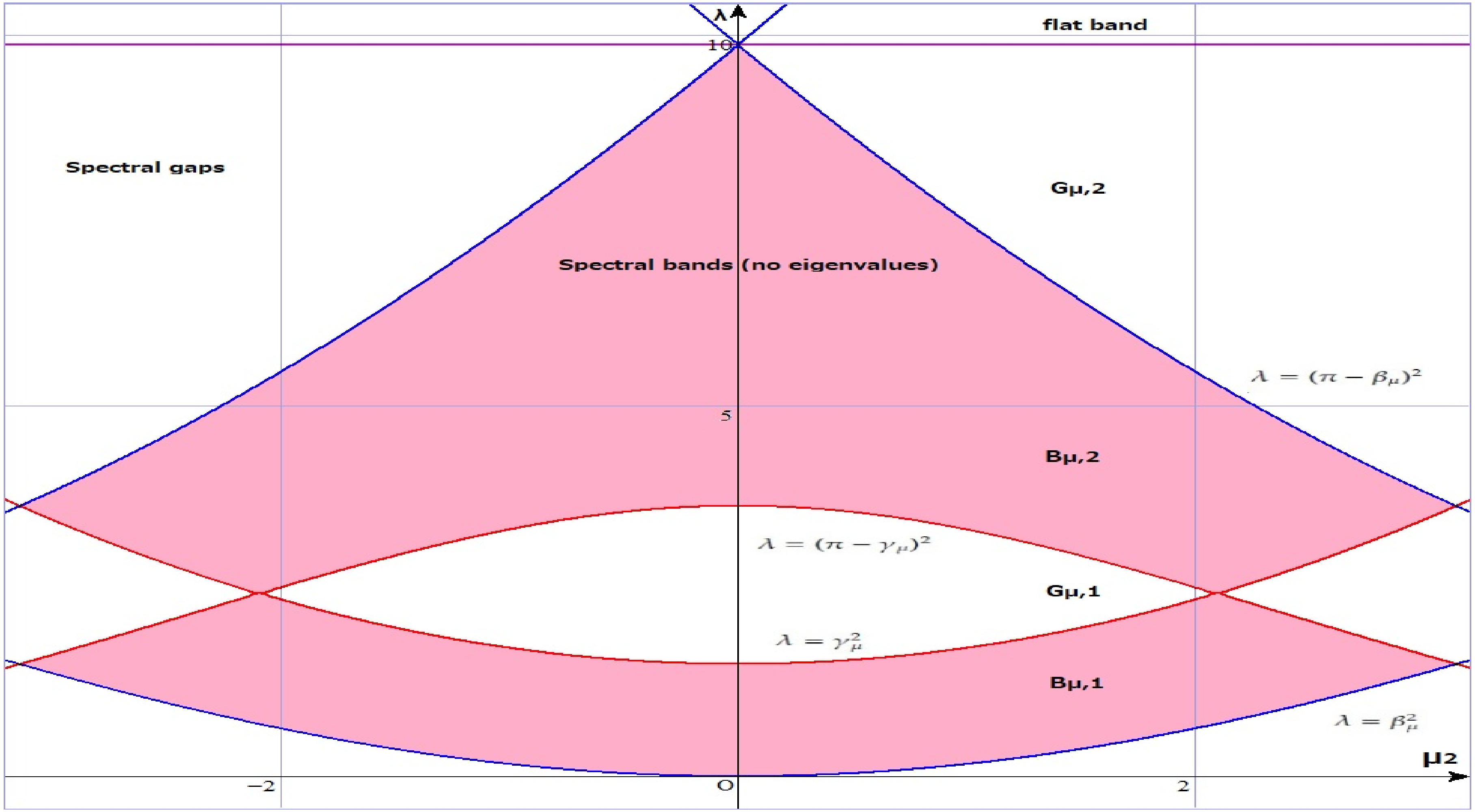


Fig. 3 The dispersion relation for H in the unperturbed case.

2 Main Results for $H^\sharp$

We put $\sigma_p^\sharp = \sigma_p(H^\sharp) \setminus \sigma_p(H)$ and call an eigenfunction corresponding to $\lambda \in \sigma_p^\sharp$ an edge state.

Theorem 2.1. *(N, to appear in "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

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

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*

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

3 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 obtain

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

where $\mu \in S^1 := [-\pi, \pi]$ and $H^\sharp(\mu)$ is a fiber operator corresponding to $H^\sharp$.

- $\lambda \in \sigma(H^\sharp)$

$$\Longleftrightarrow m(\{\mu \in S^1 | \quad \sigma(H^\sharp(\mu)) \cap (\lambda - \epsilon, \lambda + \epsilon) \neq \emptyset\}) > 0 \ (\forall \epsilon > 0).$$

- $\lambda \in \sigma_p(H^\sharp) \Longleftrightarrow m(\{\mu \in S^1 | \quad \lambda \in \sigma_p(H^\sharp(\mu))\}) > 0.$

For each quasi-momentum $\mu \in S^1 = [-\pi, \pi]$, the fiber operator $H^\sharp(\mu)$ in $L^2(\Gamma_{\mathrm{Edge},0})$ (see Fig. 4) 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 $\Gamma_{n,j}$.

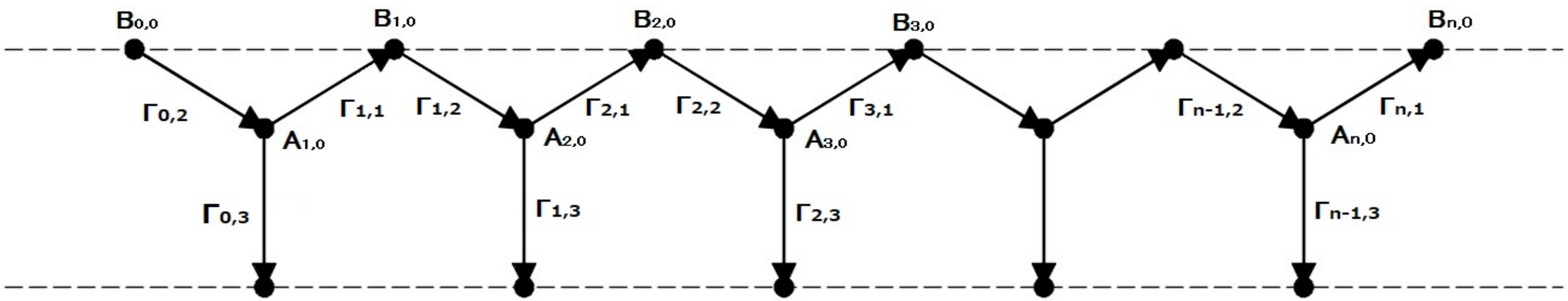
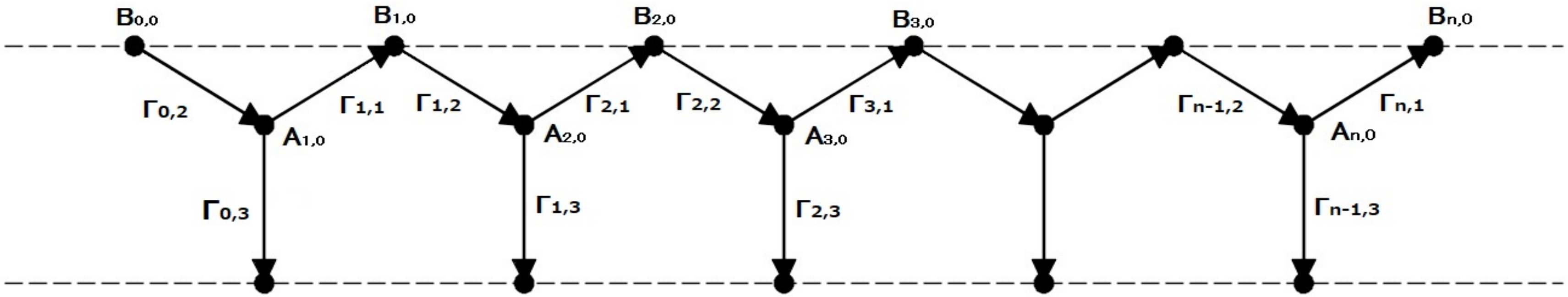


Fig. 4 The metric graph $\Gamma_{\mathrm{Edge},0}$

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 $y_{1,1}(0) = 0$.



3.1 $\sigma(H^\sharp(\mu))$ 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 prepare

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

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

$$\beta_\mu = \arccos\left\{\frac{1}{3}\left(1 + 2\cos\frac{\mu}{2}\right)\right\}, \quad \gamma_\mu = \arccos\left\{\frac{1}{3}\left|2\cos\frac{\mu}{2} - 1\right|\right\},$$

$$\xi^+_{\mu,2n-2} = \{(n-1)\pi + \beta_\mu\}^2, \quad \xi^-_{\mu,2n-1} = \{(n-1)\pi + \gamma_\mu\}^2,$$

$$\xi^+_{\mu,2n-1} = (n\pi - \gamma_\mu)^2, \quad \xi^-_{\mu,2n} = (n\pi - \beta_\mu)^2.$$

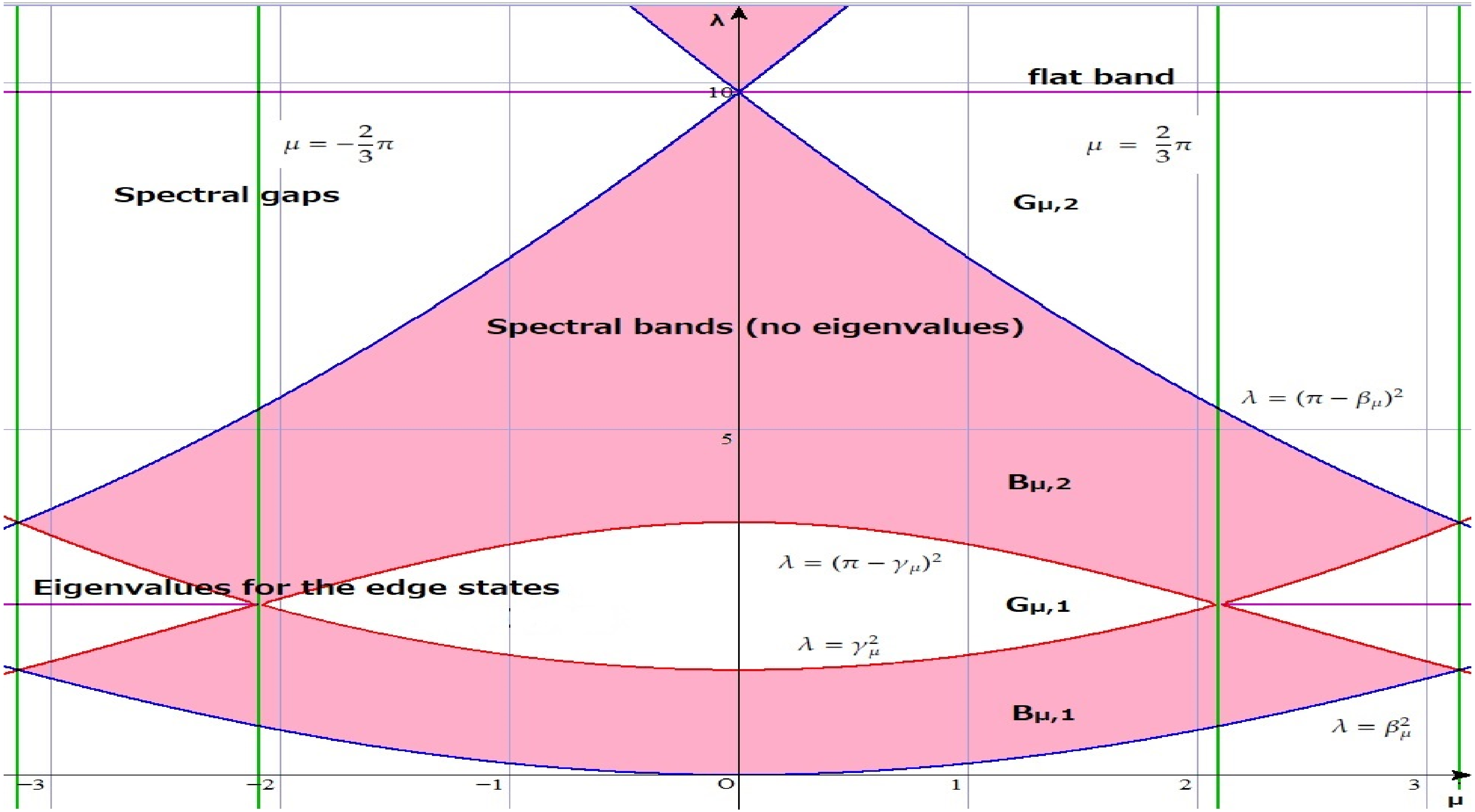


Fig. 5 The dispersion relation for $H^\sharp$ in the unperturbed case.

Theorem 3.1. *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* $\lambda \in \sigma_p(H^\sharp(\mu))$ *with infinite multiplicities.*

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

(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

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

Theoerm 3.1 yields Theorem 2.1 in the unperturbed case:

Theorem 3.2. *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* $\sigma_p^\sharp = \{\lambda \in \mathbb{R} | \ \cos \sqrt{\lambda} = 0\}$.

3.2 $\sigma(H^\sharp(\mu))$ in the perturbed case

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

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

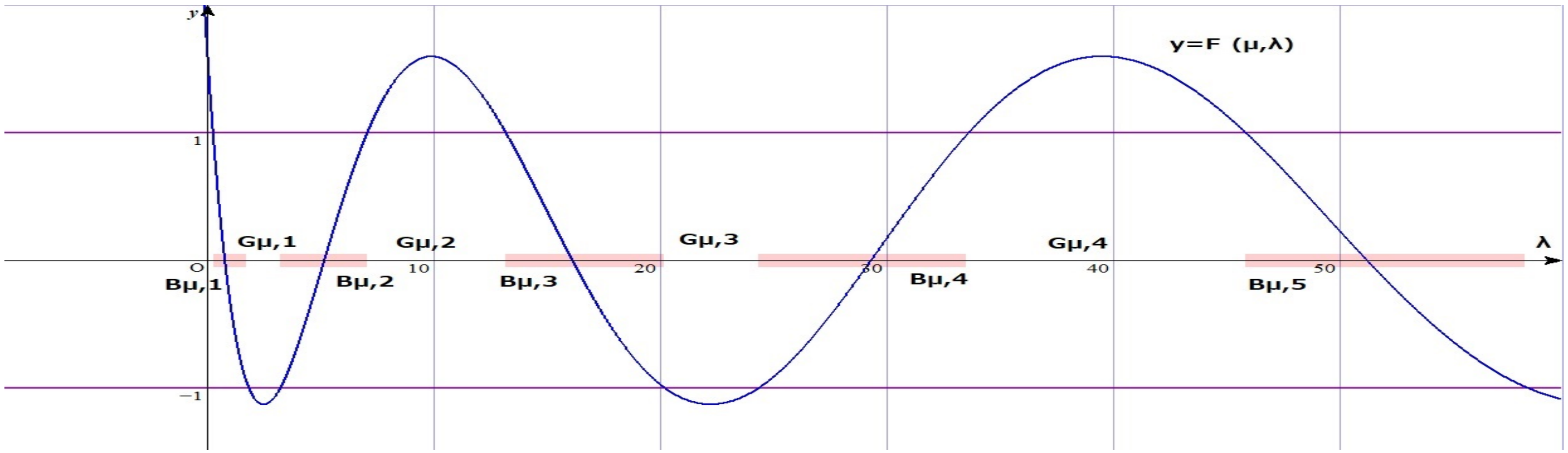
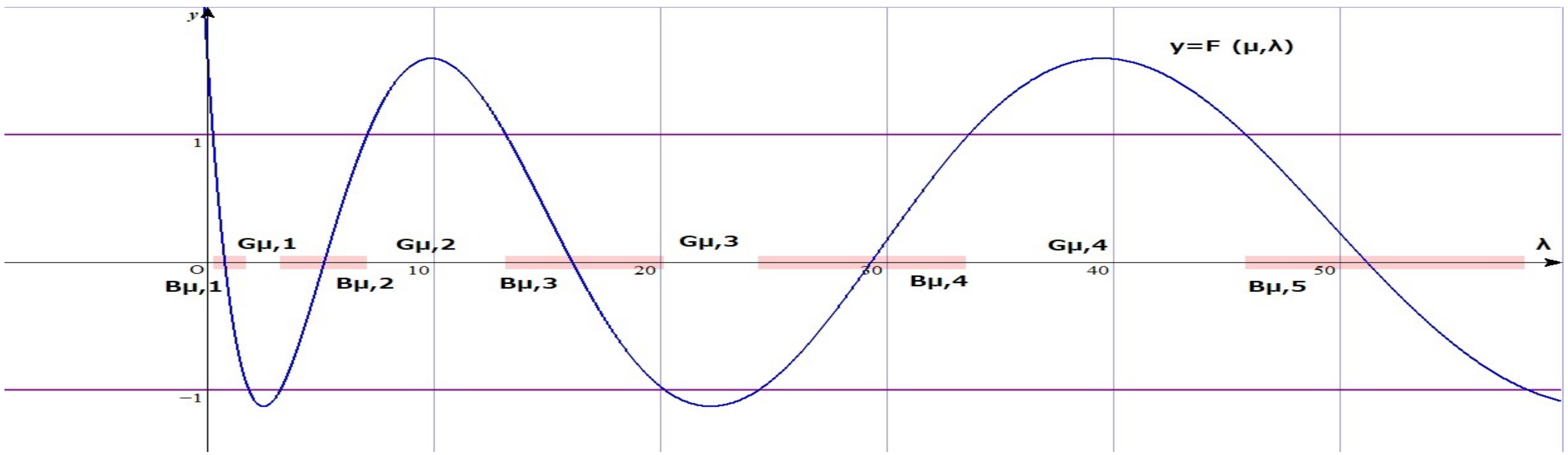


Fig. 6 A graph of the discriminant $F(\mu, \lambda)$.

The jth band $B_{\mu,j}$ and gap $G_{\mu,j}$ for $j \in \mathbb{N}$ are characterized by $F(\mu,\lambda)$, as well as $G_{\mu,0} := (-\infty, \inf B_{\mu,1})$. In particular, we have

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



Theorem 3.3. *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* $\lambda \in \sigma_p(H^\sharp(\mu))$ *with infinite multiplicities.*

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

(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 2.1;
For any $q \in L^2(0,1)$, we have

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

as well as

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

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 $H^\sharp$:

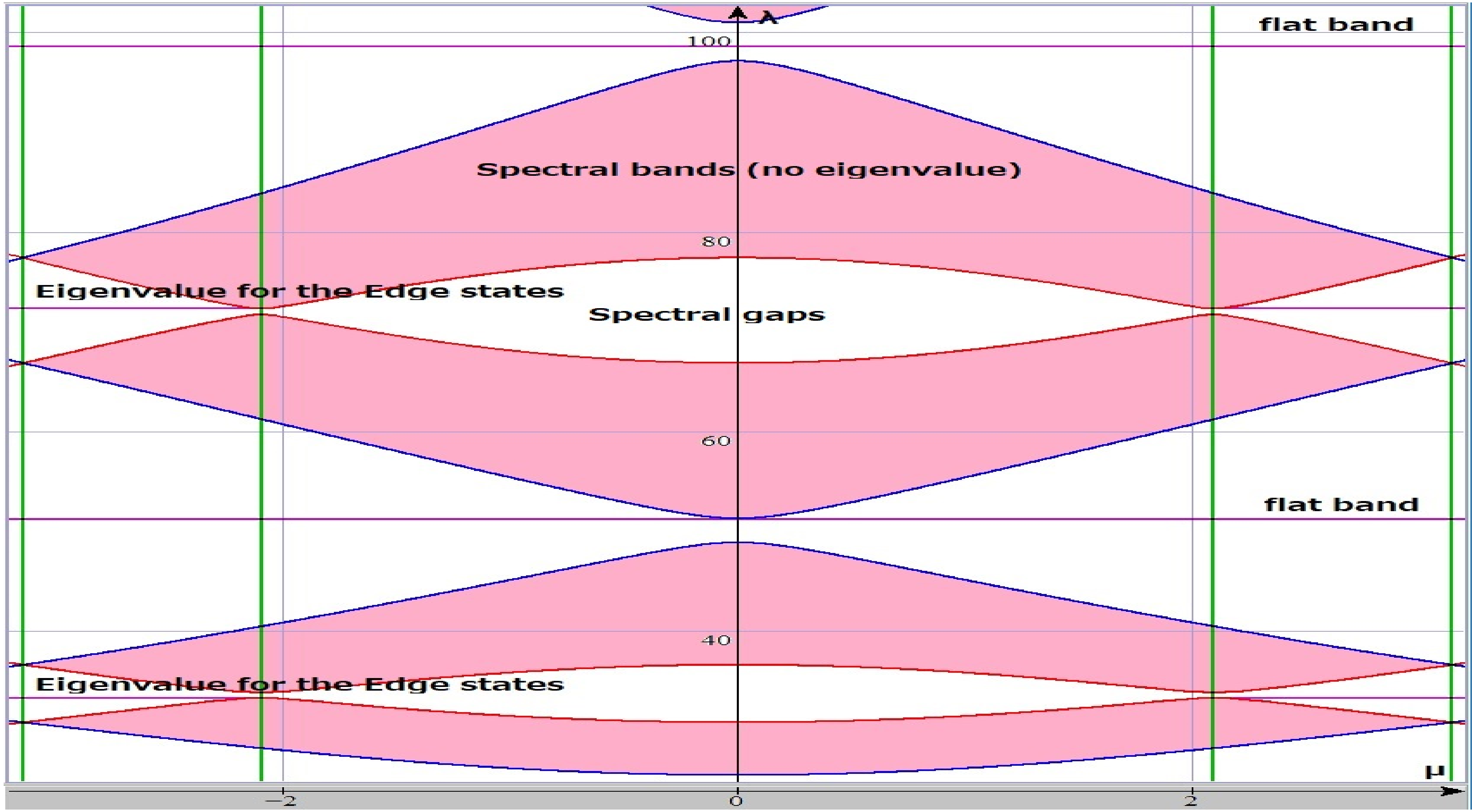


Fig. 7 The dispersion relation for $H^{\sharp}$ with a step potential.

To be continued in ...

Edge states of Schrödinger equations on graphene with zigzag boundaries, to appear in ”Results in Mathematics”.

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Thank you for your attention.

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