Eigenvalue Asymptotics near a flat band

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Flat Bands

Proposition

Let us consider a fibered operator $H_0 = \int_{\mathbb{T}^n}^{\oplus} h_0(\xi)d\xi$. *The folloqing are equivalent assertions:*

1. $\lambda \in \sigma(h_0(\xi))$ *for every* $\xi \in \mathbb{T}^n$.
2. $\lambda \in \sigma(h_0(\xi))$ *for a positive measure subset of* $\mathbb{T}^n$.
3. *There is an infinite orthonormal family of eigenfunctions of* H_0 *corresponding to the eigenvalue* λ. *(Each of which can be chosen to be finitely supported.)*

A λ satisfying any of $1-3$ is said to be a *flat band.* In particular, periodic graphs have several known examples featuring flat bands:

1. Lieb Lattice
2. Kagome Lattice
3. Super-Kagome Lattice
4. *Twisted Bilayer Graphene*

Network structure

Consider the graph X, defined with the set of vertices $\mathcal{V} = \mathbb{Z}^n$, and the set of oriented edges $\mathcal{A} = \{(x, y) \in \mathbb{Z}^n \times \mathbb{Z}^n : y = x \pm \delta_i\}$, where $\{\delta_i\}_{i=1}^n$ form the canonical basis of $\mathbb{Z}^n$. We denote an edge in $\mathcal{A}$ by $\mathrm{e} = (x, y)$ and its transpose by $\bar{\mathrm{e}} = (y, x)$. Consider the vector spaces of

$0-$*cochains* $C^0(X)$ and $1-$*cochains* $C^1(X)$ given by:

$$C^0(X) := \{f : \mathcal{V} \to \mathbb{C}\} ; \qquad C^1(X) := \{f : \mathcal{A} \to \mathbb{C} \mid f(\mathrm{e}) = -f(\bar{\mathrm{e}})\} .$$

The Hilbert spaces $\ell^2(\mathcal{V})$ and $\ell^2(\mathcal{A})$ are naturally defined by the inner products of cochains:

$$\langle f_1, f_2 \rangle_0 = \sum_{\mu \in \mathcal{V}} f_1(\mu) \overline{f_2(\mu)}; \quad \langle g_1, g_2 \rangle_1 = \frac{1}{2} \sum_{\mathrm{e} \in \mathcal{A}} g_1(\mathrm{e}) \overline{g_2(\mathrm{e})},$$

respectively.

Dirac-type operator

The coboundary operator $d : \ell^2(\mathcal{V}) \to \ell^2(\mathcal{A})$ i.e., the discrete version of the exterior derivative is defined by

$$df(\mathrm{e}) := f(\nu) - f(\mu), \quad \text{for } \mathrm{e} = (\mu, \nu) \in \mathcal{A}.$$

The adjoint $d^* : \ell^2(\mathcal{A}) \to \ell^2(\mathcal{V})$ is given by the finite sum

$$d^* g(\mu) = \sum_{j=1}^{n} g(\mu, \mu + \delta_j) + \sum_{j=1}^{n} g(\mu, \mu - \delta_j), \quad \text{for } \mu \in \mathcal{V}.$$

Then, for a positive constant m let us consider the free Dirac-type operator

$$H_0 = \begin{pmatrix} m & d^* \\ d & -m \end{pmatrix}.$$

Comments on the model

It is easy to see that

$$H_0^2 = \begin{pmatrix} \Delta_{\mathcal{V}} + m^2 & 0 \\ 0 & \Delta_{\mathcal{A}} + m^2 \end{pmatrix} ,$$

Where $\Delta_{\mathcal{V}}$ is the Laplacian describing diffusion from vertex to vertex through edges and $\Delta_{\mathcal{A}}$ is the (1-down) Laplacian describing diffusion from edge to edge through vertices. So it is natural to think of H_0 as a Dirac-type operator.

For each $\mu \in \mathbb{Z}^n$ we can construct a cycle of edges. By taking the indicator function corresponding to that cycle, we obtain f_μ such that $df_\mu = 0$. Since we can repeat this construction for every μ we obtain an infinite dimensional eigenvalue at $-m$.

Symbol of H_0

Proposition

On $\mathbb{T}^n$ define the functions $a_j(\xi) = -1 + e^{-2\pi i \xi_j}$. Then, the operator H_0 is unitarily equivalent to a matrix-valued multiplication operator in $L^2(\mathbb{T}^n; \mathbb{C}^{n+1})$ given by the real-analytic function

$$h_0(\xi) = \begin{pmatrix} m & a_1(\xi) & \dots & a_n(\xi) \\ \overline{a_1(\xi)} & -m & \dots & 0 \\ \vdots & & \ddots & \vdots \\ \overline{a_n(\xi)} & 0 & \dots & -m \end{pmatrix} .$$

From its characteristic polynomial

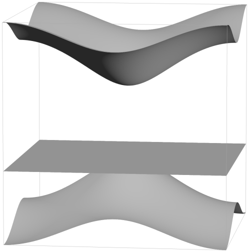
$$p_z(\xi) = (-1)^n (m+z)^{n-1} \left(m^2 - z^2 + \sum_{j=1}^{n} |a_i(\xi)|^2 \right) .$$

we can recognize the flat band at $-m$.

Spectral Structure

The analysis of its band functions permits us to show that the spectrum of H_0 is

$$\sigma(H_0) = \sigma_{ess}(H_0) = \sigma_{ac}(H_0) = [-\sqrt{m^2+4n}, -m] \bigcup [m, \sqrt{m^2+4n}].$$

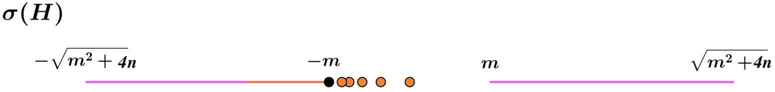


Perturbation

Let us consider $V : \mathcal{X} \to \mathbb{R}$ such that $V(\mathrm{e}) = V(\bar{\mathrm{e}})$ for every $\mathrm{e} \in A$. Given such a V, our full hamiltonian is defined by

$$H = H_0 + V \ .$$

Suppose that V decays at infinity so it defines a compact operator. Then we have that $\sigma_{\mathrm{ess}}(H_\pm) = \sigma_{\mathrm{ess}}(H_0)$. Moreover, since $m > 0$, $(-m, m)$ is a gap in the essential spectrum of H.



Then, for $\lambda \in (0, m)$ define the function

$$\mathcal{N}(\lambda) = \mathrm{Rank}\, \mathbb{1}_{(-m+\lambda,0)}(H) \ .$$

Clearly, it counts the number of discrete eigenvalues (with multiplicity) of H on the interval $(-m + \lambda, 0)$.

Admissible perturbations

Additionally, we define the following real-valued functions on $\mathbb{Z}^n$

$$v_0(\mu) := V(\mu); \quad v_j(\mu) := V(\mu\, \mathrm{e}_j), \quad 1 \leq j \leq n \ . \tag{1}$$

Let us consider the class of symbols $S^\gamma(\mathbb{Z}^n)$ given by the functions $v : \mathbb{Z}^n \to \mathbb{C}$ that satisfies for any multi-index $\alpha = (\alpha_1, \cdots, \alpha_n) \in \mathbb{N}^n$

$$|\mathrm{D}^\alpha v(\mu)| \leq C_\alpha \langle \mu \rangle^{-\gamma - |\alpha|} \ ,$$

where $\mathrm{D_j} v(\mu) := v(\mu + \delta_j) - v(\mu)$, $|\alpha| := \sum_{j=1}^n \alpha_j$, and $\mathrm{D}^\alpha := \mathrm{D}_1^{\alpha_1} ... \mathrm{D}_n^{\alpha_n}$.

Definition

We call a perturbation V *admissible* of order γ, with $n > \gamma > 0$, if $\{v_j\}_{j=0}^n \in S^\gamma(\mathbb{Z}^n)$ and for $j = 1, \ldots, n$

$$v_j(\mu) = \langle \mu \rangle^{-\gamma} (\Gamma_j + o(1)) \text{ as } \mu \to \infty, \tag{2}$$

with $\Gamma_j \neq 0$ for at least one j.

Ingredients for the asymptotics

For an admissible perturbation we define the diagonal $(n+1)\times(n+1)$ matrix Γ by

$$\Gamma_{ll} = \begin{cases} \Gamma_{l-1} & \text{if } \Gamma_{l-1} > 0 \ , \\ 0 & \text{otherwise} \ . \end{cases}$$

We also define the function $M : \mathbb{T}^n \to M_{(n+1)\times(n+1)}(\mathbb{C})$ by

$$M(\xi) := \frac{1}{r(\xi)} \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & r_1(\xi) & -a_2(\xi)\overline{a_1(\xi)} & \cdots & -a_n(\xi)\overline{a_1(\xi)} \\ 0 & -a_1(\xi)\overline{a_2(\xi)} & r_2(\xi) & \cdots & -a_n(\xi)\overline{a_2(\xi)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -a_1(\xi)\overline{a_n(\xi)} & -a_2(\xi)\overline{a_n(\xi)} & \cdots & r_n(\xi) \end{pmatrix} ,$$

where

$$r(\xi) := \sum_{j=1}^{n} |a_j(\xi)|^2 \text{ and } r_i(\xi) = r(\xi) - |a_i(\xi)|^2 = \sum_{j\neq i} |a_j|^2 \ .$$

Main Theorem

Theorem (Miranda & P. (2024))

Assume that V is an admissible perturbation of order γ. Define the constant $\mathcal{C}$ by

$$\mathcal{C} := \int_{\mathbb{T}^n} \mathrm{Tr}\left((\Gamma M(\xi))^{\frac{n}{\gamma}} \right) d\xi \ .$$

Let τ_n denote the volume of the unitary sphere in $\mathbb{R}^n$. Then, the eigenvalue counting function satisfies

$$\mathcal{N}(\lambda) = \lambda^{-\frac{n}{\gamma}} \ (\mathcal{C}\, \tau_n + o(1)), \quad \lambda \downarrow 0 \ .$$

Proof (1): Effective Hamiltonian

Proposition

Let us set $P := \mathbb{1}_{\{-m\}}(H_0)$ the projection on the flat band. Then P is unitarily equivalent to the multiplication operator by M in $L^2(\mathbb{T}^n;\mathbb{C}^{n+1})$.

Then, for each $\kappa \leq 0$ we have

$$\begin{aligned}\pm\mathcal{N}(\lambda) \leq & \pm\mathcal{N}((-m+\lambda,0); -mP + P(V \pm \kappa|V|)P) \\ & \pm\mathcal{N}((-m+\lambda,0); P^{\perp}(H_0 + (V \pm \kappa^{-1}|V|))P^{\perp}) + O(1). \quad (3)\end{aligned}$$

Lemma

$\mathcal{N}((-m+\lambda,0); P^{\perp}(H_0 + V \pm \kappa^{-1}|V|)P^{\perp}) = o(\lambda^{-n/\gamma}), \quad \lambda \downarrow 0$.

Hence we need to calculate $\mathcal{N}((\lambda,m); P(V \pm \kappa|V|)P)$

Proof (2): Eigenvalues of the effective Hamiltonian

Proposition

For an admissible V we have

$$n_+(\lambda; P(V \pm \kappa|V|)P)) = \left(\frac{1 \pm \kappa}{\lambda}\right)^{n/\gamma} \tau_n \int_{\mathbb{T}^n} \mathrm{Tr}\left((M(\xi)\Gamma M(\xi))^{n/\gamma}\right) d\xi\,(1+o(1)),\ \lambda \downarrow 0\,.$$

To obtain this proposition we first notice that after Fourier transform it corresponds to an integral operator with symbol $M\hat{V}_\kappa M$. Then we approximate on the diagonal by a suitable step functions supported on cubes. The eigenvalues of that operator can be explicitly studied, and then the proposition is recovered by taking the limit as the boxes vanish.

Finally, the main theorem is obtained by taking $\kappa \downarrow 0$.

Comparison with the Landau Hamiltonian

Theorem 2.6: *Let* k=0. *Assume that* (1.1) *holds with* $\alpha>0$. *For* $\lambda>0$ *put*

$$\nu_4^{\pm}(\lambda) = (2\pi)^{-d}\, b_1 \dots b_d \,\mathrm{vol}\left\{(x,y)\in\mathbb{R}^{2d}\equiv \mathbb{R}^m;\ \mp V(x,y) > \lambda\right\}.$$

Suppose that $\nu_4^{+}(\lambda)$ *and* $\nu_4^{-}(\lambda)$ *satisfy the condition* $\mathcal{T}$. *Moreover, assume that the estimate*

$$(2.9)_{\pm} \qquad \nu_4^{\pm}(\lambda) \ \geq\ \gamma_0 \lambda^{-2d/\alpha}, \quad \lambda\downarrow 0,$$

holds for some constant $\gamma_0>0$. *Then we have*

$$(2.10)_{\pm} \qquad N_q^{\pm}(\lambda) = \varkappa_q \nu_4^{\pm}(\lambda)(1+o(1)), \quad \lambda\downarrow 0,$$

for each Landau level Λ_q, $q\geq 1$.

Eigenvalue asymptotics for the Schrödinger operator with homogeneous magnetic potential and decreasing electric potential. I. Behaviour near the essential spectrum tips. G. Raikov, Comm. PDE **15** (3), 1990.