THE CREATION OF SPECTRAL GAPS BY GRAPH DECORATION

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Abstract. We present a mechanism for the creation of gaps in the spectra of self-adjoint operators defined over a Hilbert space of functions on a graph, which is based on the process of graph decoration. The resulting Hamiltonians can be viewed as associated with discrete models exhibiting a repeated local structure and a certain bottleneck in the hopping amplitudes.

1. Introduction

Energy spectra characterized by the presence of bands and gaps are familiar from the Bloch theory of periodic systems. In this note, we present another mechanism for the creation of spectral gaps which does not rely on translation invariance.

The band-gap spectral structure plays an important role in the theory of the solid state [1], as well as in the properties of dialectric and acustic media [2]. Of particular interest are also situations in which localized states are injected into existing gaps (see ref. [3] for a mathematical discussion with further references). These applied models are mentioned only as distant analogies; the topic we discuss pertains to spectral properties of Hamiltonians of discrete models, whose "hopping terms" can be viewed as associated with graphs exhibiting a repeated local structure and a certain bottleneck in hopping amplitudes.

To present the principle described herein it is convenient to introduce the notion of "graph decoration". Given two graphs Γ and G, we may "decorate" Γ with G by "gluing" a copy of G to each vertex v of Γ in such a way that v is identified with the appropriate copy of some distinguished vertex $\mathrm{O}_G \in G$ (see §2 for a formal definition, and figures 2 and 3 for typical examples). Given self-adjoint operators H_o on $\ell^2(\Gamma)$ and A on $\ell^2(G)$ there is a natural way to define an operator extension H of H_o and A to $\ell^2(\Gamma \triangleleft G)$ where $\Gamma \triangleleft G$ denotes the decorated graph just described. In the absence of certain degeneracy, there is a simple relation between the spectra of H and H_o, denoted here by $\sigma(H_{\dots})$, which allows us to conclude that intervals around certain energies ε_j are excluded from the spectrum of H. Specifically, there is a function γ such that

$$\sigma(H) \;=\; \gamma^{-1}\left(\sigma(H_o)\right) \ , \tag{1.1}$$

and γ is of the form

$$\gamma(E) \;=\; E + c + \sum_j w_j \, \frac{1}{\varepsilon_j - E} \ , \tag{1.2}$$

where $w_j > 0$ and $\varepsilon_j, c \in \mathbb{R}$ (see figure 1). In fact, we shall see that ε_j are exactly the eigenvalues of the operator $\widehat{P}A\widehat{P}$ where $\widehat{P}$ is the projection onto the subspace

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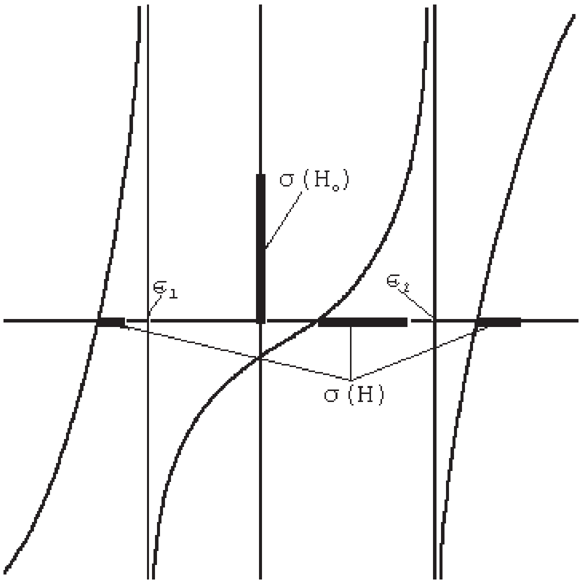

FIGURE 1. A schematic depiction of the spectral relation $\sigma(H) = \gamma^{-1}(\sigma(H_o))$.

of functions in $\ell^2(G)$ which vanish at O_G. Thus, we have the appealing picture in which the eigenenergies of the decorated graph are repelled by resonances with the "inner spectrum" of the decoration.

In §2 we define graph decoration and describe the operator extension mentioned above. In §3 we present our main result (Prop. 3.1) which describes the spectral relationship presented above in full detail. Finally, in §4 we provide several examples and applications of Prop. 3.1.

2. Graph decoration

In this section, we suppose that we are given a graph Γ and a self adjoint operator H_o on $\ell^2(\Gamma)$, the space of square summable functions on the vertices of Γ (see below). Our goal is to describe a certain class of graph extensions of Γ and a corresponding class of operator extensions of H_o.

Recall that a graph G is described by specifying two sets: (1) $V(G)$ whose elements are called vertices, and (2) $E(G)$ a set of (unordered) pairs of vertices called edges. The edges play a secondary role in our discussion, for we are mainly concerned with the Hilbert space of square summable functions mapping $V(G) \to \mathbb{C}$, which we denote $\ell^2(\Gamma)$. The situation of interest is when $E(G)$ is defined so that a given operator A on $\ell^2(G)$ is *compatible* with G, by which we mean that the off diagonal matrix elements $\langle x|A|y\rangle$ vanish whenever $\{x, y\} \notin E(G)$. [1] Correspondingly, our notation generally identifies a graph G with its vertex set: by $x \in G$ we indicate $x \in V(G)$ and we shall say that a graph is countable (finite) if $V(G)$ is countable (finite).

The graph extensions of Γ shall be obtained by "gluing" copies of a second graph G to each vertex of Γ. The extended graph may be visualized as a field in which

[1] We use the Dirac bra-ket notation for matrix elements in the standard basis $|x\rangle = \delta_x$, with $\delta_x(y)$ the Kronecker function.

are tethered many identical kites (see figures 2 and 3). Formally given any graph G with a distinguished vertex O_G we define the *decoration of* Γ *by* (G, O_G), denoted $\Gamma \triangleleft G$, to be the following graph:

1. $V(\Gamma \triangleleft G) = V(\Gamma) \times V(G)$.
2. $E(\Gamma \triangleleft G) = E_{\text{field}} \cup E_{\text{kite}}$, where:
   (a) $E_{\text{field}} = \{ \{(x, \mathrm{O}_G), (y, \mathrm{O}_G)\} \mid \{x, y\} \in E(\Gamma) \}$.
   (b) $E_{\text{kite}} = \{ \{(x, h), (x, g)\} \mid x \in V(\Gamma) \text{ and } \{h, g\} \in E(G) \}$.

We think of the space $\ell^2(\Gamma \triangleleft G)$ as the tensor product $\ell^2(\Gamma) \otimes \ell^2(G)$, which is natural since the vertex set of $\Gamma \triangleleft G$ is $V(\Gamma) \times V(G)$. The subspace of functions which are supported on $\Gamma_o = \{(x, \mathrm{O}_g) : x \in \Gamma\}$ is naturally identified with $\ell^2(\Gamma)$. We denote by P the orthogonal projection onto this space.

Let A be a self adjoint operator on $\ell^2(G)$. A natural extension of H_o to $\ell^2(\Gamma) \otimes \ell^2(G)$, incorporating A, is

$$H \ := \ PH_oP + \mathbf{1} \otimes A \ . \tag{2.1}$$

The above operator is appropriate to the geometry of graph decoration, for if H_o and A are compatible with Γ and G respectively, then H is compatible with $\Gamma \triangleleft G$.

An example of an operator of the form described in eq. (2.1) is provided by the discrete Laplacian. On any graph H the discrete Laplacian, Δ_H, is defined by

$$[\Delta_H \psi](x) \ := \sum_{y:\, \{x,y\} \in E(H)} \psi(y) - \psi(x) \ . \tag{2.2}$$

For decorated graphs, if we take $H_o = -\Delta_\Gamma$ and $A = -\Delta_G$ then the operator defined by (2.1) is $H = -\Delta_{\Gamma \triangleleft G}$.

3. A resolvent evaluation principle

We now focus on the case $|G| < \infty$ and present our main result.[2]

Proposition 3.1. *Let H be a bounded*[3] *self adjoint operator of the form described in eq.* (2.1) *with G a finite graph. If $|\mathrm{O}_G\rangle$ is a cyclic vector for A, then*

$$\sigma(H) \ = \ \gamma^{-1}\left(\sigma(H_o)\right) \ , \tag{3.1}$$

where γ is a function of the form

$$\gamma(E) \ = \ E \ + \ c \ + \sum_{j=1}^{n} w_j \frac{1}{\varepsilon_j - E} \ , \tag{3.2}$$

with $c, \varepsilon_j \in \mathbb{R}$, and $w_j > 0$.

Furthermore, whether or not $|\mathrm{O}_G\rangle$ is cyclic, there is a function γ of the form (3.2) *such that for each $x \in \Gamma$ and $z \in \mathbb{C} \setminus \mathbb{R}$*

$$\left\langle x, \mathrm{O}_G \middle| (H - z)^{-1} \middle| x, \mathrm{O}_G \right\rangle \ = \ \left\langle x \middle| (H_o - \gamma(z))^{-1} \middle| x \right\rangle \ , \tag{3.3}$$

and the spectral measure, $\widetilde{\mu}_x$, for H associated to $|x, \mathrm{O}_G\rangle$ is related to the spectral measure, μ_x, for H_o associated to $|x\rangle$ by

$$\widetilde{\mu}_x(dE) \ = \ \frac{1}{\gamma'(E)} \ \mu_x(d\gamma(E)) \ . \tag{3.4}$$

[2]This result may be easily extended to the case $|G| = \infty$ provided the spectrum of A is discrete.

[3]More generally, H may be unbounded provided the set of functions with finite support forms a core for H.

Thus

$$\gamma^{-1}(\sigma(H_o)) \subseteq \sigma(H) . \tag{3.5}$$

Remarks:

- Recall that given a self-adjoint operator K on a Hilbert space $\mathcal{K}$, the spectral measure associated to a vector $v \in \mathcal{K}$ is defined via the functional calculus and the Riesz-Markov theorem as the unique regular Borel measure, ν, such that

$$\int f(E)\nu(dE) = \langle v, f(K)v\rangle , \tag{3.6}$$

for each $f \in C_o(\mathbb{R})$, the family of continuous functions on $\mathbb{R}$ which vanish at infinity.
- Eq. (3.4) is a formal expression which indicates the following identity for the expectations of a function $f \in C_o(\mathbb{R})$:

$$\int \widetilde{\mu}_x(dE)\, f(E) = \int \mu_x(d\varepsilon) \sum_{E\in\gamma^{-1}(\varepsilon)} \frac{1}{\gamma'(E)} f(E) . \tag{3.7}$$

Proof of Proposition 3.1: The heart of Prop. 3.1 is the relation (3.3), so let us begin with a derivation of this equation. Fix $x \in \Gamma$ and $z \in \mathbb{C} \setminus \mathbb{R}$. Recall that the Green function,

$$G(y,u) := \left\langle x, \mathrm{O}_G |(H-z)^{-1}| y,u \right\rangle , \ (y,u) \in \Gamma \triangleleft G , \tag{3.8}$$

is the unique square summable solution to the equation

$$(H-z)G = |x, \mathrm{O}_G\rangle . \tag{3.9}$$

A natural guess is that the solution factors:

$$G(y,u) = g(y)\, h(u) . \tag{3.10}$$

With this ansatz, eq. (3.9) yields for g and h:

$$g(y)\,[(A-z)h](u) = 0 , \ u \neq \mathrm{O}_G , \tag{3.11a}$$

and

$$[H_o g](y)\, h(\mathrm{O}_g) + g(y)\,[(A-z)h](\mathrm{O}_g) = |x\rangle . \tag{3.11b}$$

It is now an easy exercise to solve these equations using the Green functions for H_o and A: eq. (3.11a) gives g as a function of h,

$$g(y) = \frac{1}{h(\mathrm{O}_G)} \left\langle x \right| \left(H_o + \frac{[(A-z)h](\mathrm{O}_g)}{h(\mathrm{O}_g)} \right)^{-1} \left| y \right\rangle ; \tag{3.12}$$

while eq. (3.11b) shows that h is a multiple of the Green function for A,

$$h(u) = C \left\langle \mathrm{O}_G |(A-z)^{-1}| u \right\rangle , \tag{3.13}$$

with C an arbitrary factor which drops out of the resulting solution:

$$G(y,u) = \left\langle x \right| \left(H_o + \frac{1}{\langle \mathrm{O}_G|(A-z)^{-1}|\mathrm{O}_G\rangle} \right)^{-1} \left| y \right\rangle \frac{\langle \mathrm{O}_G|(A-z)^{-1}|u\rangle}{\langle \mathrm{O}_G|(A-z)^{-1}|\mathrm{O}_G\rangle} . \tag{3.14}$$

Setting $u = \mathrm{O}_G$ and $y = x$ in this expression yields (3.3) with

$$\gamma(z) \ := \ \frac{-1}{\langle \mathrm{O}_G|(A-z)^{-1}|\mathrm{O}_G\rangle} \ . \tag{3.15}$$

Because $\dim \ell^2(G)$ is finite, γ is a rational function with finitely many simple real poles (which occur at the zeros of $\langle \mathrm{O}_G|(A-E)^{-1}|\mathrm{O}_G\rangle$). Hence, the partial fraction expansion (alternatively, the represenation theory of Herglotz functions) shows that γ is of the form displayed in eq. (3.2):

$$\gamma(z) \ = \ z \ - \ c \ + \ \sum_{j=1}^{n-1} w_j \frac{1}{\varepsilon_j - z} \ , \tag{3.16}$$

with $c, \varepsilon_j \in \mathbb{R}$ and $w_j > 0$. (The coefficient of z is one, since $z/\gamma(z) \to 1$ as $z \to \infty$.)

We now turn to the verification of the relation between the spectral measures expressed in (3.4). First consider the situation when Γ is finite. For a self-adjoint operator B on a finite dimensional vector space there is a useful formula for the spectral measure, ν_ψ, associated to a vector ψ:

$$\nu_\psi(dE) \ = \ \delta\left(\frac{-1}{\langle \psi, (B-E)^{-1}\psi\rangle}\right) dE \ , \tag{3.17}$$

where δ is the Dirac-delta "function." (This formula offers a simple route to the "spectral averaging" principle discussed in ref. [4]; its derivation is an instructive exercise which we leave to the reader.) Coupled with eq. (3.3), (3.17) easily yields:

$$\begin{aligned}\widetilde{\mu}_x(dE) \ &= \ \delta\left(\frac{-1}{\langle x, \mathrm{O}_G|(H-E)^{-1}|x, \mathrm{O}_G\rangle}\right) dE \\ &= \ \delta\left(\frac{-1}{\langle x|(H_o - \gamma(E))^{-1}|x\rangle}\right) \frac{1}{\gamma'(E)} d\gamma(E) \ = \ \frac{1}{\gamma'(E)}\mu_x(d\gamma(E)) \ . \end{aligned} \tag{3.18}$$

When Γ is infinite we must turn to a more abstract derivation of eq. (3.4). Writing each side of eq. (3.3) as a spectral integral we find that

$$\int \frac{1}{E-z} d\widetilde{\mu}_x(E) \ = \ \int \frac{1}{E-\gamma(z)} d\mu_x(E) \ . \tag{3.19}$$

Expanding the right side of this equality with partial fractions yields

$$\int \frac{1}{E-z} d\widetilde{\mu}_x(E) \ = \ \int \sum_{\lambda \in \gamma^{-1}(E)} \frac{1}{\gamma'(\lambda)} \frac{1}{\lambda - z} d\mu_x(E) \ . \tag{3.20}$$

This equation can be viewed as a special case of:

$$\int f(E)\, d\widetilde{\mu}_x(E) \ = \ \int \sum_{\lambda \in \gamma^{-1}(E)} \frac{1}{\gamma'(\lambda)} f(\lambda)\, d\mu_x(E) \ , \tag{3.21}$$

and indeed (3.20) implies (3.21), for all $f \in \mathbb{C}_o(\mathbb{R})$, since by the Stone-Weierstrass Theorem the set of finite sums of the form $\sum_j c_j \frac{1}{E-z_j}$ is dense in $\mathbb{C}_o(\mathbb{R})$. As mentioned previously, (3.21) is the statement claimed in (3.4).

Finally, the spectral inclusion $\gamma^{-1}(\sigma(H_o)) \subseteq \sigma(H)$ follows since

$$\gamma^{-1}(\sigma(H_o)) \ = \ \bigcup_{x \in \Gamma} \mathrm{supp.}(\widetilde{\mu}_x) \ , \tag{3.22}$$

which may be verified using (3.4). If $\{|x, \mathrm{O}_G\rangle\}$ is a cyclic family for H then eq. (3.22) shows further that $\gamma^{-1}(\sigma(H_o)) = \sigma(H)$. In case $|\mathrm{O}_G\rangle$ is a cyclic vector for

A, this family is easily seen to be cyclic for H. This completes the proof of the proposition. ■

We conclude this section with several remarks regarding proposition 3.1 and its proof:

1. Eigenfunctions and generalized eigenfunctions of H factor in the same way as the Green function (see eq. (3.10)). That is
$$\Psi(y,u) \;=\; \psi(y)\,\phi(u) \tag{3.23}$$
satisfies $H\Psi = E\Psi$ provided
$$\phi(u) \;=\; \frac{\left\langle \mathrm{O}_G|(A-E)^{-1}|u\right\rangle}{\left\langle \mathrm{O}_G|(A-E)^{-1}|\mathrm{O}_G\right\rangle}\;, \tag{3.24a}$$
and
$$H_o\psi = \gamma(E)\psi\;. \tag{3.24b}$$
2. The relationship between the spectrum of H_o and H is a stronger relationship than the simple inclusion $\gamma^{-1}(\sigma(H_o)) \subset \sigma(H)$: *the spectral type is preserved under the map* γ^{-1}. So, a bound state for H_o gives rise to n bound states for H. Similarly, a band of absolutely continuous spectrum for H_o gives rise to n bands of absolutely continuous spectrum for H. If H_o possesses singular continuous spectrum, then such spectrum also occurs in the spectrum of H.
3. Generically, $|\mathrm{O}_G\rangle$ is a cyclic vector for A, and $\sigma(H) \;=\; \gamma^{-1}(\sigma(H_o))$. However, even when $|\mathrm{O}_G\rangle$ is not cyclic, we may still determine the spectrum of H. We need only decompose the space $\ell^2(G)$ as a direct sum $V \oplus V^\perp$ with each summand invariant under A and $|\mathrm{O}_G\rangle$ cyclic for $A|_V$. Then,
$$\sigma(H) = \gamma^{-1}(\sigma(H_o)) \cup \sigma(A|_{V^\perp})\;, \tag{3.25}$$
which may be verified by noting that
$$H \cong \begin{pmatrix} H_o + \mathbf{1}\otimes A|_V & 0 \\ 0 & \mathbf{1}\otimes A|_{V^\perp}\end{pmatrix}\;. \tag{3.26}$$
Note that the eigenvalues in $\sigma(A|_{V^\perp})$ occur with multiplicity a multiple of $|\Gamma|$.
4. The poles ε_j of γ are eigenvalues of $\widehat{A} = \widehat{P}A\widehat{P}$, where $\widehat{P}$ is the projection of $\ell^2(G)$ onto the space of functions which vanish at O_G. To see this, recall that ε_j satisfy $\left\langle \mathrm{O}_G|(A-\varepsilon_j)^{-1}|\mathrm{O}_G\right\rangle = 0$. Thus the Green functions $\psi_j(y) \;=\; \left\langle \mathrm{O}_G|(A-\varepsilon_j)^{-1}|y\right\rangle$ themselves are eigenfunctions: $\widehat{A}\psi_j = \varepsilon_j\psi_j$. Conversely, if $|\mathrm{O}_G\rangle$ is cyclic for A then every eigenvalue of $\widehat{A}$ is a pole of γ.
5. The coefficients c and w_j in the partial fraction expansion of γ (eq. (3.2)) satisfy
$$c \;=\; -\left\langle \mathrm{O}_G\,|\,A\,|\,\mathrm{O}_G\right\rangle\;, \tag{3.27a}$$
$$\sum_{j=1}^{n} w_j \;=\; \left\langle \mathrm{O}_G\,|\,A^2\,|\,\mathrm{O}_G\right\rangle - \left\langle \mathrm{O}_G\,|\,A\,|\,\mathrm{O}_G\right\rangle^2\;, \tag{3.27b}$$
and
$$w_j \;=\; \lim_{E\to\varepsilon_j}(\varepsilon_j - E)\gamma(E) \;=\; \frac{1}{\left\langle \mathrm{O}_G|(A-\varepsilon_j)^{-2}|\mathrm{O}_G\right\rangle}\;. \tag{3.27c}$$

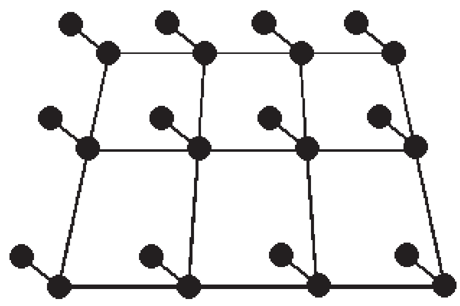

FIGURE 2. A portion of the graph discussed in §4.1 in the case $d = 2$.

The first two equalities may be verified by expanding γ in a Laurent series around 0.

4. Examples and Applications

4.1. Splitting the spectrum of the Laplacian on $\mathbb{Z}^d$. For a simple example of the phenomenon, consider the operator $H = -\Delta_{\mathbb{Z}^d \triangleleft G}$ where G is the graph consisting of two vertices $V(G) = \{0_G, 1_G\}$ and a single edge $E(G) = \{\{0_G, 1_G\}\}$ (see figure 2). As described at the end of §2, H is of the form (2.1) with $H_o = -\Delta_{\mathbb{Z}^d}$ and $A = -\Delta_G$.

The spectrum of $H_o = -\Delta_{\mathbb{Z}^d}$ is

$$\sigma(H_o) = [0, 4d] \tag{4.1}$$

and all the associated spectral measures are purely absolutely continuous. In this case, the function γ is easy to calculate:

$$\gamma(E) \ = \ -\left[\frac{1-E}{(1-E)^2-1}\right]^{-1} \ = \ E \ - \ 1 \ + \ \frac{1}{1-E}\ , \tag{4.2}$$

and the vector $|0_G\rangle$ is cyclic. Thus

$$\begin{aligned}\sigma(H) \ &= \ \left\{E \mid 0 \ \le \ E \ - \ 1 \ + \ \frac{1}{1-E} \ \le \ 4d\right\} \\ &= \ \left[0, 1 + 2d - \sqrt{1+4d^2}\right] \cup \left[2, 1 + 2d + \sqrt{1+4d^2}\right]\ ,\end{aligned} \tag{4.3}$$

and the spectral measures are purely absolutely continuous.

4.2. An example in which $|0_G\rangle$ is not cyclic. Consider now the discrete Laplacian on the graph $\mathbb{Z}^d \triangleleft G$ where G is the fully connected graph with three vertices $V(G) = \{0_G, 1_G, 2_G\}$ (see figure 3).

The involution R on $\ell^2(G)$ obtained by interchanging $|1_G\rangle$ and $|2_G\rangle$ commutes with Δ_G. Hence Δ_G leaves invariant the subspaces $V_{+(-)}$ of functions which are symmetric (anti-symmetric) with respect to this involution. A non-normalized basis of simultaneous eigenfunctions for R and $(-\Delta_G)$ consists of: $|0_G\rangle + |1_G\rangle + |2_G\rangle \in V_+$ with eigenvalue 0 , $2\,|0_G\rangle - |1_G\rangle - |2_G\rangle \in V_+$ with eigenvalue 3 , and $|1_G\rangle - |2_G\rangle \in V_-$ with eigenvalue 3.

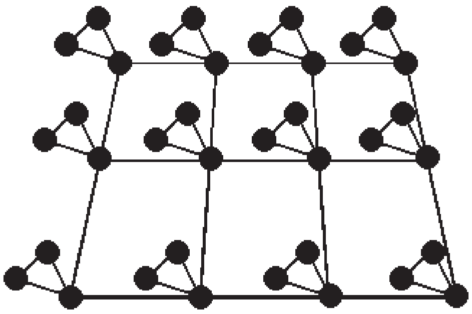

FIGURE 3. A situation in which $|O_G\rangle$ is not cyclic (§4.2).

Using this basis, it is easy to see that $|O_G\rangle$ is a cyclic vector for the restriction of Δ_G to V_+. Furthermore, we can calculate γ:

$$\gamma(E) \;=\; \frac{-1}{\frac{2}{3}\frac{1}{3-E}+\frac{1}{3}\frac{1}{0-E}} \;=\; E-2+\frac{2}{1-E}\;, \tag{4.4}$$

and note that $\sigma(-\Delta_G|_{V_-}) = \{3\}$. Thus,

$$\begin{aligned}\sigma(-\Delta_{\Gamma \triangleleft G}) \;&=\; \{3\} \cup \left\{ E \mid 0 \le E - 2 + \frac{2}{1-E} \le 4d \right\} \\ &= \left[0, \varepsilon^-\right] \cup \left[3, \varepsilon^+\right]\;,\end{aligned} \tag{4.5}$$

where $\varepsilon^\pm$ are the solutions to

$$E - 2 + \frac{2}{1-E} \;=\; 4d\,, \tag{4.6}$$

with $\varepsilon^- < 1$ and $\varepsilon^+ > 1$. The spectrum is purely absolutely continuous except for the presence of an infinitely degenerate eigenvalue at $E = 3$.

4.3. **Persistence of band edge localization.** The operator H may include disorder, in the form of a random potential at the sites of Γ_o. It is generally expected that in such a situation the spectrum of H_o will exhibit Anderson localization (*i.e.*, dense pure point spectrum) at all the spectral edges. (This has been rigorously shown to be true in various situations [2, 5, 6, 7, 8]). Let us note that the mechanism of gap creation via graph decorations preserves such band edge localization, even if the randomness is not introduced at all the sites of the decorated graph.

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