Some Results in the Spectral Theory of the Schrödinger Type Operators on the Quantum Lattice Γ^d for $d \geq 2$

by

Zackery Zane Clark

A dissertation submitted to the faculty of The University of North Carolina at Charlotte in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Applied Mathematics

Charlotte

2026

Approved by:

X

Stanislav Molchanov
Committee Chair

X

Oleg Safronov
Committee Member

X

Vlad Margarint
Comittee Member

X

Yuri Nesmelov
Graduate Faculty Representative

Table of Contents

0. Introduction

The spectral theory of the Schrödinger operators on the quantum graphs has a relatively short history. The first publication in this area can likely be contributed to P. Exner and his collaborators in the mid to late 90s, see [1], [2]. At that time, the term "quantum graph" didn't exist and P. Exner instead used the term "superlattice." For a general review of the topic plus non-complete bibliography see monograph [3].

We will study the Laplacian, related Brownian motion, and Schrödinger type operators on one of the simplest examples of a quantum or metric graph, the d-dimensional quantum lattice, Γ^d for $d \geq 2$. Γ^d is a pseudo-1-dimensional structure consisting of the vertices of $\mathbb{Z}^d$ joined to their nearest neighbors via unit intervals, $\Gamma^d = \{[n, n']: n, n' \in \mathbb{Z}^d \;\&\; d(n, n') = 1\}$. Γ^d is equipped with the Euclidean metric and the Lebesgue measure on the edges. On the quantum graph, Γ^d, the functional spaces $L^2(\cdot)$ and $C(\cdot)$ have their standard definitions but $C^2(\cdot)$ requires a new definition. On the edges of Γ^d, $\Gamma^d \backslash \mathbb{Z}^d$, $C^2(\Gamma^d \backslash \mathbb{Z}^d)$ has its standard definition, however, for a function to be in $C^2(\Gamma^d)$ the function f must be in $C^2(\Gamma^d \backslash \mathbb{Z}^d)$ and satisfy Kirchhoff's gluing condition, KGC,

$$\sum_{n':\, d(n,n')=1} \frac{\partial f}{\partial (n' - n)}(n) = 0, \qquad \forall n \in \mathbb{Z}^d \tag{0.1}$$

The Laplace operator, Δ, on Γ^d is similarly defined with the standard definition on $\Gamma^d \backslash \mathbb{Z}^d$, and condition (0.1) on $\mathbb{Z}^d$. For more formal definitions, containing Sobolev spaces on Γ^d see [3] and [4]. One of the most important applications of the spectral theory on Γ^d is that of the Laplacian, $-\Delta$, or more generalized as the Schrödinger Type Operator, H,

$$H\psi = (-\Delta + V)\psi \tag{0.2}$$

As the Hamiltonian operator, H, can be related to optical applications.

Roughly speaking, optical applications have the following description: consider a network of thin channels formed via laser drilling in an optical medium. The propagation of high frequency electromagnetic waves in this network can be described via Maxwell's equations with the appropriate selection of boundary conditions on the walls of the channels. The paper [5] (S.M, B.Vainberg, Comm.Math Ph) contains the physically important result: if the diameter of the channels, ϵ, tends towards 0, then the system of Maxwell equations can be reduced to the parabolic problem on the quantum graph,

$$\frac{\partial u}{\partial t} = Hu \tag{0.3}$$

with the generalized KGC on the vertices.

The Hamiltonian operator described in (0.2) with potential, V, concentrated on the vertices of the lattice, $\mathbb{Z}^d$, $V(s) = \sum_{n\in\mathbb{Z}^d} V(n)\delta_n(s)$, such as in the case of a crystalline structure, gives the generalized KGC of,

$$\sum_{n':\, d(n,n')=1} \frac{\partial f}{\partial(n' - n)}(n) = V(n)f(n), \qquad \forall n \in \mathbb{Z}^d \tag{0.4}$$

see further details in [4]. For the case of the Hamiltonian outlined above, this leads to a band-gap structure for the eigenvalues. In the case of simple potentials such as this, it is possible to study the number of eigenvalues in both the regions with and without bands without much difficulty. However, for more generalized potentials, the band-gap structure poses complexities which are not trivially solvable and thus estimates such as the Cwinkel-Lieb-Rozenblum and Lieb-Thirring inequalities must be relied on see further details in [5].

Regarding this dissertation, we will be exclusively considering the case of "simple" potentials concentrated on the vertices of the lattice, $\mathbb{Z}^d$, $V(s) = \sum_{n\in\mathbb{Z}^d} V(n)\delta_n(s)$, breaking our discussion up into the 3 selected potentials described below.

Section 1: $V(n) = 0$.

In this case the fundamental solution of the parabolic equation, $p(t, x, y)$, satisfies the following equation,

$$\frac{\partial p}{\partial t} = -\Delta p$$
$$p(0, x, y) = \delta_y(x)$$

and is the transition density for the Markov process, $X(t)$ for $t \geq 0$, on Γ^d. i.e. $-\Delta$ is the generator of $X(t)$, the Brownian motion on Γ^d. The central point of this section is the calculation of the resolvent $R_\lambda(x, x')$, $x, x' \in \Gamma^d$, its reduction to the lattice $\mathbb{Z}^d$, and an analysis of its temporal asymptotics.

Section 2: $V(n) = \alpha$.

Thus, the operator, H, is a perturbation of the Laplacian by a periodic δ-potential concentrated on $\mathbb{Z}^d$. The central point of this section is to reiterate and further expand upon the discussion from S.M. O.S. [] by asymptotically analyzing the spectral bands of the Hamiltonion, $H = -\Delta + V$, for $V = \alpha \sum_{n\in\mathbb{Z}^d} \delta(s - n)$.

At the physical level, a constant α corresponds to a delay in the electromagnetic waves as they pass through vertices of the graph, Γ^d. This particular model, as well as some of its generalizations, on Γ^d were previously studied by P. Exner et al, with the central result of the analysis being the existence of an infinitely repeating band gap structure within the spectrum of the Hamiltonian, H. This differs from the case of a periodic Schrödinger operator on $L^2(\mathbb{R}^d)$ for $d \geq 2$, where there are at most finitely many gaps within the spectrum see J. Karpeshina []. At the physical level, the existence of an infinitely repeating band and gap structure indicates some kind of semiconducting properties of the periodic network of thin channels in the optical medium for arbitrarily high energies.

Section 3: $V(n) = \alpha + \beta\delta_{x_i}(n)$ for $x_i \in \mathbb{Z}^d | i = 1, \dots, N$.

The central model of $V(n)$ describes the small pertubations of $V_0(n) = \alpha, n \in \mathbb{Z}^d$. The term "small" can be understood in a variety of ways. For instance,

$$V(n) = V_0(n) + \beta\zeta_n$$

where $\beta \ll 1$ and ζ_n for $n \in \mathbb{Z}^d$ are independent random variables uniformly distributed on $[0,1]$. This particular case of the Anderson model of the disordered physical system relates to the phenomenon of localization, see [4] and [5], and a similar case was analyzed in S.M. O.S[].

For our discussion we will concentrate on fast decreasing and compactly supported perturbations, $V_1(n)$,

$$V(n) = V_0(n) + V_1(n)$$

where $V_1(n)$ is non-zero only for finitely many $n \in \mathbb{Z}^d$. Specifically we will consider the case of $V_1(n) = \beta\delta_{x_i}(n)$ for $i = 1, \dots, N$ such that $x_1 = 0$ and $x_i \in \mathbb{Z}^d$ and will derive an equation for the exact number of discrete eigenvalues, $N(\beta)$, in the gaps of the spectrum.

In the case for a single rank 1 perturbation, i.e. $V_1(n) = \beta\delta_0(n)$, then for all gaps in the spectrum there exists at most 1 discrete eigenvalue. Furthermore, for dimensions less than or equal to 2, $d \leq 2$, for arbitrarily small β such that $\text{sgn}(\beta) = -\text{sgn}(\alpha)$ there exists infinitely many discrete eigenvalues in the gaps of the spectrum of $H_0 = -\Delta + \alpha \sum_{n \in \mathbb{Z}^d} \delta(s - n)$. This is opposed to the case of dimensions greater than 2, $d > 2$, which $\forall \beta \in \mathbb{R}$ there exists at most finitely many discrete eigenvalues in the gaps of the spectrum of $H_0 = -\Delta + \alpha \sum_{n \in \mathbb{Z}^d} \delta(s-n)$.

In the case of $N > 1$ which is the case for multiple rank 1 perturbations i.e. $V_1(n) = \beta\delta_{x_i}(n)$ for $i = 1, \dots, N$ such that $x_1 = 0$ and $x_i \in \mathbb{Z}^d$, the analysis is far more complex however it can be vastly simplified assuming $\forall i < j \leq N,\ d(x_i, x_j) \gg 1$. In this case of sufficiently spaced perturbations, we encounter the phenomenon known as resonance interactions.

This phenomenon of resonance interactions can be explained through the analysis of the discrete spectrums of the following 2 operators,

$$H_x(\beta) = -\Delta + \alpha \sum_{n \in \mathbb{Z}^d} \delta(s-n) + \beta\delta_x(n)$$

and

$$H_{x_1,x_2}(\beta_1, \beta_2) = -\Delta + \alpha \sum_{n \in \mathbb{Z}^d} \delta(s-n) + \beta_1\delta_{x_1}(n) + \beta_2\delta_{x_2}(n)$$

In the case of $\beta_1 \neq \beta_2$ and $d(x_1, x_2) \gg 1$, then the interactions between the perturbations are very small and the discrete spectrums follow the following relation,

$$\mathrm{Sp}\left(H_{x_1,x_2}(\beta_1, \beta_2)\right) \cong \mathrm{Sp}\left(H_{x_1}(\beta_1)\right) \cup \mathrm{Sp}\left(H_{x_2}(\beta_2)\right)$$

with exponentially small error and eigenfunctions of $H_{x_1,x_2}(\beta_1, \beta_2)$ being exponentially close to the eigenfunctions of $H_{x_1}(\beta_1)$ or $H_{x_2}(\beta_2)$. If $\beta_1 = \beta_2$ the behavior is the opposite. For arbitrarily large M such that $d(x_1, x_2) = M$, the eigenfunctions for two "almost equal" eigenvalues λ_1, λ_2 are equally distributed near points x_1 and x_2.

1. Brownian motion, $X(t)$, and transition probabilities, $p(t,x,y)$ on the quantum lattice, Γ^d

Let's start from the formal definition of the Laplacian, $-\Delta$, and the Brownian motion, $X(t)$. In the Hilbert space $L^2(\Gamma^d)$, we consider the Hamiltonian, H, generated by the quadratic form,

$$h(u) = \int_{\Gamma^d} |u'(x)|^2\, dx$$

The domain of this quadratic form, denoted $D(H)$, contains the space of continuously differential functions on the edges of Γ^d which satisfies KGC on the vertices, $C^2(\Gamma^d) \subset D(H)$,.

Symbolically we can present the self-adjoint Hamiltonian operator in the following form,

$$H(u) = -\Delta u$$

The domain of the Laplacian is similar to the Sobolov's space $W^{1,2}$ (but of course not identical due to KGC, See details for the general quantum graphs in [3] and specifically for Γ^d in [4].

Now let's consider the parabolic problem on $L^2(\Gamma^d)$:

$$\frac{\partial u}{\partial t}(t,x) = \Delta u(t,x), \qquad u(0,x) = \phi(x) \in L^2(\Gamma^d)$$

Then, the transition density, $p(t,x,y)$, of the process $X(t)$ satisfying the following relations, is the fundamental solution of the equation,

$$\frac{\partial p}{\partial t} = \Delta_x p(t,x,y) = \Delta_y p(t,x,y), \qquad p(0,x,y) = \delta_y(x) \text{ or } \delta_x(y), \qquad x,y \in \Gamma^d, t \geq 0$$

Thus, the fundamental solution defining the semigroup of bounded operators:

$$P_t\phi = e^{\Delta t}\phi = \int_{\Gamma^d} p(t,x,y)\phi(y)\,dy, \qquad \phi \in L^2(\Gamma^d), \qquad P_{t+s} = P_tP_s = P_sP_t$$

and the Markov process $X(t)$ of Γ^d (Brownian motion) such that

$$p(t,x,y) = P_x\big(X_t \in (y, y+dy)\big)$$

The physical meaning of $X(t)$ and KGC can be explained in 2 equivalent ways: the discretization approach and the continuous approach.

Discretization approach

Let's consider on each unit edge the lattice with step δ, $\frac{1}{\delta} = N$, and discrete time, t, has step size δ^2. For the symmetric random walk on $[0, \dots, N]$ with reflection at the point 0, let's denote τ_N as the initial time at which the point N is reached. Then for the generating function,

$$\phi_z(x) = E_x z^{\tau_N}$$

we have the equation,

$$\phi_z(N) = 1, \qquad \phi_z(x) = \frac{z}{2}\big(\phi(x+1) + \phi(x-1)\big), \qquad x \geq 1, \qquad \phi_z(0) = z\phi_z(1)$$

(Here we use the fact that all 2d legs at the point 0 are identical)

Using elementary calculations,

$$\phi_z(0) = \frac{2}{\left(\frac{1+\sqrt{1+z^2}}{z}\right)^N + \left(\frac{1-\sqrt{1-z^2}}{z}\right)^N}$$

Let us put $z = e^{-\lambda\delta_N^2} = e^{-\frac{\lambda}{N}}$, then,

$$E_0 e^{-\lambda\tau_{0,N}} \sim \frac{1}{\left(1+\frac{\sqrt{2\lambda}}{N}\right)^N + \left(1-\frac{\sqrt{2\lambda}}{N}\right)^N} \to e^{-\sqrt{2\lambda}}$$

but $\phi(1) = e^{-\lambda\tau_1}$ is the Laplace transform of the first exit time from $[0,1]$ of the Wiener process with reflection at 0 (or equivalently from the stun graph containing 2d unit edges from the origin with KGC). Now we have the following construction of the embedded semi-Markovian chain to the Brownian motion (Wiener process) on Γ^d. It starts from some point n_0 of $\mathbb{Z}^d$ and after some random time, $\tilde{\tau}_0$: $E_0 e^{-\lambda\tau_0} = \frac{1}{\cosh(\sqrt{2\lambda})}$, it connects to one of its 2d neighbor points, n_1: $d(n_0, n_1) = 1$, with equal probabilities $\frac{1}{2d}$. After this we repeat the same construction, etc. The distribution of τ_0 is not exponential, i.e. the corresponding process is only semi-Markovian.

Several remarks on the r.v. τ_0:

The generating function, $E_0 e^{-\lambda\tau_0} = \frac{1}{\cosh(\sqrt{2\lambda})}$ is closely related to the well known Euler numbers, E_n (See Ryz-Grad []), namely,

$$\frac{1}{\cosh(t)} = \sum_{n=0}^{\infty} \frac{E_n}{(2n)!} t^{2n}$$

The Euler numbers are integers (which is not clear in the direct approach) and,

$$\phi(\lambda) = \frac{1}{\cosh(\sqrt{2\lambda})} = \sum_{n=0}^{\infty} \frac{2^n E_n}{(2n)!} \lambda^n$$

There exists the representation of $\cosh(t)$ or $\cosh(\sqrt{2\lambda})$ into the infinite product and corresponding expansion of $\phi(\lambda) = \frac{1}{\cosh(\sqrt{2\lambda})}$ into series of the simple fraction (corollary of Euler formulas for $\cos(t), \frac{1}{\cos(t)}$:

$$\frac{1}{\cosh(\sqrt{2\lambda})} = \frac{1}{\pi}\sum_{k=1}^{\infty}(-1)^{k+1}\frac{(2k-1)\pi^2}{(2k-1)\pi^2 + 8\lambda}$$

And inverse Laplace transform gives formula for density $\pi_0(x)$ of τ_0:

$$\pi_0(x) = \sum_{k=1}^{\infty}(-1)^{k+1}\frac{(2k-1)\pi}{2}e^{-\frac{x(2k-1)^2\pi^2}{8}}$$

It is fast converging series of the exponential laws with alternating signs.) Now we'll introduce the construction of the process $X(t)$ as the combination of the symmetric random walk on $\mathbb{Z}^d$ and the semi-Markovian change of the time in this walk.

Let $\{\tau_n\}$ be the collection of the independent random variables with Laplace transform $Ee^{-\lambda\tau_0} = \frac{1}{\cosh(\sqrt{2\lambda})}$. Assuming that $X(0) = 0$. The trajectory of the $X(t)$ has the following structure. It spends time τ_0 inside the "spider", containing the point $X(0)$ and 2d unit edges connecting it to the nearest points of $\mathbb{Z}^d$, $|X(\tau_0) - X(0)| = 1$. At the moment τ_0, $X(\tau_0)$ is located with probability $\frac{1}{2d}$ at one of the nearest points of $\mathbb{Z}^d$. At this vertex we repeat the same construction. As a resulte we'll construct the symmetric random walk on $\mathbb{Z}^d$ but times between successive visits of the vertices has a distribution with Laplace transform $\phi_z(\lambda) = E_0e^{-\lambda\tau_0} = \frac{1}{\cosh(\sqrt{2\lambda})}$, which we already introduced above.

Let's calculate the resolvent of the Brownian motion process on Γ^d, $X(t)$,

$$R_\lambda(x,y) = \int_0^\infty e^{-\lambda t} p(t,x,y)\, dt$$

Here $\lambda > 0$ and (in the beginning) $x, y \in \mathbb{Z}$. Of course, $p(t,x,y) = p(t,0,y-x)$. i.e. we can use $X(0) = 0$, $y - x = z$, i.e study $p(t,0,z)$ instead of $p(t,x,y)$.

The embedded random walk on $\mathbb{Z}^d$ can visit z starting from 0 after at most $d(0,z)$ steps, i.e. $d(0,z)$ is the length of the shortest path of the random walk between 0 and z. if $z = (n_1, \dots, n_d)$ then

$$d(0,z) = \sum_{1 \le k \le d} |n_k| = \|z\|_1$$

Then,

$$R_\lambda(0,z) = \int_0^\infty e^{-\lambda t} p(t,0,z)\, dt = E_0\left(\int_0^{\tau_0} + \int_{\tau_0}^{\tau_0+\tau_1} + \cdots\right)$$

Let $q(n,0,z)$ be the transition probability for the symmetric random walk on $\mathbb{Z}^d$. It is well known that,

$$q(n,0,z) = \frac{1}{(2\pi)^d} \int_{T^d} e^{i(x,\vec{\theta})} H^n(\vec{\theta})\, d\theta$$

Here,

$$H(\vec{\theta}) = \frac{1}{d} \sum_{1 \le k \le d} \cos(\theta_k)$$

Is the characteristic function of each jump.

Now,

$$R_\lambda(0,z) = \sum_{n=d(0,z)}^{\infty} \phi^n(\lambda) \frac{1}{(2\pi)^d} \int_{T^d} e^{i(x,\vec{\theta})} H^n(\vec{\theta})\, d\theta = \frac{1}{(2\pi)^d} \int_{T^d} e^{i(x,\vec{\theta})} \left(\frac{\phi^n(\lambda) H^n(\vec{\theta})}{1 - H(\vec{\theta})\phi(\lambda)} \dots \right) d\theta$$

For transition probabilities, $q(n,0,z)$, there are asymptotic formulas based upon Cramer's form of the central limit theorem (with large deviation). Let's give the sketch of this theorem. Let $x_1, \dots, x_n$ are random variables $\left(\text{i.i.d}, P(x = \pm e_j, j = 1, \dots, d) = \frac{1}{2d} \text{ and } H(\lambda) = Ee^{(\lambda,\vec{x})} = \frac{1}{d}\sum_{1\le j\le d} \cosh(\lambda_j)\right)$. Then

$$Ee^{(\vec{\lambda}, s_n)} = Ee^{(\lambda, \sum_{1\le i\le n} x_i)} = H^n(\lambda) = e^{nR(\lambda)},$$

Where $R(\lambda) = \ln(H(\lambda))$. Note that $H(\lambda)$ is the initial characteristic function extended to the complex plane, $H(\lambda) > 0$ i.e. $R(\lambda)$ is analytic. In the new notation,

$$q(n,0,z) = P\left(\sum_{1\le i\le n} x_i = z\right)$$

But,

$$q_\lambda(n,0,z) = e^{-nR(\lambda)} q(n,0,z) e^{\lambda z}$$

It is known (but can be easily checked) that $q_\lambda(n,0,z) = q_\lambda(n,x,y), y - x = z$ of the new random walk, $x_\lambda(n)$ (Cramer's transformation).

Let's select λ from the condition, $Ex_\lambda(n) = z$. We have first

$$\sum_{z\in\mathbb{Z}^d} q_\lambda(n,0,z) e^{\mu z} = e^{n(R(\lambda+\mu) - R(\lambda))}$$

and then

$$\left(\mathrm{E}x_{\lambda}(n)\right)_{j} = \frac{d}{d\mu_f}\left(e^{n\left(R(\lambda+\mu)-R(\lambda)\right)}|_{\mu=0}\right) = n\frac{dR}{d\mu_j}, j = 1,2,\ldots$$

It means that,

$$E_0 x_{\lambda}(n) = n\nabla R(\lambda)$$

Relation $\mathrm{E}x_{\lambda}(n) = z$ now has the form

$$\nabla R(\lambda) = \frac{z}{n}$$

Let λ^* be the unique root of the equation. Then due to CLT for $x_{\lambda}(t)$,

$$q_{\lambda}(t,0,z) \sim \frac{1}{(2\pi t)^{\frac{d}{2}}} \frac{1}{\sqrt{\lambda^* \det\left[\frac{\partial^2 R}{\partial\lambda_i\,\partial\lambda_j}\right]}}$$

Or

$$q_{\lambda}(t,0,z) \sim \frac{e^{t\left(R(\lambda^*)-\left(\lambda^*,\frac{z}{t}\right)\right)}}{(2\pi t)^{\frac{d}{2}}\sqrt{\lambda^* \det\left[\frac{\partial^2 R}{\partial\lambda_i\,\partial\lambda_j}\right]}}$$

This is Cramer's formula for large deviations. In our particular case,

$$R(\lambda) = \ln\left(\frac{1}{d}\sum_{1\le j\le d}\cosh(\lambda_j)\right)$$

and the equation $\nabla R = \frac{z}{n}$ has the following form,

$$\nabla R = \left\{\frac{\sinh(\lambda_j)}{\sum_{1\le j\le d}\cosh(\lambda_j)}\right\} = \left\{\frac{z_j}{n}\right\}$$

Relabel $\sum_{1\le j\le d}\cosh(\lambda_j) = A(\vec{\lambda})$, then,

$$\sinh(\lambda_j) = \frac{z_j A(\vec{\lambda})}{n}$$

$$A(\vec{\lambda}) = \sum_{1\le j\le d}\cosh(\lambda_j) = \sum_{1\le j\le d}\sqrt{1+\sinh^2\left(\frac{z_j A(\vec{\lambda})}{n}\right)}$$

For the function $A(\vec{\lambda})$ we have scalar equation for λ^*:

$$A(\vec{\lambda}) = \sum_{1\le j\le d}\sqrt{1+\sinh^2\left(\frac{z_j A(\vec{\lambda})}{n}\right)}$$

This transcendental equation has unique solution and for small $\frac{|z|}{n}$ it can be presented in the following form.

$$A(\vec{\lambda}) \sim \frac{2n^2}{\sum_{1\le j\le d} {z_j}^2}$$

Continuous approach

Consider the generator

$$(A\psi)(x) = \sum_{x':|x'-x|=1}\psi(x') - 2d\psi(x), \qquad x', x \in \mathbb{Z}^d$$

and the corresponding random walk $X(t)$ with continuous time. Moment of the jumps of $x(t)$ form the Poisson process with parameter 2d and jump moves $x(t)$ from the point $x = x(t-0)$ to $x' = x(t+0)$, $|x'-x| = 1$ with probability $\frac{1}{2d}$. Components $x_j(t)$ of $x(t) = (x_1, \dots, x_d)(t)$ are independent random walks on $\mathbb{Z}^d$ with the generator

$$(A\psi)(x) = \frac{1}{2} \sum_{x':|x'-x|=1} \psi(x') - d\psi(x), \qquad x', x \in \mathbb{Z}^d$$

Let $p_1(t, x, x')$ be the transition matrix of 1-D random walk $x_j(t), i = 1, \dots, d$ then

$$p(t, \vec{x}, \vec{x}') = p_1(t,_1 x, x_1') \dots p_1(t, x_d, x_d')$$

And

$$\int_0^\infty e^{-\lambda t} p(t, \vec{x}, \vec{x}')\, dt = G_\lambda(x, x')$$

is the Green function of $x(t)$. We want to follow notation and formulas from Feller II [], Ryzik-Gradith [] and put $2t = s$. Then the new process $x(s) = x\left(\frac{t}{2}\right)$ will have generator

$$(A\psi)(x) = \frac{1}{2} \sum_{x':|x'-x|=1} \psi(x') - d\psi(x), \qquad x', x \in \mathbb{Z}^d$$

In Feller II (CH II) one can find the formula for the transition probabilities of $x_i(s)$:

$$p(t, x, x') = e^{-t} I_r(t), \qquad r = |x - x'|$$

i.e.

$$p(t, 0, r) = e^{-t} I_r(t)$$

Here $I_r(t)$ is the modulated Bessel function. In Ryzik-Gradith, there is a simple representation,

$$e^{-t} I_r(t) = \frac{\left(\frac{t}{2}\right)^r}{\sqrt{\pi}\,\Gamma\left(r + \frac{1}{2}\right)} \int_0^\pi e^{-2t \sin^2\left(\frac{\theta}{2}\right)} \sin^{2r}(\theta)\, d\theta$$

Then

$$p(t,0,\vec{r}) = \frac{\left(\frac{t}{2}\right)^{|\vec{r}|}}{\pi^{\frac{d}{2}}\prod_{1\le i\le d}\Gamma\left(r_i+\frac{1}{2}\right)}\int\limits_{[0,\pi]^d} e^{-2t\sum_{1\le i\le d}\sin^2\left(\frac{\theta_i}{2}\right)}\prod_{1\le i\le d}\sin^{2r_i}(\theta_i)\,d\vec{\theta}$$

Then for $\lambda > 0$ and $|\vec{r}| = \sum_{1\le i\le d} r_i$

$$G_\lambda(0,\vec{r}) = \frac{1}{2^{|\vec{r}|}\pi^{\frac{d}{2}}\prod_{1\le i\le d}\Gamma\left(r_i+\frac{1}{2}\right)}\int\limits_0^\infty\int\limits_{[0,\pi]^d} t^{|\vec{r}|}e^{-t\left(\lambda+2\sum_{1\le i\le d}\sin^2\left(\frac{\theta_i}{2}\right)\right)}\prod_{1\le i\le d}\sin^{2r_i}(\theta_i)\,d\vec{\theta}\,dt$$

Which simplifies to,

$$G_\lambda(0,\vec{r}) = \frac{\Gamma(|\vec{r}|+1)}{2^{|\vec{r}|}\pi^{\frac{d}{2}}\prod_{1\le i\le d}\Gamma\left(r_i+\frac{1}{2}\right)}\int\limits_{[0,\pi]^d}\frac{\prod_{1\le i\le d}\sin^{2r_i}(\theta_i)}{\left(\lambda+2\sum_{1\le i\le d}\sin^2\left(\frac{\theta_i}{2}\right)\right)^{|\vec{r}|+1}}\,d\vec{\theta}$$

We'll use agreement $a(r) \approx b(r)$ if $a, b > 0$ and $\frac{\ln(a(r))}{\ln(b(r))} \to 1, r \to \infty$ (logarithmical equivalence)

Then using the Stirling formula,

$$\Gamma(n+1) = n! \sim \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$$

We can reduce the Green function asymptotically to

$$G_\lambda(0,\vec{r}) \sim \frac{|\vec{r}|^{|\vec{r}|+\frac{1}{2}}}{2^{|\vec{r}|+\frac{d-1}{2}}\pi^{d-\frac{1}{2}}e^{\frac{d}{2}}}\int\limits_{[0,\pi]^d}\frac{\prod_{1\le i\le d}\left(\frac{\sin^2(\theta_i)}{r_i-\frac{1}{2}}\right)^{r_i}}{\left(\lambda+2\sum_{1\le i\le d}\sin^2\left(\frac{\theta_i}{2}\right)\right)^{|\vec{r}|+1}}\,d\vec{\theta}$$

Assuming $r_i \pm \frac{1}{2} \approx r_i$ we can further reduce this to

$$G_\lambda(0,\vec{r}) \sim \frac{1}{\pi^{d-\frac{1}{2}} e^{\frac{d}{2}}} \int_{[0,\pi]^d} \left(\frac{\prod_{1\le i\le d} \left(\frac{\sin^2(\theta_i)}{2\delta_i}\right)^{\delta_i}}{\lambda + 2\sum_{1\le i\le d} \sin^2\left(\frac{\theta_i}{2}\right)} \right)^{|\vec{r}|} d\vec{\theta}$$

Where $\delta_i = \frac{r_i}{|\vec{r}|}$ and $\sum_{1\le i\le d} \delta_i = 1$. Using logarithmic Laplace approximation we get the following relationship,

$$\ln\left(G_\lambda(0,\vec{r})\right) \le |\vec{r}| \max_{\{\theta_i\}_{1\le i\le d}} \left[\ln\left(\frac{\prod_{1\le i\le d} \left(\frac{\sin^2(\theta_i)}{2\delta_i}\right)^{\delta_i}}{\lambda + 2\sum_{1\le i\le d} \sin^2\left(\frac{\theta_i}{2}\right)} \right) \right] + \ln\left(\sqrt{\frac{\pi}{e^d}}\right)$$

This is the Lyapunov exponent $\left(G_\lambda(0,\vec{r}) \approx e^{\delta|\vec{r}|},\ \delta(\lambda) < 0\right)$. For any $a_i, b_i > 0$,

$$\prod_{1\le i\le n} a_i^{b_i} \le \sum_{i\le i\le n} a_i b_i$$

we can further reduce the above expression to,

$$\ln\left(G_\lambda(0,\vec{r})\right) \le |\vec{r}| \max_{\{\theta_i\}_{1\le i\le d}} \left[\ln\left(\frac{2\sum_{1\le i\le d} \sin^2\left(\frac{\theta_i}{2}\right)}{\lambda + 2\sum_{1\le i\le d} \sin^2\left(\frac{\theta_i}{2}\right)} \right) \right] \le |\vec{r}| \ln\left(\frac{2d}{\lambda + 2d}\right) < 0$$

In the case of $d = 1$ then this constant $\delta(\lambda)$ can be calculated explicitly as

$$\delta(\lambda) = \ln\left(\frac{1}{1 + \lambda + \sqrt{\lambda(2+\lambda)}}\right)$$

Symmetric Random walk on $\mathbb{Z}^d$ and the central limit theorem for very large deviations.

Let's recall briefly Cramer's approach for the CLT for the sums of independent identically distributed random variables (i.e. d.r.v). We'' present here the lattice r.v with values in $\mathbb{Z}^d$, $d \geq 2$. Now we formulate some definitions and assumptions. Consider the vector valued r.v.

$X(n) = [X_1(n), \dots, X_d(n)], n \geq 1$

$$P\{X(\cdot) = x\} = P(x), \qquad x \in \mathbb{Z}^d$$

For any $\lambda \in \mathbb{R}^d$, such that $|\lambda| < \delta, \delta > 0$, $E\left(e^{(\lambda,x)}\right) = e^{R(\lambda)} = \sum_{x\in\mathbb{Z}^d} e^{(\lambda,x)} P(x)$ (Cramer's condition), $R(0) = 0$.

$$E(x) = \nabla R(\lambda)|_{\lambda=0} = \sum_{x\in Z^d} xP(x) = 0 \text{ (first moment of x)} \tag{1}$$

$$\sigma_{ij} = E\left(X_i(\cdot)X_j(\cdot)\right) = \frac{\partial^2 R}{\partial\lambda_i\,\partial\lambda_j} = \begin{cases} \sigma^2 > 0 & i = j \\ 0 & i \neq j \end{cases} \tag{2}$$

$\sigma(\cdot) = \left[\sigma_{ij} |\, i, j \in \{1, \dots, d\}\right] = \sigma I_d$ (Covariance matrix of $X(\cdot)$)

The particular example

$$E\left(e^{(\lambda,x)}\right) = \frac{1}{d}\sum_{i=1}^{d} \operatorname{Cosh}(\lambda_i), R(\lambda) = \ln\left(\sum_{i=1}^{d} \operatorname{Cosh}(\lambda_i)\right) - \ln(d)$$

$$E(x) = 0, \sigma = \frac{I_d}{d} \tag{3}$$

Let $X(n), n \geq 1$ are iidrv such that

$$e^{R(\lambda)} = E\left(e^{(\lambda,x)}\right) = \sum_{x\in\mathbb{Z}^d} e^{(\lambda,x)} P(x)$$

And $Y(\lambda_0, n), n \geq 1, \lambda_0 \in \mathbb{R}^d$, $|\lambda_0| < \delta$ with distribution

$$q_{\lambda_0}(x) = \frac{e^{(\lambda_0,x)}P(x)}{e^{R(\lambda_0)}}, \qquad |\lambda| < \delta, \qquad \sum_{x\in\mathbb{Z}^d} q_\lambda(x) = 1 \tag{4}$$

Note that for fixed λ_0: $|\lambda_0| < \delta$ and small enough λ,

$$E\left(e^{(\lambda,Y(\lambda_0,\cdot))}\right) = \sum_{x\in Z^d} \frac{e^{(\lambda+\lambda_0,x)}P(x)}{e^{R(\lambda_0)}} = \frac{e^{R(\lambda+\lambda_0)}}{e^{R(\lambda_0)}}$$

(Since $R(\lambda+\lambda_0) - R(\lambda_0) = 0$, if $\lambda = 0$)

i.e.

$$E\big(Y(\lambda_0,\cdot)\big) = (\nabla R)(\lambda_0) = \left[m^{(1)}(\lambda_0,i), i\in\{1,\ldots d\}\right] \tag{5}$$

$$E[Y(\lambda_0,\cdot)\otimes Y(\lambda_0,\cdot)] = \left[\sigma_{ij}(\lambda_0)\right] = \left[\frac{\partial^2 R}{\partial^2\lambda_i} I_{i=j} + m^{(1)}(\lambda_0,i)\otimes m^{(1)}(\lambda_0,j)\right] = \left[\frac{\partial^2 R}{\partial^2\lambda_i} I_{i=j} + m_i^{(1)}(\lambda_0)m_j^{(1)}(\lambda_0)I_{i\neq j}\right]$$

Let also $P^{(n)}(x) = P\{S(n) = x\}, S(n) = x_1 + \cdots + x_n, q_\lambda^{(n)}(x) = P\{\sum(\lambda_0,x) = x\}, \sum(\lambda_0,x) = \sum_{i=1}^n Y_i(\lambda_0)$

The central point in Cramer's approach to the large deviation theorem for the sum $S(n)$ in the following formula:

$$q_{\lambda_0}^{(n)}(x) = \frac{e^{(\lambda_0,x)}P^{(n)}(x)}{e^{nR(\lambda_0)}} \tag{7}$$

Based on the multiplicative property of the exponential function and elementary calculations.

After substitution in (7) $(\lambda+\lambda_0)$ instead of $\lambda_0$and summation over $\mathbb{Z}^d$ we'll get

$$e^{nR(\lambda+\lambda_0)} = \sum_{x\in Z^d} e^{(\lambda+\lambda_0,x)}P^{(n)}(x) \tag{8}$$

Now we'll differentiate this identity over λ_i or λ_i and λ_j with substitution $\lambda = 0$. It gives

$$ne^{nR(\lambda_0)}\frac{\partial R}{\partial \lambda_i} = \sum_{x\in Z^d} x_i e^{(\lambda_0,x)} P^{(n)}(x)$$

That is

$$n\frac{\partial R}{\partial \lambda_i}(\lambda_0) = \sum_{x\in Z^d} \frac{x_i e^{(\lambda_0,x)} P^{(n)}(x)}{e^{nR(\lambda_0)}} = \sum_{x\in Z^d} x_i q_{\lambda_0}^{(n)}(x) = m_i^{(1)}(\lambda_0, n) \qquad (9)$$

Formula (9) presents the first moment of $\sum(\lambda_0, x)$.

Similarly for $i \neq j$

$$n^2\frac{\partial R}{\partial \lambda_i}(\lambda_0)\frac{\partial R}{\partial \lambda_j}(\lambda_0) = \sum_{x\in Z^d} x_i x_j q_{\lambda_0}^{(n)}(x) = m_i^{(2)}(\lambda_0, n) \qquad (10)$$

And for $i = j$

$$n^2\frac{\partial^2 R}{\partial \lambda_i\, \partial \lambda_j} = \sum_{x\in Z^d} x_i^2 q_{\lambda_0}^{(n)}(x) \qquad (11)$$

Formulas (10), (11) present the second moment of $\sum(\lambda_0, x)$

Our goal is to find the asymptotics of $P^{(n)}(x) = P\{S(n) = x\}$ of $x = O(n)$. (Large deviation. In the usual CLT for $S(n)$ we assume that $x = O(\sqrt{n})$.)

Due to Formula (7),

$$P^{(n)}(x) = \frac{q_{\lambda_0}^{(n)}(x)e^{nR(\lambda_0)}}{e^{(\lambda_0,x)}} \qquad (12)$$

Let's select parameter λ_0 for fixed $x = nx^*$, $|x^*| = O(1)$ (or may be sufficiently small.)

2. Asymptotics of the Spectral Band Gap Structure of $H = -\Delta + V$, $V(n) = \alpha$

In this section, we will discuss the infinitely repeating band gap structure of the spectrum resulting from the Schrödinger type operator,

$$H\psi(s) = \left(-\Delta + \sum_{n \in \mathbb{Z}^d} V(n)\delta(s-n)\right)\psi(s) = \lambda\psi(s), \qquad \forall s \in \Gamma^d \backslash \mathbb{Z}^d \tag{2.1}$$

with Dirichlet boundary conditions,

$$\psi(n) = \psi_n, \qquad \forall n \in \mathbb{Z}^d \tag{2.2}$$

and Kirchhoff's gluing condition, KGC,

$$\sum_{n' \colon d(n,n')=1} \frac{\partial \psi}{\partial (n'-n)}(n) = V(n)\psi(n), \qquad \forall n \in \mathbb{Z}^d \tag{2.3}$$

More specifically we aim to identify the structure of the spectrum based upon the periodic delta potential, α, and to give asymptotic approximations for the ends of each spectral band, λ_m, based upon the relationship between $|\lambda_m|$ and $\frac{|\alpha|}{2d}$.

This topic was previously analyzed in S.M. O.S. [] and thus will make up the basis for much of this section. The following lemma is a rephrasing of lemma 2.1 found in the previously mentioned paper which reduces the questions of our interest to the study of a discrete Schrödinger operator on the real axis. As stated in S.M. O.S. [] this reduction was known of at least since the publication of the paper of Von Below [8] and can also be find it in Cattaneo [9], Exner [10], and Pankrashkin [11].

Lemma 2.4. Let $\lambda \in \mathbb{R}$ satisfy the condition $\lambda \neq n^2\pi^2$ $\forall n \in \mathbb{Z}$. Let ψ satisfy equations $(2.1), (2.2),$ and (2.3), then,

$$\sum_{n':d(n,n')=1} \Psi_{n'} - A(d,k)\Psi_n = 0$$

where $A(d,k) = 2d\,C(k) + \frac{V(n)}{k}S(k)$, $C(k) = \begin{cases} \cos(k) & \lambda > 0 \\ \cosh(k) & \lambda < 0 \end{cases}$, $S(k) = \begin{cases} \sin(k) & \lambda > 0 \\ \sinh(k) & \lambda < 0 \end{cases}$, and $k = \sqrt{|\lambda|}$.

Proof:

Let ψ satisfy equations (2.1) and (2.2) then $\forall (n, n') \in \Gamma^d$ where $d(n, n') = 1$, we get the following result based upon our value of λ,

$$\psi_\lambda(x) = \frac{\Psi_n S(k\|n' - x\|) - \Psi_{n'} S(k\|n - x\|)}{S(k)}(n' - n)$$

where $S(k) = \begin{cases} \sin(k) & \lambda > 0 \\ \sinh(k) & \lambda < 0 \end{cases}$. Plugging the solution to the two-point problem into (2.3) gives,

$$\sum_{n':d(n,n')=1} \Psi_{n'} - A(d,k)\Psi_n = 0$$

where $A(d,k) = 2d\,C(k) + \frac{V(n)}{k}S(k)$, $C(k) = \begin{cases} \cos(k) & \lambda > 0 \\ \cosh(k) & \lambda < 0 \end{cases}$, and $k = \sqrt{|\lambda|}$.■

We can take the solution above and apply the Fourier transform resulting in the following inequality,

$$|A(d,k)| \leq 2d \tag{2.5}$$

Solutions to this inequality exist on a collection of disjoint intervals giving us an infinitely repeating band gap structure in the spectrum of our operator.

Corollary 2.6. The real spectrum of the Schrödinger type operator, H, $\sigma_\lambda(H) \cap \mathbb{R}$, has the following structure based upon the value of α,

$$\sigma_\lambda(H) \cap \mathbb{R} = \begin{cases} \bigcup_{m\geq 0} \left[\lambda_m, ((m+1)\pi)^2\right] & \alpha > 0 \\ [\lambda_0, \lambda_1] \cup \bigcup_{m\geq 2} \left[((m-1)\pi)^2, \lambda_m\right] & \alpha < 0 \end{cases}$$

where

$$\lambda_m = \begin{cases} -k_m^2 & m = 0 \; if \; \alpha < 0 \; and \; m = 1 \; if \; \alpha < -4d \\ k_m^2 & otherwise \end{cases}$$

for $k_m \geq 0$ the following equation is satisfied,

$$K(k_m) = \frac{C(k_m)}{S(k_m)} + \frac{\alpha}{4dk_m} - \mathrm{sgn}(\lambda)\frac{dk_m}{\alpha} = 0 \tag{2.7}$$

Proof:

By equation (2.5) we can derive an expression for the ends of the spectral bands,

$$C(k) + \frac{\alpha\, S(k)}{2dk} = \pm 1$$

Rearranging this gives,

$$C(k) + \frac{\alpha\, S(k)}{2dk} \pm 1 = 0$$

We can combine these two equations into a singular equation in the following way,

$$\left(C(k) + \frac{\alpha\, S(k)}{2dk} + 1\right)\left(C(k) + \frac{\alpha\, S(k)}{2dk} - 1\right) = 0$$

Multiplying out and reducing gives the following,

$$S(k)(4\alpha dk\, C(k) + (\alpha^2 - 4d^2\lambda)\, S(k)) = 0$$

This gives 2 equations for the edges of the spectral bands,

$$\begin{cases} S(k) = 0 \\ \dfrac{C(k)}{S(k)} - \operatorname{sgn}(\lambda)\dfrac{dk}{\alpha} + \dfrac{\alpha}{4dk} = 0 \end{cases}$$

Solving for case 1, $S(k) = 0$, only gives solutions for $\lambda > 0$, and those are,

$$k = n\pi \text{ for } n \in \mathbb{N}$$

The case of $k = 0$ is not valid due to the equation used to derive the identity. Let k_m denote a solution to case 2,

$$K(k) = \frac{C(k)}{S(k)} + \frac{\alpha}{4dk} - \operatorname{sgn}(\lambda)\frac{dk}{\alpha}$$

which shall be referred to as equation (2.7) for the remainder of the paper.

Now let's focus on the structure of the roots of (2.7), k_m. For $\lambda > 0, (2.7)$ is both continuous on each interval $(n\pi, (n+1)\pi)\ \forall n \in \mathbb{N}_0$ and has the following behavior,

$$K(k) \to \begin{cases} n = 0 & \operatorname{sgn}(\alpha + 4d)\infty \\ n > 0 & \infty \end{cases} \text{ as } k \to n\pi^+ \text{ and } K(k) \to -\infty \text{ as } k \to (n+1)\pi^-$$

Due to these limits and the continuity of $K(k)$, to prove that (2.7) has an unique solution on each such interval, $(n\pi, (n+1)\pi)\ \forall n \in \mathbb{N}_0$, it is sufficient to show that relative extrema are nonzero or nonexistent, and the function is monotonically decreasing for positive and/or negative outputs. Both of these can be shown in the following inequality,

$$K'(k) - \mathrm{sgn}(\alpha + 4d)\frac{1}{k}K(k) = \begin{Bmatrix} \alpha > -4d & -\csc^2(k) - \frac{\cot(k)}{k} - \frac{\alpha}{2dk^2} < -\frac{\alpha + 4d}{2dk^2} \\ \alpha = -4d & -\csc^2(k) + \frac{1}{k^2} - \frac{1}{4} < -\frac{7}{12} \\ \alpha < -4d & -\csc^2(k) + \frac{\cot(k)}{k} - \frac{2d}{\alpha} < -\frac{1}{6} \end{Bmatrix} < 0$$

Meaning,

$$K'(k) < \mathrm{sgn}(\alpha + 4d)\frac{1}{k}K(k)$$

Thus, relative extrema are nonzero for $\alpha \neq -4d$ and nonexistent for $\alpha = -4d$ and if $\mathrm{sgn}\big(K(k)\big) = -\mathrm{sgn}(\alpha + 4d)$ then $K(k)$ is monotonically decreasing. Thus, to guarantee a unique solution it just remains to prove that there exists a subinterval of $(n\pi, (n+1)\pi)$ such that, $\mathrm{sgn}\big(K(k)\big) = -\mathrm{sgn}(\alpha + 4d)$.

From the limit above, for all cases besides $\alpha \leq -4d$ and $n = 0$, we are guaranteed an interval such that $\mathrm{sgn}\big(K(k)\big) = -\mathrm{sgn}(\alpha + 4d)$, due to $K(k)$ ranging from $-\infty$ to ∞.

For $\alpha \leq -4d$ and $n = 0$, by the Mittag-Leffler's theorem we get the following inequality,

$$K(k) \leq \cot(k) + \frac{k}{4} - \frac{1}{k} = \left(\frac{1}{4} - \sum_{n=1}^{\infty} \frac{2}{n^2\pi^2 - k^2}\right)k \leq \left(\frac{1}{4} - \frac{2}{\pi^2}\zeta(2)\right)k = -\frac{1}{12}k < 0$$

Thus, for $\alpha < -4d$, no solutions to (2.7) exist on $(0, \pi)$.

Thus, for $\lambda > 0$,

$$\begin{Bmatrix} \alpha \leq -4d & \forall n \in \mathbb{N}, & \exists \text{a unique } k_n \in (n\pi, (n+1)\pi) \\ \alpha > -4d & \forall n \in \mathbb{N}_0, & \exists \text{a unique } k_n \in (n\pi, (n+1)\pi) \end{Bmatrix}$$

Now let's focus on $\lambda < 0$. For $\lambda < 0$, (2.7) is both continuous on the interval $(0, \infty)$ and has the following behavior,

$$\mathrm{K(k)} \to \mathrm{sgn}(\alpha + 4\mathrm{d})\infty \text{ as } \mathrm{k} \to 0^+ \text{ and } \mathrm{K(k)} \to \mathrm{sgn}(\alpha)\infty \text{ as } \mathrm{k} \to \infty$$

This gives us 3 subcases to work with, $\alpha > 0, -4\mathrm{d} \le \alpha < 0,$ and $\alpha \le -4\mathrm{d}$. In the subcase of $\alpha > 0$ we have no solutions to (2.7) as the following is true for all $\mathrm{k} > 0$,

$$\mathrm{K(k)} > 1 + \frac{\mathrm{dk}}{\alpha} + \frac{\alpha}{4\mathrm{dk}} > 1$$

In the subcase of $-4\mathrm{d} \le \alpha < 0$, we have exactly 1 solution as all relative extrema are nonzero by the following inequality,

$$\mathrm{K'(k)} - \frac{1}{\mathrm{k}}\mathrm{K(k)} = -\mathrm{csch}^2(\mathrm{k}) - \frac{\coth(\mathrm{k})}{\mathrm{k}} - \frac{\alpha}{2\mathrm{dk}^2} \le 0$$

Meaning,

$$\mathrm{K'(k)} \le \frac{1}{\mathrm{k}}\mathrm{K(k)}$$

Thus, relative extrema are nonzero and if $\mathrm{K(k)} < 0$ then $\mathrm{K(k)}$ is monotonically decreasing. Thus, solutions of (2.7) are unique for $\lambda < 0$ and $-4\mathrm{d} \le \alpha < 0$.

In the subcase of $\alpha \le -4\mathrm{d}$, we have exactly 2 solutions as, $-\mathrm{csch}^2(\mathrm{k}) + \frac{\mathrm{d}}{\mathrm{a}} - \frac{\alpha}{4\mathrm{dk}^2}$ is monotonically decreasing from ∞ to $-\infty$,

$$2\coth(\mathrm{k})\,\mathrm{csch}^2(\mathrm{k}) + \frac{\alpha}{2\mathrm{dk}^3} \le 0$$

there exists $\mathrm{k} > 0$, such that $\coth(\mathrm{k}) + \frac{\mathrm{dk}}{\alpha} + \frac{\alpha}{4\mathrm{dk}} > 0$,

$$\mathrm{K(k)} > 1 + \frac{\alpha}{4\mathrm{dk}} + \frac{\mathrm{dk}}{\alpha} = 0 \text{ at } \mathrm{k} = -\frac{\alpha}{2\mathrm{d}}$$

and

$$\coth(k) + \frac{dk}{\alpha} + \frac{\alpha}{4dk} \to -\infty \text{ as } k \to 0^+ \text{ and } \coth(k) + \frac{dk}{\alpha} + \frac{\alpha}{4dk} \to -\infty \text{ as } k \to \infty$$

Thus, for $\lambda < 0$,

$$\begin{cases} \alpha > 0 & \text{No solutions exist} \\ -4d < \alpha < 0 & \exists k_0 > 0 \text{ such that } \coth(k_0) + \frac{dk_0}{\alpha} + \frac{\alpha}{4dk_0} = 0 \\ \alpha \le -4d & \exists k_0, k_1 > 0 \text{ such that } \coth(k_0) + \frac{dk_0}{\alpha} + \frac{\alpha}{4dk_0} = \coth(k_1) + \frac{dk_1}{\alpha} + \frac{\alpha}{4dk_1} = 0 \end{cases}$$

Thus, the real part of the spectrum is as follows,

$$\sigma_\lambda(H) \cap \mathbb{R} = \begin{cases} \bigcup_{m\ge 0} \left[k_m^2, \left((m+1)\pi\right)^2\right] & \alpha > 0 \\ [-k_0^2, k_1^2] \cup \bigcup_{m\ge 2} \left[\left((m-1)\pi\right)^2, k_m^2\right] & -4d \le \alpha < 0 \\ [-k_0^2, -k_1^2] \cup \bigcup_{m\ge 2} \left[\left((m-1)\pi\right)^2, k_m^2\right] & \alpha \le -4d \end{cases}$$

Therefore, the real spectrum of the Schrödinger type operator, H, $\sigma_\lambda(H) \cap \mathbb{R}$, has the following structure based upon the value of α,

$$\sigma_\lambda(H) \cap \mathbb{R} = \begin{cases} \bigcup_{m\ge 0} \left[\lambda_m, \left((m+1)\pi\right)^2\right] & \alpha > 0 \\ [\lambda_0, \lambda_1] \cup \bigcup_{m\ge 2} \left[\left((m-1)\pi\right)^2, \lambda_m\right] & \alpha < 0 \end{cases}$$

where

$$\lambda_m = \begin{cases} -k_m^2 & m = 0 \text{ if } \alpha < 0 \text{ and } m = 1 \text{ if } \alpha < -4d \\ k_m^2 & \text{otherwise} \end{cases}$$

■

With equation (2.7), we can begin roughly analyzing the values of k_m. Resulting in the following relations based upon the analysis of the sign of both sides of the equation above.

Corollary 2.8. k_m, solutions to equation (2.7), satisfy the following identities.

For $\lambda > 0$,

$$k_m \in \begin{cases} \dfrac{|\alpha|}{2dk_m} \geq 1 & \left[m\pi + \mathrm{sgn}(\alpha)\dfrac{\pi}{2}, \left(m + \mathrm{sgn}(\alpha)\right)\pi\right) \\ \dfrac{|\alpha|}{2dk_m} \leq 1 & \left(m\pi, m\pi + \mathrm{sgn}(\alpha)\dfrac{\pi}{2}\right] \end{cases}$$

For $\lambda < 0$,

$$k_m \in \begin{cases} -4d < \alpha \leq 0 & \left[-\dfrac{\alpha}{2d}, \infty\right) \\ \alpha \leq -4d & \left[0, -\dfrac{\alpha}{2d}\right) \cup \left(-\dfrac{\alpha}{2d}, \infty\right) \end{cases}$$

Proof:

Case 1: $\lambda > 0$

(2.7) can be rearranged into the following form

$$\cot(k_m) = \frac{1}{2}\left(\frac{2dk_m}{\alpha} - \frac{\alpha}{2dk_m}\right)$$

This gives the following 5 inequalities,

$$\cot(k_m) = \begin{cases} \dfrac{|\alpha|}{2dk_m} > 1 & \begin{cases} \dfrac{1}{2}\left(\dfrac{2dk_m}{\alpha} - \dfrac{\alpha}{2dk_m}\right) < 0 & \alpha > 0 \\ \dfrac{1}{2}\left(\dfrac{2dk_m}{\alpha} - \dfrac{\alpha}{2dk_m}\right) > 0 & \alpha < 0 \end{cases} \\ \dfrac{|\alpha|}{2dk_m} = 1 & \dfrac{1}{2}\left(\dfrac{2dk_m}{\alpha} - \dfrac{\alpha}{2dk_m}\right) = 0 \\ \dfrac{|\alpha|}{2dk_m} < 1 & \begin{cases} \dfrac{1}{2}\left(\dfrac{2dk_m}{\alpha} - \dfrac{\alpha}{2dk_m}\right) > 0 & \alpha > 0 \\ \dfrac{1}{2}\left(\dfrac{2dk_m}{\alpha} - \dfrac{\alpha}{2dk_m}\right) < 0 & \alpha < 0 \end{cases} \end{cases}$$

The prior inequalities are satisfied if k_m has the following behavior,

$$k_m \in \begin{cases} \dfrac{|\alpha|}{2dk_m} \geq 1 & \left[m\pi + \operatorname{sgn}(\alpha)\dfrac{\pi}{2}, (m + \operatorname{sgn}(\alpha))\pi\right) \\ \dfrac{|\alpha|}{2dk_m} \leq 1 & \left(m\pi, m\pi + \operatorname{sgn}(\alpha)\dfrac{\pi}{2}\right] \end{cases}$$

Note: The intervals may not be in increasing order.

Case 2: $\lambda < 0$

(2.7) satisfies the following inequality,

$$K(k) > 1 + \frac{\alpha}{4dk} + \frac{dk}{\alpha}$$

This lower bound has a single root of $k = -\frac{\alpha}{2d}$. Thus, by Corollary 2.6., we get the following,

$$k_m \in \begin{cases} -4d < \alpha \leq 0 & \left[-\dfrac{\alpha}{2d}, \infty\right) \\ \alpha \leq -4d & \left[0, -\dfrac{\alpha}{2d}\right) \cup \left(-\dfrac{\alpha}{2d}, \infty\right) \end{cases}$$

■

For $\lambda > 0$, this gives us rough regions of length $\frac{\pi}{2}$ in which we can expect a solution to equation (2.7), k_m, but for more in-depth analysis we require more precise estimates of k_m. For arbitrary accuracy we can use methods such as newton's method but below we analyzed the asymptotics of the solutions using perturbation theory, the Taylor series, and corollary 2.8.

Theorem 2.9. For $\lambda > 0$, solutions to equation (2.7), k_m, have the following asymptotic structure,

$$0 \leq \frac{|\alpha|}{2dk_m} \ll 1 \qquad k_m \approx \frac{m\pi}{2} + \sqrt{\frac{m^2\pi^2}{4} + \frac{\alpha}{d}}$$

$$\frac{|\alpha|}{2dk_m} \approx 1 \qquad k_m \approx \frac{\alpha}{2(a+d)}\left(\left(m + \frac{\mathrm{sgn}(\alpha)}{2}\right)\pi + \sqrt{1 + \frac{\alpha}{d} + \left(m + \frac{\mathrm{sgn}(\alpha)}{2}\right)^2 \pi^2}\right)$$

$$\frac{|\alpha|}{2dk_m} \gg 1 \qquad k_m \approx \frac{\alpha\big(m + \mathrm{sgn}(\alpha)\big)\pi}{\alpha + 4d}$$

Proof:

Case 1: $0 \leq \frac{|\alpha|}{2dk_m} \ll 1$

Equation (2.7) can be reduced to,

$$\tan(k_m) = \frac{\alpha}{dk_m}$$

By corollary 2.8,

$$k_m \in \left(m\pi, m\pi + \mathrm{sgn}(\alpha)\frac{\pi}{2}\right]$$

Thus, $k_m \approx m\pi$, replacing k_m with $m\pi + \delta$ into the above gives the following reduced identity,

$$\tan(\delta) = \frac{\alpha}{d(m\pi + \delta)}$$

Since $0 < |\delta| \ll 1$ we can further reduce this to,

$$\delta \approx \frac{\alpha}{d(m\pi + \delta)}$$

Solving for δ and satisfying corollary 2.8 gives,

$$\delta = -\frac{m\pi}{2} + \sqrt{\frac{m^2\pi^2}{4} + \frac{\alpha}{d}}$$

Thus for $0 \leq \frac{|\alpha|}{2dk_m} \ll 1$,

$$k_m \approx \frac{m\pi}{2} + \sqrt{\frac{m^2\pi^2}{4} + \frac{\alpha}{d}}$$

Case $1.b$: $\frac{|\alpha|}{2dk_m} \gg 1$

Equation (2.7) can be reduced to,

$$\tan(k_m) = -\frac{4dk_m}{\alpha}$$

By corollary 2.8,

$$k_m \in \left[m\pi + \mathrm{sgn}(\alpha)\frac{\pi}{2}, (m + \mathrm{sgn}(\alpha))\pi\right)$$

Thus, $k_m \approx \big(m + \mathrm{sgn}(\alpha)\big)\pi$, replacing k_m with $\big(m + \mathrm{sgn}(\alpha)\big)\pi + \delta$ gives the following reduced identity,

$$\tan(\delta) = -\frac{4d\Big(\big(m + \mathrm{sgn}(\alpha)\big)\pi + \delta\Big)}{\alpha}$$

Since $0 < |\delta| \ll 1$ we can further reduce this to,

$$\delta \approx -\frac{4d\big((m + \text{sgn}(\alpha))\pi + \delta\big)}{\alpha}$$

Solving of δ gives,

$$\delta = -\frac{4d\big(m + \text{sgn}(\alpha)\big)\pi}{\alpha + 4d}$$

Thus for $\frac{|\alpha|}{2dk_m} \gg 1$,

$$k_m \approx \frac{\alpha\big(m + \text{sgn}(\alpha)\big)\pi}{\alpha + 4d}$$

(if $|\alpha| < 8dm + 4d\text{sgn}(\alpha)$ then $k_m = m\pi + \text{sgn}(\alpha)\frac{\pi}{2}$ is a better approximation)

Case 1.c: $\frac{|\alpha|}{2dk_m} \approx 1$

Equation (2.7) can be reduced to,

$$\cot(k_m) = \frac{4d^2k_m^2 - \alpha^2}{4\alpha dk_m}$$

By corollary 2.8, if $\frac{|\alpha|}{2dk_m} = 1$ then,

$$k_m = m\pi + \text{sgn}(\alpha)\frac{\pi}{2}$$

Thus, $k_m \approx m\pi + \text{sgn}(\alpha)\frac{\pi}{2}$, replacing k_m with $m\pi + \text{sgn}(\alpha)\frac{\pi}{2} + \delta$ gives the reduced identity,

$$\tan(\delta) = \frac{\alpha^2 - 4d^2\left(m\pi + \text{sgn}(\alpha)\frac{\pi}{2} + \delta\right)^2}{4\alpha d\left(m\pi + \text{sgn}(\alpha)\frac{\pi}{2} + \delta\right)}$$

Since $0 < |\delta| \ll 1$ we can further reduce this to,

$$\delta \approx \frac{\alpha^2 - 4d^2\left(m\pi + \mathrm{sgn}(\alpha)\frac{\pi}{2} + \delta\right)^2}{4\alpha d\left(m\pi + \mathrm{sgn}(\alpha)\frac{\pi}{2} + \delta\right)}$$

Solving for δ and satisfying corollary 2.8 gives,

$$\delta = \frac{-(\alpha + 2d)\left(m + \frac{\mathrm{sgn}(\alpha)}{2}\right)\pi + \alpha\sqrt{1 + \frac{\alpha}{d} + \left(m + \frac{\mathrm{sgn}(\alpha)}{2}\right)^2 \pi^2}}{2(a + d)}$$

Thus for $\frac{|\alpha|}{2dk_m} \approx 1$,

$$k_m \approx \frac{\alpha}{2(a + d)}\left(\left(m + \frac{\mathrm{sgn}(\alpha)}{2}\right)\pi + \sqrt{1 + \frac{\alpha}{d} + \left(m + \frac{\mathrm{sgn}(\alpha)}{2}\right)^2 \pi^2}\right)$$

Therefore, For $\lambda > 0$, solutions to equation (2.7), k_m, have the following asymptotic structure,

$$0 \le \frac{|\alpha|}{2dk_m} \ll 1 \qquad k_m \approx \frac{m\pi}{2} + \sqrt{\frac{m^2\pi^2}{4} + \frac{\alpha}{d}}$$

$$\frac{|\alpha|}{2dk_m} \approx 1 \qquad k_m \approx \frac{\alpha}{2(a + d)}\left(\left(m + \frac{\mathrm{sgn}(\alpha)}{2}\right)\pi + \sqrt{1 + \frac{\alpha}{d} + \left(m + \frac{\mathrm{sgn}(\alpha)}{2}\right)^2 \pi^2}\right)$$

$$\frac{|\alpha|}{2dk_m} \gg 1 \qquad k_m \approx \frac{\alpha\big(m + \mathrm{sgn}(\alpha)\big)\pi}{\alpha + 4d}$$

■

3. # of Discrete Eigenvalues for $H = -\Delta + V$, $V(n) = \alpha + \beta\delta_{x_i}(n)$ for $x_i \in \mathbb{Z}^d \mid i = 1, \dots, N$

Expanding upon our discussion in section 2, we will now consider finitely many perturbations to the potential. We will begin this analysis with the case a single rank 1 perturbation to the potential at the origin, $V(n) = \begin{cases} \alpha & n \neq 0 \\ \alpha + \beta & n = 0 \end{cases}$. From lemma 2.4, we get the following equation for this choice of potential,

$$\sum_{n':|n-n'|=1} \Psi_{n'} - A(d,k)\Psi_n = \frac{\beta\delta_0\, S(k)}{k}\Psi_n \tag{3.1}$$

where $A(d,k) = 2d\,C(k) + \frac{\alpha}{k}S(k)$, $C(k) = \begin{cases} \cos(k) & \lambda > 0 \\ \cosh(k) & \lambda < 0 \end{cases}$, and $S(k) = \begin{cases} \sin(k) & \lambda > 0 \\ \sinh(k) & \lambda < 0 \end{cases}$. We can take the solution above and apply the Fourier transform resulting in the following inequality,

$$\left(\sum_{n':|n-n'|=1} 2\cos(j_n) - A(d,k)\right)\widehat{\Psi} = \frac{\beta\, S(k)}{k}\Psi_0 \tag{3.2}$$

We can solve (3.2) in the following manner via solving for $\widehat{\Psi}$ and taking the inverse Fourier transform,

$$\psi(n) = \frac{\beta\, S(k)}{(2\pi)^d k}\int_{\tau^d} \frac{\Psi_0 e^{i\langle j,n\rangle}}{\sum_{1\le n\le d} 2\cos(j_n) - A(d,k)}\,dJ = \beta\Psi_0 G_\lambda(0,n) \tag{3.3}$$

where $\tau^d = [-\pi,\pi]^d$ and $dJ = \prod_{1\le n\le d} dj_n$. As shown in (3.3) we'll define Green's function in the following way,

$$G_\lambda(m,n) = \frac{S(k)}{(2\pi)^d k}\int_{\tau^d} \frac{e^{-i\langle J,m-n\rangle}}{\sum_{1\le n\le d} 2\cos(j_n) - A(d,k)}\,dJ \tag{3.4}$$

Plugging in 0 for n in (3.3), solving for β^{-1}, and simplifying using a u-substitution gives,

$$\frac{1}{\beta}=\frac{\operatorname{sgn}\big(A(d,k)\big)\,S(k)}{(2\pi)^{d}k}\int_{\tau^{d}}\left(\sum_{1\le n\le d}2\cos(j_n)-|A(d,k)|\right)^{-1}dJ=G_{\lambda}(0,0)\tag{3.5}$$

This gives us a restriction on the values of the perturbation, β, which will result in eigenvalues. Before we can properly count the number of eigenvalues we must first prove some seemingly unrelated identities.

Lemma 3.6. For $d,m\in\mathbb{N}$ and $M=\{M_1,\dots,M_d\}\in\mathbb{Z}^d$,

$$C_{d,m}(M)=\frac{2^m}{(2\pi)^d}\int_{\tau^d}e^{i(J,M)}\left(\sum_{1\le n\le d}\cos(j_n)\right)^m dj$$

has the following simplification,

$$C_{d,m}(M)=\begin{cases}0 & \exists n\ \dfrac{m_n-|M_n|}{2}\notin\mathbb{N}_0\\ \displaystyle\sum_{\sum_{n=1}^{d}m_n=m}\ \prod_{1\le n\le d}\frac{m!}{\left(\frac{m_n-|M_n|}{2}\right)!\left(\frac{m_n+|M_n|}{2}\right)!} & \text{otherwise}\end{cases}$$

Proof:

By symmetry,

$$C_{d,m}(M)=\frac{2^m}{(2\pi)^d}\int_{\tau^d}\prod_{1\le n\le d}\cos(M_nj_n)\left(\sum_{1\le n\le d}\cos(j_n)\right)^m dj$$

By the multinomial theorem,

$$C_{d,m}(M)=\frac{2^m m!}{(2\pi)^d}\sum_{\sum_{n=1}^{d}m_n=m}\ \prod_{1\le n\le d}\frac{1}{m_n!}\int_{-\pi}^{\pi}\cos(M_nj_n)\cos^{m_n}(j_n)\,dj_n$$

By orthogonality, this integral can be simplified in the following way,

$$\frac{1}{m_n!}\int_{-\pi}^{\pi}\cos(M_n j_n)\cos^{m_n}(j_n)\,dj_n = \begin{cases} 0 & \frac{m_n - |M_n|}{2} \notin \mathbb{N}_0 \\ \frac{2\pi}{2^{m_n}\left(\frac{m_n - |M_n|}{2}\right)!\left(\frac{m_n + |M_n|}{2}\right)!} & \text{otherwise} \end{cases}$$

Thus, the above equality can be restated as the following,

$$C_{d,m}(M) = \begin{cases} 0 & \exists n\ \frac{m_n - |M_n|}{2} \notin \mathbb{N}_0 \\ \sum_{\sum_{n=1}^{d} m_n = m}\ \prod_{1\le n\le d} \frac{m!}{\left(\frac{m_n - |M_n|}{2}\right)!\left(\frac{m_n + |M_n|}{2}\right)!} & \text{otherwise} \end{cases}$$

■

Lemma 3.7. For $\lambda \in \overline{\rho_\lambda \cap \mathbb{R}}\backslash\{0\}$, $|G_\lambda(0,0)| < \infty$ if $\begin{cases} \lambda = n^2\pi^2 \text{ for } n \in \mathbb{N} \\ |A(d,k)| > 2d & d \le 2 \\ |A(d,k)| \ge 2d & d > 2 \end{cases}$

Proof:

Case 1: $\lambda = n^2\pi^2$ for $n \in \mathbb{N}$

$$|G_\lambda(0,0)| = -\frac{\operatorname{sgn}(A(d,k))\,S(k)}{(2\pi)^d k}\int_{\tau^d}\left(|A(d,k)| - \sum_{1\le n\le d} 2\cos(j_n)\right)^{-1} dJ = 0$$

Thus, $|G_\lambda(0,0)| < \infty$ for $\lambda = n^2\pi^2$ for $n \in \mathbb{N}$.

Case 2: $\lambda \neq n^2\pi^2$ for $n \in \mathbb{N}$

As $k \neq n\pi$, $0 < \frac{|S(k)|}{(2\pi)^d k} < \infty$ and thus, will have no bearing on if $|G_\lambda(0,0)| < \infty$ allowing us to drop this factor for the following analysis. Let $|A(d,k)| \ge 2d$ and $\delta \in (0,\pi]$, then $|G_\lambda(0,0)|$ can be broken into 2 areas of integration, the ball of radius $\delta, B_\delta(0)$, and the relative compliment, $\tau^d\backslash B_\delta(0)$, giving the following,

$$\int_{\tau^d}\left(|A(d,k)| - \sum_{1\le n\le d} 2\cos(j_n)\right)^{-1} dJ = \int_{B_\delta(0)} \ldots dJ + \int_{\tau^d\setminus B_\delta(0)} \ldots dJ = I_1 + I_2$$

As $\left(|A(d,k)| - \sum_{1\le n\le d} 2\cos(j_n)\right)^{-1}$ is bounded on $\tau^d\setminus B_\delta(0)\ \forall\delta \in (0,\pi]$, I_2 is always finite, leaving the question of convergence up to the convergence of I_1. By the Taylor series of $\cos(j_n)$, we can rewrite I_1 as follows,

$$I_1 = \int_{B_\delta(0)}\left(|A(d,k)| - 2d + \sum_{1\le n\le d} j_n^2 - 2\sum_{1\le n\le d}\sum_{l=2}^{\infty}\frac{(-1)^l}{(2l)!} j_n^{2l}\right)^{-1} dj$$

This allows us to derive the following lower bound for our integral, I_1^*,

$$I_1 \ge \int_{B_\delta(0)}\left(|A(d,k)| - 2d + \sum_{1\le n\le d} j_n^2\right)^{-1} dJ = I_1^*$$

Note that I_1^* satisfies the following relationship $\forall|A(d,k)| \ge 2d\ \&\ \forall\delta \in (0,\pi]$,

$$I_1 - I_1^* \le \int_{B_\delta(0)}\left(2d - 2\sum_{1\le n\le d}\cos(j_n)\right)^{-1} - \left(\sum_{1\le n\le d} j_n^2\right)^{-1} dJ < \frac{\pi^{\frac{d}{2}}}{\left(\frac{d}{2}\right)!}\left(\frac{1}{4\sin^2\left(\frac{\delta}{2}\right)} - \frac{1}{\delta^2}\right)\delta^d < \infty$$

Thus, I_1 converges if and only if I_1^* converges. We can convert I_1^* into the following d-dimensional spherical integral,

$$I_1^* = \frac{d\pi^{\frac{d}{2}}}{\left(\frac{d}{2}\right)!}\int_0^\delta \frac{r^{d-1}}{r^2 + |A(d,k)| - 2d} dr = \frac{d\pi^{\frac{d}{2}}}{\left(\frac{d}{2}\right)!}\int_0^\delta \frac{r^{d-1}}{r^2 + c} dr$$

Using partial fractions we get the following identity,

$$\int_0^{\delta} \frac{r^{d-1}}{r^2+c}\,dr = \int_0^{\delta} \frac{(-c)^{\left\lfloor \frac{d-1}{2} \right\rfloor} r^{d-1-2\left\lfloor \frac{d-1}{2} \right\rfloor}}{r^2+c} + \sum_{i=1}^{\left\lfloor \frac{d-1}{2} \right\rfloor} r^{d-1-2i}(-c)^{i-1}\,dr$$

Plugging in this identity into the equation for I_1^* and solving gives the following result,

$$I_1^* = \frac{d\pi^{\frac{d}{2}}}{\left(\frac{d}{2}\right)!}\left(I(d,k) + \sum_{i=1}^{\left\lfloor \frac{d-1}{2} \right\rfloor} \frac{\delta^{d-2i}(2d-|A(d,k)|)^{i-1}}{d-2i} \right)$$

where $I(d,k) = \begin{cases} \frac{(2d-|A(d,k)|)^{\frac{d}{2}-1}}{2} \ln\left(1+\frac{\delta^2}{|A(d,k)|-2d}\right) & d=2n \\ \frac{(2d-|A(d,k)|)^{\frac{d-1}{2}}}{\sqrt{|A(d,k)|-2d}} \arctan\left(\frac{\delta}{\sqrt{|A(d,k)|-2d}}\right) & d=2n+1 \end{cases}$.

Thus, we have two distinct behaviors based upon the value of $|A(d,k)|$.

When $|A(d,k)| > 2d$, we get the following relationship for all d,

$$I_1^* = \frac{d\pi^{\frac{d}{2}}}{\left(\frac{d}{2}\right)!}\left(I(d,k) + \sum_{i=1}^{\left\lfloor \frac{d-1}{2} \right\rfloor} \frac{\delta^{d-2i}(2d-|A(d,k)|)^{i-1}}{d-2i} \right) < \infty$$

When $|A(d,k)| = 2d$, we get the following relationships for $d > 2$ and $d \leq 2$,

$$I_1^* = \frac{d\pi^{\frac{d}{2}}}{\left(\frac{d}{2}\right)!}\int_0^{\delta} r^{d-3}\,dr = \begin{cases} \frac{d\pi^{\frac{d}{2}}}{(d-2)\left(\frac{d}{2}\right)!}\delta^{d-2} < \infty & d>2 \\ \frac{d\pi^{\frac{d}{2}}}{\left(\frac{d}{2}\right)!}\left(\ln(\delta) - \lim_{t\to 0^+}\ln(t)\right) = \infty & d=2 \\ \frac{d\pi^{\frac{d}{2}}}{\left(\frac{d}{2}\right)!}\left(-\frac{1}{\delta} + \lim_{t\to 0^+}\frac{1}{t}\right) = \infty & d=1 \end{cases}$$

Thus,

$$I_1 < \infty \text{ if } \begin{cases} |A(d,k)| > 2d & d \le 2 \\ |A(d,k)| \ge 2d & d > 2 \end{cases}$$

Therefore, for $\lambda \in \overline{\rho_\lambda \cap \mathbb{R}} \backslash \{0\}$, $|G_\lambda(0,0)| < \infty$ if $\begin{cases} \lambda = n^2\pi^2 \text{ for } n \in \mathbb{N} \\ |A(d,k)| > 2d & d \le 2 \\ |A(d,k)| \ge 2d & d > 2 \end{cases}$. ■

Lemma 3.8. For $M = \{M_1, \dots, M_d\} \in \mathbb{Z}^d$,

$$G_\lambda(0,M) = \frac{S(k)}{(2\pi)^d k} \int_{\tau^d} \frac{e^{i(J,M)}}{\sum_{1\le n\le d} 2\cos(j_n) - A(d,k)} dJ$$

has the following analytic solution,

$$-\frac{S(k)}{A(d,k)k} \sum_{m=0}^{\infty} \frac{C_{d,m}(M)}{A(d,k)^m} = -\frac{S(k)}{A(d,k)k} \sum_{m=0}^{\infty} \frac{(2m + \|M\|)!}{A(d,k)^{2m+\|M\|}} \sum_{\sum_{n=1}^{d} m_n = m} \prod_{1\le n\le d} \frac{1}{m_n!\,(m_n + |M_n|)!}$$

Proof:

By Lemma 3.7,

$$|G_\lambda(0,M)| \le |G_\lambda(0,0)| < \infty \text{ if } \begin{cases} |A(d,k)| > 2d & d \le 2 \\ |A(d,k)| \ge 2d & d > 2 \end{cases}$$

Since $\frac{|\sum_{1\le n\le d} 2\cos(j_n)|}{|A(d,k)|} < 1 \ \forall J = \{j_1, j_2, \dots, j_d\}$ such that $J \ne 0$ and $J \notin \partial\tau^d$, we can rewrite $G_\lambda(0,M)$ in the following way,

$$G_\lambda(0,M) = -\frac{1}{(2\pi)^d k} \frac{S(k)}{A(d,k)} \int_{\tau^d} \sum_{m=0}^{\infty} e^{i(J,M)} \left(\frac{\sum_{1\le n\le d} 2\cos(j_n)}{A(d,k)} \right)^m dJ$$

As this integral is finite by Lemma 3.7, the Fubini–Tonelli theorem states that the integral and summation can be interchanged giving,

$$-\frac{S(k)}{A(d,k)k}\sum_{m=0}^{\infty}\frac{1}{A(d,k)^m}\frac{2^m}{(2\pi)^d}\int_{\tau^d} e^{i(J,M)}\left(\sum_{1\le n\le d}\cos(j_n)\right)^m dJ = -\frac{S(k)}{A(d,k)k}\sum_{m=0}^{\infty}\frac{C_{d,m}(M)}{A(d,k)^m}$$

where $C_{d,m}(M) = \frac{2^m}{(2\pi)^d}\int_{\tau^d} e^{i(J,M)}(\sum_{1\le n\le d}\cos(j_n))^m\, dJ$. By Lemma 3.7, the above equality can be restated as the following,

$$G_\lambda(0,M) = -\frac{S(k)}{A(d,k)k}\sum_{m=0}^{\infty}\frac{(2m+\|M\|)!}{A(d,k)^{2m+\|M\|}}\sum_{\sum_{n=1}^{d} m_n=m}\prod_{1\le n\le d}\frac{1}{m_n!\,(m_n+|M_n|)!}$$

Therefore, for $M = \{M_1, \dots, M_d\} \in \mathbb{Z}^d$,

$$G_\lambda(0,M) = \frac{S(k)}{(2\pi)^d k}\int_{\tau^d}\frac{e^{i(J,M)}}{\sum_{1\le n\le d} 2\cos(j_n) - A(d,k)}\, dJ$$

has the following analytic solution,

$$-\frac{S(k)}{A(d,k)k}\sum_{m=0}^{\infty}\frac{C_{d,m}(M)}{A(d,k)^m} = -\frac{S(k)}{A(d,k)k}\sum_{m=0}^{\infty}\frac{(2m+\|M\|)!}{A(d,k)^{2m+\|M\|}}\sum_{\sum_{n=1}^{d} m_n=m}\prod_{1\le n\le d}\frac{1}{m_n!\,(m_n+|M_n|)!}$$

■

Lemma 3.9. For $\lambda \in \rho_\lambda \cap \mathbb{R}$, $G_\lambda(0,0)$ is monotonically decreasing with respect to λ.

Proof:

For $\lambda \in \rho_\lambda \cap \mathbb{R}$, the integrand of $G_k(0,0)$ is absolutely continuous $\forall J = \{j_1, j_2, \dots, j_d\} \in \tau^d$. Thus, by the fundamental theorem of calculus and Leibniz integral rule, the derivative of $G_\lambda(0,0)$ with respect to λ can be reduced to the following,

$$\frac{d\big(G_\lambda(0,0)\big)}{d\lambda} = \int_{\tau^d}\frac{\mathrm{sgn}(\lambda)(\sum_{1\le n\le d}\cos(j_n))\big(k\,C(k) - S(k)\big) - d\,\mathrm{sgn}(\lambda)\big(k - S(k)C(k)\big)}{(2\pi)^d k^3\big(\sum_{1\le n\le d} 2\cos(j_n) - A(d,k)\big)^2}\, dJ$$

$\forall k \geq 0$ the following inequality holds,

$$|kC(k) - S(k)| \leq \mathrm{sgn}(\lambda)\big(k - S(k)C(k)\big)$$

Thus, $\forall k \geq 0$ & $\forall c \in [-d, d]$,

$$c\big(k\,C(k) - S(k)\big) - d\,\mathrm{sgn}(\lambda)\big(k - S(k)C(k)\big) \leq 0$$

Therefore, $G_\lambda(0,0)$ is monotonically decreasing with respect to λ.■

Theorem 3.10. For $\lambda \in \rho_\lambda \cap \mathbb{R}$ and $\alpha, \beta \in \mathbb{R}$, the number of discrete eigenvalues which solves (3.5), $N(\beta)$, is given by the following,

If $-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2 < \pi^2$, then,

$$N(\beta) \leq 1$$

If $-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2 \geq \pi^2$, then,

$$N(\beta) \approx \frac{1}{\pi}\sqrt{-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2}$$

where the error is less than 1,

$$\left|\frac{1}{\pi}\sqrt{-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2} - N(\beta)\right| < 1$$

Note: $\forall \beta \in \mathbb{R}$ such that $\mathrm{sgn}(\beta) = -\mathrm{sgn}(\alpha)$, $N(\beta) = \infty$ for $d \leq 2$ and $N(\beta) < \infty$ for $d > 2$.

Proof:

Using (2.7) we can derive the following expression assuming $S(k) \neq 0$ and $|A(d,k)| = 2d$,

$$-\frac{S(k)}{A(d,k)k} = -\frac{\alpha}{2d^2}\frac{1}{\lambda + \left(\frac{\alpha}{2d}\right)^2} \tag{3.11}$$

By Lemmas 3.7 through 3.9., the monotone convergence theorem, and (3.11), we have the following identity,

$$\lim_{\lambda \to \lambda_n} G_\lambda(0,0) = -\frac{\alpha}{d}\frac{1}{\lambda_n + \left(\frac{\alpha}{2d}\right)^2}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} \tag{3.12}$$

which is finite for $d > 2$ and is $-\mathrm{sgn}\left(\frac{\alpha}{\lambda_n + \left(\frac{\alpha}{2d}\right)^2}\right)\infty$ for $d \leq 2$.

By Corollary 2.6, Lemma 3.9., and (3.12), then for all intervals in $\rho_\lambda \cap \mathbb{R}$, $G_\lambda(0,0)$ can be bounded in the following way,

$$G_\lambda(0,0) \in \left(0, -\frac{\alpha}{d}\frac{1}{\lambda_n + \left(\frac{\alpha}{2d}\right)^2}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}}\right) \tag{3.13}$$

Note: The intervals may not be in increasing order.

For (3.5) to satisfy (3.13), the perturbation, β, must satisfy the following,

$$\mathrm{sgn}(\beta) = -\mathrm{sgn}\left(\frac{\alpha}{\lambda_n + \left(\frac{\alpha}{2d}\right)^2}\right) \tag{3.14}$$

Solving 3.13 for λ_n using (3.14), gives the following,

$$\lambda_n \in \left(-\left(\frac{\alpha}{2d}\right)^2, -\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2\right) \tag{3.15}$$

Note: The intervals may not be in increasing order.

If $-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}}-\left(\frac{\alpha}{2d}\right)^2<\pi^2$ then by corollary 2.6 and (3.15), $N(\beta)\leq 1$.

If $-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}}-\left(\frac{\alpha}{2d}\right)^2\geq\pi^2$ then by corollary 2.6 and (3.15), we find the following relationship to the number of discrete eigenvalues which solve (3.5),

$$\lambda_{N(\beta)-\frac{1+\mathrm{sgn}(\alpha)}{2}}<-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}}-\left(\frac{\alpha}{2d}\right)^2<\lambda_{N(\beta)+\frac{1-\mathrm{sgn}(\alpha)}{2}} \tag{3.16}$$

By corollary 2.6, we can extend (3.16) in the following way,

$$(N(\beta)-1)^2\pi^2<-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}}-\left(\frac{\alpha}{2d}\right)^2<(N(\beta)+1)^2\pi^2$$

We can rearrange this inequality into the following expression,

$$\left|\frac{1}{\pi}\sqrt{-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}}-\left(\frac{\alpha}{2d}\right)^2}-N(\beta)\right|<1 \tag{3.17}$$

Thus,

$$N(\beta)\approx\frac{1}{\pi}\sqrt{-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}}-\left(\frac{\alpha}{2d}\right)^2} \tag{3.18}$$

■

Repeating our calculations for the case of a single perturbation for some finite collection of perturbations separated by $||M_0||$,

$$V(n) = \begin{cases} \alpha & n \notin Z \\ \alpha + \beta & n \in Z \end{cases}$$

where,

$$Z = \left\{ x_i \in \mathbb{Z}^d \middle| i = 1, \dots, N,\ x_1 = 0, \text{and } \forall i < j \leq N,\ d\left(x_i, x_j\right) > \|M_0\| \right\}$$

gives the following by Lemma 2.4,

$$\sum_{n' : |n - n'| = 1} \Psi_{n'} - A(d,k)\Psi_n = \Psi_n \frac{\beta\, S(k)}{k} \sum_{x_i \in Z} \delta_{x_i} \tag{3.19}$$

Taking the Fourier transform of both sides and simplifying, gives the following,

$$\left(\sum_{n' : |n - n'| = 1} 2\cos(j_n) - A(d,k) \right) \widehat{\Psi} = \frac{\beta\, S(k)}{k} \sum_{x_i \in Z} \Psi_{x_i} e^{-i\langle J, x_i \rangle} \tag{3.20}$$

We can solve (3.20) in the following manner via solving for $\widehat{\Psi}$ and taking the inverse Fourier transform,

$$\psi(n) = \frac{\beta\, S(k)}{(2\pi)^d k} \int_{\tau^d} \frac{\sum_{x_i \in Z} \Psi_{x_i} e^{i\langle J, n - x_i \rangle}}{\sum_{1 \leq n \leq d} 2\cos(j_n) - A(d,k)} dJ = \beta \sum_{x_i \in Z} \Psi_{x_i} G_\lambda(n, x_i) \tag{3.21}$$

where $\tau^d = [-\pi, \pi]^d$ and $dJ = \prod_{1 \leq n \leq d} dj_n$. Putting everything to 1 side gives,

$$\psi(n) - \beta \sum_{x_i \in Z} \psi(x_i) G_\lambda(n, x_i) = 0 \tag{3.22}$$

Theorem 3.23. For $d \geq 3$, $\lambda \in \rho_\lambda \cap \mathbb{R}$ and $\alpha, \beta \in \mathbb{R}$, if $\|M_0\| \gg 1$, the number of discrete eigenvalues which solves (3.22), $N(\beta)$, is given by the following,

If $-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2 < \pi^2$, then,

$$N(\beta) \leq N$$

If $-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2 \geq \pi^2$, then,

$$N(\beta) \approx \frac{N}{\pi}\sqrt{-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2}$$

where the error is less than N,

$$\left|\frac{N}{\pi}\sqrt{-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2} - N(\beta)\right| < N$$

Proof:

Plugging in $n = x_i \ \forall x_i \in Z$ into (3.22) gives the following system of equations,

$$\begin{bmatrix} 1-\beta G_\lambda(x_1,x_1) & \cdots & -\beta G_\lambda(x_1,x_N) \\ \vdots & \ddots & \vdots \\ -\beta G_\lambda(x_N,x_1) & \cdots & 1-\beta G_\lambda(x_N,x_N) \end{bmatrix} \begin{bmatrix} \Psi_{x_1} \\ \vdots \\ \Psi_{x_N} \end{bmatrix} = A \begin{bmatrix} \Psi_{x_1} \\ \vdots \\ \Psi_{x_N} \end{bmatrix} = 0 \tag{3.24}$$

Since $\{\Psi_{x_i}\}_{i<N}$ are arbitrary, this equality is only zero if $\det(A) = 0$. Via symmetry $G_\lambda(x_i, x_j) = G_\lambda(x_j, x_i) \ \forall i, j \in \{1, \dots, N\}$, we can rewrite the matrix "A" in the following way,

$$A = \begin{bmatrix} 1-\beta G_\lambda(0,0) & \cdots & -\beta G_\lambda(x_1,x_N) \\ \vdots & \ddots & \vdots \\ -\beta G_\lambda(x_1,x_N) & \cdots & 1-\beta G_\lambda(0,0) \end{bmatrix} \tag{3.25}$$

Meaning the determinant can be simplified in the following way assuming $1-\beta G_k(0,0) \neq 0$,

$$\det(A) = \left(1-\beta G_k(0,0)\right)^N \det\left(\begin{bmatrix} 1 & \cdots & -\frac{\beta G_k(0, x_1 - x_N)}{1-\beta G_k(0,0)} \\ \vdots & \ddots & \vdots \\ -\frac{\beta G_k(0, x_1 - x_N)}{1-\beta G_k(0,0)} & \cdots & 1 \end{bmatrix}\right) = 0 \quad (3.26)$$

By Lemmas 3.7 and 3.8, for $M \in \mathbb{Z}^d$, as $\|M\| \to \infty, G_\lambda(0, M) \to 0$ thus $\forall \epsilon > 0\ \exists \|M_0\| \in \mathbb{N}$ such that $\forall M \in \mathbb{Z}^d$ such that $\|M\| \geq \|M_0\|$, $|G_\lambda(0, M)| < \epsilon \ll \left|\frac{1}{\beta} - G_\lambda(0,0)\right|$. Making (3.26) into,

$$\det(A) \approx \left(1-\beta G_\lambda(0,0)\right)^N \det\left(\begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix}\right) = \left(1-\beta G_\lambda(0,0)\right)^N = 0 \qquad (3.27)$$

Therefore, by theorem 3.10,

If $-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2 < \pi^2$, then,

$$N(\beta) \leq N$$

If $-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2 \geq \pi^2$, then,

$$N(\beta) \approx \frac{N}{\pi}\sqrt{-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2}$$

where the error is less than N,

$$\left|\frac{N}{\pi}\sqrt{-\frac{\alpha\beta}{d}\sum_{m=0}^{\infty}\frac{C_{d,m}(0)}{(2d)^{m+1}} - \left(\frac{\alpha}{2d}\right)^2} - N(\beta)\right| < N$$

■

Bibliography

[1] Need to find

[2] Need to find

[3] Berkolaiko, Gregory, and Peter Kuchment. Introduction to Quantum Graphs. American Mathematical Society, 2013.

[4] Need to find

[5] Need to find

[6] Molchanov, Stanislav, and Boris Vainberg. "On general Cwikel–Lieb–Rozenblum and Lieb–Thirring inequalities." Around the Research of Vladimir Maz'ya III: Analysis and Applications. New York, NY: Springer New York, 2009. 201-246.

[7] Lieb, E., Thirring, W.: Inequalities for the moments of the eigenvalues of the Schrödinger Hamiltonian and their relation to Sobolev inequalities. In: Studies in Mathematical Physics: Essays in Honor of Valentine Bargmann, pp. 269– 303, Princeton Univ. Press, Princeton, (1976)

[8] J. Von Below: A characteristic equation associated to an eigenvalue problem on c^2-networks, Linear Algebra and its Applications 71 (1985), 309-325

[9] C. Cattaneo: The spectrum of the continuous Laplacian on a graph, Monat. fur Math. ¨ 124 (1997), 215–235.

[10] P. Exner: Topologically induced spectral behavior: the example of quantum graphs, preprint (2020)

[11] K. Pankrashkin: Unitary dimension reduction for a class of self-adjoint extensions with applications to graph-like structures J. Math. An. Appl. 396, no 2 (2012), 640-655.