# Sum of lowest eigenvalues of the Discrete Laplacian

by

Grethe Hystad

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A Dissertation Submitted to the Faculty of the

Department of Mathematics

In Partial Fulfillment of the Requirements
For the Degree of

Masters of Science

In the Graduate College

The University of Arizona

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# ACKNOWLEDGMENTS

I would like to thank my advisor Dr. Daniel Ueltschi for his help, patient and expertise. I will also thank my committee members Dr. Leonid Friedlander and Dr. Thomas G. Kennedy for their advice and corrections. Further, I will thank Arthur Lim for his help with the drawings. I will also thank Jim, Tina and my family for their support.

# Dedication

to

* my grandmother Gudrun Schie

* my grandmother Lise Hystad

* my aunt Ruth Westlie

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# ABSTRACT

In this paper, we will explore the lower bound for the sum of the $N$ lowest eigenvalues of the Discrete Laplacian defined on a finite subset of the infinite lattice. We will see the connection between the Discrete and Continuum Laplacian. We will show that the sum of the $N$ lowest eigenvalues of the Discrete Laplacian converges to the sum of the $N$ lowest eigenvalues of the Continuum Laplacian in the continuum limit.

# Sum of lowest eigenvalues of the Discrete Laplacian

Grethe Hystad, M.S.
The University of Arizona, 2006

Director: Daniel Ueltschi

In this paper, we will explore the lower bound for the sum of the $N$ lowest eigenvalues of the Discrete Laplacian defined on a finite subset of the infinite lattice. We will see the connection between the Discrete and Continuum Laplacian. We will show that the sum of the $N$ lowest eigenvalues of the Discrete Laplacian converges to the sum of the $N$ lowest eigenvalues of the Continuum Laplacian in the continuum limit.

# 1. Introduction

## 1.1. Brief history

In 1912, H. Weyl proved that

$$\lambda_k \simeq 4\pi\Gamma\left(\frac{d}{2}+1\right)^{\frac{2}{d}}\left(\frac{k}{|D|}\right)^{\frac{2}{d}}$$

as $k \to \infty$ where $\lambda_k$ is the $k$-th eigenvalue for the Dirichlet boundary problem on a bounded domain $D$ in $\mathbb{R}^d$ with volume $|D|$ [1]. In 1960, Pólya followed by proving that,

$$\lambda_k \geq 4\pi\Gamma\left(\frac{d}{2}+1\right)^{\frac{2}{d}}\left(\frac{k}{|D|}\right)^{\frac{2}{d}}$$

for any $k$ and for any domain $D$ that tiles $\mathbb{R}^d$ [1]. Subsequently, in 1983, Li and Yau [1] proved that for any bounded domain $D$ in $\mathbb{R}^d$,

$$\sum_{i=1}^{N}\lambda_i \geq 4\pi\Gamma\left(\frac{d}{2}+1\right)^{\frac{2}{d}}|D|^{-\frac{2}{d}}\frac{d}{d+2}N^{1+\frac{2}{d}}. \tag{1.1}$$

The last inequality can also be written as

$$S_N = \sum_{i=1}^{N}\lambda_i \geq |D|e(\rho)$$

where $e(\rho)$ denotes the ground state energy density of non-interacting electrons in the continuum with density $\rho = \frac{N}{|D|}$.

In 1955 and 1956, Payne, Polya and Weinberger proved that the ratio of the first two eigenvalues for the Dirichlet problem on a bounded domain in the plane is given by

$$\frac{\lambda_2}{\lambda_1} \leq 3. \tag{1.2}$$

[2]. Further, they conjectured that

$$\frac{\lambda_2}{\lambda_1} \leq \frac{\lambda_2}{\lambda_1}|_{D=disk} \approx 2,539. \tag{1.3}$$

Later, Thompson generalized the result in (1.2) to dimension $d$. He obtained

$$\frac{\lambda_2}{\lambda_1} \leq 1 + \frac{4}{d}$$

[2]. Thompson also extended their conjecture in (1.3) to

$$\frac{\lambda_2}{\lambda_1} \leq \frac{\lambda_2}{\lambda_1}|_{|D|=d-dim.ball} = (j_{d/2,1}/j_{d/2-1,1})^2$$

[2]. Here $j_{p,k}$ denotes the $k^{th}$ positive zero of the Bessel function $J_p(x)$. In 1992, Ashbaugh and Benguria [2] proved the general Payne-Polya-Weinberger conjecture. They proved that the ratio of the first two Dirichlet eigenvalues of the Laplacian on a domain $D \subset \mathbb{R}^d$ is given by

$$\frac{\lambda_2}{\lambda_1} \leq \frac{\lambda_2}{\lambda_1}|_{|D|=d-dim.ball} = \frac{j^2_{d/2,1}}{j^2_{d/2-1,1}}.$$

Later, in 1994, Ashbaugh and Benguria [3] proved that for any integer, $k \geq 1$,

$$\frac{\lambda_{2^k}}{\lambda_1} < \left(\frac{\lambda_2}{\lambda_1}|_{|D|=d-dim.ball}\right)^k = \left(\frac{j^2_{d/2,1}}{j^2_{d/2-1,1}}\right)^k. \tag{1.4}$$

This result is much better than the bound

$$\frac{\lambda_{m+1}}{\lambda_m} \leq 1 + \frac{4}{d}$$

and

$$\frac{\lambda_m}{\lambda_1} \leq \left(1 + \frac{4}{d}\right)^{m-1}$$

of Payne-Polya-Weinberger (for two dimensions) and Thompson (for $d$ dimensions) [3], [4]. The ratio result in (1.4) also gives lower bounds for the counting function $N(\lambda)$. $N(\lambda)$ denotes the number of eigenvalues less than or equal to $\lambda$. For $\lambda \geq \lambda_1$, $d \geq 2$ one obtains from (1.4) [3]

$$N(\lambda) \geq 2^{\lfloor \log(\lambda/\lambda_1)/log(j^2_{n/2,1}/j^2_{n/2-1,1}) \rfloor}.$$

Here $\lfloor x \rfloor$ denotes the largest integer less than or equal to $x$.

We also have the celebrated Faber-Krahn inequality which is concerning the lowest eigenvalue of the Laplacian with Dirichlet boundary condition, on a bounded domain in $\mathbb{R}^d (d \geq 2)$ : In $d$ dimensions the inequality is

$$\lambda_1 \geq \left( \frac{B_d}{|D|} \right)^{\frac{2}{d}} j^2_{d/2-1,1},$$

where $B_d$ is the volume of the $d$- dimensional unit ball [4], [5].

In 1991, Laptev [6] proved that for an open set $D \subset \mathbb{R}^d$ of finite measure, $|D| < \infty$,

$$N(\lambda) \leq \lambda^{\frac{d}{2}} L_d^{cl} \left( 1 + \frac{2}{d} \right)^{\frac{d}{2}} |D|$$

with

$$L_d^{cl} = 2^{-d} \pi^{-\frac{d}{2}} / \Gamma \left( 1 + \frac{d}{2} \right).$$

He noticed that this is equivalent to (1.1) proved by Li and Yau. Let $\omega_1, \omega_2, ....$ be the orthonormal basis of eigenfunctions of the Dirichlet Laplacian with respective eigenvalues $0 < \lambda_1 < \lambda_2 \leq ....$ Consider the convex function

$$\varphi_\lambda(t) = (\lambda - t)_+ = \left\{ \begin{array}{ll} \lambda - t, & \text{if } t < \lambda; \\ 0, & \text{if } t \geq \lambda; \end{array} \right\}$$

Laptev [6] proved that for $\lambda > 0$,

$$\sum_k (\lambda - \lambda_k)_+ \geq (\lambda - \lambda_1)_+^{1+\frac{d}{2}} L_d^{cl} \frac{2}{d+2} \overline{\omega}^{-2},$$

where $\overline{\omega} = \sup_{x \in D} |\omega_1(x)|$. When $\lambda = \lambda_2$, Laptev [6] showed that

$$\lambda_2 - \lambda_1 \leq \left( L_d^{cl} \frac{2}{d+2} \right)^{\frac{-2}{d}} \overline{\omega}^{\frac{4}{d}}.$$

Furthermore, Laptev [6] showed that for any $\lambda > \lambda_1$,

$$N(\lambda) \geq (\lambda - \lambda_1)^{\frac{d}{2}} L_d^{cl} \frac{2}{d+2} \overline{\omega}^{-2}.$$

In 2002, Melas [7] improved the lower bound in (1.1) of Li and Yau . He proved that

$$S_N \geq |D|e(\rho) + M_d N \frac{|D|}{I(D)},$$

where $M_d$ is a constant that depends only on the dimension and

$$I(D) = \min_{a \in D} \int_D |x - a|^2 dx$$

is the 'moment of inertia of $D$.'

Richardson [8] developed in his work in 1917 a new method to deduce results of boundary problems for ordinary elliptic partial equations and tried this method on new boundary problems for the hyperbolic equation. In his method he divided the region into equal rectangles by a lattice and studied the difference equations approximating to the differential equation at the lattice points. He let the mesh of the lattice approach smaller and smaller values. He showed for the elliptic partial differential equation that the lattice functions approach uniformly a function that is continuous with continuous derivatives of as high order as those possessed by the coefficients of the equation.

Weinberger [9] found in 1956 upper and lower bounds for the lowest eigenvalue, $\lambda$, of the Laplacian on the membrane $D$ with Dirichlet boundary conditions, by finite difference methods. He considered the square lattice with mesh size $a > 0$. He obtained the lower bound on a grid that was slightly larger than the domain $D$ and the upper bound on a grid that was smaller than or equal to $D$. He found arbitrary close upper and lower bound for $\lambda$ on certain domains. He did this by solving a single finite difference problem with the mesh size $a$, sufficiently small. In other words, the lower and upper bound of $\lambda$ were the lowest lattice eigenvalues.

Lyusternik [10] considered in 1958 questions related to difference approximations of the Laplace operator in two dimensions. He studied the convergence of eigenvalues and eigenvectors of the Laplacian with zero boundary condition for arbitrary parallelogram network approximations. The convergence is in terms of uniform convergence on the closure of the domain. He also extended the simplest difference approximations to more general difference approximations. In this sense he showed that the solutions of the difference approximation of the Dirichlet's problem converges to the solution of the corresponding boundary value problem for the differential equation.

Courant, Friedrichs and Lewy [11] treated in 1928 the boundary and eigenvalue problems for elliptic difference equations and the initial value problem for hyperbolic parabolic difference equations. They showed that the solutions of the difference equations converge to the solutions of the differential equations. They also showed that the elliptic equations, i.e. difference quotients of arbitrary high order converge to the differential quotients.

Freericks, Lieb, Ueltschi [12] proved in 2002 and Ueltschi [13] in 2004 that the sum, $S_N^{(a)}$, of the $N$ lowest eigenvalues of the Discrete Laplacian defined on a finite subset $\Lambda \subset (a\mathbb{Z})^d$, where $a > 0$ is the mesh of the lattice, is bounded below by a term proportional to the volume of the domain, $\Lambda$, ('bulk term') and a term proportional to the boundary of $\Lambda$ ('boundary correction'). Ueltschi's [13] paper in 2004 was an improvement of the 'boundary correction' in [12].

They proved that for every $N \geq 1$,

$$S_N^{(a)} \geq |\Lambda| a^d e^{(a)}(\rho^{(a)}) + C\, B(\Lambda) a^d (\rho^{(a)})^{\frac{2}{d}+1}, \tag{1.5}$$

where $B(\Lambda) = |\{(x,y) : x \in \Lambda, y \in \Lambda^C, |x-y| = a\}|$, $\rho^{(a)} = \frac{N}{|\Lambda| a^d}$ denotes the lattice density, $e^{(a)}(\rho^{(a)})$ is the ground state energy density of non-interacting electrons with density, $\rho$, in $(a\mathbb{Z})^d$, and $C$ is a constant. They proved that $C$ is strictly positive for all densities. They found an explicit value of $C$ only for small densities.

Electrons on solid are described by wave functions, $\varphi(x)$, which are normalized complex valued functions in the state space $l^2(\Lambda)$, where $\Lambda$ is a subset of the infinite lattice. The Discrete Laplacian, $-\Delta^{(a)}$, represents their kinetic energy. The eigenvalue equation for one particle at site $x$ is given by $-\Delta^{(a)}\varphi(x) = E\varphi(x)$, where $E$ represents the eigenvalues and $\varphi(x)$ the respective eigenfunctions of $-\Delta^{(a)}$. The lowest eigenvalue represents the ground state energy of the electron. When we have $N$ non-interacting electrons, the state space is $l^2(\Lambda^N)$ and the kinetic energy is given by $-\sum_{j=1}^{N}\Delta_j^{(a)}$, where $-\Delta_j^{(a)}$ is the Discrete Laplacian. It turns out that to minimize the ground state energy of $N$ non-interacting electrons amounts to minimizing the sum of the $N$ lowest eigenvalues of the Discrete Laplacian defined on $\Lambda$.

## 1.2. Motivation and introduction

The motivation for this thesis is to explore the lower bound in (1.5) and to see the connection between the discrete case and the continuum case. In chapter 4 we will be looking at the sum of the $N$ lowest eigenvalues of the Discrete Laplacian and we will show that it converges to the sum of the $N$ lowest eigenvalues of the Continuum Laplacian in the continuum limit. In chapter 5 we will see that when we take the continuum limit of the bound in (1.5) we recover the 'bulk term' in the continuum, while the 'boundary correction' unfortunately tends to zero. The discrete case is, therefore, more general than the continuum case. In the future we hope that we can find a lower bound for the sum of the $N$ lowest eigenvalues of the Discrete Laplacian that involves a 'boundary correction' that is different from zero in the continuum limit. In other words, one of the reasons for looking at the discrete case is that we hope to find a 'boundary correction' for the continuum case in the continuum limit. This problem is still open.

In chapter 6 we will use the bathtub principle [14] with gradient to prove one of the lemmas in the paper of Melas [7](lemma 1). Melas improved the lower bound in the continuum. The use of the bathtub principle will somewhat simplify the proof of the lemma he applied to prove the lower bound. We obtained the same results as

Melas. In chapter 7 we will follow the paper of [12] and [13] to show that the sum of the $N$ lowest eigenvalues of the Discrete Laplacian defined on a finite subset, $\Lambda$, of the torus is bounded below by a term proportional to the volume of $\Lambda$. In chapter 8 we will show for small densities and for $L$ large enough, where $L$ is the size of the torus, that the lower bound also involves a term proportional to the boundary of $\Lambda$. In chapter 9 we will use the results of Goldbaum [15] to discuss a method to find an explicit value of the 'boundary correction' for all densities for the Discrete Laplacian defined on a finite subset of the torus. This problem is still unsolved.

Remark: In chapter 8, page 61 we have not proved lemma 12(b) yet, due to lack of time. In chapter 9, page 68 we have not proved the bound for the terms in lemma 13 yet, due to lack of time.

# Part I

## 2. The Continuum Laplacian.

Let $D \subset \mathbb{R}^d$ be an open, bounded domain. Let $\Delta$ denote the Laplace operator $\displaystyle\sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2}$. We are interested in the Dirichlet problem on D. We have that $\lambda$ is a Dirichlet eigenvalue of $D$ if there exists a function $f \in C^2(D) \cap C^0(\overline{D})$ satisfying the equation:

$$-\Delta f = \lambda f \quad \text{in} \quad D$$

$$f = 0 \quad \text{on} \quad \partial D,$$

where $\partial D$ is the boundary of $D$ [16].

Recall that the Sobolev space, $H^1(D)$, is the space of $L^2(D)$ functions with distributional gradient, $\nabla f$, in $L^2(D)$. We also recall that the subspace, $H_0^1(D)$, of $H^1(D)$, is the completion of $C_c^\infty(D)$, the space of smooth functions with compact support, in the $H^1$-norm. That means that we can interpret $H_0^1(D)$ as the space of functions in $H^1(D)$ that vanish on the boundary of $D$ [17]. Equivalently, we have

$$H_0^1(D) = \{f \in L^2(D) : |k|\widehat{f}(k) \in L^2(\mathbb{R}^d)\}.$$

The eigenvalues of the above defined problem are characterized [14] by the following minimization criterion.

$$\lambda_1 = \inf \int_D |\nabla \phi(x)|^2 \, dx.$$

Here the infimum is taken over all normalized functions in $H_0^1(D)$ in the $L^2$-norm. Let us denote the first $(k-1)$ eigenfunctions by $f_1, ..., f_{k-1} \in H_0^1(D)$. The $k^{th}$ eigenvalue exists as a minimizer of the Dirichlet integral

$$\lambda_k = \inf \int_D |\nabla \phi(x)|^2 \, dx,$$

where the infimum is taken over all normalized functions $\phi \in H_0^1(D)$ in the $L^2$-norm which are perpendicular to $f_1, ...., f_{k-1}$. For $f \in L^1(D)$, the Fourier transform is given by

$$\widehat{f}(k) = \int_D f(x) e^{ikx}\, dx, \quad k \in \mathbb{R}^d.$$

and the Inverse Fourier transform is

$$f(x) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \widehat{f}(k) e^{-ikx}\, dk, \quad x \in D.$$

Note that by Schwarz's inequality $L^2(D) \subseteq L^1(D)$.

We can for $f \in H_0^1(D)$ define the total energy $E(f)$ to be the kinetic energy $E(f) = \int_D |\nabla f(x)|^2\, dx$ [14]. We have for any $f \in H_0^1(D)$,

$$E(f) = \int_D |\nabla f(x)|^2\, dx = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} |k|^2 |\widehat{f}(k)|^2\, dk.$$

The second equality is proved by applying Plancherel's identity. The proof can be found in [1] or in [14].

We denote the sum of the N lowest eigenvalues by $S_N = \sum_{1=1}^{N} \lambda_i$.

Let the density, $\rho$, of $N$ non-interacting electrons in the continuum be given by $\rho = \frac{N}{|D|}$, where $|D|$ is the volume of $D$.

Let $\varepsilon_F(\rho)$ denote the Fermi level which is determined by the relation

$$\rho = \frac{1}{(2\pi)^d} \int_{|k|^2 < \varepsilon_F(\rho)} dk.$$

Let $e(\rho)$ denote the ground-state energy density of non-interacting electrons with density, $\rho$, in the limit of infinite volume. It is given by

$$e(\rho) = \frac{1}{(2\pi)^d} \int_{|k|^2 < \varepsilon_F(\rho)} |k|^2\, dk.$$

This expression can be understood as follows: In the continuum limit $a \to 0$, we define the torus, $T_L$, of length $L > 1$ for even $L$, by

$$T_L = \left\{ x \in \mathbb{R}^d : -\frac{L}{2} \leq x_j \leq \frac{L}{2} \quad \forall j = 1, ..., d \right\}$$

[18]. The dual, $T_L^*$, of $T_L$ is defined by

$$T_L^* = \left\{ k \in \frac{2\pi}{L} \mathbb{Z}^d : -\infty < k_j < \infty \quad \forall j = 1, ..., d \right\}.$$

Let $D = T_L$. Define $K_{L,N'}$ as the set with $N'$ elements with lowest $|k|^2$. The energy per site of a density $\rho = \frac{N'}{L^d}$ of free electrons in $T_L$ is given by $e_L(\rho)$, where

$$e_L(\rho) = \frac{1}{L^d} \sum_{K_{L,N'}} |k|^2.$$

When we take the thermodynamic limit $L \to \infty$ we get the following Riemann sum,

$$\begin{aligned}
\lim_{L\to\infty} e_L(\rho) &= \lim_{L\to\infty} \frac{1}{(2\pi)^d} \sum_{K_{L,N'}} \left(\frac{2\pi}{L}\right)^d |k|^2 \\
&= \frac{1}{(2\pi)^d} \int_{|k|^2<\varepsilon_F(\rho)} |k|^2, dk \\
&= e(\rho)
\end{aligned}$$

It can be checked that

$\varepsilon_F(\rho) = 4\pi\rho^{\frac{2}{d}}\Gamma\left(\frac{d}{2}+1\right)^{\frac{2}{d}}$ and

$e(\rho) = 4\pi\rho^{1+\frac{2}{d}}\frac{d}{d+2}\Gamma\left(\frac{d}{2}+1\right)^{\frac{2}{d}}$,

We notice that $\varepsilon_F(\rho) = \frac{d}{d\rho}e(\rho)$.

## 3. The Discrete Laplacian

The results we obtain for the Discrete Laplacian are more general than those for the Continuum Laplacian since we will recover the results for the Continuum Laplacian in the continuum limit.

Define $\Lambda = (a\mathbb{Z})^d \bigcap D^0$, where $a > 0$ is the mesh of the lattice and where $D^0$ is the set of all $x \in D$ where we can place a cubic cell of size $2a$ centered around $x$ such that the cubic cell is contained in $D$. That means that the lattice, $\Lambda$, is excluded around the boundary of $D$ with a width of at least $a$.

Let $\Delta^{(a)}$ denote the Discrete Laplacian. Let $\varphi$ be a normalized, complex valued function in $l^2(\Lambda)$.

**Definition.** For $\varphi \in l^2(\Lambda)$, the Discrete Laplace operator $-\Delta^{(a)}$ can be written

$$[-\Delta^{(a)}\varphi](x) = -\frac{1}{a^2} \sum_{y\in\Lambda, |x-y|=a} \varphi(y) + \frac{2d\varphi(x)}{a^2}, \quad \forall x \in \Lambda.$$

Here it is understood that $\varphi(x) = 0$ outside $\Lambda$. In 1-dimension, the Lattice Laplacian can be represented by the following $(|\Lambda| \times |\Lambda|)$- matrix with respect to the basis $\frac{1}{a}\delta_x(y)$ for $x, y \in \Lambda$:

$$\frac{1}{a^2}\begin{pmatrix} 2 & -1 & 0 & ... & 0 \\ -1 & 2 & -1 & ... & ... \\ 0 & ... & ... & ... & 0 \\ : & ... & -1 & 2 & -1 \\ : & ... & 0 & -1 & 2 \end{pmatrix}$$

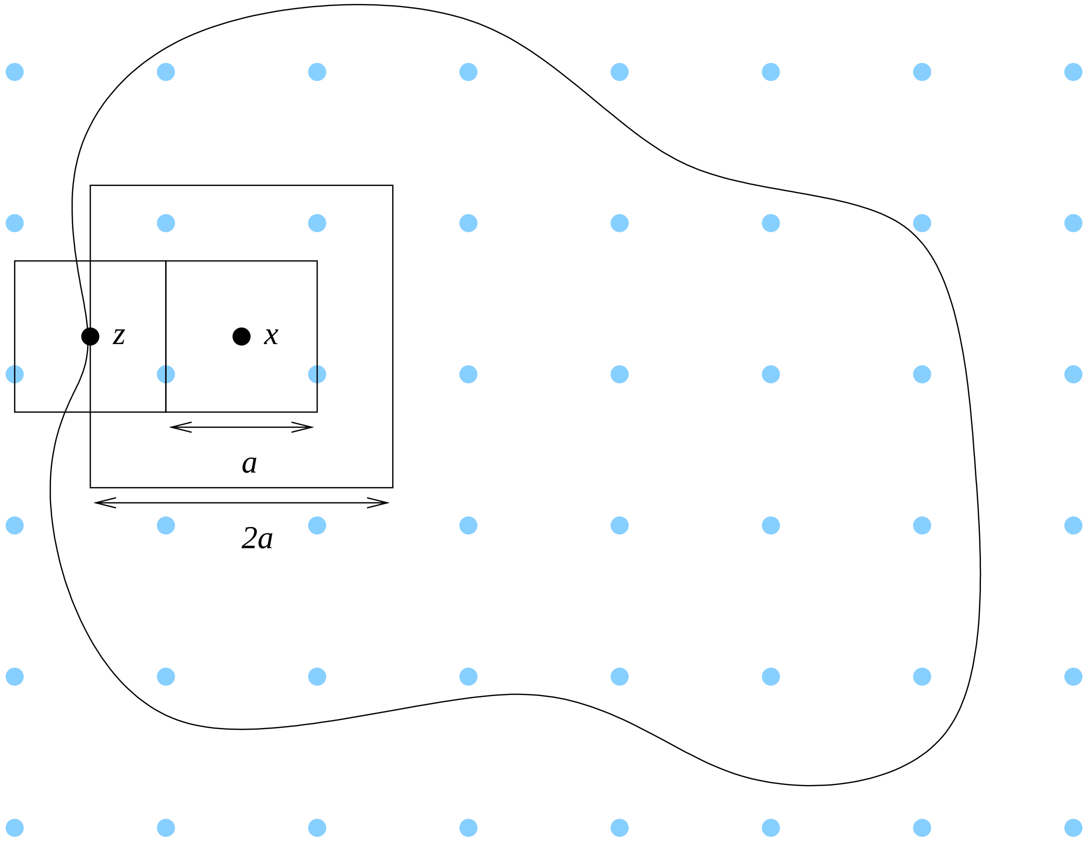

FIGURE 3.1. This picture shows the domain $D$ and the lattice in two dimensions. We can put a unit cube of size $2a$ centered around $x \in D$. That means that $\Lambda$ must be placed to the right for the point $x$.

**Definition.** For $\varphi \in l^p(\Lambda)$,we define the $l^p$ norm by

$$\|\varphi\|_{l^p(\Lambda)} = \left( a^d \sum_{x \in \Lambda} |\varphi(x)|^p \right)^{\frac{1}{p}}.$$

The factor $a^d$ is a scaling factor such that in the continuum limit we will get the $L^p$-norm. For $\varphi \in l^2(\Lambda)$, the Fourier transform is given by

$$\widehat{\varphi}(k) = a^d \sum_{x \in \Lambda} \varphi(x) e^{ikx}, \quad k \in \left[ -\frac{\pi}{a}, \frac{\pi}{a} \right]^d$$

and the inverse transform is

$$\varphi(x) = \frac{1}{(2\pi)^d} \int_{[-\frac{\pi}{a}, \frac{\pi}{a}]^d} \widehat{\varphi}(k) e^{-ikx} dk, \quad x \in \Lambda.$$

It can be checked that for $\varphi \in l^2(\Lambda)$

$$\langle \varphi, -\Delta^{(a)}\varphi \rangle = a^{d-2} \sum_{\substack{\{x,y\}\subset (a\mathbb{Z})^d \\ |x-y|=a}} |\varphi(x) - \varphi(y)|^2 \tag{3.1}$$

which shows that $-\Delta^{(a)} \geq 0$. It is obvious that $-\Delta^{(a)}$ is a self adjoint operator on $l^2[(a\mathbb{Z})^d]$. Define

$$\varepsilon_k^{(a)} = \frac{1}{a^2}\sum_{v=1}^{d}[2 - 2\cos(ak_v)], \quad k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]^d.$$

Notice that $\varepsilon_k^{(a)} \to |k|^2$ as $a \to 0$. For $\varphi \in l^2(\Lambda)$, we have

$$\langle \varphi, -\Delta^{(a)}\varphi \rangle = \frac{1}{(2\pi)^d}\int_{\left[-\frac{\pi}{a}, \frac{\pi}{a}\right]^d} \varepsilon_k^{(a)} |\widehat{\varphi}(k)|^2 \, dk.$$

Since

$$[(\widehat{-\Delta^{(a)}\varphi})(k)] = \varepsilon_k^{(a)}\widehat{\varphi}(k),$$

we obtain the result above by applying Plancherel's identity.

The spectrum of $-\Delta^{(a)}$ on $\Lambda$ is contained in $[0, \frac{4d}{a^2}]$ [12]. We denote the eigenvalues of $-\Delta^{(a)}$ on $\Lambda$ by $\lambda_1^{(a)} \leq \lambda_2^{(a)} \leq ... \leq \lambda_{|\Lambda|}^{(a)}$.

Define $S_N^{(a)}$ to be the ground state energy of N electrons on $\Lambda$, which corresponds to the sum of the N lowest eigenvalues of the Discrete Laplace operator on $\Lambda$, i.e $S_N^{(a)} = \sum_{j=1}^{N} \lambda_j^{(a)}$.

We let $\rho^{(a)} = \frac{N}{a^d|\Lambda|}$ denote the lattice density, where $|\Lambda|$ is the number of sites of $\Lambda$. Notice that $\rho^{(a)} \downarrow \rho$ as $a \to 0$, where we recall that $\rho$ is the density in the continuum. Let $\varepsilon_F^{(a)}(\rho^{(a)})$ denote the lattice Fermi level which is determined by the relation

$$\rho^{(a)} = \frac{1}{(2\pi)^d}\int_{\varepsilon_k^{(a)} < \varepsilon_F^{(a)}(\rho^{(a)})} dk, \quad k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]^d.$$

Let $e^{(a)}(\rho^{(a)})$ denote the ground-state energy density of non-interacting electrons in the infinite volume $(a\mathbb{Z})^d$ with density, $\rho^{(a)}$, which is given by

$$e^{(a)}(\rho^{(a)}) = \frac{1}{(2\pi)^d}\int_{\varepsilon_k^{(a)} < \varepsilon_F^{(a)}(\rho^{(a)})} \varepsilon_k^{(a)} \, dk, \quad k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]^d.$$

It can be checked that $\varepsilon_F^{(a)}(\rho^{(a)}) = \frac{d}{d\rho^{(a)}} e^{(a)}(\rho^{(a)})$.

# 4. Convergence of lattice eigenvalues.

In this chapter we will show that for any open, bounded domain D, the sum of the N lowest eigenvalues of the Discrete Laplacian defined on $\Lambda$ converges to the sum of the N lowest eigenvalues of the Continuum Laplacian defined on D.

Recall from chapter (2) that the Dirichlet eigenvalues are characterized by

$$\lambda_k = \inf \int_D |\nabla\phi(x)|^2 \, dx$$

where the infimum is taken over all normalized functions $\phi \in H_0^1(D)$ in the $L^2$-norm, perpendicular to the first $(k-1)$ eigenfunctions $f_1, ..., f_{k-1} \in H_0^1(D)$. The sum of the N lowest eigenvalues in the continuum is given by

$$S_N = \inf_{\substack{\phi_1,\dots,\phi_N \\ \|\phi_j\|_{L^2}=1, \langle\phi_i,\phi_j\rangle=0}} \sum_{j=1}^{N} \int_D |\nabla\phi_j|^2 \, dx.$$

where the infimum is taken over N orthonormal functions in $H_0^1(D)$ in the $L^2$-norm. Similarly, the sum of the N lowest eigenvalues on the lattice is given by

$$S_N^{(a)} = \inf_{\substack{\varphi_1,\dots,\varphi_N \\ \|\phi_j\|_{l^2}=1, \langle\varphi_i,\varphi_j\rangle=0}} \sum_{j=1}^{N} \langle\varphi_j, -\Delta^{(a)}\varphi_j\rangle,$$

where the infimum is taken over N orthonormal functions in $l^2(\Lambda)$.

**Theorem 1.** *For any open, bounded domain D, and any $N \geq 1$,*

$$\lim_{a\to 0} S_N^{(a)} = S_N.$$

In this chapter we will prove this theorem. The proof of this theorem will be done in two stages. First we will prove that $S_N \geq \limsup_{a\to 0} S_N^{(a)}$. We will do this by defining a lattice function $f^{(a)} \in l^2(\Lambda)$ from a given function $f \in H_0^1(D)$ such that

$\lim_{a\to 0}\langle f^{(a)}, -\Delta^{(a)} f^{(a)}\rangle = \int_D |\nabla f|^2$. The value of $\int_D |\nabla f|^2$ is larger than the minimum eigenvalue on the lattice. When we have N such eigenfunctions $f_1, ...., f_N$ in $H_0^1(D)$ such that $S_N = \sum_{j=1}^N \int_D |\nabla f_j|^2$, we will need to orthonormalize the corresponding lattice functions $f_1^{(a)}, ..., f_N^{(a)}$. We will do this by applying the Gram-Schmidt process. By combining these results, we will obtain a lower bound.

The second stage is to prove that $S_N \leq \liminf_{a\to 0} S_N^{(a)}$. We will do this by defining a function $\varphi^{(a)}$ in $H_0^1(D)$ from a given function $\varphi \in l^2(\Lambda)$. Now, $\langle \varphi, -\Delta^{(a)}\varphi\rangle$ is larger than the minimum eigenvalue in the continuum so we will obtain an upper bound. When we have $N$ such eigenfunctions $\varphi_1, ...., \varphi_N$ in $l^2(\Lambda)$ such that $S_N^{(a)} = \sum_{j=1}^N \langle \varphi_j, -\Delta^{(a)}\varphi_j\rangle$ we will need to orthonormalize the corresponding functions $\varphi^{(a)}, ...., \varphi_N^{(a)}$ in the continuum. Again we will apply the Gram-Schmidt process. By combining these results, we will obtain an upper bound.

**Proposition 1.** *For any open, bounded domain $D$, and any $N \geq 1$,*

$$S_N \geq \limsup_{a\to 0} S_N^{(a)}.$$

The strategy is to construct a function $f^{(a)} \in l^2(\Lambda)$ from a given function
$f \in H_0^1(D)$ such that

$$\lim_{a\to 0} \|f^{(a)}\|_{l^2} = \|f\|_{L^2} \tag{4.1}$$

and

$$\lim_{a\to 0}\langle f^{(a)}, -\Delta^{(a)} f^{(a)}\rangle = \|\nabla f\|_{L^2}. \tag{4.2}$$

Before giving the proof of proposition 1, we will define the function $f^{(a)}$ and prove that $f^{(a)}$ satisfies (4.1) and (4.2).

**Definition.** For a given function $f \in L^1(D)$, we define a function $f^{(a)} \in l^2(\Lambda)$ by

$$f^{(a)}(x) = \frac{1}{a^d}\int_{C^{(a)}(x)} f(y)\, dy, \qquad x \in \Lambda,$$

where $C^a(x)$ is a cubic cell of size $a > 0$ centered around $x \in (a\mathbb{Z})^d$.

Let $f^{(a)}(x) = 0$ for $x \in (a\mathbb{Z})^d \setminus \Lambda$. We extend $f^{(a)} \in l^2(\Lambda)$ to a piecewise constant function in $L^2(D)$ by letting $f^{(a)}(y) = f^{(a)}(x)$ for all $y \in C^{(a)}(x)$. Note that

$$\|f^{(a)}\|^2_{l^2(\Lambda)} = \sum_{x\in\Lambda} \int_{C^a(x)} |f^{(a)}(y)|^2 \, dy = \|f^{(a)}\|^2_{L^2(D)}.$$

Recall that we defined $\Lambda = (a\mathbb{Z})^d \bigcap D^0$, where $D^0$ is the set of all $x \in D$ where we can place a cubic cell of size $2a$ centered around $x$ such that the cubic cell is contained in $D$. That means that there exists $z \in D$ such that $z$ is not included in a unit cube, $C^a(x)$, centered around $x \in \Lambda$.

Let $D'$ be the set of all $y \in D$ such that $y$ is included in a unit cube, $C^a(x)$, centered around $x \in \Lambda$. The distance from $y$ in $D'$ to the boundary of $D$ is at least $\frac{a}{2}$.

**Lemma 1.** *If $f \in L^2(D)$ then,*

$$\|f^{(a)}\|_{l^2(\Lambda)} \leq \|f\|_{L^2(D)}.$$

**Proof.** By Schwarz's inequality,

$$\begin{aligned} |f^{(a)}(x)|^2 &\leq \frac{1}{a^{2d}} \int_{C^a(x)} |f(y)|^2 \, dy \int_{C^a(x)} dy \\ &= \frac{1}{a^d} \int_{C^a(x)} |f(y)|^2 \, dy. \end{aligned}$$

Hence

$$\|f^{(a)}\|^2_{l^2(\Lambda)} \leq \int_{D'} |f(y)|^2 \, dy \leq \|f\|^2_{L^2(D)}.$$

□

**Lemma 2.** *If $f \in L^2(D)$, then*

$$\lim_{a\to 0} \|f^{(a)}\|_{l^2(\Lambda)} = \|f\|_{L^2(D)}.$$

**Proof.** Since $L^2(D)$ is the closure of $C_c^\infty(D)$ in the $L^2$-norm, we will first prove this lemma for a smooth function with compact support. For a general function $f \in L^2(D)$, we will approximate $f$ with a function $g$ in $C_c^\infty(D)$.

Since $\|f^{(a)}\|_{l^2(\Lambda)} = \|f^{(a)}\|_{L^2(D)}$, we can prove the lemma if we can show that $\lim_{a\to 0} \|f^{(a)}\|_{L^2(D)} = \|f\|_{L^2(D)}$.

First, let $f \in C_c^\infty(D)$. We have

$$\|f^{(a)} - f\|_{L^2(D)} = \|f^{(a)} - f\|_{L^2(D')} + \|f^{(a)} - f\|_{L^2(D\setminus D')}. \tag{4.3}$$

The latter term converges to 0 when $a \to 0$ since $D' \setminus D$ tends to 0. We calculate the first term in (4.3). By Schwarz's inequality,

$$\begin{aligned} |f^{(a)}(x) - f(x)|^2 &\leq \frac{1}{a^{2d}} \int_{C^a(x)} |f(y) - f(x)|^2 \, dy \int_{C^a(x)} dy \\ &= \frac{1}{a^d} \int_{C^a(x)} |f(y) - f(x)|^2 \, dy \\ &\leq \frac{1}{a^d} \int_{C^a(x)} a^2 \sup_{y' \in C^a(x)} |\nabla f(y')|^2 \, dy. \end{aligned}$$

Then

$$\|f^{(a)} - f\|^2_{L^2(D')} \leq a^2 \sup_{y' \in C^a(x)} |\nabla f(y')|^2 |D'|.$$

The latter term converges to 0 when $a \to 0$. Hence for $f \in C_c^\infty(D)$ we obtain $\lim_{a\to 0} \|f^{(a)}\|_{L^2(D)} = \|f\|_{L^2(D)}$.

Now let $f$ be any function in $L^2(D)$. We have

$$\|f^{(a)} - f\|_{L^2(D)} \leq \|f^{(a)} - g^{(a)}\|_{L^2(D)} + \|g^{(a)} - g\|_{L^2(D)} + \|g - f\|_{L^2(D)},$$

where $g \in C_c^\infty(D)$ is the $L^2$-norm approximation of $f$, i.e $\|f - g\|_{L^2(D)} < \epsilon$ for $\epsilon > 0$. By Lemma 1, $\|f^{(a)} - g^{(a)}\|_{L^2(D)} = \|f^{(a)} - g^{(a)}\|_{l^2(\Lambda)} \leq \|f - g\|_{L^2(D)} < \epsilon$. Furthermore, we proved above that $\lim_{a\to 0} \|g^{(a)}\|_{L^2(D)} = \|g\|_{L^2(D)}$. This implies that $\|f^{(a)} - f\|_{L^2(D)} \to 0$ as $a \to 0$. Hence for any function $f \in L^2(D)$ we obtain $\lim_{a\to 0} \|f^{(a)}\|_{L^2(D)} = \|f\|_{L^2(D)}$. $\square$

Let $\nabla^{(a)}$ denote the discrete gradient, where $\nabla^{(a)}\varphi = (\nabla_1^{(a)}\varphi, ...., \nabla_d^{(a)}\varphi)$ for $\varphi \in l^2(\Lambda)$. Define

$$\Lambda' \equiv \{y \in (a\mathbb{Z}^d) : \mathrm{dist}(y, \Lambda) \leq a\}.$$

The $i^{th}$ directional gradient is given by

$$\nabla_i^{(a)}\varphi(x) = \frac{\varphi(x + a\, e_i) - \varphi(x)}{a},$$

where $e_i$ is the unit vector in the $i^{th}$ direction and $x \in \Lambda'$. For $\varphi \in l^2(\Lambda')$, we have

$$\langle \varphi, -\Delta^{(a)}\varphi\rangle = \sum_{i=1}^{d} \|\nabla_i^{(a)}\varphi\|^2_{l^2(\Lambda')} = \|\nabla^{(a)}\varphi\|^2_{l^2(\Lambda')}.$$

This can be shown by letting $y = x + ae_i$. Since $\varphi(x)$ is zero outside $\Lambda$, we have

$$\begin{aligned} \sum_{i=1}^{d} \|\nabla_i^{(a)}\varphi\|^2_{l^2(\Lambda')} &= \sum_{i=1}^{d} a^d \sum_{x\in\Lambda'} \frac{|\varphi(x+ae_i) - \varphi(x)|^2}{a^2} \\ &= a^{d-2} \sum_{\substack{\{x,y\}\subset(a\mathbb{Z})^d \\ |x-y|=a}} |\varphi(y) - \varphi(x)|^2 \\ &= \langle \varphi, -\Delta^{(a)}\varphi\rangle. \end{aligned}$$

For $f \in H_0^1(D)$ we denote the $i^{th}$ directional gradient by $\nabla_i f$.

**Lemma 3.** *If* $f \in H_0^1(D)$, *then*

$$\lim_{a\to 0} \|\nabla^{(a)} f^{(a)}\|^2_{l^2(\Lambda')} = \|\nabla f\|^2_{L^2(D)}.$$

**Proof.** We need to show that for each $i = 1, ...., d$,

$$\lim_{a\to 0} \|\nabla_i^{(a)} f^{(a)}\|_{l^2(\Lambda')} = \|\nabla_i f\|_{L^2(D)}.$$

From lemma 2, we have

$$\lim_{a\to 0} \|(\nabla_i f)^{(a)}\|_{l^2(\Lambda)} = \|\nabla_i f\|_{L^2(D)},$$

so we need to show that for each $i = 1, ..., d$,

$$\lim_{a\to 0} \|(\nabla_i^{(a)} f^{(a)})\|_{l^2(\Lambda')} = \lim_{a\to 0} \|(\nabla_i f)^{(a)}\|_{l^2(\Lambda)}. \tag{4.4}$$

We will first prove (4.4) for a smooth function with compact support, since $H_0^1(D)$ is the closure of $C_c^\infty(D)$ in the $H^1$-norm. For a general function $f \in H_0^1(D)$, we will approximate $f$ with a function $g$ in $C_c^\infty(D)$. Notice that $\Lambda' \setminus \Lambda \to 0$ as $a \to 0$.

First, let $f \in C_c^\infty(D)$. We have for $x \in \Lambda$,

$$\nabla_i^{(a)} f^{(a)}(x) = \frac{f^{(a)}(x + a\,e_i) - f^{(a)}(x)}{a} = \frac{1}{a^d} \int_{C^a(x)} \frac{f(y + a\,e_i) - f(y)}{a}\, dy,$$

so we get

$$|\nabla_i^{(a)} f^{(a)}(x) - (\nabla_i f)^{(a)}(x)| = \frac{1}{a^d} \left| \int_{C^a(x)} \left[ \frac{f(y + a\,e_i) - f(y)}{a} - \nabla_i f(y) \right] dy \right| .$$

By applying the first order Taylor's formula we obtain

$$\lim_{a \to 0} \|\nabla_i^{(a)} f^{(a)}\|_{l^2} = \lim_{a \to 0} \|(\nabla_i f)^{(a)}\|_{l^2} \quad \text{for} \quad f \in C_c^\infty(D).$$

Now, let $f$ be any function in $H_0^1(D)$ and suppose that $g \in C_c^\infty(D)$ is the approximation of $f$ in the $H^1$-norm. Recall that the $H^1$-norm is given by

$$\|f\|_{H^1(D)} = \left( \int_D |f(x)|^2 dx + \int_D |\nabla f(x)|^2 dx \right)^{\frac{1}{2}} .$$

Then $\|\nabla f - \nabla g\|_{L^2(D)} < \epsilon$ for $\epsilon > 0$. By lemma 1,

$$\|(\nabla_i f)^{(a)} - (\nabla_i g)^{(a)}\|_{l^2(\Lambda)} \le \|\nabla_i f - \nabla_i g\|_{L^2(D)} \le \|\nabla f - \nabla g\|_{L^2(D)} < \epsilon.$$

Furthermore, by Jensen's inequality and the Fundamental theorem of calculus for distributions,

$$\begin{aligned}
&\left| \nabla_i^{(a)} f^{(a)}(x) - \nabla_i^{(a)} g^{(a)}(x) \right|^2 \\
&\le \frac{1}{a^d} \int_{C^a(x)} \left| \frac{f(y + a\,e_i) - f(y) - (g(y + a\,e_i) - g(y))}{a} \right|^2 dy \\
&= \frac{1}{a^d} \int_{C^a(x)} \left| \int_0^1 [\nabla_i f(y + t\,a\,e_i) - \nabla_i g(y + t\,a\,e_i)]\, dt \right|^2 dy \\
&\le \frac{1}{a^d} \int_{C^a(x)} \int_0^1 \left| \nabla_i f(y + t\,a\,e_i) - \nabla_i g(y + t\,a\,e_i) \right|^2 dt\, dy
\end{aligned}$$

.

Next,

$$\begin{aligned}
&\|\nabla_i^{(a)} f^{(a)} - \nabla_i^{(a)} g^{(a)}\|^2_{l^2(\Lambda)} \\
&\leq \int_D \int_0^1 \left|\nabla_i f(y + t\, a\, e_i) - \nabla_i g(y + t\, a\, e_i)\right|^2 \, dt\, dy \\
&= \int_0^1 \int_D \left|\nabla_i f(y + t\, a\, e_i) - \nabla_i g(y + t\, a\, e_i)\right|^2 \, dy\, dt < \epsilon^2.
\end{aligned}$$

Here $\nabla_i f(y + t\, a\, e_i) = \nabla_i g(y + t\, a\, e_i) = 0$ for $(y + t\, a\, e_i)$ located outside $D$. Now, by proceeding as in lemma 2, the lemma is proved for any function $f \in H_0^1(D)$. □

**Proof of proposition 1.** We will first prove the proposition for $N = 1$.

Let $f_1 \in H_0^1(D)$ be the eigenvector of $-\Delta$ with minimum eigenvalue (which is equal to $S_1$), and let $f_1^{(a)}$ be the function in $l^2(\Lambda)$ as defined above. The minimum eigenvalue on the lattice is equal to $S_1^{(a)}$. By lemma 3,

$$S_1 = \|\nabla f_1\|^2_{L^2(D)} = \lim_{a \to 0} \|\nabla^{(a)} f_1^{(a)}\|^2_{l^2(\Lambda')} = \lim_{a \to 0} \frac{\|\nabla^{(a)} f_1^{(a)}\|^2_{l^2(\Lambda')}}{\|f_1^{(a)}\|^2_{l^2(\Lambda')}} \|f_1^{(a)}\|^2_{l^2(\Lambda')}.$$

By lemma 2,

$$\lim_{a \to 0} \|f_1^{(a)}\|^2_{l^2(\Lambda')} = \|f_1\|^2_{L^2(D)} = 1$$

while

$$\frac{\|\nabla^{(a)} f_1^{(a)}\|^2_{l^2(\Lambda')}}{\|f_1^{(a)}\|^2_{l^2(\Lambda')}} \geq S_1^{(a)}.$$

We take lim sup since we do not know yet if $S_1^{(a)}$ converges as $a \to 0$. We obtain

$$S_1 \geq \limsup_{a \to 0} S_1^{(a)},$$

so the proposition is proved for $N = 1$.

Now let $\lambda_1, ..., \lambda_N$ denote the $N$ lowest eigenvalues of $-\Delta$ with corresponding eigenfunctions $f_1, ..., f_N \in H_0^1(D)$ respectively. Let $f_1^{(a)}, ..., f_N^{(a)}$ be functions in $l^2(\Lambda)$ obtained from the continuum functions $f_1, ..., f_N$ respectively as defined in this section. We will use the Gram-Schmidt process in order to orthonormalize the lattice functions $f_1^{(a)}, ..., f_N^{(a)}$.

Define

$\psi_1^{(a)} = \dfrac{f_1^{(a)}}{\|f_1^{(a)}\|_{l^2(\Lambda)}}$. Having defined $\psi_1^{(a)}, ..., \psi_{N-1}^{(a)}$ set

$\psi_N^{(a)} = \dfrac{\psi_N'^{(a)}}{\|\psi_N'^{(a)}\|_{l^2(\Lambda)}}$ with $\psi_N'^{(a)} = f_N^{(a)} - \sum_{i=1}^{N-1} \langle f_N^{(a)}, \psi_i^{(a)} \rangle \psi_i^{(a)}$.

Then $\psi_1^{(a)}, ..., \psi_N^{(a)}$ are orthonormal functions in $l^2(\Lambda)$. We will need the following lemma:

**Lemma 4.** $\forall N \in \mathbb{N}$,

$(a)$ $\lim_{a \to 0} \|\psi_i'^{(a)}\|_{l^2(\Lambda)} = 1 \quad \forall i \leq N.$

$(b)$ $\lim_{a \to 0} \langle f_i^{(a)}, \psi_j'^{(a)} \rangle = 0 \quad \forall i > j \leq N.$

$(c)$ $\lim_{a \to 0} \|\nabla^{(a)} \psi_i'^{(a)}\|_{l^2(\Lambda')} = \lim_{a \to 0} \|\nabla^{(a)} f_i^{(a)}\|_{l^2(\Lambda')} \quad \forall i \leq N.$

**Proof.** We will prove the lemma by induction. The statement is true for $N = 1$. Suppose the statement is true for $N = M$.

Part $(a)$. Recall that $\|f^{(a)}\|_{l^2(\Lambda)} = \|f^{(a)}\|_{L^2(D)}$. We have,

$$\begin{aligned}\left| \|\psi_{M+1}'^{(a)}\|_{l^2(\Lambda)} - 1 \right| &= \left| \|\psi_{M+1}'^{(a)}\|_{l^2(\Lambda)} - \|f_{M+1}\|_{L^2(D)} \right| \\ &\leq \|f_{M+1}^{(a)} - f_{M+1}\|_{L^2(D)} - \sum_{i=1}^{M} \left| \langle f_{M+1}^{(a)}, \psi_i^{(a)} \rangle \right| \|\psi_i^{(a)}\|_{L^2(D)}.\end{aligned}$$

The latter term converges to 0 as $a \to 0$ by lemma 2 and by the assumption.

Part $(b)$. We have for $i > M + 1$,

$$\langle f_i^{(a)}, \psi_{M+1}'^{(a)} \rangle \leq \langle f_i^{(a)}, f_{M+1}^{(a)} \rangle - \langle f_i^{(a)}, \sum_{k=1}^{M} \langle f_{M+1}^{(a)}, \psi_k^{(a)} \rangle \psi_k^{(a)} \rangle.$$

The latter term converges to 0 as $a \to 0$ by the polarization identity and by the assumption.

Part $(c)$. We have

$$\left| \|\nabla^{(a)} \psi_{M+1}'^{(a)}\|_{l^2(\Lambda')} - \|\nabla^{(a)} f_{M+1}^{(a)}\|_{l^2(\Lambda')} \right| \leq \sum_{j=1}^{M} \left| \langle f_{M+1}^{(a)}, \psi_j^{(a)} \rangle \right| \|\nabla^{(a)} \psi_j^{(a)}\|_{l^2(\Lambda')}.$$

The latter term converges to 0 as $a \to 0$ by the assumption. $\square$

Now we will prove the proposition for any $N \geq 1$. By using the same method as for the case $N = 1$ and applying lemma 4 we obtain

$$\begin{aligned} S_N = \sum_{i=1}^{N} \lambda_i = \sum_{i=1}^{N} \|\nabla f_i\|^2_{L^2(D)} &= \lim_{a\to 0} \sum_{i=1}^{N} \|\nabla^{(a)} f_i^{(a)}\|^2_{l^2(\Lambda')} \\ &= \lim_{a\to 0} \sum_{i=1}^{N} \|\nabla^{(a)} \psi_i^{(a)}\|^2_{l^2(\Lambda')} \end{aligned}$$

where

$$\sum_{i=1}^{N} \|\nabla^{(a)} \psi_i^{(a)}\|^2_{l^2(\Lambda')} \geq S_N^{(a)}.$$

We do not know yet if $S_N^{(a)}$ converges so we take $\limsup$. Hence we obtain

$$S_N \geq \limsup_{a\to 0} S_N^{(a)}.$$

$\square$

**Proposition 2.** *For any open, bounded domain $D$, and any $N \geq 1$,*

$$S_N \leq \liminf_{a\to 0} S_N^{(a)}.$$

The strategy is as follows. For a given function $\varphi \in l^2(\Lambda)$, we will construct a function $\varphi^{(a)} \in H_0^1(D)$ such that $\lim_{a\to 0} \|\varphi^{(a)}\|_{L^2} = 1$ and $\|\nabla \varphi^{(a)}\|_{L^2} \leq \|\nabla^{(a)} \varphi\|_{l^2}$. Before we give the proof of Proposition 2, we will construct the function $\varphi^{(a)}$.

Let $C^a(x)$ be a cubic cell of size $a > 0$, centered around $x \in D$. For any $\varphi \in l^2(\Lambda)$, we will extend $\varphi$ to a piecewise constant function in $L^2(D)$ by letting $\varphi(y) = \varphi(x)$ for $x \in \Lambda$ and for all $y \in C^a(x)$. We will let $\varphi$ vanish on $(a\mathbb{Z})^d \setminus \Lambda$. In order to smoothen the function $\varphi$, we will define the following convolution:

**Definition.** For any $x \in D$, and $\varphi \in l^2(\Lambda)$ we define

$$\varphi^{(a)}(x) = \frac{1}{a^d} \int_{C^a(x)} \varphi(y)\, dy = \left[\frac{1}{a^d} \chi_{C^a(0)} * \varphi\right](x), \tag{4.5}$$

where $\chi_{C^a(0)}$ is the characteristic function on $C^a(0)$.

Note that $\varphi^{(a)}(x) = \varphi(x)$ when $x \in \Lambda$. We also note that by the definition of $\Lambda$, $\varphi^{(a)}(x)$ vanishes on the boundary of D and outside D. In addition, $\varphi^{(a)}(x)$ will tend to zero when x approaches the boundary of D. It is proved in [19] that $\varphi^{(a)}$ is jointly continuous in $a > 0$ and $x$.

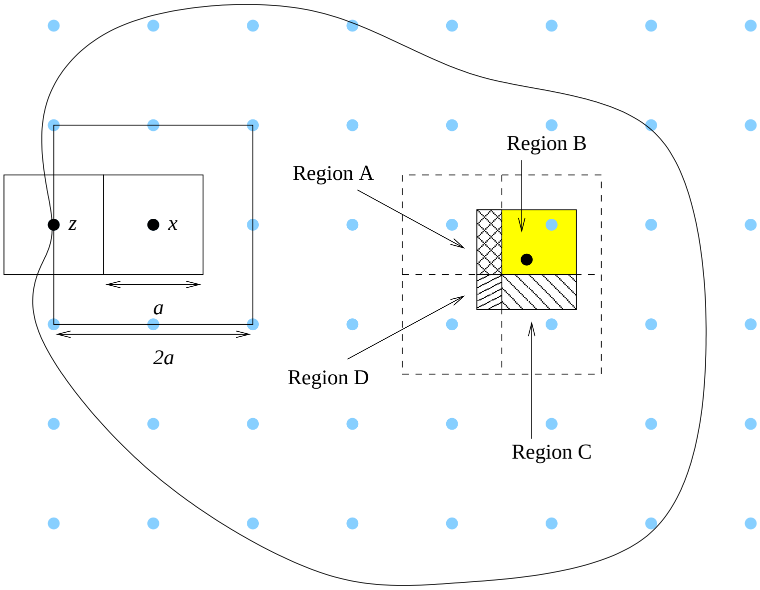

Figure 4.1. This picture shows the domain $D$ and the lattice in two dimensions. We can place a unit cube of size $2a$ centered around the point $x$. In this case the point $x$ is located on the lattice which means that this is the closest we can put any of the points of $\Lambda$ to the boundary of $D$. For the right part of the picture; if the point is located at the black dot in region $B$, the value of $\varphi^{(a)}$ at that point is defined as the average value of $\varphi$ on the region $A, B, C, D$. The value of $\varphi^{(a)}$ defined at the boundary point $z$ will be zero since the unit cube centered around $z$ will not intersect any unit cube centered around points in $\Lambda$.

**Lemma 5.**

$$\varphi^{(a)} \in H_0^1(D) \quad \textit{for any} \quad a > 0.$$

**Proof of lemma 5.** We have that $\varphi^{(a)}(x)$ is jointly continuous in $a > 0$ and $x$, and that $\varphi^{(a)}(x)$ goes to zero when x approaches the boundary of D. Therefore, it is enough to show that $\varphi^{(a)} \in H^1(D)$. We also have that $\varphi^{(a)} \in L^2(D)$, so we only have to prove that $\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} |k|^2 |\widehat{\varphi^{(a)}}(k)|^2 < \infty$.

The Fourier transform of $\varphi^{(a)}$ is given by

$$\widehat{\varphi^{(a)}}(k) = \frac{1}{a^d} \widehat{\chi}_{C^a(0)}(k) \widehat{\varphi}(k), \tag{4.6}$$

where

$$\frac{1}{a^d} \widehat{\chi}_{C^a(0)}(k) = \prod_{i=1}^{d} \left( \frac{\sin\left(\frac{a\,k_i}{2}\right)}{\frac{a\,k_i}{2}} \right). \tag{4.7}$$

Now suppose that we can prove that if $0 \le a_i \le b_i, \quad i = 1, ..., d$ then

$$\prod_{i=1}^{d} \frac{a_i}{b_i} \le \frac{\sum_{i=1}^{d} a_i}{\sum_{i=1}^{d} b_i}. \tag{4.8}$$

Then by letting $a_i = |\sin \frac{ak_i}{2}|^2$ and $b_i = \left|\frac{ak_i}{2}\right|^2$, we obtain from (4.7)

$$|k|^2 \prod_{i=1}^{d} \frac{\left|\sin\left(\frac{a\,k_i}{2}\right)\right|^2}{\left|\frac{a\,k_i}{2}\right|^2} \le \frac{4}{a^2} \sum_{i=1}^{d} \left|\sin \frac{ak_i}{2}\right|^2 \le \frac{4d}{a^2}. \tag{4.9}$$

By Parseval's identity and (4.6), (4.7), (4.9), we have

$$\begin{aligned} \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} |k|^2 \, |\widehat{\varphi^{(a)}}(k)|^2 \, dk &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} |\widehat{\varphi(k)}|^2 |k|^2 \prod_{i=1}^{d} \frac{\left|\sin\left(\frac{a\,k_i}{2}\right)\right|^2}{\left|\frac{a\,k_i}{2}\right|^2} \, dk \\ &\le \frac{4d}{a^2} \int_D |\varphi(x)|^2 \, dx. \end{aligned}$$

Hence, $\varphi^{(a)} \in H_0^1(D)$ for any $a > 0$. □

Now will prove the statement in (4.8)

**Lemma 6.** *Suppose that* $0 \le a_i \le b_i$ *for* $i = 1, ..., d$. *Then*

$$\prod_{i=1}^{d} \frac{a_i}{b_i} \le \frac{\sum_{i=1}^{d} a_i}{\sum_{i=1}^{d} b_i}.$$

**Proof.** Since $\frac{a_i}{b_i} \le 1$, the logarithm is negative. By using that fact and Jensen's inequality we obtain

$$\begin{aligned}\log \prod_{i=1}^{d} \frac{a_i}{b_i} = \sum_{i=1}^{d} \log \frac{ai}{b_i} &\le \sum_{i=1}^{d} \frac{b_i}{\sum_j b_j} \log \frac{a_i}{b_i} \\ &\le \log \sum_{i=1}^{d} \frac{b_i}{\sum_j b_j} \frac{a_i}{b_i} \\ &= \log \frac{\sum_i a_i}{\sum_i b_i}.\end{aligned}$$

□

Recall that for $\varphi \in l^2(\Lambda)$, $\|\varphi\|_{l^2(\Lambda)} = \|\varphi\|_{L^2(D)}$.

**Lemma 7.** *If* $\varphi \in l^2(\Lambda)$, *then*

$$\|\varphi - \varphi^{(a)}\|^2_{L^2(D)} \le a^d \sum_{\substack{x,y\in\Lambda \\ |x-y|_\infty = a}} |\varphi(x) - \varphi(y)|^2 \le a^2\, C_d \langle \varphi, -\Delta^{(a)} \varphi \rangle, \tag{4.10}$$

where the constant $C_d$ depends on the dimension.

**Proof of lemma 7.** The first inequality in (4.10) can be calculated by applying Jensen's inequality. We obtain

$$\begin{aligned}\|\varphi - \varphi^{(a)}\|^2_{L^2(D)} &= \int_D \left|\varphi(x) - \varphi^{(a)}(x)\right|^2 dx \\ &= \int_D \left| \frac{1}{a^d} \int_{C^a(x)} [\varphi(x) - \varphi(y)]\, dy \right|^2 dx \\ &\le \int_D \int_{C^a(x)} \frac{1}{a^d} |\varphi(x) - \varphi(y)|^2\, dy\, dx \\ &= \sum_{x,y\in\Lambda} |\varphi(x) - \varphi(y)|^2 \frac{1}{a^d} \int_{C^a(x)} \int_{C^a(y)} \chi_{\left[|x'-y|'_\infty \le \frac{a}{2}\right]}\, dx'\, dy' \\ &\le a^d \sum_{\substack{x,y\in\Lambda \\ |x-y|_\infty = a}} |\varphi(x) - \varphi(y)|^2.\end{aligned}$$

We will calculate $C_2$; Recall that

$$\langle \varphi, -\Delta^{(a)}\varphi\rangle = a^{d-2} \sum_{\substack{\{x,y\}\subset (a\mathbb{Z})^d \\ |x-y|=a}} |\varphi(x)-\varphi(y)|^2.$$

We have

$$\begin{aligned} \sum_{x,y\in\Lambda, |x-y|_\infty = a} |\varphi(x)-\varphi(y)|^2 = & \sum_{\substack{x,y\in\Lambda \\ |x-y|=a}} |\varphi(x)-\varphi(y)|^2 \\ & + \sum_{\substack{x,y\in\Lambda \\ |x-y|_2=\sqrt{2}a}} |\varphi(x)-\varphi(y)|^2. \end{aligned} \tag{4.11}$$

Since

$$|m+n|^2 \leq 2^2 \max\{|m|^2, |n|^2\} \leq 2^2(|m^2|+|n|^2),$$

we have

$$|\varphi(x)-\varphi(y)|^2 \leq 2^2\left(|\varphi(x)-\varphi(z)|^2 + |\varphi(z)-\varphi(y)|^2\right).$$

By using this, the term in (4.11) can be calculated:

$$\begin{aligned} & \sum_{\substack{x,y\in\Lambda \\ |x-y|_2=\sqrt{2}a}} |\varphi(x)-\varphi(y)|^2 \\ \leq\ & 2^2 \sum_{\substack{x,z,y\in\Lambda \\ |x-z|=a, |z-y|=a}} \left[ |\varphi(x)-\varphi(z)|^2 + |\varphi(z)-\varphi(y)|^2 \right] \\ \leq\ & 4\cdot 2^2 \left[ \sum_{\substack{x,z\in\Lambda \\ |x-z|=a}} |\varphi(x)-\varphi(z)|^2 + \sum_{\substack{z,y\in\Lambda \\ |y-z|=a}} |\varphi(z)-\varphi(y)|^2 \right] \\ \leq\ & 16\cdot 2 \left[ \sum_{\substack{\{x,z\}\subset(a\mathbb{Z})^d \\ |x-z|=a}} |\varphi(x)-\varphi(z)|^2 + \sum_{\substack{\{z,y\}\subset(a\mathbb{Z})^d \\ |y-z|=a}} |\varphi(z)-\varphi(y)|^2 \right]. \end{aligned}$$

Hence, we obtain $C_2 = 66$. We can use the same method to find $C_d$ for other dimensions than $d = 2$. □

**Lemma 8.** *If* $\varphi \in l^2(\Lambda)$, *then*

$$\|\nabla_i \varphi^{(a)}\|_{L^2(D)} \leq \|\nabla_i^{(a)} \varphi\|_{L^2(D)} \quad \forall \quad 1 \leq i \leq d.$$

**Proof of lemma 8.** We will prove the lemma for $i = 1$. Let $C_1^a(x)$ be the $(d-1)$ dimensional cube centered at $x$ in the direction perpendicular to $e_1$. We have for $\varphi \in l^2(\Lambda)$,

$$[\nabla_1 \varphi^{(a)}](x) = \frac{1}{a^d} \int_{C_1^a(x)} \left[ \varphi\left( y + \frac{1}{2} a\, e_1 \right) - \varphi(y - \frac{1}{2}\, ae_1) \right] dy_2 ... dy_d.$$

By Jensen's inequality,

$$\begin{aligned}
\|\nabla_1 \varphi^{(a)}\|_{L^2(D)}^2 &= \int_D \left| \int_{C_1^a(x)} \frac{\left[\varphi(y + \frac{1}{2}\, ae_1) - \varphi(y - \frac{1}{2}\, ae_1)\right]}{a} \frac{dy_2 ... dy_d}{a^{d-1}} \right|^2 dx \\
&\leq \int_{\mathbb{R}^d} \int_{C_1^a(x)} \left| \frac{\left[\varphi(y + \frac{1}{2}\, ae_1) - \varphi(y - \frac{1}{2}\, ae_1)\right]}{a} \right|^2 \frac{dy_2 ... dy_d}{a^{d-1}}\, dx \\
&= \int_{\mathbb{R}^d} \left| [\nabla_1^{(a)} \varphi](y) \right|^2 dy \int_{C_1^a(y)} \frac{dx_2 ... dx_d}{a^{d-1}} \\
&= \|\nabla_1^{(a)} \varphi\|_{L^2(D)}^2.
\end{aligned}$$

$\square$

**Proof of proposition 2.** We will prove

$$S_N \leq \liminf_{a \to 0} S_N^{(a)}.$$

We will first prove the proposition for $N = 1$. Let $\varphi \in l^2(\Lambda)$ be the eigenvector of $-\Delta^{(a)}$ with minimum eigenvalue (which is equal to $S_1^{(a)}$), and let $\varphi^{(a)}$ be the function in $H_0^1(D)$ as defined above. The minimum eigenvalue in the continuum is equal to $S_1$. Then by lemma 8,

$$\begin{aligned}
S_1^{(a)} = \|\nabla^{(a)} \varphi_1\|_{l^2(\Lambda')}^2 &\geq \|\nabla \varphi_1^{(a)}\|_{L^2(D)}^2 \\
&= \frac{\|\nabla \varphi_1^{(a)}\|_{L^2(D)}^2}{\|\varphi_1^{(a)}\|_{L^2(D)}^2} \|\varphi_1^{(a)}\|_{L^2(D)}^2 \\
&\geq S_1 \|\varphi_1^{(a)}\|_{L^2(D)}^2.
\end{aligned}$$

The term $\|\varphi_1^{(a)}\|_{L^2(D)}^2$ converges to 1 as $a \to 0$ : By lemma 7,

$$\left|\|\varphi_1^{(a)}\|_{L^2(D)} - 1\right| = \left|\|\varphi_1^{(a)}\|_{L^2(D)} - \|\varphi_1\|_{l^2(\Lambda)}\right| \leq \|\varphi_1^{(a)} - \varphi_1\|_{L^2(D)} \leq a\sqrt{C_d \lambda_1^{(a)}}.$$

By proposition 1,

$$\limsup_{a\to 0} \left|\|\varphi_1^{(a)}\|_{L^2(D)} - 1\right| \leq \lim_{a\to 0} a\sqrt{C_d\lambda_1} = 0.$$

So the proposition is proved for $N = 1$.

Now, let $\lambda_1^{(a)}, ..., \lambda_N^{(a)}$ denote the $N$ lowest lattice eigenvalues with corresponding eigenfunctions $\varphi_1, ..., \varphi_N \in l^2(\Lambda)$ respectively. Let $\varphi_1^{(a)}, ..., \varphi_N^{(a)}$ be functions in $H_0^1(D)$ obtained from the lattice functions $\varphi_1, ..., \varphi_N$ respectively as defined is this section. We will use the Gram-Schmidt process in order to orthonormalize the continuum functions $\varphi_1^{(a)}, ...., \varphi_N^{(a)}$. Define

$\psi_1^{(a)} = \dfrac{\varphi_1^{(a)}}{\|\varphi_1^{(a)}\|_{L^2(D)}}$. Having defined $\psi_1^{(a)}, ..., \psi_{N-1}^{(a)}$, set

$$\psi_N^{(a)} = \frac{\psi_N'^{(a)}}{\|\psi_N'^{(a)}\|_{L^2(D)}} \text{ with } \psi_N'^{(a)} = \varphi_N^{(a)} - \sum_{i=1}^{N-1} \langle \varphi_N^{(a)}, \psi_i^{(a)} \rangle \psi_i^{(a)}.$$

Then $\psi_1^{(a)}, ..., \psi_N^{(a)}$ are orthonormal functions in $H_0^1(D)$. We will need the following lemma:

**Lemma 9.** $\forall N \in \mathbb{N}$,

(a) $\lim_{a\to 0} \|\psi_i'^{(a)}\|_{L^2(D)} = 1 \quad \forall i \leq N.$

(b) $\lim_{a\to 0} \langle \varphi_i^{(a)}, \psi_j'^{(a)} \rangle = 0 \quad \forall i > j \leq N.$

(c) $\lim_{a\to 0} \|\nabla \psi_i'^{(a)}\|_{L^2(D)} = \lim_{a\to 0} \|\nabla \varphi_i^{(a)}\|_{L^2(D)} \quad \forall i \leq N.$

**Proof.** We will prove the lemma by using induction. The statement is true for $N = 1$. Suppose the statement is true for $N = M$.

Part $(a)$. We have

$$\begin{aligned}\left| \|\psi'^{(a)}_{M+1}\|_{L^2(D)} - 1 \right| &= \left| \|\psi'^{(a)}_{M+1}\|_{L^2(D)} - \|\varphi_{M+1}\|_{l^2(\Lambda)} \right| \\ &\leq \|\varphi^{(a)}_{M+1} - \varphi_{M+1}\|_{L^2(D)} - \sum_{i=1}^{M} \left| \langle \varphi^{(a)}_{M+1}, \psi^{(a)}_i \rangle \right| \|\psi^{(a)}_i\|_{L^2(D)}.\end{aligned}$$

The latter term converges to 0 as $a \to 0$ by proposition 1 and by the assumption.

Part $(b)$. We have for $i > M+1$,

$$\langle \varphi^{(a)}_i, \psi'^{(a)}_{M+1} \rangle \leq \langle \varphi^{(a)}_i, \varphi^{(a)}_{M+1} \rangle - \langle \varphi^{(a)}_i \sum_{k=1}^{M} \langle \varphi^{(a)}_{M+1}, \psi^{(a)}_k \rangle \psi^{(a)}_k \rangle.$$

The latter term converges to 0 as $a \to 0$ by the polarization identity and by the assumption.

Part $(c)$. We have

$$\left| \|\nabla \psi'^{(a)}_{M+1}\|_{L^2(D)} - \|\nabla \varphi^{(a)}_{M+1}\|_{L^2(D)} \right| \leq \sum_{j=1}^{M} \left| \langle \varphi^{(a)}_{M+1}, \psi^{(a)}_j \rangle \right| \|\nabla \psi^{(a)}_j\|_{L^2(D)}.$$

The latter term converges to 0 as $a \to 0$ by proposition 1 and by the assumption. □

Now we will prove proposition 2 for any $N \geq 1$. We have by lemma 8,

$$\begin{aligned}S^{(a)}_N = \sum_{i=1}^{N} \lambda^{(a)}_i &= \sum_{i=1}^{N} \|\nabla^{(a)} \varphi_i\|^2_{l^2(\Lambda')} \\ &\geq \sum_{i=1}^{N} \|\nabla \varphi^{(a)}_i\|^2_{L^2(D)}.\end{aligned}$$

When we take the $\liminf$ of the expression above we obtain, by applying the same method as for the case $N = 1$, and lemma 9:

$$\liminf_{a \to 0} S^{(a)}_N \geq \liminf_{a \to 0} \sum_{i=1}^{N} \|\nabla \psi^{(a)}_i\|^2_{L^2(D)} \geq S_N.$$

□

## 5. On the lower bound for the sum of lowest eigenvalues.

Freericks, Lieb, Ueltschi [12] proved in 2002, that the sum of the $N$ lowest eigenvalues of the Discrete Laplacian defined on a finite subset, $\Lambda$, of the infinite lattice is bounded below by a term proportional to the volume of the domain ('bulk term') and a term proportional to the boundary ('boundary correction'). In 2004, Ueltschi [13] improved the 'boundary correction'.

Freericks, Lieb, Ueltschi [12] and Ueltschi [13] proved the following theorem :

**Theorem 2.** *For every* $N \geq 1$,

$$S_N^{(a)} \geq |\Lambda| a^d e^{(a)}(\rho^{(a)}) + C\, B(\Lambda) a^d (\rho^{(a)})^{\frac{2}{d}+1},$$

*where* $B(\Lambda) = |\{(x,y) : x \in \Lambda, y \in \Lambda^C, |x-y| = a\}|$, $\rho^{(a)} = \frac{N}{|\Lambda| a^d}$ *denotes the lattice density,* $e^{(a)}(\rho^{(a)})$ *denotes the lattice energy density of non-interacting electrons with density* $\rho$, *in the limit of infinite volume,* $|\Lambda|$ *is the volume of* $\Lambda$ *and* $C$ *is a constant.*

They proved that the constant, $C$, is strictly positive for all densities, but only for small densities do they have an explicit value of $C$.

In this section we will give the proof of the 'bulk term,' i.e we will show that for any $N \geq 1$

$$S_N^{(a)} \geq |\Lambda| a^d e^{(a)}(\rho^{(a)}).$$

Furthermore, we will show that the 'bulk term' in the lower bound for the sum of the $N$ lowest eigenvalues of the Discrete Laplacian converges to the 'bulk term' in the lower bound for the sum of the $N$ lowest eigenvalues of the Continuum Laplacian when $a \to 0$ while the 'boundary correction' tends to zero. The Discrete case is, therefore, more general than the continuum case. Recall from the previous chapter that we recovered $S_N$ from $S_N^{(a)}$ in the continuum limit. In other words, we will recover

$S_N \geq |D| e(\rho)$ in the continuum limit $a \to 0$ where $e(\rho)$ denotes the energy density in the continuum of density $\rho = \frac{N}{|D|}$, in the limit of infinite volume.

**Proof of Theorem 2 without the boundary correction .** The proof follows that of Freericks, Lieb and Ueltschi's [12] and Lieb and Loss's [14].

Recall that the Fourier transform of $\varphi \in l^2(\Lambda)$ is defined by:

$$\widehat{\varphi}(k) = a^d \sum_{x \in \Lambda} e^{ikx} \varphi(x), \qquad k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]^d.$$

and the inverse-transform is

$$\varphi(x) = \frac{1}{(2\pi)^d} \int_{[-\frac{\pi}{a}, \frac{\pi}{a}]^d} \widehat{\varphi}(k) e^{-ikx}\, dk, \qquad x \in \Lambda$$

A function $\varphi \in l^2(\Lambda)$ can be considered to be in $l^2[(a\mathbb{Z})^d]$ by letting $\varphi = 0$ outside $\Lambda$. The energy of a particle in a state $\varphi_i \in l^2(\Lambda)$ is given by

$$\lambda_j^{(a)} = \langle \varphi_j, -\Delta^{(a)} \varphi_j \rangle = \frac{1}{(2\pi)^d} \int_{[-\frac{\pi}{a}, \frac{\pi}{a}]^d} \varepsilon_k^{(a)}\, |\widehat{\varphi_j}(k)|^2\, dk.$$

This can be proved by applying Plancherel's identity, since we have $[-(\widehat{\Delta^{(a)} \varphi_j})(k)] = \varepsilon_k^{(a)} \widehat{\varphi_j}(k)$.

Eigenfunctions with different eigenvalues are orthonormal and we can take the eigenfunctions with the same eigenvalues to be orthonormal so that we have an orthonormal set. We have that the energy $S_N^{(a)}(\varphi_1, ..., \varphi_N)$ of N orthonormal functions $\varphi_1, ...., \varphi_N \in l^2(\Lambda)$ is given by

$$S_N^{(a)}(\varphi_1, ..., \varphi_N) = \frac{1}{(2\pi)^d} \int_{\left[-\frac{\pi}{a}, \frac{\pi}{a}\right]^d} \varepsilon_k^{(a)} \varrho(k),$$

where

$$\varrho(k) = \sum_{j=1}^{N} |\widehat{\varphi_j}(k)|^2.$$

The function $\varrho(k)$ satisfies the following equations:

$$\frac{1}{(2\pi)^d} \int_{[-\frac{\pi}{a}, \frac{\pi}{a}]^d} \varrho(k) dk = N. \tag{5.1}$$

$$0 \leq \varrho(k) \leq a^d|\Lambda|. \tag{5.2}$$

The first equation follows from Parseval's identity and the fact that $\varphi_j$ is a normalized function.

Since the eigenfunctions, $\varphi_i$, are orthonormal in $l^2(\Lambda)$, they can be completed to form an orthonormal basis, $\{\varphi_i\}_{i=1}^{\infty}$, in $l^2[(a\mathbb{Z})^d]$. Define the function $f_k : (a\mathbb{Z})^d \to \mathbb{C}$ by $f_k(x) = e^{-ikx}\chi_\Lambda(x)$, where $\chi_\Lambda(x)$ is the characteristic function on $\Lambda$ and $k \in [-\frac{\pi}{a}, \frac{\pi}{a}]^d$. Then $\widehat{\varphi_j}(k) = \langle \varphi_j, f_k \rangle$. The upper bound of $\varrho$ can be found by using Bessel's inequality. We have

$$\varrho(k) = \sum_{j=1}^{N} |\widehat{\varphi_j}(k)|^2 = \sum_{j=1}^{N} |\langle \varphi_j, f_k \rangle|^2 \leq \|f_k\|^2_{l^2(\Lambda)} = a^d|\Lambda|.$$

We minimize $S_N^{(a)}(\varphi_1, ..., \varphi_N)$ over all $\varrho$ that satisfies the two conditions (5.1) and (5.2). Thus the ground state energy, $S_N^{(a)}$, of N orthonormal functions $\varphi_1, ...., \varphi_N$ is bounded below by

$$S_N^{(a)} \geq \inf_{\substack{\varrho : 0 \leq \varrho \leq |\Lambda| a^d \\ \frac{1}{(2\pi)^d}\int_{[-\frac{\pi}{a},\frac{\pi}{a}]^d} \varrho(k) = N}} \frac{1}{(2\pi)^d} \int_{[-\frac{\pi}{a},\frac{\pi}{a}]^d} \varrho(k)\, \varepsilon_k^{(a)}\, dk. \tag{5.3}$$

By applying the 'bathtub principle' [14] (See figure 5.1), we find the minimizer $\varrho_{min}$. It is given by

$$\varrho_{min}(k) = \begin{cases} |\Lambda| a^d, & \text{if } \varepsilon_k^{(a)} < \varepsilon_F^{(a)}(\rho^{(a)}) \\ 0, & \text{elsewhere} \end{cases} \tag{5.4}$$

Recall that the lattice Fermi level $\varepsilon_F^{(a)}(\rho^{(a)})$ is given by the following identity

$$\rho^{(a)} = \frac{1}{(2\pi)^d} \int_{\varepsilon_k^{(a)} < \varepsilon_F^{(a)}(\rho^{(a)})} dk.$$

Recall that the energy per site of a density $\rho^{(a)}$ of free electrons in $(a\mathbb{Z})^d$ is given by

$$e^{(a)}(\rho^{(a)}) = \frac{1}{(2\pi)^d} \int_{\varepsilon_k^{(a)} < \varepsilon_F^{(a)}(\rho^{(a)})} \varepsilon_k^{(a)} dk. \tag{5.5}$$

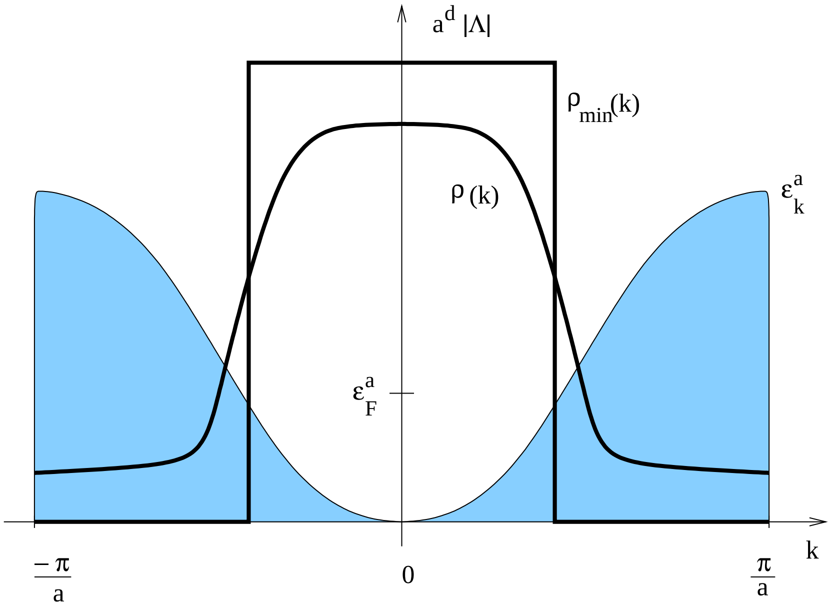

FIGURE 5.1. Bathtub principle. The figure shows the minimizer $\varrho_{min}(k)$ in one dimension.

By (5.3), (5.4) and (5.5) we get

$$S_N^{(a)} \geq |\Lambda| a^d e^{(a)}(\rho^{(a)}).$$

□

Now we will show that when we take the continuum limit $a \to 0$ of the right hand side of the inequality

$$S_N^{(a)} \geq |\Lambda| a^d e^{(a)}(\rho^{(a)}) + C\, B(\Lambda) a^d (\rho^{(a)})^{\frac{2}{d}+1},$$

we obtain $e(\rho)|D|$. To show this, we will need the next lemma which gives the relationship between $e(\rho^{(a)})$ and $e^{(a)}(\rho^{(a)})$ and between $\varepsilon_F(\rho^{(a)})$ and $\varepsilon_F^{(a)}(\rho^{(a)})$.

**Lemma 10.** *For any $\rho^{(a)}$ such that $\frac{1}{3}a^2\varepsilon_F^{(a)}(\rho^{(a)}) \leq 1$,we have*

*(a)* $\varepsilon_F(\rho^{(a)}) - \frac{1}{12}a^2\varepsilon_F^2(\rho^{(a)}) \leq \varepsilon_F^{(a)}(\rho^{(a)}) \leq \varepsilon_F(\rho^{(a)})$.

*(b)* $e(\rho^{(a)}) - \frac{4}{3}a^2\pi^2\frac{d}{d+4}\Gamma\left(\frac{d}{2}+1\right)^{\frac{4}{d}} {\rho^{(a)}}^{1+\frac{4}{d}} \leq e^{(a)}(\rho^{(a)}) \leq e(\rho^{(a)})$.

**Proof of lemma 10 (a).** It can be checked that $k^2 - \frac{1}{12}k^4 \leq 2 - 2\cos k \leq k^2$ and $|k|^4 \geq \sum_{i=1}^{d} k_i^4$. Then $|k|^2 - \frac{a^2}{12}|k|^4 \leq \varepsilon_k^{(a)} \leq |k|^2$. Recall that

$$\varepsilon_F(\rho^{(a)}) = 4\pi\,\Gamma\left(\frac{d}{2}+1\right)^{\frac{2}{d}} \rho^{(a)\,\frac{2}{d}} \tag{5.6}$$

and

$$\rho^{(a)} = \frac{1}{(2\pi)^d}\int_{\varepsilon_k^{(a)}<\varepsilon_F^{(a)}(\rho^{(a)})} dk.$$

We have

$$\frac{1}{(2\pi)^d}\int_{|k|^2<\varepsilon_F^{(a)}(\rho^{(a)})} dk \leq \rho^{(a)} \leq \frac{1}{(2\pi)^d}\int_{|k|^2-\frac{a^2}{12}|k|^4<\varepsilon_F^{(a)}(\rho^{(a)})} dk. \tag{5.7}$$

From the first inequality in (5.7) it follows that

$$\varepsilon_F^{(a)}(\rho^{(a)}) \leq \varepsilon_F(\rho^{(a)}).$$

In the latter integral in (5.7) we integrate over those $k's$ such that

$$|k|^2 \leq \frac{1-\sqrt{1-\frac{1}{3}\,a^2\varepsilon_F^{(a)}(\rho^{(a)})}}{\frac{a^2}{6}},$$

provided that $\frac{1}{3}a^2\,\varepsilon_F^{(a)}(\rho^{(a)}) \leq 1$. Then

$$\frac{1-\sqrt{1-\frac{1}{3}\,a^2\varepsilon_F^{(a)}(\rho^{(a)})}}{\frac{a^2}{6}} \geq \varepsilon_F(\rho^{(a)})$$

which implies that

$$-1+\frac{1}{3}a^2\,\varepsilon_F(\rho^{(a)}) - \frac{1}{36}a^4\varepsilon_F^2(\rho^{(a)}) \leq a^2\,\frac{1}{3}\varepsilon_F^{(a)}(\rho^{(a)}) - 1.$$

This proves (a). □

**Proof of lemma 10 (b).** By part (a), we have

$$e^{(a)}(\rho^{(a)}) = \int_0^{\rho^{(a)}} \varepsilon_F^{(a)}(t)\,dt \leq \int_0^{\rho^{(a)}} \varepsilon_F(t)\,dt = e(\rho^{(a)}).$$

We also have that

$$e^{(a)}(\rho^{(a)}) \geq \int_0^{\rho^{(a)}} \left[\varepsilon_F(t) - \frac{1}{12} a^2 \, \varepsilon_F^2(t)\right] \, dt.$$

By using the expression for $\varepsilon_F(t)$ given in (5.6), we obtain (b). $\square$

Recall that Freericks, Lieb, Ueltschi [12] and Ueltschi [13] proved that for any open, bounded domain $D$, and for every $N \geq 1$, and density $\rho^{(a)}$,

$$S_N^{(a)} \geq e^{(a)}(\rho^{(a)})|\Lambda|a^d + C\, B(\Lambda) a^d (\rho^{(a)})^{\frac{2}{d}+1} \tag{5.8}$$

where $B(\Lambda) = |\{(x,y) : x \in \Lambda, y \in \Lambda^C, |x-y| = a\}|$, and $C$ is a constant. When we take the continuum limit $a \to 0$ of (5.8) we obtain

$$S_N \geq e(\rho)|D|.$$

This is shown as follows: Since $\rho^{(a)} \to \rho$ we obtain by applying lemma 10,

$\lim_{a \to 0} e^{(a)}(\rho^{(a)}) = e(\rho).$

Hence, in the continuum limit $a \to 0$ we obtain

$$e^{(a)}(\rho^{(a)})|\Lambda|a^d \to e(\rho)|D|$$

and

$$C\,(\rho^{(a)})^{\frac{2}{d}+1} B(\Lambda) a^d = C\,(\rho^{(a)})^{\frac{2}{d}+1} \left[\frac{|\partial D|}{a^{d-1}} - o(1)\right] a^d \to 0.$$

We proved in Theorem 1 in section 4 that $S_N^{(a)} \to S_N$ when $a \to 0$. Thus, when we take the continuum limit $a \to 0$ of (5.8) we obtain $S_N \geq e(\rho)|D|$.

## 6. APPLICATION OF THE BATHTUB PRINCIPLE WITH GRADIENT TO THE PAPER OF MELAS.

In 2002, Melas [7] improved the lower bound for the sum of the $N$ lowest eigenvalues of the continuum Laplacian. Melas [7] proved that for any open bounded set $D \subseteq \mathbb{R}^d$ and any $k \geq 1$,

$$S_N \geq |D|e(\rho) + M_d N \frac{|D|}{I(D)},$$

where $I(D)$ denotes the 'moment of inertia of $D$,' that is $I(D) = \min_{a \in D} \int_D |x-a|^2 \, dx$, and the constant, $M_d$, depends on the dimension.

Let $\varrho(k) = \sum_{j=1}^{N} |\widehat{\varphi_j}(k)|^2$, where $\varphi_j(k)$ are the eigenfunctions of $-\Delta$ with corresponding eigenvalues $\lambda_j$. Recall from chapter 5 that in the discrete case we have $0 \leq \varrho(k) \leq a^d |\Lambda|$ and $\frac{1}{(2\pi)^d} \int_{[-\frac{\pi}{a}, \frac{\pi}{a}]^d} \varrho(k) \, dk = N$. We also recall that

$$S_N^{(a)} \geq \inf_{\varrho} \frac{1}{(2\pi)^d} \int_{[-\frac{\pi}{a}, \frac{\pi}{a}]^d} \varrho(k) \varepsilon_k^{(a)} \, dk,$$

where the infimum is taken over all $\varrho$ that satisfy these two constraints above. In the continuum case, the analog results are

$$0 \leq \varrho(k) \leq \frac{1}{(2\pi)^d} |D| \tag{6.1}$$

and

$$\int_{R^d} \varrho(k) \, dk = N. \tag{6.2}$$

Melas [7] also proved that

$$|\nabla \varrho(k)| \leq \frac{2}{(2\pi)^d} \sqrt{|D| I(D)} \tag{6.3}$$

which is the key-idea in improving the lower bound for $S_N$.

Melas [7] found and proved a lower bound for $S_N$ under the constraint in (6.1), (6.2) and (6.3). In his proof, Melas applied and proved a lemma finding a lower bound for the infimum $\int_{\mathbb{R}^d} |x|^2 g(x)\,dx$ over nonnegative, measurable functions $g$ on $\mathbb{R}^d$ under the constraint $0 \le g(x) \le 1, \quad |\nabla g(x)| \le \alpha, \quad \int_{\mathbb{R}^d} g(x)\,dx = G$, where $\alpha, G$ are positive constants.

In this chapter, the problem will be solved in a somewhat different way by using the bathtub principle with gradient [14]. The use of the bathtub principle will somewhat simplify the proof of the lemma done in the paper of Melas [7]. We will use the bathtub principle since the problem we are trying to solve is a minimization problem satisfying the conditions given therein.

We will first explain and give the proof of the bathtub principle with gradient. We will need the following lemma.

**Lemma 11.** *Let* $(\Omega, \sum, \mu)$ *be a measure space and let* $f$ *be any nonnegative, measurable function on* $\Omega$*. Then for any* $t \ge 0$

$$\int_\Omega f(x)\,d\mu(x) = \int_0^\infty \mu(\{x : f(x) > t\})\,dt.$$

**Proof.** We can write

$$f(x) = \int_0^\infty \chi_{[0,f(x)]}(t)\,dt.$$

Then by Tonelli, we have

$$\begin{aligned} \int_\Omega f(x)\,d\mu(x) &= \int_\Omega \int_0^\infty \chi_{[0,f(x)]}(t)\,dt\,d\mu(x) && (6.4)\\ &= \int_0^\infty \int_\Omega \chi_{[0,f(x)]}(t)\,d\mu(x)\,dt && (6.5)\\ &= \int_0^\infty \mu\{x : f(x) > t\}\,dt. && (6.6) \end{aligned}$$

□

We consider a measurable function $f : [0,\infty) \to [0,\infty)$ such that $r^{d-1} f(r)$ is strictly increasing; we define the functional

$$F(g) = \int_{\mathbb{R}^d} f(|x|) g(x)\,dx.$$

We are looking for the minimum of $F$ over nonnegative, measurable functions $g$ on $\mathbb{R}^d$ satisfying the constraint

$$0 \leq g(x) \leq 1, |\nabla g(x)| \leq \alpha, \int_{\mathbb{R}^d} g(x)\, dx = G,$$

where $\alpha$ and $G$ are given constants.

**Theorem 3** (Bathtub principle with gradient)**.** *There exists a unique minimizing function $g$ to the problem above. It is spherically symmetric. It is given by one of the following alternatives, where we let $|S_{d-1}|$ denote the volume of the unit sphere in $d$ dimensions.*

*(a)If $G\alpha^d \leq \frac{|S_{d-1}|}{d(d+1)}$, we have*

$$g(x) = \left\{ \begin{array}{ll} \alpha(r_2 - |x|), & \textit{if } |x| \leq r_2; \\ 0, & \textit{if } |x| \geq r_2; \end{array} \right\}$$

*and $r_2$ satisfies $r_2^{d+1} = \frac{d(d+1)G}{\alpha|S_{d-1}|}$.*

*(b)If $G\alpha^d > \frac{|S_{d-1}|}{d(d+1)}$, we have*

$$g(x) = \left\{ \begin{array}{ll} 1, & \textit{if } |x| \leq r_1; \\ 1 - \alpha(|x| - r_1), & \textit{if } r_1 \leq |x| \leq r_2; \\ 0, & \textit{if } |x| \geq r_2 \end{array} \right\}$$

*and $r_1, r_2$ satisfy $r_2 = r_1 + \frac{1}{\alpha}$, and $\int_{\mathbb{R}^d} g(x)\, dx = G$.*

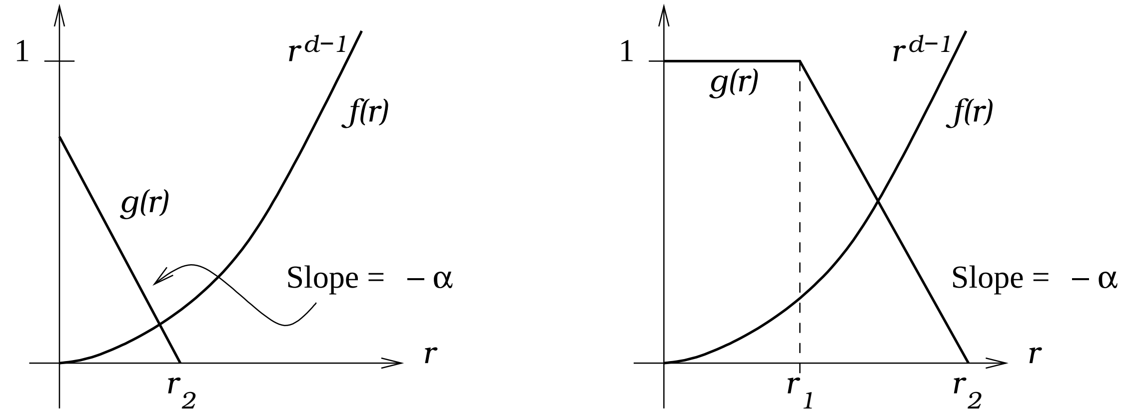

FIGURE 6.1. These pictures show the minimizer $g$ in one dimension. The first picture is the case $G\alpha^d \leq \frac{|S_{d-1}|}{d(d+1)}$. The second picture is the case $G\alpha^d > \frac{|S_{d-1}|}{d(d+1)}$.

**Proof.** Given $g$, let $g'$ be the spherically symmetric function obtained by averaging g over angular variables.

The averaged function, $g'$, satisfies the same conditions as $g$, and $F(g) = F(g')$. It is therefore enough to minimize $F$ over spherically symmetric functions. In spherical coordinates, we have

$$F(g) = |S_{d-1}| \int_0^\infty r^{d-1} f(r) g(r)\, dr.$$

Now we will follow the structure in the proof of the bathtub principle given in [20]. Given $g : [0,\infty) \to [0,1]$, we define the measure $d\mu_g = |S_{d-1}| g(r) r^{d-1} \mu$, where $\mu$ is the Lebesgue measure. Then $\mu_g([0,\infty)) = |S_{d-1}| \int_0^\infty g(r) r^{d-1} d\mu(r) = G$.

By lemma 11 we have,

$$\begin{aligned} F(g) = \int f(r)\, d\mu_g(r) &= \int_0^\infty \mu_g(\{r : f(r) > t\})\, dt \\ &= \int_0^\infty [G - \mu_g(\{r : f(r) \leq t\})]\, dt. \end{aligned}$$

To minimize $F$ it is sufficient to minimize the decreasing function $\mu_g(\{r : f(r) > t\})$ for each $t$. That is equivalent to maximize the increasing function

$\mu_g(\{r : f(r) \leq t\})$, i.e we want to maximize the integral of

$$\mu_g(\{r : f(r) \leq t\}) = |S_{d-1}| \int_0^{r(t)} r^{d-1} g(r)\, dr.$$

The maximizing measure is obtained when $g = 1$ so we would like to have $g = 1$ on a large set as possible. On the other hand we need $g$ to satisfy $|\nabla g(x)| \leq \alpha$. For any $t$, the function, $g$, given in the theorem is the optimal function, and it is the unique optimizer.

There cannot exist an optimizer that is not spherically symmetric; Suppose $g$ is not spherically symmetric, then

$$\sup_{x \in \mathbb{R}^d} |\nabla g'(x)| < \sup_{x \in \mathbb{R}^d} |\nabla g(x)|.$$

The maximal gradient of $g'$ is then strictly less than $\alpha$ so $g'$ cannot be a minimizer. But since $F(g) = F(g')$, $g$ is not a minimizer either. $\square$

Define the class, $\zeta$, of measurable functions, $g$, on $\mathbb{R}^d$ by,

$$\zeta = \left\{ g : 0 \leq g(x) \leq 1, |\nabla g(x)| \leq \alpha, \int_{\mathbb{R}^d} g(x) = G \right\}.$$

**Corollary 1.** *We have that*

$$I = \inf_{g \in \zeta} \int_{\mathbb{R}^d} |x|^2 g(x)\, dx,$$

*is given by one of the following alternatives.*

(a) *If* $G\alpha^d \leq \frac{|S_{d-1}|}{d(d+1)}$, *then*

$$I = \frac{(|S_{d-1}|\alpha)^{\frac{-2}{d+1}}}{(d+2)(d+3)} \left[Gd(d+1)\right]^{\frac{d+3}{d+1}},$$

*where* $|S_{d-1}|$ *is the volume of the unit sphere in* $d$ *dimensions.*

(b) *If* $G\alpha^d > \frac{|S_{d-1}|}{d(d+1)}$, *then*

$$I \geq |S_{d-1}|^{\frac{-2}{d}} \frac{1}{d+2} (dG)^{\frac{d+2}{d}} + \frac{G}{6(d+2)\alpha^2},$$

*where* $|S_{d-1}|$ *is the volume of the unit sphere in* $d$ *dimensions.*

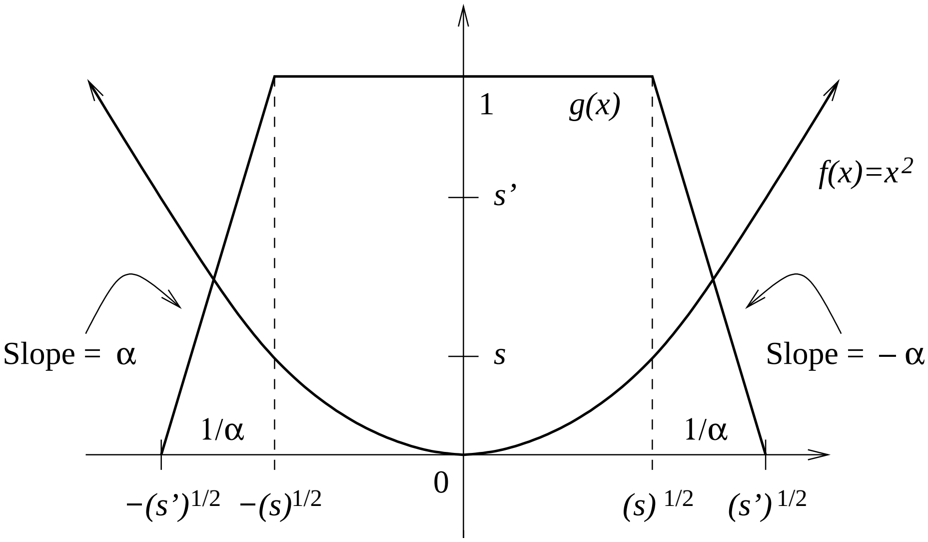

FIGURE 6.2. Bathtub Principle with gradient: The figure shows the minimizer $g(x)$ in one dimension for the problem in the corollary to Theorem 3. Here, $s'^{\frac{1}{2}} = r_2$ and $s^{\frac{1}{2}} = r_1$.

**Proof of corollary 1(a).** The minimizer $g$ is given by

$$g(x) = [\alpha\,(r_2 - |x|)]\chi_{(0,r_2)|x|}.$$

We have

$$\begin{aligned} I &= \int_{\mathbb{R}^d} |x|^2 g(x)\,dx \\ &= |S_{d-1}| \int_0^{r_2} r^2 r^{d-1} \alpha(r_2 - r)\,dr \\ &= \frac{|S_{d-1}|\alpha}{(d+2)(d+3)} r_2^{d+3}. \end{aligned}$$

By inserting $r_2 = \left(\frac{Gd(d+1)}{|S_{d-1}|\alpha}\right)^{\frac{1}{d+1}}$ into the equation above we obtain

$$I = \frac{(|S_{d-1}|\alpha)^{\frac{-2}{d+1}}}{(d+2)(d+3)} \left(Gd(d+1)\right)^{\frac{d+3}{d+1}}.$$

□

**Proof of corollary 1(b).** The minimizer $g$ is given by

$$g(x) = \chi_{(0,r_1)|x|} + [1 - \alpha(|x| - r_1)]\chi_{(r_1,r_2)|x|}.$$

We have

$$\begin{aligned} G &= \int_{\mathbb{R}^d} g(x)\,dx \\ &= |S_{d-1}| \int_0^{r_1} r^{d-1}\,dr + |S_{d-1}| \int_{r_1}^{r_2} (-\alpha r + \alpha\, r_1 + 1) r^{d-1}\,dr \\ &= \frac{|S_{d-1}|}{d} r_1^d + |S_{d-1}| \left[ \frac{-\alpha}{d+1}(r_2^{d+1} - r_1^{d+1}) + \frac{\alpha\, r_1 + 1}{d}(r_2^d - r_1^d) \right]. \end{aligned}$$

By simplifying

$$G = \frac{|S_{d-1}|\alpha}{d(d+1)} \left( r_2^{d+1} - r_1^{d+1} \right). \tag{6.7}$$

Next,

$$\begin{aligned} I &= \int_{\mathbb{R}^d} |x|^2 g(x)\,dx \\ &= |S_{d-1}| \int_0^{r_1} r^2 r^{d-1}\,dr + |S_{d-1}| \int_{r_1}^{r_2} r^2(-\alpha\, r + \alpha\, r_1 + 1) r^{d-1}\,dr \\ &= |S_{d-1}| \left[ \frac{r_1^{d+2}}{d+2} - \frac{\alpha}{d+3}(r_2^{d+3} - r_1^{d+3}) + \frac{(\alpha\, r_1 + 1)}{d+2}(r_2^{d+2} - r_1^{d+2}) \right]. \end{aligned}$$

By simplifying the expression above we obtain:

$$I = \frac{|S_{d-1}|\alpha}{(d+2)(d+3)} \left[ r_2^{d+3} - r_1^{d+3} \right]. \tag{6.8}$$

From (6.7), we have

$$dG = |S_{d-1}| \int_{r_1}^{r_2} r^d \alpha\,dr. \tag{6.9}$$

Similarly, from (6.8), we have

$$I(d+2) = |S_{d-1}| \int_{r_1}^{r_2} r^{d+2} \alpha\,dr \tag{6.10}$$

Now, by following Melas paper [7], we let $\tau > 0$ be chosen later and integrate the inequality

$$\alpha d r^{d+2} - \alpha(d+2)\tau^2 r^d + \alpha 2\tau^{d+2} \geq \alpha 2\tau^d (r - \tau)^2$$

over $[r_1, r_2]$ with respect to $r$ to get, where we use (6.9) and (6.10):

$$\begin{aligned} d(d+2)\frac{I}{|S_{d-1}|} - (d+2)\tau^2\frac{dG}{|S_{d-1}|} + 2\tau^{d+2} &\geq \alpha 2\tau^d \int_{r_1}^{r_1+\frac{1}{\alpha}} (r-\tau)^2\, dr \\ &\geq \alpha 2\tau^d \int_{-\frac{1}{2\alpha}}^{\frac{1}{2\alpha}} t^2\, dt \\ &= \frac{\tau^d}{6\alpha^2}, \end{aligned}$$

Now, choosing $\tau = \left(\frac{dG}{|S_{d-1}|}\right)^{\frac{1}{d}}$,

$$I \geq |S_{d-1}|^{\frac{-2}{d}} \frac{1}{d+2}(dG)^{\frac{d+2}{d}} + \frac{G}{6(d+2)\alpha^2}.$$

We obtain the same lower bound as Melas [7] for the case $G\alpha^d > \frac{|S_{d-1}|}{d(d+1)}$. $\square$

# Part II

## 7. THE DISCRETE LAPLACIAN ON A SUBSET OF A FINITE TORUS

In this chapter we want to show that the sum of the $N$ lowest eigenvalues of the Discrete Laplacian on a subset, $\Lambda$, of a finite torus is bounded below by a term proportional to the volume of the domain $\Lambda$. The proof will follow that of Freericks, Lieb, Ueltschi's [12] in the case of the infinite lattice and Lieb and Loss's [14] in the case of the continuum. For simplicity we will let $a = 1$.

We will introduce some new notations. Let $L > 1$, be the size of the $d$-dimensional torus, where $L$ is even. The torus can be defined as the following set [18]:

$$T_L = \left\{ x \in \mathbb{Z}^d : -\frac{L}{2} \leq x_j \leq \frac{L}{2}, \quad \forall j = 1, ..., d \right\}.$$

The dual $T_L^*$ of $T_L$ is given by

$$T_L^* = \left\{ k \in \frac{2\,\pi}{L} \mathbb{Z}^d : -\pi \leq k_i \leq \pi \quad \forall i = 1, ..., d \right\}.$$

We will define the Discrete Laplacian, $-\Delta$, whose action on a normalized function $\varphi$ in $l^2(\Lambda)$ is

$$-\Delta\varphi(x) = -\sum_{y \in \Lambda, |x-y|=1} \varphi(y) + 2d\varphi(x), \quad x \in \Lambda.$$

Define $S_N$ to be the ground state energy of $N$ non-interacting electrons in $\Lambda$, which corresponds to the sum of the N lowest eigenvalues of the Discrete Laplacian on $\Lambda$.

Define $e_L(\rho)$ to be the ground state energy density of non-interacting electrons on the torus with density $\rho = \frac{N}{|\Lambda|}$, where $|\Lambda|$ is the volume of $\Lambda$.

**Theorem 4.** *For every $N \geq 1$ and even $L > 1$,*

$$S_N \geq e_L(\rho)|\Lambda|.$$

**Proof.** Let $\lambda_1 \leq \lambda_2 \leq .... \leq \lambda_{|\Lambda|}$ denote the eigenvalues of $-\Delta$ with corresponding eigenfunctions $\varphi_1, ..., \varphi_{|\Lambda|}$.

For $\Lambda = T_L$, it is well known that the eigenvalues are given by

$$\varepsilon_k = \sum_{v=1}^{d} [2 - 2\cos(k_v)]$$

with corresponding normalized eigenfunctions $\varphi_k(x) = \frac{1}{L^{\frac{d}{2}}} e^{ikx}$, where $k \in T_L^*$ and $x \in \Lambda$.

Let $N' = \lfloor \rho L^d \rfloor$ which is the integer part of $\rho L^d$. Here $N'$ denotes the number of eigenvalues defined on the torus, $T_L$.

Define $K_{L,N'} \subset T_L^*$ as the set containing $N'$ elements with lowest $\varepsilon_k$.

The energy per site of a density, $\rho$, of free electrons on $T_L$ is given by $e_L(\rho)$, where

$$e_L(\rho) = \sum_{k \in K_{L,N'}} \frac{1}{L^d} \varepsilon_k \quad \text{for} \quad \rho = \frac{N'}{L^d}$$

and in the case where $L^d \rho$ is not an integer, we define $e_L(\rho)$ by letting

$$e_L(\rho) = e_L\left(\frac{N'}{L^d}\right) \quad \text{if} \quad \frac{N'}{L^d} \leq \rho < \frac{N'+1}{L^d}.$$

Let $e(s)$ denote the ground state energy density of non-interacting electrons in the infinite volume $\mathbb{Z}^d$. In the thermodynamic limit $L \to \infty$ we get the following Riemann sum:

$$\begin{aligned} \lim_{L\to\infty} e_L(s) &= \lim_{L\to\infty} \frac{1}{(2\pi)^d} \sum_{k \in K_{L,N'}} \left(\frac{2\pi}{L}\right)^d \varepsilon_k \\ &= \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d, \varepsilon_k < \varepsilon_F^1(s)} \varepsilon_k \, dk \\ &= e(s). \end{aligned}$$

The lattice Fermi level, $\varepsilon_F^1(s)$, is chosen such that $s = \frac{1}{(2\pi)^d} \int_{\varepsilon_k < \varepsilon_F^1(s)} dk$.

For $\widehat{\phi}, \widehat{\psi} : T_L^* \to \mathbb{C}$, we define

$$\langle \widehat{\phi}, \widehat{\psi} \rangle_{T^*L} = \frac{1}{L^d} \sum_{k \in T_L^*} \overline{\widehat{\phi}(k)} \widehat{\psi}(k).$$

From [18] we have

$$\langle \widehat{\phi}, \widehat{\psi} \rangle_{T^*L} = \langle \phi, \psi \rangle_{l^2(\Lambda)}. \tag{7.1}$$

The Fourier transform of $\varphi \in l^2(\Lambda)$ is given by

$$\widehat{\varphi}(k) = \sum_{x \in \Lambda} e^{ikx} \varphi(x), \qquad k \in T_L^*$$

and the inverse transform is

$$\varphi(x) = \frac{1}{L^d} \sum_{k \in T_L^*} \widehat{\varphi}(k) e^{-ikx}, \qquad x \in \Lambda.$$

A function $\varphi \in l^2(\Lambda)$ can be considered to be in $l^2(T_L)$ by letting $\varphi = 0$ outside $\Lambda$. The energy of a particle in a state $\varphi_j \in l^2(\Lambda)$ is given by

$$\lambda_j = \langle \varphi_j, -\Delta \varphi_j \rangle = \frac{1}{L^d} \sum_{k \in T_L^*} \varepsilon_k \, |\widehat{\varphi_j}(k)|^2 \, dk.$$

This can be showed as follows. We have $[-\widehat{(\Delta\varphi_j)}(k)] = \varepsilon_k \widehat{\varphi_j}(k)$. Then from (7.1)

$$\begin{aligned} \langle \varphi_j, -\Delta \varphi_j \rangle &= \langle \widehat{\varphi_j}, -\widehat{\Delta \varphi_j} \rangle_{T_L^*} \\ &= \frac{1}{L^d} \sum_{k \in T_L^*} \varepsilon_k \, |\widehat{\varphi_j}(k)|^2 \, dk. \end{aligned}$$

Eigenfunctions with different eigenvalues are orthonormal and we can take the eigenfunctions with the same eigenvalues to be orthonormal so that we have an orthonormal set. We have that the energy $S_N(\varphi_1, ..., \varphi_N)$ of $N$ orthonormal functions $\varphi_1, ...., \varphi_N \in l^2(\Lambda)$ is given by

$$S_N(\varphi_1, ..., \varphi_N) = \frac{1}{L^d} \sum_{k \in T_L^*} \varepsilon_k \, \varrho(k),$$

where

$$\varrho(k) = \sum_{j=1}^{N} |\widehat{\varphi_j}(k)|^2.$$

The function $\varrho(k)$ satisfies the following two expressions:

$$\frac{1}{L^d} \sum_{k \in T_L^*} \varrho(k) \, dk = N. \tag{7.2}$$

$$0 \leq \varrho(k) \leq |\Lambda|. \tag{7.3}$$

Equation (7.2) follows from Parseval's identity and the fact that $\varphi_j$ is a normalized function.

Equation (7.3) can be proved as follows. Since the eigenfunctions, $\varphi_i$, are orthonormal in $l^2(\Lambda)$, they can be completed to form an orthonormal basis, $\{\varphi_i\}_{i=1}^{\infty}$, in $l^2(T_L)$. Define the function $f_k : (T_L) \to \mathbb{C}$ by $f_k(x) = e^{-ikx}\chi_\Lambda(x)$, where $\chi_\Lambda(x)$ is the characteristic function on $\Lambda$ and $k \in T_L^*$. Then $\widehat{\varphi_j}(k) = \langle \varphi_j, f_k \rangle$. The upper bound of $\varrho$ can be found by using Bessel's inequality. We have

$$\varrho(k) = \sum_{j=1}^{N} |\widehat{\varphi_j}(k)|^2 = \sum_{j=1}^{N} |\langle \varphi_j, f_k \rangle|^2 \leq \|f_k\|^2_{l^2(\Lambda)} = |\Lambda|.$$

We minimize $S_N(\varphi_1, ..., \varphi_N)$ over all $\varrho$ that satisfies the two conditions in (7.2) and (7.3). Thus, the ground state energy, $S_N$, of N orthonormal functions $\varphi_1, ...., \varphi_N$ is bounded below by

$$S_N \geq \inf_{\substack{\varrho : 0 \leq \varrho \leq |\Lambda| \\ \frac{1}{L^d}\sum_{k \in T_L^*} \varrho(k) = N}} \frac{1}{L^d} \sum_{k \in T_L^*} \varrho(k)\, \varepsilon_k \, dk.$$

Let $\delta = \rho L^d - N'$. Then $0 \leq \delta < 1$. By the 'bathtub principle' [14], we find the minimizer to be given by:

$$\varrho_{min}(k) = \begin{cases} |\Lambda|, & \text{if } k \in K_{L,N'} \\ \delta|\Lambda|, & \text{if } k \in K_{L,N'+1} \backslash K_{L,N'} \text{ where } 0 \leq \delta < 1 \text{ .} \\ 0, & \text{else} \end{cases}$$

Therefore, the sum of the N lowest eigenvalues, $S_N$, with density, $\rho = \frac{N}{|\Lambda|}$, is bounded below by the following term:

$$S_N \geq |\Lambda| \frac{1}{L^d} \sum_{k \in K_{L,N'}} \varepsilon_k = e_L(\rho)|\Lambda|.$$

□

## 8. Lower bound involving the boundary for low densities

In the previous section we proved that the sum, $S_N$, of the $N$ lowest eigenvalues of $-\Delta$ defined on a finite subset, $\Lambda$, of the torus is bounded below by a term proportional to the volume of the domain $\Lambda$ ('bulk term '). Now we want to strengthen the lower bound and show that if the density is small enough and $L$ large enough, the lower bound also involves a term proportional to the boundary of the domain $\Lambda$ ('boundary correction').

We want to find a lower bound for $S_N$ on the form

$$S_N \geq e(\rho)|\Lambda| + C_1 \rho^{\frac{2}{d}+1} B(\Lambda) - C_2 \frac{|\Lambda|}{L^2},$$

where

$$B(\Lambda) = |\{(x,y) : x \in \Lambda, y \in \Lambda^C, |x-y| = 1\}|$$

is the number of bounds connecting $\Lambda$ with $\Lambda^c$, and $C_1, C_2$ are constants. Recall that $e(\rho)$ represents the energy density on the lattice in the limit of infinite volume.

**Theorem 5.** *If* $\rho \leq \frac{\left[8\pi\left(1+\frac{1}{32d^3}\right)\right]^{-\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}$, *we have for* $N \geq 1$ *and* $L$ *large enough,*

$$S_N \geq e(\rho)|\Lambda| + \frac{1}{2(4d)^3}\xi(\rho)B(\Lambda) - \left(1 - \frac{1}{2(4d)^3}\frac{B(\Lambda)}{|\Lambda|}\right) d4\pi^2 \frac{|\Lambda|}{L^2},$$

*where* $\xi(\rho) = \rho\varepsilon_F(\rho) - e(\rho)$.

The proof is inspired by the papers of Freericks, Lieb, Ueltschi [12] and Ueltschi [13] in the case of the infinite lattice.

**Proof.** Let $\lambda_j$ be the $j^{th}$ eigenvalue of $-\Delta$ corresponding to the eigenfunction, $\varphi_j$, and let $\hat{\varphi}_j$ be the Fourier transform of $\varphi_j$. Recall that the sum $S_N(\varphi_1, ...., \varphi_{|\Lambda|})$ of N orthonormal functions is given by

$$S_N(\varphi_1, ...., \varphi_{|\Lambda|}) = \frac{1}{L^d} \sum_{k \in T_L^*} \varrho(k)\, \varepsilon_k$$

with

$$\varrho(k) = \sum_{j=1}^{N} |\widehat{\varphi_j}(k)|^2.$$

We proved in the last section that

$$0 \leq \varrho(k) \leq |\Lambda|.$$

We want to strengthen the lower bound of $S_N$ by strengthening the upper bound of $\varrho(k)$ to

$$\varrho(k) \leq |\Lambda| - \text{const} \cdot \, B(\Lambda).$$

By letting $y = x + e$, where $e$ is the unit vector, we can write the Discrete Laplacian, which acts on a normalized square summable, complex-valued function $\varphi$ on $\Lambda$ as

$$-\Delta\varphi(x) = -\sum_{e:x+e\in\Lambda} \varphi(x+e) + 2d\varphi(x), \quad x \in \Lambda.$$

We have the eigenvalue equation

$$-\Delta\varphi_j(x) = \lambda_j \varphi_j(x) \qquad \forall x \in \Lambda.$$

A function in $l^2(\Lambda)$ can be considered to be in $l^2(T_L)$ by letting $\varphi(x)$ be zero outside $\Lambda$. The following equation is then valid $\forall x \in T_L$:

$$-\sum_{e:x+e\in T_L} \varphi_j(x+e) + \chi_{\Lambda^C}(x) \sum_{e:x+e\in\Lambda} \varphi_j(x+e) + 2d\varphi_j(x) \;\;=\;\; \lambda_j\varphi_j(x), \quad (8.1)$$

where $\chi_{\Lambda^C}(x)$ is the characteristic function on $\Lambda^c$. The middle term is necessary in order for the equation to be zero on both sides for sites outside $\Lambda$ that are neighbors of sites in $\Lambda$.

Let $\partial\Lambda$ be the set of sites of $\Lambda$ that are neighbors to the complement of $\Lambda$.

$$\partial\Lambda = \{x \in \Lambda : \text{dist}(x, \Lambda^C) = 1\}.$$

By taking the Fourier transform of both sides of the equation (8.1), we get

$$\varepsilon_k \widehat{\varphi_j}(k) + \langle b_k, \varphi_j \rangle = \lambda_j \widehat{\varphi_j}(k), \qquad (8.2)$$

where $b_k$ is the boundary vector:

$$b_k(x) = \chi_{\partial\Lambda}(x)e^{-ikx} \sum_{e:x+e\notin\Lambda} e^{-ik\,e}$$

Define $K_\rho = \{k \in [-\pi,\pi]^d : \varepsilon_k < \varepsilon_F(\rho\}$.

**Lemma 12.**

*(a) If $\rho \leq \frac{|B_d|}{(2\sqrt{2}\pi)^d}$, where $|B_d|$ denotes the volume of the unit ball in $d$ dimensions, then*
*$K_\rho \subset \left(-\frac{\pi}{4}, \frac{\pi}{4}\right)^d$.*

*(b) If $\rho \leq \frac{|B_d|}{(2\sqrt{2}\pi)^d} - C_{L,\rho}$, where $|B_d|$ denotes the volume of the unit ball in $d$ dimensions, then $K_{L,N'} \subset \left(-\frac{\pi}{4}, \frac{\pi}{4}\right)^d$, where $C_{L,\rho}$ is a constant such that $C_{L,\rho} \to 0$ as $L \to \infty$.*

(No proof of lemma (12(b) yet.)

**Proof of lemma 12 (a).** We have that

$$\frac{|B_d|}{(2\sqrt{2}\pi)^d} \geq \rho \geq \frac{1}{(2\pi)^d}|B_d|\varepsilon_F(\rho)^{\frac{d}{2}}.$$

Hence

$$\varepsilon_F(\rho) \leq \frac{1}{2}. \tag{8.3}$$

We have that $1 - \frac{x^2}{2} \leq \cos(x) \leq 1 - \frac{4}{\pi^2}x^2$, which implies that

$$\frac{8}{\pi^2}|k|_2^2 \leq \varepsilon_k \leq |k|_2^2, \tag{8.4}$$

where $|k|_2^2 = k_1^2 + .... + k_d^2$. From (8.3) and (8.4), we obtain

$$\frac{8}{\pi^2}|k|_2^2 \leq \varepsilon_k < \frac{1}{2}$$

Therefore,

$$|k|_\infty \leq |k|_2 < \frac{\pi}{4}.$$

□

It can be checked that

$$B(\Lambda) \leq \|b_k\|^2 \leq 2dB(\Lambda), \tag{8.5}$$

where the lower bound holds at least when $|k|_\infty \leq \frac{\pi}{4}$.

By completeness of the set of eigenvectors, $\{\varphi_j\}$, we have

$$\varrho(k) = \sum_{j=1}^{N} |\widehat{\varphi_j}(k)|^2 = |\Lambda| - \sum_{j=N+1}^{|\Lambda|} |\widehat{\varphi_j}(k)|^2. \tag{8.6}$$

From equation (8.2) we obtain

$$|\widehat{\varphi_j}(k)|^2 = \frac{|\langle b_k, \varphi_j\rangle|^2}{(\lambda_j - \varepsilon_k)^2} \geq \frac{1}{(4d)^2}|\langle b_k, \varphi_j\rangle|^2 \qquad \text{where} \quad \lambda_j \leq 4d. \tag{8.7}$$

Recall from (3.1) that we have

$$\langle b_k, -\Delta b_k\rangle = \sum_{\substack{\{x,y\}\subset\mathbb{Z}^d \\ |x-y|=1}} |b_k(x) - b_k(y)|^2. \tag{8.8}$$

By noticing that each site x of $\partial\Lambda$ has at least one neighbor y outside $\Lambda$ and the boundary vector, $b_k$, is zero there, it can be checked that

$$\sum_{\substack{\{x,y\}\subset\mathbb{Z}^d \\ |x-y|=1}} |b_k(x) - b_k(y)|^2 \geq \|b_k\|^2. \tag{8.9}$$

Now consider all domain $\Lambda$ and all $N^o$ such that $\lambda_{N^o} \leq \frac{1}{2}$ and $\lambda_{N^o+1} > \frac{1}{2}$. Let us first consider the case $N \leq N^o$. By using (8.8) and (8.9) we obtain

$$\begin{aligned} 4d \sum_{j=N^o+1}^{|\Lambda|} |\langle b_k, \varphi_j\rangle|^2 &\geq \sum_{j=N^o+1}^{|\Lambda|} |\langle b_k, \varphi_j\rangle|^2 \lambda_j & (8.10) \\ &\geq \langle b_k, -\Delta b_k\rangle - \sum_{j=1}^{N^o} |\langle b_k, \varphi_j\rangle|^2 \lambda_j & (8.11) \\ &\geq \frac{\|b_k\|^2}{2}. & (8.12) \end{aligned}$$

From the first part of (8.5) and the result above, we obtain for $|k|_\infty \leq \frac{\pi}{4}$

$$\sum_{j=N+1}^{|\Lambda|} \frac{1}{(4d)^2}|\langle b_k, \varphi_j\rangle|^2 \geq \frac{\|b_k\|^2}{2(4d)^3} \geq \frac{B(\Lambda)}{2(4d)^3}. \tag{8.13}$$

Hence, from (8.6), (8.7) and (8.13), we get

$$\varrho(k) \leq |\Lambda| - \frac{B(\Lambda)}{2(4d)^3}.$$

Now, define $\alpha = \frac{1}{2(4d)^3}\frac{B(\Lambda)}{|\Lambda|}$. Then we can write

$$\varrho(k) \leq (1-\alpha)|\Lambda|.$$

We will now go through the same steps as we did in chapter 7. We will find a minimizer for the lower bond of $S_N$, given by

$$S_N \geq \inf_{\substack{0\leq\varrho\leq|\Lambda|(1-\alpha) \\ \frac{1}{L^d}\sum_{k\in T_L^*}\varrho(k)=N}} \frac{1}{L^d}\sum_{k\in T_L^*}\varrho(k)\,\varepsilon_k. \tag{8.14}$$

Define $K_{L,M'} \subset T_L^*$ as the set containing $M'$ elements with lowest $\varepsilon_k$. We choose $M'$ to be the largest integer such that $M' \leq \frac{\rho L^d}{1-\alpha}$, i.e $M' = \lfloor \frac{\rho L^d}{1-\alpha} \rfloor$.
Let $\delta = \frac{\rho L^d}{1-\alpha} - M'$. Then $0 \leq \delta < 1$. By applying the 'bathtub principle' [14] we obtain the following minimizer:

$$\varrho_{min}(k) = \begin{cases} (1-\alpha)|\Lambda|, & \text{if } k \in K_{L,M'} \\ \delta(1-\alpha)|\Lambda|, & \text{if } k \in K_{L,M'+1}\backslash K_{L,M'}, \text{ for } 0\leq\delta<1 \\ 0, & \text{else} \end{cases}.$$

We define the energy per site of density $\frac{\rho}{1-\alpha}$ of free electrons in $T_L$ by

$$e_L(\tfrac{\rho}{1-\alpha}) = \frac{1}{L^d}\sum_{k\in K_{L,M'}}\varepsilon_k \quad \text{for} \quad \frac{M'}{L^d} \leq \frac{\rho}{(1-\alpha)} < \frac{M'+1}{L^d}.$$

When we take the thermodynamic limit $L \to \infty$ of $e_L(\frac{\rho}{1-\alpha})$, we obtain the energy density in the infinite lattice which is given by

$$e(\tfrac{\rho}{1-\alpha}) = \frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d,\varepsilon_k<\varepsilon_F(\frac{\rho}{1-\alpha})}\varepsilon_k\,dk.$$

We will write the sum in (8.14) in terms of integrals which will give us an expression that it is easier to work with. We will do this in the following way. We will decompose the dual $T_L^*$ of $T_L$ into cells of volume $\left(\frac{2\pi}{L}\right)^d$, centered around elements of $T_L^*$. We let $C_k$ denote the cell around $k$, where we have $\varepsilon(k) = \varepsilon_k$. We will extend $\varepsilon_k$ to be constant on the entire cell, $C_k$. Let us call this extended function $\varepsilon_L(k)$. Thus $\varepsilon_L(k) = \varepsilon(k)$ whenever $k \in T_L^*$. Then we have from (8.14):

$$S_N \geq \frac{1}{(2\pi)^d} \sum_{k\in T_L^*} \varrho_{min}(k) \int_{C_k} \varepsilon_L(\xi)\, d\xi. \tag{8.15}$$

Replace the piecewise constant function, $\varepsilon_L(\xi)$, by a linear approximation for $\varepsilon(\xi)$ inside $C_k$. Let us call this function $\tilde{\varepsilon}_L(\xi)$. We have

$$\frac{1}{(2\pi)^d} \sum_{k\in T_L^*} \varrho_{min}(k) \int_{C_k} \varepsilon_L(\xi)\, d\xi = \frac{1}{(2\pi)^d} \sum_{k\in T_L^*} \varrho_{min}(k) \int_{C_k} \tilde{\varepsilon}_L(\xi)\, d\xi.$$

The error is of second order;

$$\left| \int_{C_k} [\tilde{\varepsilon}_L(\xi) - \varepsilon(\xi)]\, d\xi \right| \leq R_1(\xi, k)|C_k|,$$

where $R_1(\xi, k)$ is the remainder in the first order Taylor's formula. We have for $v = 1, ..., d,$

$$\frac{\partial^2 \varepsilon(\xi)}{\partial \xi_v^2} = 2\cos(a\, \xi_v).$$

$$\frac{\partial^2 \varepsilon(\xi)}{\partial \xi_i \partial \xi_v} = 0 \quad \text{for} \quad i \neq v.$$

Since $|\cos(\xi_v)|$ is bounded by 1 for all $\xi_v$, we have

$$|R_1(\xi, k)| \leq \frac{1}{2} \sum_{v=1}^{d} 2(\xi_v - k_v)^2 \leq d \left(\frac{2\pi}{L}\right)^2 = d\, \frac{4\pi^2}{L^2}.$$

We have

$$\left| \int_{C_k} \tilde{\varepsilon}_L(\xi) - \varepsilon(\xi)\, d\xi \right| \leq \int_{C_k} |R_1(\xi, k)|\, d\xi \leq d\, 4\pi^2 \frac{|C_k|}{L^2}, \tag{8.16}$$

where $|C_k| = \left(\frac{2\pi}{L}\right)^d$. Now by (8.16) we obtain

$$\begin{aligned} S_N &\geq \frac{1}{(2\pi)^d} \sum_{k \in T_L^*} \varrho_{min}(k) \int_{C_k} \tilde{\varepsilon}_L(\xi)\, d\xi && (8.17) \\ &\geq \frac{1}{(2\pi)^d} \sum_{k \in T_L^*} \varrho_{min}(k) \int_{C_k} \varepsilon(\xi)\, d\xi - \frac{1}{(2\pi)^d} \sum_{k \in T_L^*} \varrho_{min}(k)\, d 4\pi^2 \frac{|C_k|}{L^2} && (8.18) \end{aligned}$$

The last term in (8.18) can be calculated as follows:

$$\frac{1}{(2\pi)^d} \sum_{k \in T_L^*} \varrho_{min}(k) d4\pi^2 \frac{|C_k|}{L^2} \leq |\Lambda|(1-\alpha) d4\pi^2 \frac{1}{L^2}. \tag{8.19}$$

Thus by combining (8.18) and (8.19) we obtain the following lower bound:

$$\begin{aligned} S_N &\geq \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \varrho_{min}(k)\, \varepsilon_k\, dk - d\, 4\pi^2 \frac{1}{L^2} |\Lambda|(1-\alpha) && (8.20) \\ &\geq |\Lambda|(1-\alpha) e\left(\frac{\rho}{1-\alpha}\right) - d\, 4\pi^2 \frac{1}{L^2} |\Lambda|(1-\alpha). \end{aligned}$$

We are interested in finding a lower bound for $S_N$ for density, $\rho$, so we need to convert $e(\frac{\rho}{1-\alpha})$ into an expression involving $e(\rho)$. We start by introducing the function $\xi(\rho)$ which is given by

$$\xi(\rho) = \rho \varepsilon_F(\rho) - e(\rho).$$

Let

$$\psi(\alpha) = (1-\alpha) e(\tfrac{\rho}{1-\alpha}).$$

We have that the derivative, $\psi'$, of $\psi$ is given by

$$\psi'(\alpha) = \xi(\tfrac{\rho}{1-\alpha}),$$

where we used that the derivative of $e(s)$ is equal to $\varepsilon_F(s)$. Since $\psi(\alpha)$ is convex as a function of $\alpha$, we have a supporting line at 0, i.e

$$\psi(\alpha) \geq \psi(0) + \psi'(0)(\alpha - 0) = e(\rho) + \xi(\rho)(\alpha - 0).$$

Thus from (8.20) and the equation above we obtain

$$S_N \geq e(\rho)|\Lambda| + \alpha \xi(\rho)|\Lambda| - (1-\alpha) d4\pi^2 \frac{|\Lambda|}{L^2},$$

where

$$\alpha = \frac{1}{2(4d)^3}\frac{B(\Lambda)}{|\Lambda|}.$$

So we have shown that for all domains $\Lambda$ and for all $N \leq N^o$, such that $\lambda_{N^o} \leq \frac{1}{2}$ and $\lambda_{N^o+1} > \frac{1}{2}$ that we have

$$S_N \geq e(\rho)|\Lambda| + \frac{1}{2(4d)^3}\xi(\rho)B(\Lambda) - \left(1 - \frac{1}{2(4d)^3}\frac{B(\Lambda)}{|\Lambda|}\right) d4\pi^2\frac{|\Lambda|}{L^2}. \tag{8.21}$$

Now consider the situation where we have (8.21) proved but $N \geq N^o$. Write $\rho^o = \frac{N^o}{|\Lambda|}$. Then

$$\begin{aligned} S_N &= \sum_{j=1}^{N^o}\lambda_j + \sum_{j=N^o+1}^{N}\lambda_j \\ &= e(\rho^o)|\Lambda| + \frac{1}{2(4d)^3}\xi(\rho^o)B(\Lambda) - \left(1 - \frac{1}{2(4d)^3}\frac{B(\Lambda)}{|\Lambda|}\right) d4\pi^2\frac{|\Lambda|}{L^2} \\ &+ \frac{1}{2}|\Lambda|(\rho - \rho^o), \end{aligned}$$

where we bound the second sum by using $\lambda_j \geq \frac{1}{2}$. The right side of the expression above is larger than

$$e(\rho)|\Lambda| + \frac{1}{2(4d)^3}\xi(\rho)B(\Lambda) - \left(1 - \frac{1}{2(4d)^3}\frac{B(\Lambda)}{|\Lambda|}\right) d4\pi^2\frac{|\Lambda|}{L^2}$$

provided that

$$\begin{aligned} e(\rho^o) + \frac{1}{2(4d)^3}\xi(\rho^o)\frac{B(\Lambda)}{|\Lambda|} + \frac{1}{2}(\rho - \rho^o) \\ \geq e(\rho) + \frac{1}{2(4d)^3}\xi(\rho)\frac{B(\Lambda)}{|\Lambda|}. \end{aligned}$$

Let $f(\rho) = \frac{1}{2}\rho - e(\rho) - \frac{1}{64d^2}\xi(\rho)$. (Notice that $\frac{1}{64d^2}$ is an upper bound for $\alpha$ since $\frac{B(\Lambda)}{|\Lambda|} \leq 2d$.) It is enough to check that the function $f(\rho)$ is increasing in $\rho$. Recall from lemma 10 in chapter 5 that

$$\varepsilon_F^1(\rho) \leq \varepsilon_F(\rho) = 4\pi\rho^{\frac{2}{d}}\Gamma\left(\frac{d}{2}+1\right)^{\frac{2}{d}}, \tag{8.22}$$

where $\varepsilon_F(\rho)$ denotes the Fermi level in the continuum. Then

$$\frac{d}{d\rho}\varepsilon_F^1(\rho) \leq \frac{8\pi}{d}\rho^{\frac{2}{d}-1}\Gamma\left(\frac{d}{2}+1\right)^{\frac{2}{d}}. \tag{8.23}$$

By inserting (8.22) and (8.23) into (8.24), we obtain

$$\begin{aligned} \frac{d}{d\rho}f(\rho) &= \frac{1}{2} - \varepsilon_F^1(\rho) - \frac{1}{64d^2}\rho\frac{d}{d\rho}\varepsilon_F^1(\rho) && (8.24) \\ &\geq \frac{1}{2} - 4\pi\Gamma\left(\frac{d}{2}+1\right)^{\frac{2}{d}}\rho^{\frac{2}{d}}\left(1+\frac{1}{32d^3}\right). && (8.25) \end{aligned}$$

Thus, for $\rho \leq \frac{\left[8\pi\left(1+\frac{1}{32d^3}\right)\right]^{-\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}$ the function, $f(\rho)$, is increasing. Thus, we have proved for all $N \geq 1$ and for $\rho \leq \frac{\left[8\pi\left(1+\frac{1}{32d^3}\right)\right]^{-\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}$ with $L$ large enough,

$$S_N \geq e(\rho)|\Lambda| + \frac{1}{2(4d)^3}\xi(\rho)B(\Lambda) - \left(1 - \frac{1}{2(4d)^3}\frac{B(\Lambda)}{|\Lambda|}\right)d4\pi^2\frac{|\Lambda|}{L^2}.$$

□

# 9. LOWER BOUND INVOLVING THE BOUNDARY

In this chapter we will describe a different method for finding the lower bound for the sum, $S_N$, of the $N$ lowest eigenvalues. Again we will show that $S_N$ is bounded below by a term proportional to the volume of the domain of $\Lambda$ ('bulk term'). The 'bulk term' depends on the size of the torus. We will explain a method to show that the lower bound also involves a term proportional to the boundary of $\Lambda$ ('boundary term ').The method will work for all densities, but so far we are unable to prove this. We will follow the paper of Goldbaum [15] where he considered the case $\rho = \frac{1}{2}$ for the infinite lattice.

Let $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_{|\Lambda|}$, be the eigenvalues of the Discrete Laplacian ,$-\Delta$, with corresponding eigenfunctions $\varphi_1, ...., \varphi_{|\Lambda|}$.

Let $b_k(x) = \chi_{\partial\Lambda}(x) e^{-ikx} \sum\limits_{e: x+e \notin \Lambda} e^{-ike}$ be the boundary vector.

Recall that the energy density of free electrons on the torus is given by $e_L(\rho) = \dfrac{1}{L^d} \sum\limits_{k \in K_{L,N'}} \varepsilon_k$, where $K_{L,N'}$ denotes the set of $N'$ elements of $T_L^*$ with lowest $\varepsilon_k$. We have $\lim\limits_{L\to\infty} e_L(\rho) = e(\rho)$. Recall that $\varepsilon_F^1(\rho)$ denotes the lattice Fermi level determined from the relation $\rho = \frac{1}{(2\pi)^d} \int_{\varepsilon_k < \varepsilon_F^1(\rho)} dk$.

**Lemma 13.** *For $N \geq 1$ and even $L > 1$,*

$$S_N \geq e_L(\rho)|\Lambda| + \frac{1}{2}\frac{1}{(4d)^4}\frac{1}{L^d} \sum_{k \in T_L^*} |\varepsilon_k - \varepsilon^{1}{}_F^{(L)}(\rho)| \; \|(-\Delta - \lambda N) b_k\|^2 \tag{9.1}$$
$$- \frac{1}{2}\frac{1}{(4d)^3}\frac{1}{L^d} \sum_{k \in T_L^*} (\varepsilon_k - \varepsilon^{1}{}_F^{L}(\rho)) \langle b_k, (-\Delta - \lambda_N) b_k \rangle,$$

**Proof of lemma 13.** Recall from the previous chapter that we have

$$|\widehat{\varphi}(k)|^2 = \frac{|\langle b_k, \varphi_j\rangle|^2}{(\lambda_j - \varepsilon_k)^2} \geq \frac{1}{(4d)^2} |\langle b_k, \varphi_j \rangle|^2. \tag{9.2}$$

Let

$$\varrho(k) = \sum_{j=1}^{N} |\widehat{\varphi_j}(k)|^2.$$

We have

$$S_N - |\Lambda| e_L(\rho) = \frac{1}{L^d} \sum_{k \in T_L^*} \varepsilon_k [\varrho(k) - |\Lambda| \chi_{K_{L,N'}(k)}]. \tag{9.3}$$

Since $\sum \varrho(k) = \sum \chi_{K_{L,N'}(k)}$, we can shift $\varepsilon_k$ by any constant in (9.3). Replacing $\varepsilon_k$ by $\varepsilon_k - \varepsilon 1_F^L(\rho)$, we obtain

$$S_N - |\Lambda| e_L(\rho) = \frac{1}{L^d} \sum_{k \in T_L^*} \left| \varepsilon_k - \varepsilon 1_F^L(\rho) \right| (\Delta_+(k) + \Delta_-(k)), \tag{9.4}$$

where

$$\Delta_+(k) = (|\Lambda| - \varrho(k)) \chi_{[K_{L,N'}]}(k)$$

and

$$\Delta_-(k) = \varrho(k) \chi_{[T_L^* \setminus K_{L,N'}]}(k).$$

From (9.2) we obtain

$$\Delta_+(k) \geq \frac{1}{(4d)^2} \|P_+ b_k\|^2 \quad \text{if} \quad k \in K_{L,N'}.$$

$$\Delta_-(k) \geq \frac{1}{(4d)^2} \|P_- b_k\|^2 \quad \text{if} \quad k \in T_L^* \setminus K_{L,N'},$$

where $P_- b_k$ and $P_+ b_k$ denote the projectors onto the subspace spanned by the eigenfunctions $\varphi_1, ..., \varphi_N$ and $\varphi_{N+1}, ..., \varphi_{|\Lambda|}$ respectively. From Goldbaum [15] we have the following estimates of $\|P_+ b_k\|$ and $\|P_- b_k\|$.

$$\|P_+ b_k\|^2 = \sum_{j=N+1}^{|\Lambda|} |\langle b_k, \varphi_j \rangle|^2 \geq \sum_{j=N+1}^{|\Lambda|} |\langle b_k, \varphi_j \rangle|^2 \frac{\lambda_j - \lambda_N}{4d - \lambda_N} \tag{9.5}$$

$$= \frac{1}{2} \left[ \sum_{j=1}^{|\Lambda|} |\langle b_k, \varphi_j \rangle|^2 \frac{|\lambda_j - \lambda_N|}{4d - \lambda_N} + \sum_{j=1}^{|\Lambda|} |\langle b_k, \varphi_j \rangle|^2 \frac{\lambda_j - \lambda_N}{4d - \lambda_N} \right] \tag{9.6}$$

$$\geq \frac{1}{2} \left\| \frac{-\Delta - \lambda_N}{4d - \lambda_N} \, b_k \right\|^2 + \frac{1}{2} \left\langle b_k, \frac{-\Delta - \lambda_N}{4d - \lambda_N} \, b_k \right\rangle. \tag{9.7}$$

Similarly we obtain

$$\|P_{-}b_k\|^2 \geq \frac{1}{2}\left\|\frac{-\Delta - \lambda_N}{\lambda_N} b_k\right\|^2 - \frac{1}{2}\left\langle b_k, \frac{-\Delta - \lambda_N}{\lambda_N}\, b_k\right\rangle.$$

Then we obtain the lower bound

$$\begin{aligned}
&S_N - |\Lambda| e_L(\rho) \\
&\geq \frac{1}{2}\frac{1}{(4d)^4}\frac{1}{L^d}\sum_{k\in T_L^*}\left|\varepsilon_k - \varepsilon^{1}{}^{L}_{F}(\rho)\right| \|(-\Delta - \lambda_N)b_k\|^2 \\
&- \frac{1}{2}\frac{1}{(4d)^3}\frac{1}{L^d}\sum_{k\in T_L^*}\left(\chi_{[\varepsilon_k < \varepsilon^{1}{}^{L}_{F}(\rho)]}(k) - \chi_{[\varepsilon_k > \varepsilon^{1}{}^{L}_{F}(\rho)]}(k)\right)|\varepsilon_k - \varepsilon^{1}{}^{L}_{F}(\rho)|\langle b_k, (-\Delta - \lambda_N)b_k\rangle
\end{aligned}$$

with

$$\left(\chi_{[\varepsilon_k < \varepsilon^{1}{}^{L}_{F}(\rho)]}(k) - \chi_{[\varepsilon_k > \varepsilon^{1}{}^{L}_{F}(\rho)]}(k)\right)\left|\varepsilon_k - \varepsilon^{1}{}^{L}_{F}(\rho)\right| = -(\varepsilon_k - \varepsilon^{1}{}^{L}_{F}(\rho)),$$

so the lemma is proved. □

Now we will explain how we can use lemma 13. We will explain the situation $L \to \infty$ but the boundary term can be calculated for all even $L > 1$.

When we take the limit $L \to \infty$ of the expression in (9.1) we obtain

$$\begin{aligned}
S_N \geq e(\rho)|\Lambda| &+ \frac{1}{2}\frac{1}{(4d)^4}\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d} |\varepsilon_k - \varepsilon^1_F(\rho)| \|(-\Delta - \lambda_N)b_k\|^2\, dk \\
&- \frac{1}{2}\frac{1}{(4d)^3}\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d} (\varepsilon_k - \varepsilon^1_F(\rho))\langle b_k, (-\Delta - \lambda_N)b_k\rangle\, dk.
\end{aligned}$$

We will now follow Goldbaum's paper [15]. The boundary term can be calculated if we can show that the terms $\|(-\Delta - \lambda_N)b_k\|^2$ and $\langle b_k, (-\Delta - \lambda_N)b_k\rangle$ are proportional to the boundary of $\Lambda$ for $k$ in a strip that contains the Fermi surface, $\varepsilon^1_F(\rho)$, of $\rho$. We will first explain how we can show that the term $|(-\Delta - \lambda_N)b_k\|^2$ is proportional to the boundary of $\Lambda$ for $k$ in a strip that contains the Fermi surface, $\varepsilon^1_F(\rho)$, of $\rho$.

**A bound for** $\|(-\Delta - \lambda_N)b_k\|^2$.

We would like to show that there exists some $k$ in the Fermi surface, $\varepsilon_k = \varepsilon^1_F(\rho)$, of $\rho$ such that $\|(-\Delta - \lambda_N)b_k\|^2$ does not vanish. Yet, we are not able to find these

$k's$ for all densities and all dimensions. We are able to find $k$ for d=2 for part of the intermediate density. For higher dimensions it is even harder to find the correct $k's$.

We will here look at the case $d = 2$. We will follow Goldbaum's paper [15]. He considered the case $\rho = \frac{1}{2}$ $(\varepsilon_F^1 = 2d)$. We have

$$\begin{aligned}
&[(-\Delta - \lambda_N)b_k](x) \\
= &-\sum_e b_k(x+e) + (2d-\lambda_N)b_k(x) \\
= &\, e^{-ikx}\left[(2d-\lambda_N)\chi_{\partial\Lambda}(x)\sum_{e':x+e'\notin\Lambda} e^{-ike'} - \sum_{e:x+e\in\partial\Lambda}\ \sum_{e':x+e+e'\notin\Lambda} e^{-ik(e+e')}\right].
\end{aligned}$$

We sum over exponentials over some of the nearest neighbors $x + e'$ and over some of the second nearest neighbors $x + e + e'$. The diagrams on page 72 and 73 illustrate which terms which will be in the sum. They show the real part of the terms for each site, for particular values of $k$. We will try to find values of $k$ such that all of the terms have either positive or negative real part such that they are not cancelled out by each other. Note that we do not consider the imaginary part of the terms since these terms will cancel each other out.

Because of symmetry, we can calculate the bound for density $\rho$ or $1 - \rho$. We will calculate the bound for density $1 - \rho$ which will make $\lambda_N \geq 2d$.

Let the notation $e \| i$ means that $e$ is parallel to the $i^{th}$ direction. For $x \in \Lambda$ let us introduce the matrix $[Q_x]_{ij}$ with integer entries $q_{x,ij}$.

$$[Q_x]_{ij} = q_{x,ij} = \sharp\{(e,e') : e\|i, e'\|j, x+e \in \partial\Lambda, x+e+e' \notin \Lambda.\}$$

We will consider the two cases; $tr\, Q_x \neq 0$ and $tr\, Q_x = 0$, $Q_x \neq 0$.

For the case $d = 2$, and density, $\rho$, such that $4 < \varepsilon_F(\rho) < 6$, we will average $\|(-\Delta - \lambda_N)b_k\|^2$ over two different values of $k$; $k_1, k_2$ in the Fermi surface. The value of $k_2$ is obtained by inversion of coordinates of $k_1$. By considering the average value, we can, for the case $tr\, Q_x \neq 0$, cancel out the terms which involve the second nearest neighbors when $e$ is not equal to $e'$, and control the sign of the other terms (see diagram 9.3). When $tr\, Q_x = 0$, we can control the signs of the terms which involve the nearest neighbors (see diagram 9.4).

We have

$$\frac{1}{2}\sum_{i=1}^{2} |[(-\Delta - \lambda_N)b_{k_i}](x)|^2 \geq \left| \frac{1}{2}\sum_{i=1}^{2}[(-\Delta - \lambda_N)b_{k_i}](x) \right|^2.$$

When $tr\, Q_x \neq 0$, we sum over the vectors $k_1 = (\frac{\pi}{2}, \frac{\pi}{2} + y)$ and $k_2 = (\frac{\pi}{2} + y, -\frac{\pi}{2})$ for $0 \leq y < \frac{\pi}{2}$, where $y$ is determined by the density. We obtain

$$\frac{1}{2}\sum_{i=1}^{2} |[(-\Delta - \lambda_N)b_{k_i}](x)|^2 \geq \frac{1}{4}| - 1 - \cos(2y)|^2.$$

When $tr\, Q_x = 0$ while $Q_x \neq 0$, we sum over the vectors $k_1 = (\pi, \pi - y)$ and $k_2 = (\pi - y, \pi)$ for $\frac{\pi}{2} < y \leq \pi$, where $y$ is determined by the density. We obtain

$$\frac{1}{2}\sum_{i=1}^{2} |[(-\Delta - \lambda_N)b_{k_i}](x)|^2 \geq |\cos(y)|^2.$$

The results are illustrated in the diagrams 9.1-9.4. We obtain for $d = 2$ and density, $\rho$, such that $4 < \varepsilon_F^1(\rho) < 6$, the following diagrams. We first consider the case when $tr\, Q_x \neq 0$.

$$\begin{array}{rrlll}
 & & \circ\ -\cos(2y) & & \\
 & +\cos(y)\ \circ & \circ\ -\sin(y) & \circ\ -\cos(y) & \\
-1\ \circ & 0\ \circ & \bullet\ \mathrm{x} & \circ\ 0 & \circ\ -1 \\
 & -\cos(y)\ \circ & \circ\ -\sin(y) & \circ\ +\cos(y) & \\
 & & \circ\ -\cos(2y) & &
\end{array}$$

Figure 9.1

$$\begin{array}{rrlll}
 & & \circ\ -1 & & \\
 & -\cos(y)\ \circ & \circ\ 0 & \circ\ +\cos(y) & \\
-\cos(2y)\ \circ & -\sin(y)\ \circ & \bullet\ \mathrm{x} & \circ\ -\sin(y) & \circ\ -\cos(2y) \\
 & +\cos(y)\ \circ & \circ\ 0 & \circ\ -\cos(y) & \\
 & & \circ\ -1 & &
\end{array}$$

Figure 9.2

$$\begin{array}{ccccc}
 & & \circ\ -1-\cos(2y) & & \\
 & 0\ \circ & \circ\ -\sin(y) & \circ\ 0 & \\
-1-\cos(2y)\ \circ & -\sin(y)\ \circ & \bullet\ \mathrm{x} & \circ\ -\sin(y) & \circ\ -1-\cos(2y) \\
 & 0\ \circ & \circ\ -\sin(y) & \circ\ 0 & \\
 & & \circ\ -1-\cos(2y) & &
\end{array}$$

Figure 9.3

Figure 9.1 Diagram of nearest and second nearest neighbors when $k_1 = \left(\frac{\pi}{2}, \frac{\pi}{2} + y\right)$ for $0 \leq y < \frac{\pi}{2}$.
Figure 9.2 Diagram of nearest and second nearest neighbors when $k_2 = \left(\frac{\pi}{2} + y, -\frac{\pi}{2}\right)$ for $0 \leq y < \frac{\pi}{2}$. Figure 9.3 Diagram of nearest and second nearest neighbors when we add together the entries in diagram 9.1 and 9.2.

Since $tr\, Q_x \neq 0$, then at least one of the terms with $-1 - \cos(2y)$ in diagram 9.3 must exists. Since the entries (except the zero ones) in the diagram 9.3 are negative for $0 \leq y < \frac{\pi}{2}$, they are not cancelled out by each other.

Next, consider the case when $tr\, Q_x = 0$ while $Q_x \neq 0$. By adding the diagrams for the vectors $k_1 = (\pi, \pi - y)$ and $k_2 = (\pi - y, \pi)$ for $\frac{\pi}{2} < y \leq \pi$ we obtain the following diagram:

$$\begin{array}{ccccc}
 & & \circ & & \\
 & 2\cos(y)\ \circ & \circ\ -1-\cos(y) & \circ\ 2\cos(y) & \\
\circ & -1-\cos(y)\ \circ & \bullet\ \mathrm{x} & \circ\ -1-\cos(y) & \circ \\
 & 2\cos(y)\ \circ & \circ\ -1-\cos(y) & \circ\ 2\cos(y) & \\
 & & \circ & &
\end{array}$$

Figure 9.4
Figure 9.4 Diagram of the nearest and second nearest neighbors when we add together the vectors $k_1 = (\pi, \pi - y)$ and $k_2 = (\pi - y, \pi)$ for $\frac{\pi}{2} < y \leq \pi$.

Since $Q_x \neq 0$, then at least one of the terms in diagram 9.4 with $2\cos(y)$ must exists. Since all the entries in the diagram 9.4 are negative for $\frac{\pi}{2} < y \leq \pi$, they are not cancelled out by each other.

When other densities or dimensions are considered, we might have to average over more than two combinations of inversions of the coordinates of $k$ in the Fermi surface. If we average over all combinations of inversions of $k_i$ in the Fermi surface we obtain

$$\frac{1}{2^d}\sum_{i=1}^{2^d} |[(-\Delta-\lambda_N)b_{k_i}](x)|^2 \geq \left|\frac{1}{2^d}\sum_{i=1}^{2^d}[(-\Delta-\lambda_N)b_{k_i}](x)\right|^2 .$$

Goldbaum [15] then conclude that if we can find such $k_i$ in the Fermi surface as described in this section, and if $tr\, Q_x \neq 0$ we have

$$\|(-\Delta-\lambda_N)b_{k_i}\|^2 \geq \text{const}\cdot \#\{x\in\Lambda, tr\, Q_x \neq 0\}.$$

Similarly, if $tr\, Q_x = 0, Q_x \neq 0$ we have

$$\|(-\Delta-\lambda_N)b_{k_i}\|^2 \geq \text{const}\cdot \#\{x\in\Lambda, tr\, Q_x = 0 \quad \text{and} \quad Q_x \neq 0\}.$$

From [15] we also have

$$\#\{x\in\Lambda, Q_x\neq 0\} \geq \alpha|\partial\Lambda|,$$

where $\alpha$ is a constant and $\partial\Lambda$ is the boundary of $\Lambda$. Now, from lemma A.1 in [12] we have

$$\left\|\nabla\|(-\Delta-\lambda_N)b_k\|^2\right\| \leq 2^9 d^{\frac{11}{2}}|\partial\Lambda|.$$

Hence, for $k$ in a strip that contains the Fermi surface, $\varepsilon_F^1(\rho)$ of $\rho$, we obtain

$$\|(-\Delta-\lambda_N)b_k\|^2 \geq C_1|\partial\Lambda|,$$

where $C_1$ is a constant. Recall

$$\begin{aligned} S_N \geq e(\rho)|\Lambda| &+ \frac{1}{2}\frac{1}{(4d)^4}\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d}|\varepsilon_k-\varepsilon_F^1(\rho)|\|(-\Delta-\lambda_N)b_k\|^2 dk \\ &- \frac{1}{2}\frac{1}{(4d)^3}\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d}(\varepsilon_k-\varepsilon_F^1(\rho))\langle b_k,(-\Delta-\lambda_N)b_k\rangle\, dk. \end{aligned}$$

Now the first term in the expression above can be written:

$$\begin{aligned} &\frac{1}{2}\frac{1}{(4d)^4}\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d}|\varepsilon_k-\varepsilon_F^1(\rho)|\|(-\Delta-\lambda_N)b_k\|^2 dk \\ &\geq \frac{1}{2}\frac{1}{(4d)^4}\frac{1}{(2\pi)^d}C_1|\partial\Lambda|\int_{S_1}|\varepsilon_k-\varepsilon_F^1(\rho)|\, dk, \end{aligned}$$

where we integrate over a strip, $S_1$, that contains the Fermi surface, $\varepsilon_F^1(\rho)$, of $\rho$. The integral $\int_{S_1} |\varepsilon_k - \varepsilon_F^1(\rho)|\, dk$ is uniformly bounded in $\Lambda$. (Due to lack of time we have not calculated this integral yet.)

Now suppose that we can find a vector $k$, such that, for density, $\rho$, we have $\varepsilon_k = \varepsilon_F^1(\rho)$ and $\|(-\Delta - \lambda_N)b_k\|^2 \geq \alpha|\partial\Lambda|$, for some constant $\alpha$. Then we have to consider two possible cases:

$$-\frac{1}{2}\frac{1}{(4d)^3}\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]} (\varepsilon_k - \varepsilon_F^1(\rho))\langle b_k, (-\Delta - \lambda_N)b_k\rangle\, dk \geq 0$$

$$-\frac{1}{2}\frac{1}{(4d)^3}\frac{1}{(2\pi)^d}\int_{[-\pi.pi]} (\varepsilon_k - \varepsilon_F^1(\rho))\langle b_k, (-\Delta - \lambda_N)b_k\rangle\, dk < 0.$$

We should be concerned with the last case since the value of this term could cancel out the contribution from the term

$$\frac{1}{2}\frac{1}{(4d)^4}\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d} |\varepsilon_k - \varepsilon_F^1(\rho)|\|(-\Delta - \lambda_N)b_k\|^2 dk.$$

We have not worked out this yet due to lack of time. Goldbaum [15] consider the case $\rho = \frac{1}{2}$ ($\varepsilon_F^1(\rho) = 2d$). He let $k' = k + (\pi, \pi, ...., \pi)$. Then he proves that

$$\varepsilon_{k'} = 2d.$$

$$\|(-\Delta - 2d)b_k\|^2 = \|(-\Delta - 2d)b_{k'}\|^2.$$

$$\langle b_k, (-\Delta - 2d)b_k\rangle = -\langle b_{k'}, (-\Delta - 2d)b_{k'}\rangle \geq 0.$$

He shows that

$$\left\|\frac{\partial}{\partial k_j}\langle b_k, (-\Delta - 2d)b_k\rangle\right\| \leq 6\alpha d^3|\partial\Lambda|,$$

where $\alpha$ is a constant. Then he shows that

$$C_2\|(-\Delta - 2d)b_k\|^2 + C_3\langle b_k, (-\Delta - 2d)b_k\rangle \geq C_4|\partial\Lambda|$$

for $k$ in a strip that contains the Fermi surface $\varepsilon_F = 2d$, where $C_2, C_3, C_4$ are constants.

# 10. CONCLUSION

In this paper, we showed that the sum of the $N$ lowest eigenvalues of the Discrete Laplacian converges to the sum of the $N$ lowest eigenvalues of the Continuum Laplacian in the continuum limit.

(Freericks, Lieb, Ueltschi) [12] and (Ueltschi)[13] showed that the sum of the $N$ lowest eigenvalues of the Discrete Laplacian defined on a finite subset of the infinite lattice is bounded below by a term proportional to the volume of the domain ('bulk term') plus a term proportional to the boundary ('boundary correction'). They found an explicit value of the 'boundary correction' for small densities.

We showed that the 'bulk term' in the lower bound for the sum of the $N$ lowest eigenvalues of the Discrete Laplacian converges to the 'bulk term ' in the lower bound for the sum of the $N$ lowest eigenvalues of the Continuum Laplacian while the 'boundary correction' tends to zero.

In the future, we hope that we can find an explicit value of the 'boundary correction ' for all densities. We also hope that we can find a lower bound for the sum of the $N$ lowest eigenvalues of the Discrete Laplacian defined on a finite subset of the infinite lattice that involves a 'boundary correction' that is different from zero in the continuum limit.

When we started looking at the paper of Melas [7] we hoped that proving lemma 1 in [7] by using the bathtub principle with gradient would give us a better lower bound for the sum of the $N$ lowest eigenvalues of the Continuum Laplacian than the one Melas [7] found. Instead, we got the same result as Melas [7].

Goldbaum [15] found an explicit value of the 'boundary correction' for the sum of the $N$ lowest eigenvalues of the Discrete Laplacian defined on a finite subset of the infinite lattice. He found this for two dimensions and for density equal to $\frac{1}{2}$. He claimed that this method would work for all densities and all dimensions. However, to find the correct vectors on the Fermi-level for all densities and all dimensions turned out to be a difficult task. On the other hand, to find these vectors will be the main task that remains before we can compute the value of the ‘boundary correction’ explicitly for all densities and all dimensions.

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