The Density of States in a Quasi-Gap

by

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As members of the Final Examination Committee, we certify that we have read the dissertation prepared by **JEFFREY LEE SELDEN**

entitled **THE DENSITY OF STATES IN A QUASI-GAP**

and recommend that it be accepted as fulfilling the dissertation requirement for the Degree of **DOCTOR OF PHILOSOPHY**

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DEDICATIONS

To my parents,

Gary and Leellyn Selden,

to my wife,

Nicole Lamartine.

and to the memory of my canine companion,

Kramer.

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Abstract

This dissertation studies the asymptotic behavior for the integrated density of states function for operators associated with the propagation of classical waves in a high-contrast, periodic, two-component medium. Consider a domain Ω_+ contained in the hypercube $[0, 2\pi)^n$. We define a function χ_τ which takes the value 1 in Ω_+ and the value τ in $[0, 2\pi)^n \setminus \Omega_+$. We extend this setup periodically to $\mathbb{R}^n$ and define the operator $L_\tau = -\nabla \chi_\tau \nabla$. As $\tau \to \infty$, it is known that the spectrum of L_τ exhibits a band-gap structure and that the spectral density accumulates at the upper endpoints of the bands. We establish the existence and some important properties of a rescaled integrated density of states function in the large coupling limit which describes the non-trivial asymptotic behavior of this spectral accumulation.

1. Introduction and Background

1.1. Physical Motivations

Quantum theory tells us that an electron in a solid material is confined to take on certain prescribed energy values. These values make up the energy spectrum of the electron and an enormous amount of insight into the behavior of matter can be obtained by examining the different spectra which arise. Solid materials have an underlying crystalline structure which introduces a certain periodicity into the equation governing the behavior of the electron, i.e., Schrödinger's equation (see [2, 4]). The result is the so-called band-gap structure in the energy spectrum of the electron. Basically, allowed values of energy for the electron lie in energy bands separated by gaps, i.e., regions of forbidden energy for the electron.

This band-gap structure for the electron model gives rise to the incredibly successful theory of semiconductors, which has led many physicists and mathematicians to explore other situations with the hopes of finding analogous behavior and applications. In the foregoing situation, the Schrödinger operator was an example of a second-order differential operator and one can wonder about the effects of periodicity upon the spectrum of other second-order differential operators, e.g., those occurring in classical electrodynamics or acoustics. Although these operators are different in some fundamental ways, the presence of periodicity makes possible the existence of band-gap structures (via Bloch-Floquet Theory). If one can show that gaps exist, then one would also like to understand the structure of the spectrum within the bands. This is done using the integrated density of states function. This function can be thought of as measuring the local concentration of the spectrum. In other words, if there are a lot of possible electron states with energy values localized about a certain energy value, then the way we would see this concentration is via this integrated density of states function.

The structure of the dissertation is as follows. The remainder of this chapter will be devoted to an introduction of the problem and bring us up to the state of the art. Chapter 2 will contain the computations and reformulations necessary for the proof of the main theorem, which is the focus of Chapter 3. Chapter 4 contains further properties of the integrated density of states function and an examination of some of its asymptotic behavior.

1.2. Divergence-type operators in periodic media

In this section, we will cast the particular problem for study in a more precise mathematical form. We will articulate the assumptions to be used throughout the remainder and discuss the relevant results leading up to and including the main results of this dissertation.

Consider the periodic lattice $L = 2\pi\mathbb{Z}^n$ contained in $\mathbb{R}^n$. Let Q denote our fundamental cell $(0, 2\pi]^n$. Consider a connected domain Ω_+ which is properly contained in Q and has a smooth boundary Γ. We will also assume that Ω_+ is such that $\Omega_- = Q \setminus \Omega_+$ is connected. Now let $\Omega = \{\Omega_+ + 2\pi m : m \in \mathbb{Z}^n\}$. This set Ω is clearly periodic with respect to the lattice L by construction and will play a crucial role in our work. Figure 1.1 presents the idea of the situation in two dimensions. Let $\tau > 0$. We consider the quadratic form

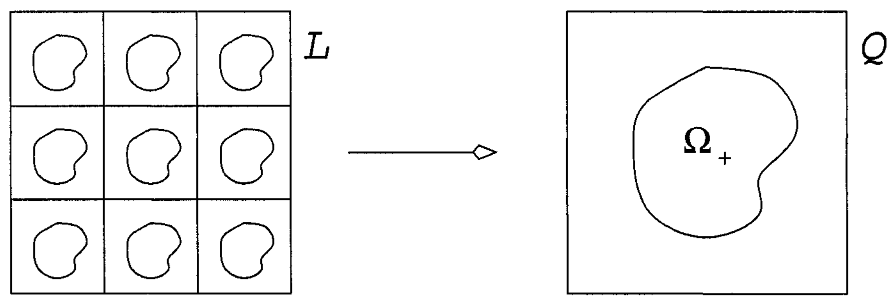
$$q_\tau(u) = \int_{\mathbb{R}^n} \chi_\tau(x)|\nabla u|^2 dx, \tag{1.1}$$

where

$$\chi_\tau(x) = \begin{cases} 1, & \text{if } x \in \Omega; \\ \tau & \text{otherwise} \end{cases}, \tag{1.2}$$

and where the form domain is the Sobolev space $\mathcal{H}^1(\mathbb{R}^n)$. For every τ, the corresponding quadratic form defines a unique self-adjoint operator L_τ in $L^2(\mathbb{R}^n)$ [11] which we

FIGURE 1.1. The Lattice L and Fundamental Cell Q



can write formally in divergence form as

$$L_\tau = -\nabla \chi_\tau(x) \nabla. \tag{1.3}$$

When τ is very large, there is a large difference in the refractive index between Ω and $\mathbb{R}^n \setminus \Omega$. In some sense, it is "easier" for waves to propagate inside Ω than outside Ω. In the large coupling limit, i.e., as τ goes to infinity, it is expected that there is a connection between the spectrum of L_τ and the spectrum of the Dirichlet Laplacian in Ω. Since Ω is made up of countably many copies of Ω_+, the spectrum of the Dirichlet Laplacian in Ω is a pure point spectrum, i.e.,

$$0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \dots,$$

where these values are the eigenvalues of the Dirichlet Laplacian in Ω_+. For Ω, however, the multiplicity of each of these eigenvalues is infinite. To set notation, let ψ_j be the normalized eigenfunction corresponding to λ_j for the Dirichlet Laplacian in Ω_+. Following [10, 9], we will now make two assumptions.

Genericity Assumption 1. *The spectrum of the Dirichlet Laplacian in Ω_+ is simple, i.e.,*

$$0 < \lambda_1 < \lambda_2 < \lambda_3 < \dots.$$

Genericity Assumption 2. *For each j,*

$$\int_{\Omega_+} \psi_j(x)dx \neq 0,$$

i.e., no eigenfunction of the Dirichlet Laplacian in Ω_+ averages to 0.

The genericity of the first condition is confirmed in [1, 15]. A proof of the genericty of the second condition can be found in the appendix to [9]. We should note that while these conditions are generically true, some of the following results will work in a broader context. To be more specific, we can consider the case when we are looking at a single eigenvalue λ_j of the Dirichlet Laplacian in Ω_+ which is simple and for which $\int_{\Omega_+} \psi_j(x)dx \neq 0$. For instance, the first eigenvalue, λ_1, always fulfills these criteria. As such, the following results that deal with specific eigenvalues of the Dirichlet Laplacian will yield information even if the genericity assumptions given above are not satisfied for all j.

For the remainder of this paper, we will assume that $\Gamma = \partial\Omega_+$ is smooth, though this level of regularity for the boundary is not needed for the following theorem of Hempel and Lienau.

Theorem 1. *[10] Under genericty assumptions 1 and 2 as given above, there exists a sequence ν_k that interlaces with λ_k,*

$$0 = \nu_1 < \lambda_1 < \nu_2 < \lambda_3 < \nu_3 < \dots,$$

such that for every $K > 0$ and for sufficiently large values of τ the spectrum of L_τ in $(-\infty, K)$ is:

1. *purely absolutely continuous,*

2. *consists of a finite number of non-overlapping bands*

3. converges to

$$(-\infty, K) \cap \left(\bigcup_{j=1}^{\infty} [\nu_j, \lambda_j] \right)$$

as $\tau \to \infty$.

The techniques employed in the proof of this result in [10] involve the convergence of quadratic forms. In [9], Friedlander employs a different technique resulting in the smoothness requirement on Γ but also providing a different viewpoint from which to examine the character of the spectrum of L_τ. If we let $m_\tau((-\infty, \lambda)) = m_\tau(\lambda)$ be the integrated density of states for L_τ, cf. Section 2.2, then the following theorem provides us with a more detailed understanding of the behavior of the spectrum for large τ.

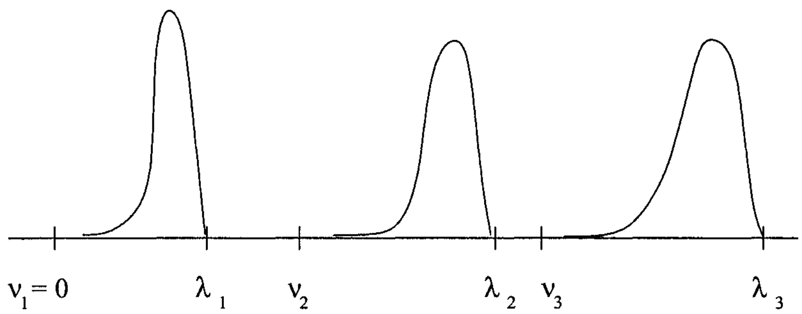
Theorem 2. *[9] Under the genericity assumptions 1 and 2 as given above, for any* γ *such that* $0 \leq \gamma < 1$ *and for any positive constant* C,

$$m_\tau(\lambda_j - C\tau^{-\gamma}) = j - 1 + \mathcal{O}(\tau^{-n(1-\gamma)/2}), \quad \tau \to \infty. \tag{1.4}$$

In a very precise way, this theorem is saying that the spectrum of L_τ accumulates near λ_j for large τ. The result is the formation in the large coupling limit of a quasi-gap between consecutive Dirichlet eigenvalues. This quasi-gap has two sections with distinctly different characteristics. One of the constituents is the gap coming from Theorem 1. We will call this piece the true gap of the quasi-gap and it consists roughly of the interval between λ_{j-1} and ν_j, where we have used the word "roughly" to indicate that there may be some spectrum in a neighborhood of ν_j for any finite value of τ. The other piece of the quasi-gap will be called the spectral band and consists roughly of the interval between ν_j and λ_j, where the word "roughly" is again used to indicate that these endpoints may not be precise. The basic ideas discussed above are contained in Figure 1.2.

The true gap contains no spectrum whatsoever, modulo the caveat about the upper endpoint being somewhat "fuzzy". The spectral band contains spectral points for all

FIGURE 1.2. The Density of States Function in the Quasi-Gaps



τ and is the focus of this dissertation. Theorem 2 tells us that the spectrum inside the band accumulates at λ_j, where we rely on the integrated density of states function for our spectral information. This dissertation studies the asymptotic behavior of the density of states function in the large coupling limit. The main result is as follows.

Theorem 3. *Under the genericity assumptions 1 and 2 as given above and for all* $x > 0$,

$$f_j(x) := \lim_{\tau \to \infty} m_\tau \left(\lambda_j - \frac{x}{\tau} \right) \tag{1.5}$$

exists.

The proof of this theorem will provide us with the means for establishing some of the properties of the $f_j(x)$, as well as the asymptotic behavior of these functions as $x \to \infty$.

2. Bloch-Floquet Theory and Dirichlet-to-Neumann Operators

The proof of Theorem 3 and the resulting properties of the $f_j(x)$ require a certain amount of machinery. This chapter will consist of the definitions, techniques and lemmas needed for these proofs. It should be noted that all of these facts can be found in the references, e.g., [9, 5, 6, 12, 14]. They are included here for the convenience of the reader, though some proofs will be relegated to the more thorough treatments given in the references.

The structure of this chapter is as follows. The first section will describe Bloch-Floquet theory as it applies to the problem at hand. The second section will give an introduction to the integrated density of states function. The third and fourth sections will be the introduction of the Dirichlet-to-Neumann (DtN) operators and a discussion of how these operators can be used, along with Bloch-Floquet theory, to recast the original problem in a new light. The result will be an operator denoted by $N(\tau, \lambda, k)$, whose examination will be the final section of Chapter 2.

2.1. The Bloch-Floquet Decomposition

Mathematicians and physicists often use symmetry to reduce a problem's difficulty or to formulate an ansatz for the structure of a solution. In the case of a periodic differential operator on $\mathbb{R}^n$, this approach allows one to use the periodicity to transform the original operator into a family of operators, the properties of which are well-understood. The first use of this symmetry for solving differential equations is credited to the mathematician G. Floquet in [7]. Without knowledge of Floquet's work, F. Bloch developed the theory 45 years later to study the behavior of electrons in a crystal [3]. As a result, the theory bears either name depending on the inclination of the user. To avoid having to make the choice, we will refer to it as Bloch-Floquet theory, where we have used alphabetical ordering. The references consulted most for the following section were [5, 14, 12]. Detailed treatments of Bloch-Floquet theory can be found in any of these, though Reed and Simon [14] consider only Schrödinger operators. The structure of what follows is taken from the article by Figotin and Kuchment [5] and is presented here only for reasons of self-containment.

Recall that we are considering the lattice $L = 2\pi\mathbb{Z}^n$ contained in $\mathbb{R}^n$, to which there are associated transformations of $\mathbb{R}^n$ which preserve this lattice, i.e., shifts by elements of $2\pi\mathbb{Z}^n$. These transformations naturally induce actions on $L^2(\mathbb{R}^n)$, which we can write down explicitly as

$$(\mathcal{T}_g f)(x) = f(x+g), \tag{2.1}$$

where $f \in L^2(\mathbb{R}^n)$ and $g \in 2\pi\mathbb{Z}^n$. These transformations form a commutative group $\mathcal{G} \cong 2\pi\mathbb{Z}^n$. The invariance of the Lebesgue measure on $\mathbb{R}^n$ implies that each $\mathcal{T}_g$ maps $L^2(\mathbb{R}^n)$ isometrically into $L^2(\mathbb{R}^n)$. In addition, since the norm for the first Sobolev space on $\mathbb{R}^n$ satisfies

$$\begin{aligned} ||(\mathcal{T}_g f)||^2_{\mathcal{H}^1} &= ||f(x+g)||^2_{L^2} + ||\nabla(f(x+g))||^2_{L^2} \\ &= ||f(x)||^2_{L^2} + ||\nabla f(x)||^2_{L^2} \\ &= ||f||^2_{\mathcal{H}^1}, \end{aligned} \tag{2.2}$$

each $\mathcal{T}_g$ maps $\mathcal{H}^1(\mathbb{R}^n)$ isometrically into $\mathcal{H}^1(\mathbb{R}^n)$. Recall that the domain of the original quadratic form q_τ, see(1.1), is $\mathcal{H}^1(\mathbb{R}^n)$. For $f, h \in \mathcal{H}^1(\mathbb{R}^n)$,

$$\begin{aligned} q_\tau(T_g f, T_g h) &= \int_{\mathbb{R}^n} \chi_\tau(x)\nabla f(x+g)\cdot\overline{\nabla h(x+g)}dx \\ &= \int_{\mathbb{R}^n} \chi_\tau(x-g)\nabla f(x)\cdot\overline{\nabla h(x)}dx \\ &= \int_{\mathbb{R}^n} \chi_\tau(x)\nabla f(x)\cdot\overline{\nabla h(x)}dx \\ &= q_\tau(f,h), \end{aligned} \tag{2.3}$$

where we have made use of the fact that χ_τ is 2π-periodic in x. The preceding computation shows that q_τ, and thus L_τ, is invariant with respect to the action of the group $\mathcal{G}$. As a result, L_τ can be decomposed in the following way according to standard arguments that can be found in [12, 5]. Let $K := [-1/2, 1/2)^n$. We define a family of quadratic forms depending on $k \in K$ by

$$q_{\tau,k}(u) = \int_Q \chi_\tau(x)|\nabla u|^2 dx, \tag{2.4}$$

where $u \in \mathcal{H}^1(Q)$ and satisfies the quasi-periodic boundary conditions, i.e., for all $j = 1, \ldots, n$ and $m \in \mathbb{Z}^n$,

$$\begin{aligned} u(x + 2\pi m) &= e^{2\pi i k \cdot m} u(x), \\ \frac{\partial u}{\partial x_j}(x + 2\pi m) &= e^{2\pi i k \cdot m} \frac{\partial u}{\partial x_j}(x). \end{aligned} \tag{2.5}$$

Each $q_{\tau,k}$ determines a unique self-adjoint operator which we call $L_\tau(k)$. Then we have

$$L_\tau \cong \int_K^\oplus L_\tau(k) dk, \tag{2.6}$$

where we are to understand this as a direct fiber decomposition (see [14]). The elements of K are usually referred to as quasimomenta. For each k, the operator $L_\tau(k)$ is elliptic and has a discrete spectrum of eigenvalues of finite multiplicity which we can write as an increasing sequence. Let's denote these eigenvalues, which depend upon τ and k, by

$$\mu_1(\tau, k) \le \mu_2(\tau, k) \le \mu_3(\tau, k) \le \mu_4(\tau, k) \le \ldots.$$

As a result of the decomposition (2.6), the spectrum of L_τ has the very special form

$$\sigma(L_\tau) = \bigcup_{k \in \left[-\frac{1}{2}, \frac{1}{2}\right)^n} \sigma(L_\tau(k)). \tag{2.7}$$

A thorough understanding of the spectrum of L_τ can be gotten by examining the spectra of the $L_\tau(k)$, which effectively transforms a problem on all of $\mathbb{R}^n$ to a family of spectral problems in a hypercube.

The spectral problem for the $L_\tau(k)$ can be characterized in a different (and useful) way. The equivalent problem is to find a function u on Q that satisfies

$$\begin{cases} \Delta u + \lambda u = 0, & x \in \Omega_+ \\ \tau\Delta u + \lambda u = 0, & x \in \Omega_-^{int}, \end{cases} \tag{2.8}$$

along with the quasi-periodic boundary conditions (2.5) and the transmission boundary conditions

$$u_+(x) = u_-(x), \quad \frac{\partial u}{\partial n_+}(x) + \tau \frac{\partial u}{\partial n_-}(x) = 0, \quad x \in \Gamma, \tag{2.9}$$

where $u_\pm(x)$ are the limiting values of $u(x)$ from $\Omega_\pm$ and $n_\pm$ is the normal vector on Γ pointing out of $\Omega_\pm$. The first transmission condition is simply continuity across the boundary, which is required of any function in $\mathcal{H}^1(Q)$. To see how the second transmission conditions arise, we need only apply integration-by-parts to the $q_{\tau,k}$, i.e.,

$$\begin{aligned} q_{\tau,k}(f,g) &= \int_Q \chi_\tau(x) \nabla f \cdot \overline{\nabla g} dx \\ &= \int_{\Omega_+} \nabla f \cdot \overline{\nabla g} dx + \tau \int_{\Omega_-} \nabla f \cdot \overline{\nabla g} dx \\ &= \int_{\Omega_+} (\Delta f) \overline{g} dx + \int_\Gamma \left(\frac{\partial f}{\partial n_+} \right) \overline{g} dS + \tau \int_{\Omega_-} (\Delta f) \overline{g} dx \\ &\quad + \tau \int_\Gamma \left(\frac{\partial f}{\partial n_-} \right) \overline{g} dS + \int_{\partial Q} \left(\frac{\partial f}{\partial \nu} \right) \overline{g} dS', \end{aligned} \tag{2.10}$$

where ν is the outward-pointing normal vector on ∂Q. Since f and g are in the domain of $q_{\tau,k}$, they satisfy the quasi-periodic boundary conditions (2.5). This fact implies that

$$\int_{\partial Q} \left(\frac{\partial f}{\partial \nu} \right) \overline{g} dS' = 0. \tag{2.11}$$

This leaves us with the Laplacian on $\Omega_\pm$ and two integrals over Γ. In order to be left with the desired operator on Q, we require the two boundary integrals to sum to zero, i.e.,

$$\int_\Gamma \left(\frac{\partial f}{\partial n_+}\right) \overline{g} dS + \tau \int_\Gamma \left(\frac{\partial f}{\partial n_-}\right) \overline{g} dS = 0. \tag{2.12}$$

It is now easy to see that this final equation defines the transmission conditions described above.

2.2. The Integrated Density of States Function

As mentioned in the introduction, the standard way to study the spectrum of an operator such as L_τ is with the integrated density of states function. One can gain insight into the information provided by this function by thinking of it as the limit of a normalized counting function. This idea is presented nicely in [14]. We will follow the treatment given therein, as well as the more physically-oriented treatment in [2]. Let us begin by considering a finite subdomain of $\mathbb{R}^n$. For convenience, we will take this subdomain to be of a special form. Recall that $Q = (0, 2\pi]^n$ is the fundamental cell for our lattice. The subdomain Q_d is a conglomerate cube of fundamental cells which measures $2\pi d$ on each side. In other words, we build up a cube with volume $(2\pi d)^n$ using d^n copies of the fundamental cell Q. We will now denote by L_τ^d the restriction of the operator L_τ to Q_d with the so-called Born-von Karman boundary conditions. These boundary conditions arise from the identification of opposing sides of Q^d, which results in the formation of an n-dimensional torus. This identification is equivalent to imposing the following periodicity on a function $\psi(x)$,

$$\psi(x + 2\pi dm) = \psi(x), \quad \text{where } m \in \mathbb{Z}^n. \tag{2.13}$$

Since L_τ^d is a self-adjoint, second-order, elliptic operator on a finite domain, it follows that it has a discrete spectrum tending to infinity, which we can denote by

$$0 \leq \lambda_1^d \leq \lambda_2^d \leq \ldots \tag{2.14}$$

It therefore makes sense to consider a normalized counting function

$$m_{\tau,d}(\lambda) = \frac{\#\{j : \lambda_j^d \leq \lambda\}}{d^n}. \tag{2.15}$$

This quantity measures the number of eigenvalues per unit volume, and hence it is referred to as the integrated density of states function. The obvious problem with the above function is that it does not take the entire lattice into account. To remedy this situation, we can take d to be larger and larger, thereby accounting for more and more of the lattice. So we consider

$$m_\tau(\lambda) = \lim_{d\to\infty} m_{\tau,d}(\lambda). \tag{2.16}$$

It is well-known that this limit exists for operators of the sort with which we are dealing. So the function $m_\tau(\lambda)$ is well-defined. This function is the integrated density of states function for the original spectral problem, though its current form is less explicit than we would like. To remedy this, we can use Bloch-Floquet theory to rewrite each $m_{\tau,d}(\lambda)$ in a new form, leading us to a more convenient characterization of $m_\tau(\lambda)$.

It can be shown (see [14, 2]) that any function ψ satisfying the Born-von Karman boundary conditions (2.13) can be expressed as

$$\psi(x) = \sum_k c_k \psi_k(x), \tag{2.17}$$

where k is of the form

$$k = \left(\frac{a_1}{2d}, \dots, \frac{a_n}{2d}\right), \quad \text{where } a_i \in \mathbb{Z}, -d \leq a_i \leq d-1, \tag{2.18}$$

and each $\psi_k(x)$ satisfies

$$\psi_k(x + 2\pi m) = e^{2\pi i k\cdot m}\psi_k(x), \quad \text{where } m \in \mathbb{Z}^n. \tag{2.19}$$

Taking into account the restriction on k, it is clear that the ψ_k satisfy the Born-von Karman boundary conditions on Q_d. This restriction on k comes from the finiteness of the domain Q_d and the Born-von Karman boundary conditions (see [2]). Due to this decomposition, we need to analyze the action of the operator L_τ^d on each ψ_k. Recall that $L_\tau(k)$ is an operator fiber in the direct integral decomposition of L_τ, cf. (2.6). It follows that $L_\tau^d\psi_k$ is equivalent to letting $L_\tau(k)$ act on ψ_k and then extending the result to Q_d using the quasi-periodic boundary conditions (2.5). Since the space of functions in Q which satisfy the quasi-periodic boundary conditions for a particular value of k is invariant under the action of $L_\tau(k)$, we have that

$$L_\tau\psi = \sum_k c_k L_\tau(k)\psi_k = \sum_k c_k\phi_k, \tag{2.20}$$

where the ϕ_k also satisfy (2.19). As a result, if $L_\tau\psi = \lambda_j\psi$, then

$$L_\tau\psi = \sum_k c_k L_\tau(k)\psi_k = \lambda_j \sum_k c_k\psi_k \tag{2.21}$$

implies that $L_\tau(k)\psi_k = \lambda_j\phi_k$ for some k satisfying (2.18). For each such k, we will have a different eigenfunction and the corresponding eigenvalue will be an eigenvalue of $L_\tau(k)$. As before, we denote these eigenvalues by $\mu_j(\tau, k)$. Therefore,

$$\#\{j : \lambda_j \le \lambda\} = \#\{j, k : \mu_j(\tau, k) \le \lambda\}, \tag{2.22}$$

where we keep in mind that k must be of the form (2.18), i.e., it depends explicitly on the value of d. The right-hand side of the above equality can be rewritten as

$$\#\{j, k : \mu_j(\tau, k) \le \lambda\} = \sum_{j=1}^{\infty}\sum_k \chi_{C(j,\lambda)}(k), \tag{2.23}$$

where $\chi_{C(j,\lambda)}$ is the indicator function for the set $C(j, \lambda) = \{k : \mu_j(\tau, k) \le \lambda\}$. So we can express the integrated density of states $m_{\tau,d}(\lambda)$ as

$$m_{\tau,d}(\lambda) = \sum_{j=1}^{\infty} \frac{\sum_k \chi_{C(j,\lambda)}(k)}{d^n}. \tag{2.24}$$

We can make use of (2.18) to calculate that the volume of k-space per allowed value of k is

$$\Delta k = \frac{1}{d^n}. \tag{2.25}$$

As a result, we have that

$$m_{\tau,d}(\lambda) = \sum_{j=1}^{\infty} \sum_{k} \chi_{C(j,\lambda)}(k) \Delta k. \tag{2.26}$$

If we take the limit as $d \to \infty$, then this sum can be interpreted as a Riemann sum, i.e.,

$$\lim_{d\to\infty} \sum_{j=1}^{\infty} \sum_{k} \chi_{C(j,\lambda)}(k) \Delta k = \sum_{j=1}^{\infty} \int_K \chi_{C(j,\lambda)}(k) dk. \tag{2.27}$$

For the details concerning convergence issues, see [14]. Another way to write that particular integral is

$$\int_K \chi_{C(j,\lambda)}(k) dk = meas\left\{k \in K : \mu_j(\tau, k) \leq \lambda\right\} \tag{2.28}$$

Hence, according to (2.16), the integrated density of states function for the operator L_τ is given by

$$m_\tau(\lambda) = \sum_{j=1}^{\infty} meas\left\{k \in K : \mu_j(\tau, k) \leq \lambda\right\}. \tag{2.29}$$

When we look at $m_\tau(\lambda)$ as a function of λ, it provides us with an idea of where "most" of the spectrum lies. More precisely, $m_\tau(\lambda)$ measures the mass of the spectrum of L_τ below λ. Formula (4.1) of [9] tells us that for large enough τ and $\lambda_{j-1} < \lambda < \lambda_j$, we can rewrite the integrated density of states as

$$m_\tau(\lambda) = j - 1 + vol\left\{k \in K : \mu_j(\tau, k) \leq \lambda\right\}. \tag{2.30}$$

Basically, if $\lambda_{j-1} < \lambda < \lambda_j$, we can find a large τ so that for $p \leq j$, the p^{th} summand in (2.29) is 1, and for $p > j$, the measure of the corresponding set in (2.29) is 0. This leaves the case when $p = j$, which corresponds to the last term in (2.30). The proof of Theorem 2 in [9] boils down to estimating this volume.

2.3. The Dirichlet-to-Neumann Operators

The technique employed here to study $m_\tau(\lambda)$ in more detail involves Dirichlet-to-Neumann operators. This setup will follow that given by Friedlander in [9]. Recall that $\Omega_- = Q\backslash\Omega_+$. Let $n_\pm$ denote the outward-pointing normal vectors on Γ as defined in the previous section. Let ϕ be a smooth function defined on Γ. We will define two different DtN operators. For the first one, let $P_+(\lambda)$ be the Poisson operator which assigns to ϕ the function v_+, where

$$\begin{cases} \Delta v_+(x) + \lambda v_+(x) = 0, & x \in \Omega_+ \\ v_+(x) = \phi(x), & x \in \Gamma. \end{cases} \tag{2.31}$$

Let j_+ denote the operator which takes the normal derivative on Γ with respect to n_+, i.e., $j_+ = \partial/\partial n_+$. Then our first DtN operator is

$$N_+(\lambda)\phi = j_+ P_+(\lambda)\phi = \frac{\partial v_+}{\partial n_+}. \tag{2.32}$$

This operator is not well-defined if the Poisson operator is multi-valued, i.e., if λ belongs to the spectrum of the Dirichlet Laplacian in Ω_+. To see this, suppose that there exists a nonzero u such that $\Delta u + \lambda u = 0$ on Ω_+ and $u = 0$ on Γ. Now suppose that $v_+ = P_+(\lambda)\phi$. Clearly, the function $u + v_+$ will also be a solution to (2.31), but the normal derivatives of v_+ and $u + v_+$ will not be the same unless $j_+ u = 0$. Since this would imply that u is also a Neumann eigenfunction, it cannot happen. So $N_+(\lambda)$ is defined only for λ not in the Dirichlet spectrum of the Laplacian in Ω_+.

Now let $P_-(\lambda, k)$ be the Poisson operator which assigns to ϕ the function v_- where

$$\begin{cases} \Delta v_- + \lambda v_- = 0, & x \in \Omega_-^{int} \\ v_-(x) = \phi(x), & x \in \Gamma \\ v_- \text{ satisfies (2.5).} & \end{cases} \tag{2.33}$$

Let j_- denote the operator which takes the normal derivative on Γ with respect to n_-, i.e., $j_- = \partial/\partial n_-$. Our second DtN operator is

$$N_-(\lambda, k)\phi = j_- P_-(\lambda, k)\phi = \frac{\partial v_-}{\partial n_-}. \tag{2.34}$$

This operator is well-defined so long as λ is not in the spectrum of the Laplacian in Ω_- with Dirichlet boundary conditions on Γ and the quasi-periodic boundary conditions on ∂Q. Let us take a moment to handle this issue. For each k, the smallest eigenvalue $\alpha(k)$ of the Laplacian in Ω_- with Dirichlet boundary conditions on Γ and the quasi-periodic boundary conditions on ∂Q corresponding to k is positive. This follows from the fact that constants cannot satisfy the boundary conditions. If we think of k as lying on a torus, it is easy to see that $\alpha(k)$ is a continuous function on a compact set. It therefore has a uniform, positive lower bound. As long as λ is less than this lower bound, $N_-(\lambda, k)$ will be well-defined.

The properties of these DtN operators are of great importance in what follows, so let us spend some time talking about them. Again, the following is covered in [9] and is included here for the convenience of the reader. First of all, $N_+(\lambda)$ and $N_-(\lambda, k)$ are elliptic pseudodifferential operators of order 1. Their principal symbols are the same and equal to $|\xi'|$, where (x', ξ') is a point in the cotangent bundle on Γ. One of the key facts about these operators is their differentiability with respect to λ. By this, it is meant that the difference quotient has a limit in the operator norm topology. To see this, we will do the computations for $N_+(\lambda)$. The operator $N_-(\lambda, k)$ can be handled almost in exactly the same way. Using the definition of N_+, we can write the difference quotient as

$$\begin{aligned} \frac{N_+(\mu) - N_+(\lambda)}{\mu - \lambda} &= \frac{1}{\mu - \lambda} j_+ \left(P_+(\mu) - P_+(\lambda)\right) \\ &= \frac{1}{\mu - \lambda} j_+ \left(-(\mu - \lambda) R_+(\mu) P_+(\lambda)\right) \\ &= -j_+ R_+(\mu) P_+(\lambda), \end{aligned} \tag{2.35}$$

where $R_+(\lambda) = (\Delta + \lambda)^{-1}$ is the resolvent for the Laplacian on Ω_+ with Dirichlet boundary conditions on Γ and we have made use of the fact that

$$\begin{aligned}(\Delta+\mu)\left(P_+(\mu)-P_+(\lambda)\right) &= -(\Delta+\mu)P_+(\lambda) \\ &= -(\mu-\lambda)P_+(\lambda)-(\Delta+\lambda)P_+(\lambda) \\ &= -(\mu-\lambda)P_+(\lambda). \end{aligned} \tag{2.36}$$

If we denote the limit of the derivative of N_+ with respect to λ by $\dot{N}_+(\lambda)$, it follows that

$$\dot{N}_+(\lambda) = -j_+R_+(\lambda)P_+(\lambda) \tag{2.37}$$

If we take $\phi \neq 0$, then

$$\begin{aligned}\left(\dot{N}_+(\lambda)\phi,\phi\right) &= -\int_\Gamma (j_+R_+(\lambda)P_+(\lambda)\phi)\overline{\phi}dS \\ &= -\int_{\Omega_+}(\Delta+\lambda)(R_+(\lambda)P_+(\lambda)\phi)\overline{P_+(\lambda)\phi}dS \\ &= -\int_{\Omega_+}|P_+(\lambda)\phi|^2\,dS<0. \end{aligned} \tag{2.38}$$

So $\dot{N}_+(\lambda)$ is a negative operator. None of the above computations depend in a crucial way on our choice of $N_+(\lambda)$ over $N_-(\lambda,k)$ and one can easily calculate that $\dot{N}_-(\lambda,k) = -j_-R_-(\lambda)P_-(\lambda)$ is also a negative operator.

Also important for our cause is the dependence of $N_-(\lambda,k)$ upon the quasimomenta variable k. In particular, we will be interested in the case when $\lambda = 0$, i.e., $N_-(0,k)$. In its current form, the k-dependence for this operator appears in the boundary conditions. As in [5, 9], we can use a simple transformation to alleviate this problem. Suppose that $u(x)$ is a function on Ω_- which satisfies the quasi-periodic boundary conditions (2.5). Define

$$v(x) = e^{-ikx}u(x). \tag{2.39}$$

It is easy to see that this transformation takes $u(x)$ to a function which satisfies periodic boundary conditions on ∂C. Therefore, we can think of $v(x)$ as a function on the n-dimensional torus, T^n, minus Ω_+. Since we will be dealing with Poisson operators, we will want to know what happens to a harmonic function. To that end, suppose that $\Delta u(x) = 0$ for some $u(x)$ on Ω_-. Then

$$\begin{aligned} \Delta u(x) &= \Delta e^{ikx} e^{-ikx} u(x) \\ &= \Delta e^{ikx} v(x) \\ &= e^{ikx} \left(-|k|^2 v(x) + \Delta v(x) + 2ik \cdot \nabla v(x) \right). \end{aligned} \tag{2.40}$$

Since this must be equal to 0, we get the partial differential equation for $v(x)$,

$$\Delta v(x) + 2ik \cdot \nabla v(x) - |k|^2 v(x) = 0 \tag{2.41}$$

Using the same trick,

$$\begin{aligned} j_- u(x) &= j_- \left(e^{ikx} e^{-ikx} u(x) \right) \\ &= j_- \left(e^{ikx} v(x) \right) \\ &= e^{ikx} \left(ik \cdot n_-(x) v(x) + j_- v(x) \right), \end{aligned} \tag{2.42}$$

where $n_-(x)$ is the normal vector to Γ at $x \in \Gamma$. We are now in a position to transform $N_-(0,k)$. Let ϕ be a function on Γ. Let $u(x) = P_-(0,k)\phi(x)$ and $v(x) = e^{-ikx}u(x)$. Using (2.42), it follows that

$$\begin{aligned} N_-(0,k)\phi(x) &= j_- u(x) \\ &= e^{ikx} ik \cdot n_-(x) v(x) + e^{ikx} j_- v(x) \\ &= ik \cdot n_-(x)\phi(x) + e^{ikx} j_- \tilde{P}(k) e^{-ikx} \phi(x), \end{aligned} \tag{2.43}$$

where $\tilde{P}(k)$ is the Poisson operator associated to (2.41). It clearly follows that

$$N_-(0,k) = e^{ikx} \tilde{N}(k) e^{-ikx} + ik \cdot n_-(x), \tag{2.44}$$

where $\tilde{N}(k) = j_- \tilde{P}(k)$ is the DtN operator corresponding to (2.41). The last term in (2.44) is as nice a function of k as one could hope for. As a result, we are left to examine the first term. The exponentials are analytic with respect to k, so only the Poisson operator $\tilde{P}(k)$ needs to be studied further. Consider the difference $\tilde{P}(k_1) - \tilde{P}(k_2)$ for some complex k_1 and k_2. Consider the operator

$$\tilde{L}(k) = \Delta + 2ik \cdot \nabla - |k|^2$$

along with Dirichlet boundary conditions on Γ. Then

$$\begin{aligned}\tilde{L}(k_2)\left(\tilde{P}(k_1) - \tilde{P}(k_2)\right) &= \tilde{L}(k_2)\tilde{P}(k_1) \\ &= \Delta\tilde{P}(k_1) + 2ik_2 \cdot \nabla\tilde{P}(k_1) - |k_2|^2\tilde{P}(k_1) \\ &= (k_1 - k_2)\left(-2i\nabla\tilde{P}(k_1) + (k_1 + k_2)\tilde{P}(k_1)\right)\end{aligned}$$

It follows that

$$\tilde{P}(k_1) - \tilde{P}(k_2) = (k_1 - k_2)\tilde{L}(k_2)^{-1}\left(-2i\nabla\tilde{P}(k_1) + (k_1 + k_2)\tilde{P}(k_1)\right). \tag{2.45}$$

This formula gives us a couple of nice results. First, if we consider only real values of k, then (2.45) implies that $\tilde{N}(k)$ has a derivative in k in the sense that the difference quotient

$$\frac{\tilde{N}(k_1) - \tilde{N}(k_2)}{k_1 - k_2}$$

converges to the n-tuple of bounded operators

$$D_k\tilde{N}(k) = 2j_-\tilde{L}(k)^{-1}(-i\nabla + k)\,\tilde{P}(k) \tag{2.46}$$

in the norm operator topology as $k_1 \to k_2$. Coupled with (2.44), this implies that $N_-(0, k)$ is differentiable with respect to k (in the same sense as $\tilde{N}(k)$). To find an explicit formula for the derivative of $N_-(0, k)$, we will have to do a little more work. Using (2.44), we can write

$$\begin{aligned}D_kN_-(0, k) &= D_k\left(e^{ikx}\tilde{N}(k)e^{-ikx} + ik \cdot n_-(x)\right) \\ &= D_k\left(e^{ikx}\tilde{N}(k)e^{-ikx}\right) + in_-(x) \\ &= ixe^{ikx}\tilde{N}(k)e^{-ikx} + e^{ikx}D_k\tilde{N}(k)e^{-ikx} \\ &\quad -ie^{ikx}\tilde{N}(k)xe^{-ikx} + in_-(x).\end{aligned} \tag{2.47}$$

We can use (2.46) to write

$$e^{ikx} D_k \tilde{N}(k) e^{-ikx} = e^{ikx} \left(2j_- \tilde{L}(k)^{-1} (-i\nabla + k) \tilde{P}(k) \right) e^{-ikx}. \tag{2.48}$$

Notice that $e^{ikx} \tilde{L}(k)^{-1} e^{-ikx} = L_-(k)^{-1}$, where $L_-(k)$ is the Dirichlet Laplacian on Ω_- with quasi-periodic boundary conditions, and $e^{ikx} \tilde{P}(k) e^{-ikx} = P_-(0,k)$. In addition, $e^{ikx} (-i\nabla + k) e^{-ikx} = \nabla$. So we can rewrite the above as

$$\begin{aligned} e^{ikx} D_k \tilde{N}(k) e^{-ikx} &= e^{ikx} \left(2j_- e^{-ikx} L_-(k)^{-1} \nabla P_-(0,k) \right) \\ &= -ik \cdot n_-(x) L_-(k)^{-1} \nabla P_-(0,k) \\ &\quad -2ij_- L_-(k)^{-1} \nabla P_-(0,k) \\ &= -2ij_- L_-(k)^{-1} \nabla P_-(0,k). \end{aligned} \tag{2.49}$$

Bringing all of this back to bear on $D_k N_-(0,k)$, we get

$$\begin{aligned} D_k N_-(0,k) &= i(x N_-(0,k) - N_-(0,k) x) \\ &\quad -2ij_- L_-(k)^{-1} \nabla P_-(0,k) + in_-(x). \end{aligned} \tag{2.50}$$

This expression for the derivative of $N_-(0,k)$ will prove very useful later on. In addition, it is not hard to see that the expression for $D_k N_-(0,k)$ is a smooth operator-valued function of k, which allows us to conclude that $N_-(0,k)$ is also a smooth operator-valued function of k.

The equation (2.45) can be used again to gain even more insight into the dependence of $N_-(0,k)$ upon k. Consider the variable k as a complex parameter. The domain of the Poisson operator $\tilde{P}(k)$ is independent of the parameter k. Let ϕ be a function on Γ. Fix a complex k_0 and choose some index α such that $1 \leq \alpha \leq n$. We will now vary only k_α, which reduces the situation to that of a single complex variable. We can use (2.45) to conclude that

$$\lim_{k_\alpha \to k_{\alpha 0}} \frac{\tilde{P}(k_\alpha)\phi - \tilde{P}(k_{\alpha 0})\phi}{k_\alpha - k_{\alpha 0}} = \tilde{L}(k_{\alpha 0})^{-1} \left(-2i\nabla \tilde{P}(k_{\alpha 0})\phi + (2k_{\alpha 0}) \tilde{P}(k_{\alpha 0})\phi \right), \tag{2.51}$$

which shows that $\tilde{P}(k)\phi$ is analytic as a function of the single complex variable k_α. As a result, for any k_α, $\tilde{P}(k)$ is an analytic family of type A with respect to k_α (see [11]). Using (2.44), we conclude that $N_-(0,k)$ is also an analytic family of type A with respect to any k_α. This is a very strong condition which will provide us with some crucial proofs in the proceeding.

2.4. Reformulating with the DtN Operators

We have spent some time describing the Bloch-Floquet decomposition of L_τ and introducing the DtN operators, but now we must make the connection between these two ideas. To do so, we follow Friedlander [9] in defining the following operator. Let

$$N(\tau,\lambda,k) = N_+(\lambda) + \tau N_-(\tau^{-1}\lambda, k). \tag{2.52}$$

Here we have incorporated both of the DtN operators along with τ into a single operator which will have a very important connection with L_τ. To see this, recall the following observation made in [9].

Claim 1. *$\lambda \in \sigma(L_\tau(k))$ if and only if $N(\tau,\lambda,k)$ has a nontrivial null space.*

Suppose that $\lambda \in \sigma(L_\tau(k))$, i.e., there is a function u satisfying (2.5),(2.8), and (2.9). When we apply $N(\tau,\lambda,k)$ to the restriction of u to Γ, we get

$$\begin{aligned} N(\tau,\lambda,k)u &= N_+(\lambda)u + \tau N_-(\tau^{-1}\lambda,k)u \\ &= j_+P_+(\lambda)u + \tau j_-P_-(\tau^{-1}\lambda,k)u. \end{aligned} \tag{2.53}$$

We see from (2.8) that $P_+(\lambda)u = u$ and $P_-(\tau^{-1}\lambda,k)u = u$. It follows that

$$N(\tau,\lambda,k)u = j_+u + \tau j_-u = 0, \tag{2.54}$$

by (2.9) and so $N(\tau,\lambda,k)$ has a nontrivial null space. Conversely, suppose that $N(\tau,\lambda,k)$ has a nontrivial null space, i.e., there exists a function ϕ on Γ such that

$$N(\tau,\lambda,k)\phi = N_+(\lambda)\phi + \tau N_-(\tau^{-1}\lambda,k)\phi = 0. \tag{2.55}$$

We can define a function u on Q by setting $u = P_+(\lambda)\phi$ for $x \in \Omega_+$ and $u = P_-(\tau^{-1}\lambda, k)\phi$ for $x \in \Omega_-$. We need to show that u satisfies (2.5),(2.8), and (2.9). By virtue of $P_-(\tau^{-1}\lambda, k)$, u will satisfy the quasi-periodic boundary conditions (2.5) and the two equations in (2.8). If we write down (2.9), we get

$$\begin{aligned} \frac{\partial u}{\partial n_+}(x) + \tau\frac{\partial u}{\partial n_-}(x) &= j_+P_+(\lambda)u + \tau j_-P_-(\tau^{-1}\lambda, k)u \\ &= N_+(\lambda)\phi + \tau N_-(\tau^{-1}\lambda, k)\phi \\ &= 0, \end{aligned} \tag{2.56}$$

by (2.54). So the claim is true. Consequently, we have a new way of looking at the spectral problem for L_τ, i.e., examining the conditions surrounding a 0-eigenvalue of $N(\tau, \lambda, k)$.

2.5. Preparing the DtN operators

In this section, we will manipulate $N(\tau, \lambda, k)$ so as to make it more amenable for our purposes. To do this, we will consider $N(\tau, \lambda, k)$ as it is defined and establish certain facts about the operators. Secondly, we will rescale $N(\tau, \lambda, k)$, which will put us into a position to capture the asymptotic behavior near λ_j as $\tau \to \infty$.

2.5.1. Some General Facts About $N(\tau, \lambda, k)$

Recall that $\{\lambda_j\}_{j=1}^{\infty}$ denotes the set of Dirichlet eigenvalues for the Laplacian in Ω_+. We can choose corresponding Dirichlet eigenfunctions ψ_j such that they span $L^2(\Omega_+)$. From now on, we will consider the case when $\lambda \in (\lambda_{j-1}, \lambda_j)$. Let ϕ be a smooth function on Γ. Since we want to be able to compute explicitly with $N_+(\lambda)$, we will write down a particular Poisson operator. Let ν satisfy $\Delta\nu = 0$ on Ω_+ and $\nu|_\Gamma = \phi$. In other words, ν is the harmonic extension of ϕ to Ω_+. Then our Poisson operator $P_+(\lambda)$ is

$$P_+(\lambda)\phi(x) = \nu(x) + w(x), \tag{2.57}$$

where

$$w(x) = -\lambda \sum_j \frac{1}{\lambda - \lambda_j} \left(\nu(x), \psi_j(x)\right) \psi_j(x). \tag{2.58}$$

It is clear from this formula that $P_+(\lambda)\phi$ restricts to ϕ on Γ. To see that $\Delta P_+(\lambda)\phi + \lambda P_+(\lambda)\phi = 0$, we need only do a simple computation.

$$\begin{aligned} -\Delta P_+(\lambda)\phi &= -\Delta(\nu + w) \\ &= -\Delta\left(-\lambda \sum_j \frac{1}{\lambda - \lambda_j} (\nu, \psi_j)\, \psi_j\right) \\ &= \lambda \sum_j \frac{-\lambda_j}{\lambda - \lambda_j} (\nu, \psi_j)\, \psi_j. \end{aligned} \tag{2.59}$$

We can rewrite $\frac{-\lambda_j}{\lambda - \lambda_j}$ as $1 - \frac{\lambda}{\lambda - \lambda_j}$. So

$$\begin{aligned} -\Delta P_+(\lambda)\phi &= \lambda \sum_j \left(1 - \frac{\lambda}{\lambda - \lambda_j}\right) (\nu, \psi_j)\, \psi_j \\ &= \lambda \left(\sum_j (\nu, \psi_j)\, \psi_j + \sum_j \frac{-\lambda}{\lambda - \lambda_j} (\nu, \psi_j)\, \psi_j\right) \\ &= \lambda(\nu + w) \end{aligned} \tag{2.60}$$

where we have made use of the completeness of the Dirichlet eigenfunctions. It follows from the definition of $N_+(\lambda)$ (2.32) that we can write

$$N_+(\lambda)\phi(x) = N_+(0)\phi(x) - \lambda \sum_k \frac{1}{\lambda - \lambda_k} \left(\nu(x), \psi_k(x)\right) \frac{\partial \psi_k}{\partial n_+}(x). \tag{2.61}$$

For the given value of j, it is clear from this formula that the coefficient in front of the function $\frac{\partial \psi_j}{\partial n_+}$ blows up as λ gets close to λ_j. However, that is the only part of the formula which has a singularity at λ_j. All of the other terms in (2.61) are regular at λ_j.

Now we turn our attention to $\tau N_-(\tau^{-1}\lambda, k)$, which contains all of the τ-dependence present in the operator $N(\tau, \lambda, k)$. We are interested in the large coupling limit, i.e.,

$\tau \to \infty$. As in [9], we will use the differentiability of $N_-(\lambda, k)$ with respect to λ to expand $N_-(\tau^{-1}\lambda, k)$ in a Taylor series about 0. We have the expansion

$$N_-(\tau^{-1}\lambda, k) = N_-(0,k) + \tau^{-1}\lambda \dot{N}_-(0,k) + \mathcal{O}(\tau^{-2}), \quad \tau \to \infty, \tag{2.62}$$

uniformly in $k \in \left[-\frac{1}{2}, \frac{1}{2}\right)^n$. Multiplying this expansion by τ, we get

$$\tau N_-(\tau^{-1}\lambda, k) = \tau N_-(0,k) + \lambda \dot{N}_-(0,k) + \mathcal{O}(\tau^{-1}), \quad \tau \to \infty. \tag{2.63}$$

It follows that we can write

$$N(\tau, \lambda, k) = N_+(\lambda) + \tau N_-(0,k) + \lambda \dot{N}_-(0,k) + \mathcal{O}(\tau^{-1}), \quad \tau \to \infty. \tag{2.64}$$

This is the form we will use in what follows.

2.5.2. Rescaling $N(\tau, \lambda, k)$

Theorem 2 tells us that the spectrum of L_τ is accumulating near λ_j as $\tau \to \infty$ and that any rescaling which moves with speed less than τ^{-1} toward λ_j will not be able to capture any nontrivial asymptotic behavior. Fix $x > 0$ and consider the rescaling

$$\begin{aligned} N(\tau, \lambda_j - x\tau^{-1}, k) = \; & N_+(\lambda_j - x\tau^{-1}) + \tau N_-(0,k) \\ & + (\lambda_j - x\tau^{-1})\dot{N}(0,k) + \mathcal{O}(\tau^{-1}), \end{aligned} \tag{2.65}$$

as τ goes to ∞, where we have used (2.64). From equation (2.61), we know that $N_+(\lambda_j - x\tau^{-1})$ when applied to a function ϕ is given by

$$\begin{aligned} N_+(\lambda_j - x\tau^{-1})\phi = N_+(0)\phi + \left(\frac{\lambda_j - x\tau^{-1}}{\lambda_j}\right) \frac{-\tau}{x} \left(\frac{\partial \psi_j}{\partial n_+}, \phi\right) \frac{\partial \psi_k}{\partial n_+} \\ + \sum_{k \neq j} \left(\frac{\lambda_j - x\tau^{-1}}{\lambda_k}\right) \frac{1}{\lambda_j - x\tau^{-1} - \lambda_k} \left(\frac{\partial \psi_k}{\partial n_+}, \phi\right) \frac{\partial \psi_k}{\partial n_+}. \end{aligned} \tag{2.66}$$

It is clear from the above that only one term in the sum has order τ. All other terms will be bounded in τ. Hence, in the large τ limit, it is enough to think of $N_+(\lambda_j - x\tau^{-1})$ as a rank one operator given by $(-\tau/x)\left(\partial\psi_j/\partial n_+, \cdot\right)\partial\psi_j/\partial n_+$. The other term of order τ in (2.65) is $N_-(0,k)$. These two terms will dominate the behavior of $N(\tau, \lambda_j - x\tau^{-1}, k)$ as $\tau \to \infty$. As a result, let

$$A(x,k) = \frac{-1}{x}\left(\frac{\partial \psi_j}{\partial n_+}, \cdot\right)\frac{\partial \psi_j}{\partial n_+} + N_-(0,k), \tag{2.67}$$

and let $B(x,\tau,k) = N(\tau, \lambda_j - x\tau^{-1}, k) - A(x,k)$. Then we can rewrite

$$N(\tau, \lambda_j - x\tau^{-1}, k) = \tau A(x,k) + B(x,\tau,k), \qquad \tau \to \infty, \tag{2.68}$$

where $B(x,\tau,k)$ is an operator which is uniformly bounded in τ and k [8, 9]. It is important to point out that A is independent of τ. Recall that $N_-(0,k)$ is a holomorphic family of operators with respect to each k_i for $i = 1, \ldots, n$, and so the same can be said about $A(x,k)$ since the rank 1 perturbation is independent of k.

Before we state the key existence theorem, it will be convenient to deal with the set of k such that the bottom of the spectrum of $A(x,k)$ is 0. Define

$$Z(x) = \left\{k \in K = \left[-\frac{1}{2}, \frac{1}{2}\right)^n : A(x,k) \text{ has a nontrivial null-space}\right\}. \tag{2.69}$$

Clearly, the set $Z = Z(x)$ includes the set of k where 0 is the bottom of the spectrum. We have the following lemma.

Lemma 1. *For $x > 0$, $meas(Z) = 0$.*

Proof: Let $k \in Z$. Then there exists a $\phi(k) \neq 0$ such that $A(x,k)\phi(k) = 0$. If we expand this last equality using the definition of $A(x,k)$, we get

$$-\frac{1}{x}\left(\frac{\partial \psi_j}{\partial n_+}, \phi(k)\right)\frac{\partial \psi_j}{\partial n_+} + N_-(0,k)\phi(k) = 0. \tag{2.70}$$

We can assume that $k \neq 0$ since single points will not affect the measure of Z. Then $N_-(0,k)$ is invertible and we can rewrite (2.70) as

$$N_-(0,k)^{-1}\frac{\partial \psi_j}{\partial n_+} = \frac{x\phi(k)}{\left(\frac{\partial \psi_j}{\partial n_+}, \phi(k)\right)}. \tag{2.71}$$

Taking the inner product of both sides of (2.71) with $\partial\psi_j/\partial n_+$ gives

$$\left(N_-(0,k)^{-1}\frac{\partial\psi_j}{\partial n_+},\frac{\partial\psi_j}{\partial n_+}\right)=x. \tag{2.72}$$

So if $k\in Z$, then we have (2.72). Now suppose that k is such that (2.72) is satisfied. Let

$$\phi(k):=N_-(0,k)^{-1}\frac{\partial\psi_j}{\partial n_+}.$$

A simple computation shows that

$$A(x,k)\phi(k)=-\frac{1}{x}\left(\frac{\partial\psi_j}{\partial n_+},N_-(0,k)^{-1}\frac{\partial\psi_j}{\partial n_+}\right)\frac{\partial\psi_j}{\partial n_+}+\frac{\partial\psi_j}{\partial n_+}=0,$$

where we have used (2.72) to cancel the x. As a result, $k\in Z$. So if we ignore $k=0$, we have another characterization of Z using (2.72), in which the only k dependence appears in the operator $N_-(0,k)^{-1}$. Recall that $N_-(0,k)$ is a holomorphic family of type A and that $N_-(0,k)$ is a positive operator for $k\neq 0$. It follows that $N_-(0,k)^{-1}$ is also a holomorphic family of type A for $k\neq 0$ (see [11]). This implies that

$$F(k):=\left(N_-(0,k)^{-1}\frac{\partial\psi_j}{\partial n_+},\frac{\partial\psi_j}{\partial n_+}\right)-x \tag{2.73}$$

is a holomorphic function for $k\neq 0$ in a complex neighborhood of K. The zero set of $F(k)$ restricted to K is the set Z. Since $N_-(0,0)$ has 0 as an eigenvalue and $\partial\psi_j/\partial n_+$ is not orthogonal to constants, $F(k)$ blows up as $|k|$ gets close to 0. This implies that $F(k)$ cannot be identically zero for all $k\in K$. Recall that the zero set of any nonzero analytic function of a single variable is countable and hence has 1-dimensional measure equal to 0. We proceed with induction on the dimension n. Suppose now that if we restrict an analytic function to a given $(n-1)$-dimensional hyperplane on which the function is not identically zero, then the $(n-1)$-dimensional measure of the zero set of this function is equal to 0. Observe that the analytic function $F(k_1,0,\ldots,0)$ can only have a countable number of zeros on the set $(-1/2,0)\cup(0,-1/2]$. We can use this set to parameterize K as $(-1/2,-1/2]\times(-1/2,1/2]^{n-1}$. Except for a countable number of instances, the function $F(k)$ will have a nonzero value on each $(n-1)$-dimensional hyperplane. The inductive hypothesis along with Fubini's theorem imply that the measure of Z is 0. Q.E.D.

3. Proof of Theorem 3

Lemma 1 allows us to forget about any k for which 0 is an eigenvalue of $A(x,k)$. In particular, we can ignore those k for which the bottom of the spectrum of $A(x,k)$ is 0. Now we are ready to prove Theorem 3.

Proof of Theorem 3: Recall formula (2.30) which was taken from [9] and gave us a nice expression for the integrated density of states function, i.e.,

$$m_\tau(\lambda) = j - 1 + vol\,\{k \in K : \mu_j(\tau,k) \leq \lambda\}.$$

Claim 1 allows us to connect the last term of the above expression with the DtN operators in the following way. Let $E(\tau, \lambda_j - x\tau^{-1})$ denote the set of all $k \in K$ such that there exists a non-zero function ϕ for which $(N(\tau, \lambda_j - x\tau^{-1}, k)\phi, \phi) \leq 0$. Then we can write the integrated density of states as

$$m_\tau(\lambda_j - x\tau^{-1}) = j - 1 + vol(E(\tau, \lambda_j - x\tau^{-1})). \tag{3.1}$$

It is clear from (3.1) that to establish the existence of (1.5) it will suffice to show that

$$\lim_{\tau \to \infty} vol(E(\tau, \lambda_j - x\tau^{-1})) \tag{3.2}$$

exists. To do this, we will provide the value of the limit and show that (3.2) is equal to it. Recall formula (2.68) which rewrites $N(\tau, \lambda_j - x\tau^{-1}, k)$ using A and B. Define

$$E^{as}(x) \quad = \quad \{k \in K : \exists \phi \text{ s.t. } (A(x,k)\phi, \phi) < 0\}.$$

A quick word of explanation should aid in the understanding of the choice of $E^{as}(x)$. It is clear from the structure of $N(\tau, \lambda_j - x\tau^{-1}, k)$ that $A(x,k)$ will play the most important part in the large τ limit since it is of the highest order in τ. Lemma 1 tells us that if we are concerned with volumes, it will be sufficient to concern ourselves with the negativity of the order τ part only. This is precisely what motivates the definition of $E^{as}(x)$. We claim that

$$\lim_{\tau\to\infty} vol\left(E(\tau,\lambda_j - x\tau^{-1})\right) = vol\left(E^{as}(x)\right). \tag{3.3}$$

To see this, let $k \in E^{as}(x)$. By definition there exists ϕ such that

$$(A(x,k)\phi,\phi) < 0.$$

Since $B(x,\tau,k)$ is bounded in τ, it follows that there exists a $T > 0$ such that for $\tau > T$,

$$(N(\tau,\lambda_j - x\tau^{-1},k)\phi,\phi) = \tau\,(A(x,k)\phi,\phi) + (B(x,\tau,k)\phi,\phi) < 0.$$

This in turn implies that $k \in E(\tau,\lambda_j - x\tau^{-1})$ for $\tau > T$. So every point of $E^{as}(x)$ belongs to $E(\tau,\lambda_j - x\tau^{-1})$ as $\tau \to \infty$. Conversely, suppose that $k \notin E^{as}(x)$. Then for all ϕ it must be true that

$$(A(x,k)\phi,\phi) \geq 0.$$

Since we are really interested in volumes, Lemma 1 implies that we can ignore the equality and consider only the case when for all ϕ,

$$(A(x,k)\phi,\phi) > 0.$$

Choose any ϕ. Then $(A(x,k)\phi,\phi) > \epsilon(k)$ for some positive value ϵ which depends upon k. Since B is uniformly bounded in τ and k, there exists a $T > 0$ such that for $\tau > T$,

$$(N(\tau,\lambda_j - x\tau^{-1},k)\phi,\phi) = \tau\,(A(x,k)\phi,\phi) + (B(x,\tau,k)\phi,\phi) > 0.$$

So $k \notin E(\tau,\lambda_j - x\tau^{-1})$ for $\tau > T$. In this way, we see that any $k \notin E^{as}(x)$ either belongs to a set with measure 0 or does not belong to $E(\tau,\lambda_j - x\tau^{-1})$ as $\tau \to \infty$. Now let $\chi_\tau(k)$ denote the characteristic function on $E(\tau,\lambda_j - x\tau^{-1})$ and $\chi_{as}(x)$ denote the characteristic function on $E^{as}(k)$. The above shows that $\chi_\tau(k)$ converges pointwise to $\chi_{as}(k)$ as $\tau \to \infty$. The Lebesgue Dominated Convergence Theorem implies (3.3). Q.E.D.

4. Properties and Asymptotics of the $f_j(x)$

4.1. Some properties of the $f_j(x)$

Theorem 3 ensures the existence of

$$f_j(x) = \lim_{\tau \to \infty} m_\tau(\lambda_j - x\tau^{-1}), \tag{4.1}$$

but the method of proof provides us with even more information. We can better our situation by combining (3.1) with (3.3) to write

$$f_j(x) = j - 1 + vol(E^{as}(x)). \tag{4.2}$$

We will use (4.2) to examine $f_j(x)$, but first we need the following lemma.

Lemma 2. *There exist $M > 0$ and $m \geq 0$ such that*

$$m \leq \left(N_-(0,k)\frac{\partial \psi_j}{\partial n_+}, \frac{\partial \psi_j}{\partial n_+}\right) \leq M.$$

Proof: Let $\eta(k) = \left(N_-(0,k)\frac{\partial \psi_j}{\partial n_+}, \frac{\partial \psi_j}{\partial n_+}\right)$. In Section 2.3, we showed that $N_-(0,k)$ is differentiable, and hence continuous, as a function of k. This implies that $\eta(k)$ is continuous as a function of k. Let $p \in T^n$, where T^n is the n-fold torus. The operator $N_-(0,p)$ is defined in the obvious fashion, i.e., with the quasi-periodic boundary conditions corresponding to p. Now define

$$\tilde{\eta}(p) = \left(N_-(0,p)\frac{\partial \psi_j}{\partial n_+}, \frac{\partial \psi_j}{\partial n_+}\right).$$

This is a function on a manifold and therefore local coordinates can be used to verify that it is continuous. We can make use of the continuity of $N_-(0,k)$ with respect to k again to conclude that $\tilde{\eta}$ is continuous in any local coordinate chart. As a result,

$\tilde{\eta}$ is bounded above and below. Since $\eta(k)$ is continuous on $K = [-1/2, 1/2)^n$ and when restricted to $k \in K \setminus (-1/2, \ldots. -1/2)$ is equal to $\tilde{\eta}$, $\eta(k)$ must be bounded on K. So there exist $m, M \in \mathbb{R}$ such that

$$m \leq \eta(k) \leq M,$$

for all $k \in K$. Q.E.D.

Note that if $\partial\psi_j/\partial n_+$ is constant, then $m = 0$. Otherwise, m will be strictly greater than 0. Now we are prepared to state the first result about $f_j(x)$.

Lemma 3. *There exists $\kappa_j > 0$ such that for $x < \kappa_j$,*

$$f_j(x) = j.$$

Proof: First of all, let

$$\kappa_j = \frac{\left|\left|\frac{\partial\psi_j}{\partial n_+}\right|\right|^4}{M},$$

where M is the maximum from Lemma 2. Suppose that $x < \kappa_j$. Pick any k. Then

$$x < \frac{\left|\left|\frac{\partial\psi_j}{\partial n_+}\right|\right|^4}{M} \leq \frac{\left|\left|\frac{\partial\psi_j}{\partial n_+}\right|\right|^4}{\left(N_-(0,k)\frac{\partial\psi_j}{\partial n_+}, \frac{\partial\psi_j}{\partial n_+}\right)}. \tag{4.3}$$

A little algebraic manipulation leads us from (4.3) to

$$-\frac{1}{x}\left|\left|\frac{\partial\psi_j}{\partial n_+}\right|\right|^4 + \left(N_-(0,k)\frac{\partial\psi_j}{\partial n_+}, \frac{\partial\psi_j}{\partial n_+}\right) < 0,$$

which upon inspection is seen to be exactly the requirement for membership to that very elite set known as $E^{as}(x)$. Since this was independent of the choice for k,

$$E^{as}(x) = K.$$

So $vol(E^{as}(x)) = 1$. Making use of (4.2), we immediately see that

$$f_j(x) = j - 1 + 1 = j,$$

for $x < \kappa_j$. Q.E.D.

Lemma 3 implies that there is a gap in the spectrum from $\lambda_j - \kappa_j \tau^{-1}$ to λ_j. This gap can really only be seen in the rescaling that was done above, yet its presence seems interesting nonetheless.

Lemma 4. *The function $f_j(x)$ is non-increasing when $x > \kappa_j$.*

Proof: It suffices to show that $E^{as}(x_2) \subset E^{as}(x_1)$ when $x_1 < x_2$. Let $k \in E^{as}(x_2)$. Then there exists ϕ such that $(A(x_2, k)\phi, \phi) < 0$. Expanding this, we have

$$-\frac{1}{x_2}\left(\frac{\partial \psi_j}{\partial n_+}, \phi\right)^2 + (N_-(0,k)\phi, \phi) < 0. \tag{4.4}$$

Since $-\frac{1}{x_1} < -\frac{1}{x_2}$, it follows that

$$(A(x_1,k)\phi,\phi) = -\frac{1}{x_1}\left(\frac{\partial \psi_j}{\partial n_+}, \phi\right)^2 + (N_-(0,k)\phi, \phi) < 0. \tag{4.5}$$

So $k \in E^{as}(x_1)$. Q.E.D.

Lemma 5. *For any j,*

$$\lim_{x\to\infty} f_j(x) = j - 1.$$

Proof: Lemma 4 combined with (4.2) imply that the limit as x goes to infinity exists and is greater than or equal to $j-1$. Let's consider $A(x,k)$ only, as it will be sufficient for our purposes. Let $\delta > 0$. For $|k| > \delta$, the operators $N_-(0,k)$ have a uniform lower bound $d = d(\delta) > 0$, we have that

$$\begin{aligned}(A(x,k)\phi,\phi) &= \frac{-1}{x}\left(\frac{\partial\psi_j}{\partial n_+},\phi\right)^2 + (N_-(0,k)\phi,\phi) \\ &\geq \frac{-1}{x}\left|\left|\frac{\partial\psi_j}{\partial n_+}\right|\right|^2 ||\phi||^2 + d\,||\phi||^2 \\ &= \left(\frac{-1}{x}\left|\left|\frac{\partial\psi_j}{\partial n_+}\right|\right|^2 + d\right)||\phi||^2 \qquad (4.6)\end{aligned}$$

It is clear from (4.6) that $(A(x,k)\phi,\phi) > 0$ when

$$x > \frac{\left|\left|\frac{\partial\psi_j}{\partial n_+}\right|\right|^2}{d}.$$

But if this is the case, then any k for which $|k| > \delta$ cannot possibly be in $E^{as}(x)$. Since δ is arbitrary, the characteristic function of $E^{as}(x)$, $\chi_{as}(k)$, converges pointwise almost everywhere to 0 as $x \to \infty$. It follows that

$$\lim_{x\to\infty} f_j(x) = j - 1 + \lim_{x\to\infty} vol(E^{as}(x)) = j - 1 \qquad (4.7)$$

Q.E.D.

4.2. Asymptotics for $f_j(x)$ as $x \to \infty$

The preceding results give a clearer picture of the density of states function in this setting at the upper end of the spectral band in the large coupling limit. Lemma 5 begins the next step of examining the behavior of the $f_j(x)$ as $x \to \infty$. A better understanding of this behavior will make up the remainder of this dissertation.

Lemma 5 implies that

$$vol(E^{as}(x)) \to 0 \quad \text{as} \quad x \to \infty. \qquad (4.8)$$

We would like to know more about the behavior of these volumes as $x \to \infty$. Recall that one of the key players in the definition of the f_j was the non-negative Dirichlet-to-Neumann operator $N_-(0,k)$. For k such that $|k| \geq \eta > 0$, these operators are uniformly bounded from below. We can see how this fact is crucial when $x \to \infty$ if we use (4.2) to write down the $f_j(x)$, i.e.,

$$f_j(x) = j - 1 + vol(E^{as}(x)),$$

where

$$E^{as}(x) = \left\{ k \in K = \left[-\frac{1}{2}, \frac{1}{2}\right)^n : \exists \phi \text{ s.t. } (A(x,k)\phi, \phi) < 0 \right\}, \tag{4.9}$$

and

$$(A(x,k)\phi, \phi) = -\frac{1}{x}\left(\frac{\partial \psi_j}{\partial n_+}, \phi\right)^2 + (N_-(0,k)\phi, \phi)\,. \tag{4.10}$$

It is clear from (4.10) and the preceding discussion about $N_-(0,k)$ that the quantity $(N_-(0,k)\phi, \phi)$ must go to 0 as $x \to \infty$ in order for any particular k to be in $E^{as}(x)$ for large x. As a result, we expect the contributions to the volume of $E^{as}(x)$ for large x to come from small k (in the norm sense). The only value of k for which $N_-(0,k)$ has 0 as an eigenvalue is $k = 0$. In this case, the eigenspace is one-dimensional and consists of the constant functions. Recall that $N_-(0,k)$ depends smoothly on k. So for small k, we can expand $N_-(0,k)$ in a Taylor series about $k = 0$. We get

$$\begin{aligned} N_-(0,k) &= N_-(0,0) + \sum_{\alpha=1}^{n} D_\alpha N_-(0,0) k_\alpha \\ &\quad + \sum_{\alpha \leq \beta} \left(1 - \frac{\delta_{\alpha,\beta}}{2}\right) D_{\alpha,\beta} N_-(0,0) k_\alpha k_\beta + o(|k|^2), \end{aligned} \tag{4.11}$$

where $D_\alpha = \partial/\partial k_\alpha$ and $D_{\alpha,\beta} = D_\alpha D_\beta$. We are interested in the constant function 1, and so we write down

$$(N_-(0,k)1,1) = \sum_{\alpha \leq \beta} \left(1 - \frac{\delta_{\alpha,\beta}}{2}\right) (D_{\alpha,\beta} N_-(0,0)1,1)\, k_\alpha k_\beta + o(|k|^2), \tag{4.12}$$

where we have made use of two facts. First, $N_-(0,0)1 = 0$. Second, the vector $D_\alpha N_-(0,0)1$ lies in the subspace orthogonal to constants. A proof of this last fact can be found in [9], but we will include it here for the convenience of the reader. We will need to introduce the normalized eigenfunction $\ell(k)$ for $N_-(0,k)$, where

$$N_-(0,k)\ell(k) = \omega(k)\ell(k), \quad \ell(0) = 1. \tag{4.13}$$

Recall that $N_-(0,0)$ has 0 as its lowest eigenvalue and that it has multiplicity equal to 1, i.e., it is simple. As a result, for $|k|$ sufficiently small, the eigenvalue $\omega(k)$ will be simple and hence differentiable with respect to any k_α. When we differentiate the above expression with respect to k_α, we get

$$D_\alpha N_-(0,k)\ell(k) + N_-(0,k)D_\alpha\ell(k) = (D_\alpha\omega(k))\,\ell(k) + \omega(k)D_\alpha\ell(k). \tag{4.14}$$

Since $N_-(0,k)$ is positive for $k \neq 0$, the value $k = 0$ is a minimum for $\omega(k)$ with respect to k. This implies that $D_\alpha\omega(0) = 0$ for all α. Setting $k = 0$ in (4.14), we conclude that

$$D_\alpha N_-(0,0)1 = -N_-(0,0)D_\alpha\ell(0). \tag{4.15}$$

And since the image of $N_-(0,0)$ is orthogonal to constants, the same can be said about the vector $D_\alpha N_-(0,0)1$. So $(D_\alpha N_-(0,k)1, 1) = 0$ for each α. Let

$$S(k) = \sum_{\alpha\leq\beta}\left(1 - \frac{\delta_{\alpha,\beta}}{2}\right)(D_{\alpha,\beta}N_-(0,0)1, 1)\,k_\alpha k_\beta, \tag{4.16}$$

where this is nothing more than a homogeneous polynomial of order 2 in n variables. It is important to show that $S(k)$ is a positive definite quadratic form. This can be done using formula (4.17) in [9], i.e.,

$$(D_{\alpha,\beta}N_-(0,0)1, 1) = 2\,(N_-(0,0)x_\alpha, x_\beta) + 4\delta_{\alpha,\beta}|\Omega_+| + 2\delta_{\alpha,\beta}|\Omega_-|, \tag{4.17}$$

where x_j is the j^{th} coordinate function. We can rewrite $S(k)$ as

$$\begin{aligned} S(k) = {} & \textstyle\sum_{\alpha=1}^{n}\left((N_-(0,0)x_\alpha, x_\alpha) + 2|\Omega_+| + |\Omega_-|\right)k_\alpha k_\alpha \\ & +2\textstyle\sum_{\alpha<\beta}(N_-(0,0)x_\alpha, x_\beta)\,k_\alpha k_\beta. \end{aligned} \tag{4.18}$$

The terms involving the volumes of $\Omega_{\pm}$ can be dropped since they are clearly positive. The result can be written as

$$\sum_{\alpha=1}^{n}(N_{-}(0,0)(k_{\alpha}x_{\alpha}),(k_{\alpha}x_{\alpha}))+2\sum_{\alpha<\beta}(N_{-}(0,0)(k_{\alpha}x_{\alpha}),(k_{\beta}x_{\beta}))\,. \tag{4.19}$$

Noting that $N_{-}(0,0)$ is self-adjoint and strictly positive when acting on functions other than constants, we can quickly conclude that (4.19) is a positive quantity since it is equal to

$$\left(N_{-}(0,0)\left(\sum_{\alpha=1}^{n}k_{\alpha}x_{\alpha}\right),\left(\sum_{\alpha=1}^{n}k_{\alpha}x_{\alpha}\right)\right)>0. \tag{4.20}$$

As a result, $S(k)>0$ and hence is a positive definite quadratic form. Let $\Psi=\left(\frac{\partial\psi_j}{\partial n_+},1\right)^2$ and define

$$\mathcal{S}=\{k\in\mathbb{R}^n : S(k)<\Psi\}\,. \tag{4.21}$$

The fact that $S(k)$ is positive definite ensures that $vol(\mathcal{S})<\infty$.

With all of this said, we are now in a position to state the asymptotics of $f_j(x)$ as $x\to\infty$.

Lemma 6. *$f_j(x)\sim j-1+x^{-\frac{n}{2}}vol(\mathcal{S})$ as $x\to\infty$.*

Proof: Due to the form of the $f_j(x)$ as given in (4.2), we are only interested in $vol(E^{as}(x))$ as $x\to\infty$. This quantity goes to 0 in the limit, so we can rescale. We will replace k by $\tilde{k}=k\sqrt{x}$. We have

$$vol(E^{as}(x)) \;=\; \int_K \chi_{E^{as}(x)}(k)dk, \tag{4.22}$$

where $\chi_{E^{as}(x)}(k)$ is the characteristic function for the set $E^{as}(x)$. With our rescaling in mind, we compute that

$$\begin{aligned} x^{n/2}vol(E^{as}(x)) &= \int_K x^{n/2}\chi_{E^{as}(x)}(k)dk \\ &= \int_{\sqrt{x}K}\chi_{E^{as}(x)}\left(\frac{\tilde{k}}{\sqrt{x}}\right)d\tilde{k}. \end{aligned} \tag{4.23}$$

We can reinterpret the final expression on the right as defining the volume of the set

$$\tilde{E}^{as}(x) = \left\{ \tilde{k} \in \left[-\frac{\sqrt{x}}{2}, \frac{\sqrt{x}}{2} \right)^n : \exists \phi \text{ s.t. } \left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right) \phi, \phi \right) < 0 \right\}. \tag{4.24}$$

To see this, suppose that $\tilde{k} \in \sqrt{x}K$ is such that $\tilde{k}/\sqrt{x} = k \in E^{as}(x)$. Then the definition of $E^{as}(x)$ implies that there exists a ϕ such that $(A(x,k)\phi, \phi) < 0$. Suppose we can show that

$$vol(\tilde{E}^{as}(x)) \sim vol(\mathcal{S}) \quad \text{as} \quad x \to \infty, \tag{4.25}$$

where $\mathcal{S}$ is defined in (4.21). Then the lemma would follow from (4.2), (4.23) and (4.25). So we have only to show the validity of (4.25).

Let $\tilde{k} \in \mathcal{S}$. Then $S(\tilde{k}) < \Psi$. For sufficiently large values of x, we can make use of (4.12) and (4.16) to expand

$$\begin{aligned} \left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right) 1, 1 \right) &= -\frac{1}{x}\Psi + \left(N_- \left(0, \frac{\tilde{k}}{\sqrt{x}}\right) 1, 1 \right) \\ &= -\frac{1}{x}\Psi + S\left(\frac{\tilde{k}}{\sqrt{x}}\right) + o\left(\frac{|\tilde{k}|^2}{x}\right), \end{aligned} \tag{4.26}$$

as $x \to \infty$. Since S is a homogeneous polynomial of order 2, we know that

$$S\left(\frac{\tilde{k}}{\sqrt{x}}\right) = \frac{1}{x} S(\tilde{k}). \tag{4.27}$$

As a result, there exists a sufficiently large X such that for $x > X$, $\tilde{k} \in \sqrt{x}K$ and $\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right) 1, 1\right) < 0$. This implies that $\tilde{k} \in \tilde{E}^{as}(x)$ as $x \to \infty$.

Suppose now that $\tilde{k} \notin \mathcal{S}$. Then $S(\tilde{k}) \geq \Psi$. Since S is a polynomial and we are concerned with volumes, we can ignore the cases when $S(\tilde{k}) = \Psi$. Consider

$$\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right) \phi, \phi \right) = -\frac{1}{x} \left(\frac{\partial \psi_j}{\partial n_+}, \phi \right)^2 + \left(N_- \left(0, \frac{\tilde{k}}{\sqrt{x}}\right) \phi, \phi \right). \tag{4.28}$$

We need to establish that the above will be greater than 0 for sufficiently large x no matter what ϕ is. For this, we will begin by considering the case when $\phi = 1$. We make use of (4.26) and the assumption that $S(\tilde{k}) > \Psi$ to conclude that

$$\begin{aligned}\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right)1, 1\right) &= -\frac{1}{x}\Psi + S\left(\frac{\tilde{k}}{\sqrt{x}}\right) + o\left(\frac{|\tilde{k}|^2}{x}\right) \\ &= \frac{1}{x}\left(-\Psi + S(\tilde{k})\right) + o\left(\frac{|\tilde{k}|^2}{x}\right) \\ &> 0, \end{aligned} \tag{4.29}$$

as $x \to \infty$. Therefore the constant function results in $(A\left(x, \tilde{k}/\sqrt{x}\right)1, 1) > 0$ for $x > X$, where X is some sufficiently large positive number.

The next collection of ϕ that we will consider have the form $\phi = 1 + \phi_n$. Suppose that $||\phi_n|| < \epsilon$, where the value of $\epsilon > 0$ will be determined in a moment. We have

$$\begin{aligned}\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right)(1+\phi_n), (1+\phi_n)\right) = \quad & \left(A\left(x, \tfrac{\tilde{k}}{\sqrt{x}}\right)1, 1\right) \\ & +2\left(A\left(x, \tfrac{\tilde{k}}{\sqrt{x}}\right)1, \phi_n\right) \\ & +\left(A\left(x, \tfrac{\tilde{k}}{\sqrt{x}}\right)\phi_n, \phi_n\right), \end{aligned} \tag{4.30}$$

where we have made use of the fact that A is self-adjoint. The second term on the right-hand side can be bounded below in the following way. By definition,

$$\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right)1, \phi_n\right) = -\frac{1}{x}\left(\frac{\partial \psi_j}{\partial n_+}, 1\right)\left(\frac{\partial \psi_j}{\partial n_+}, \phi_n\right) + \left(N_-\left(0, \frac{\tilde{k}}{\sqrt{x}}\right)1, \phi_n\right). \tag{4.31}$$

Using the Cauchy-Schwarz inequality, we know that

$$\left(\frac{\partial \psi_j}{\partial n_+}, \phi_n\right) \leq \left|\left|\frac{\partial \psi_j}{\partial n_+}\right|\right| \, ||\phi_n|| \tag{4.32}$$

and

$$\left(N_-\left(0, \frac{\tilde{k}}{\sqrt{x}}\right)1, \phi\right) \geq -\left|\left|N_-\left(0, \frac{\tilde{k}}{\sqrt{x}}\right)1\right|\right| \, ||\phi_n||. \tag{4.33}$$

Since $N_{-}(0,0)1 = 0$ and $N_{-}(0,k)$ is continuous with respect to k, there exists an $M > 0$ such that

$$\left\| N_{-}\left(0, \frac{\tilde{k}}{\sqrt{x}}\right) 1 \right\| < M, \tag{4.34}$$

for all $x > X$. Using these facts along with the assumption that $||\phi_n|| < \epsilon$, we can bound (4.31) from below, i.e.,

$$\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right) 1, \phi_n \right) \geq -\frac{1}{x}\left(\frac{\partial \psi_j}{\partial n_+}, 1\right) \left\| \frac{\partial \psi_j}{\partial n_+} \right\| \epsilon - M\epsilon. \tag{4.35}$$

In a similar way, we will deal with the third term, i.e.,

$$\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right) \phi_n, \phi_n \right) = -\frac{1}{x}\left(\frac{\partial \psi_j}{\partial n_+}, \phi_n\right)^2 + \left(N_{-}\left(0, \frac{\tilde{k}}{\sqrt{x}}\right) \phi_n, \phi_n \right). \tag{4.36}$$

Since $N_{-}(0,k)$ is a nonnegative operator, we can forget about the last term in (4.36) as we are looking for lower bounds. For the first term in (4.36), we can again make use of the Cauchy-Schwarz inequality. The result is that

$$\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right) \phi_n, \phi_n \right) \geq -\frac{1}{x}\left\| \frac{\partial \psi_j}{\partial n_+} \right\|^2 \epsilon^2. \tag{4.37}$$

It follows from (4.35) and (4.37) that

$$\begin{aligned} \left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right) (1+\phi_n), (1+\phi_n) \right) \geq & \left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right) 1, 1 \right) \\ & -\frac{1}{x}\left(\frac{\partial \psi_j}{\partial n_+}, 1\right) \left\| \frac{\partial \psi_j}{\partial n_+} \right\| \epsilon - M\epsilon - \frac{1}{x}\left\| \frac{\partial \psi_j}{\partial n_+} \right\|^2 \epsilon^2. \end{aligned} \tag{4.38}$$

The selection of the value of ϵ should be such that it makes the right-hand side of the above expression greater than 0. Such an ϵ can be found since for $x > X$, $\left(A\left(x, \tilde{k}/\sqrt{x}\right) 1, 1\right) > 0$. It follows that for $x > X$, the quantity

$$\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right) (1+\phi_n), (1+\phi_n) \right) \tag{4.39}$$

will be positive for any ϕ_n which is orthogonal to constants and has norm less than ϵ.

We will now consider functions $\phi = 1 + \phi_n$, where ϕ_n is orthogonal to constants and $||\phi_n|| \geq \epsilon$. We will again be considering the quantity

$$\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right)(1+\phi_n), (1+\phi_n)\right) = -\frac{1}{x}\left(\frac{\partial \psi_j}{\partial n_+}, 1+\phi_n\right)^2 + \left(N_-\left(0, \frac{\tilde{k}}{\sqrt{x}}\right)(1+\phi_n), (1+\phi_n)\right). \quad (4.40)$$

Recall that $N_-(0,0)$ has a simple eigenvalue at 0 which corresponds to an eigenspace spanned by the constant function 1. Therefore, the variational characterization of the eigenvalues of $N_-(0,0)$ tells us that

$$(N_-(0,0)(1+\phi_n), (1+\phi_n)) \geq (N_-(0,0)\phi_n, \phi_n) \geq C||\phi_n||^2, \quad (4.41)$$

where $C > 0$ and ϕ_n is any function which is orthogonal to constants. Let us note that C is independent of ϕ_n. Continuity of this variational characterization implies that for a sufficiently large x,

$$\left(N_-\left(0, \frac{\tilde{k}}{\sqrt{x}}\right)(1+\phi_n), (1+\phi_n)\right) \geq C'||\phi_n||^2, \quad (4.42)$$

where $C' > 0$ is possibly different from C but is also independent of ϕ_n. This implies that

$$\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right)(1+\phi_n), (1+\phi_n)\right) \geq -\frac{1}{x}\left|\left|\frac{\partial \psi_j}{\partial n_+}\right|\right|^2 (1+\epsilon)^2 + C'\epsilon^2, \quad (4.43)$$

where we have used the Cauchy-Schwarz inequality and our assumption that $||\phi_n|| \geq \epsilon$. It is clear from this expression that there exists a sufficiently large value of x that will make this positive for any ϕ_n which is orthogonal to constants and has norm greater than or equal to ϵ. It should be noted that any function ϕ which is not itself orthogonal to constants can be normalized in such a way so as to be written as $1+\phi_n$. As a result, any such ϕ has been dealt with in the above arguments.

The only functions ϕ which are not handled with the above arguments are those such that $\phi = \phi_n$, i.e., ϕ is orthogonal to constants. For this, we note that

$$\left(A\left(x, \frac{\tilde{k}}{\sqrt{x}}\right)\phi_n, \phi_n\right) \geq -\frac{1}{x}\left|\left|\frac{\partial \psi_j}{\partial n_+}\right|\right|^2 ||\phi_n||^2 + C'||\phi_n||^2, \tag{4.44}$$

which will be positive for a sufficiently large value of x. To find a sufficiently large value of x that will work for any ϕ, we simply take the maximum of the three values determined by the three types of ϕ, i.e., $\phi = 1$, $\phi = 1 + \phi_n$, where ϕ_n is orthogonal to constants and have norm greater than ϵ, and $\phi = \phi_n$. Therefore, we have dealt with all possible ϕ in a uniform manner. It follows that if $\tilde{k} \notin \mathcal{S}$ then $\tilde{k} \notin \tilde{E}^{as}(x)$ as $x \longrightarrow \infty$. So $vol(\mathcal{S}) \sim vol(\tilde{E}^{as}(x)$ as $x \longrightarrow \infty$ and the proof of the lemma is complete. Q.E.D.

References

[1] J. Albert, *Generic properties of eigenfunctions of elliptic partial differential operators*, Trans. Amer. Math. Soc. **238** (1978), 341–354.

[2] N.W. Ashcroft and N.D. Mermin, *Solid state physics*, Holt, Rinehart and Winston, New York-London, 1976.

[3] F. Bloch, *Über die quantenmechanik der elektronen in kristallgittern*, Zeit. für Physik **52** (1928), 555–600.

[4] R. H. Bube, *Electronic properties of crystalline solids*, Academic Press, New York-London, 1974.

[5] A. Figotin and P. Kuchment, *Band-gap structure of spectra of periodic dielectric and acoustic media. i: Scalar model*, SIAM Journal in Applied Mathematics **56** (1996), 68–88.

[6] ———, *Spectral properties of classical waves in high-contrast periodic media*, SIAM Journal in Applied Mathematics **58** (1998), 683–702.

[7] G. Floquet, *Sur les equations differentielles lineaires a coefficients periodiques*, Ann. Ecole Norm. **12** (1883), 47–89.

[8] L. Friedlander, *Some inequalities between dirichlet and neumann eigenvalues*, Arch. Rational Mech. Anal. **116** (1991), 153–160.

[9] ———, *On the density of states of periodic media in the large coupling limit*, Commun. Partial Diff. Equations **27** (2002), 355–380.

[10] R. Hempel and K. Lienau, *Spectral properties of periodic media in the large coupling limit*, Commun. Partial Diff. Equations **25** (2000), 1445–1470.

[11] Tosio Kato, *Perturbation theory for linear operators*, Die Grundlehren der mathematischen Wissenschaften, Band 132, Springer-Verlag New York, Inc., New York, 1966.

[12] P. Kuchment, *Floquet theory for partial differential equations*, Birkhäuser: Base, 1993.

[13] A. I. Markushevich, *Theory of functions of a complex variable*, vol. 1-3, Chelsea Publishing Company, New York, 1985.

[14] M. Reed and B. Simon, *Methods of modern mathematical physics, vol. iv. analysis of operators*, Academic Press: New York, 1976.

[15] K. Uhlenbeck, *Generic properties of eigenfunctions*, Amer. J. Math. **98** (1976), 1059–1078.