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THEORY OF BLOCH WAVES.(U)

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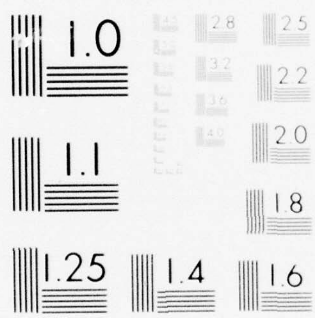

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THEORY OF BLOCH WAVES

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ABSTRACT

The Bloch waves of the one-electron theory of electronic states in crystals are the eigenfunctions of a family of unbounded selfadjoint operators $H(p)$ that depend holomorphically on the wave momentum $p = (p_1, p_2, p_3) \in R^3$. $H(p)$ has a discrete spectrum, with corresponding complete orthonormal sequences of eigenfunctions, and it is customary to denote such a sequence by $\{\psi_n(p)\}$ and speak of "the" Bloch waves. However, the eigenfunctions are not unique and a separate choice is required for each p. The customary definition therefore rests on the axiom of choice and can provide no information about the p-dependence of the Bloch waves. Some information is essential for applications. A minimal requirement is p-measurability. In this paper the operators $K(p) = (H(p) + \gamma_0^2)^{-2}$ are shown to form a family of Fredholm integral operators that is holomorphic for $p \in C^3$, $|\mathrm{Im}\ p| < \gamma_0$. The classical theory of Fredholm minors is then used to construct families of Bloch waves $\psi_n(p)$ which are holomorphic on the complement of a closed nullset.

CONTENTS

1. INTRODUCTION AND STATEMENT OF RESULTS

The main features of the electronic states of crystalline solids have been deduced from the one-electron model [26, Ch. 3]. The principal operator of the theory is the one-electron Hamiltonian

$$H = -\Delta + V \tag{1.1}$$

where Δ is the Laplace operator in three-dimensional Euclidean space E^3 and V denotes multiplication by the real-valued crystal potential which has the periodicity of the crystal lattice. It will be convenient to describe H by means of a fixed system of lattice coordinates. Thus if $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ is a lattice basis in E^3 then the position vectors $\vec{q}$ of points in E^3 may be identified with the coordinate triples $q = (q^1, q^2, q^3) \in R^3$ defined by

$$\vec{q} = \sum_{j=1}^{3} q^j \vec{a}_j \tag{1.2}$$

Δ has the representation

$$\Delta = \sum_{j,k=1}^{3} g^{jk} \frac{\partial^2}{\partial q^j \partial q^k} \tag{1.3}$$

where g^{jk} are the contravariant components of the metric tensor for the coordinates q^j. V is represented by a real-valued function V(q) of the coordinates and the periodicity condition becomes

$$V(q + m) = V(q) \text{ for all } q \in R^3 \text{ and } m \in Z^3 \tag{1.4}$$

where Z denotes the set of integers. A unit cell in the crystal is described by the unit cube

$$\Omega = \{q \in R^3:\ -1/2 < q^1, q^2, q^3 < 1/2\} \tag{1.5}$$

in the coordinate space. It is assumed throughout the paper that $V(q) \in L_2(\Omega)$; i.e., $V(q)$ is Lebesgue measurable in Ω and

$$\|V\|^2_{L_2(\Omega)} = \int_\Omega |V(q)|^2\, dq < \infty \tag{1.6}$$

where $dq = dq^1 dq^2 dq^3$ denotes Lebesgue measure in R^3. The Hamiltonian H is identified with the selfadjoint realization of the differential operator $-\Delta + V(q)$ in $L_2(R^3)$. Its domain $D(H) = L_2^2(R^3)$ is the Sobolev space of functions $u(q)$ whose distribution derivatives $D^\alpha u(q) = \partial^{\alpha_1+\alpha_2+\alpha_3} u(q)/\partial q_1^{\alpha_1} \partial q_2^{\alpha_2} \partial q_3^{\alpha_3} \in L_2(R^3)$ for $0 \le \alpha_1 + \alpha_2 + \alpha_3 \le 2$.

H is known to have a continuous band spectrum. Moreover, a spectral representation of H can be based on the theory of the generalized eigenfunctions known as Bloch waves. The literature contains several proofs of the completeness of families of Bloch waves that fulfill certain regularity conditions (usually unspecified) concerning their dependence on the wave momentum $p \in R^3$. It is surprising that the literature contains no proof of the existence of such families although their existence has been asserted. The purpose of the present paper is to close this gap in the theory by giving an explicit construction of families of Bloch waves that have adequate regularity properties.

The paper is organized as follows. In the remainder of this section the Bloch waves are defined and the principal results of the paper are formulated. Section 2 contains a discussion of related literature. Section 3 presents a construction of a holomorphic family K(p) of Fredholm integral operators in $L_2(\Omega)$ whose eigenfunctions are precisely the Bloch waves for H. In section 4 the Fredholm determinant of K(p) is used to construct the Bloch wave eigenvalues or energy band functions. In section 5 the Fredholm minors of K(p) are used to construct families of Bloch waves that are "almost" holomorphic functions of p; i.e., holomorphic on the complement of a closed nullset in R^3. Section 6 contains proofs of the lemmas formulated in the preceding sections.

The selfadjointness of the Hamiltonian H follows from

Lemma 1.1. $D(H) = L_2^2(R^3) \subset D(V)$ and there exists a constant $C > 0$ such that for all $u \in D(H)$ and $r \geq 1$

$$(1.7) \qquad \|Vu\|^2_{L_2(R^3)} \leq C\|V\|^2_{L_2(\Omega)}\, r^{-1/2}\, (\|\Delta u\|^2_{L_2(R^3)} + r^2\|u\|^2_{L_2(R^3)})$$

It is well known that $H_0 = -\Delta$ acting on the domain $D(H_0) = L_2^2(R^3)$ is a selfadjoint non-negative operator in $L_2(R^3)$ (see e.g. [24]). Hence Lemma 1.1 and theorems of T. Kato [12, pp. 287-291] imply

Lemma 1.2. $H = -\Delta + V = H_0 + V$, acting on the domain $D(H) = L_2^2(R^3)$, is a selfadjoint operator in $L_2(R^3)$. Moreover, H is bounded below.

Note that a constant potential satisfies (1.4), (1.6). Thus if $H \geq -\alpha$ $(\alpha > 0)$ then replacing $V(q)$ by $V(q) + \alpha$ gives a new Hamiltonian that satisfies

$$(1.8) \qquad H \geq 0$$

In the remainder of the paper it is assumed that H satisfies (1.8).

The Bloch waves for H are the solutions of the equation

$$(1.9) \qquad H\psi(q) \equiv -\Delta\psi(q) + V(q)\psi(q) = \lambda\psi(q),\ q \in R^3$$

that have the form

$$(1.10) \qquad \psi(q) = e^{2\pi i\, p\cdot q}\ \phi(q),\ q \in R^3$$

where $p \in R^3$, $p \cdot q = \Sigma_{j=1}^{3} p_j q^j$ and $\phi(q)$ is a non-zero function having the periodicity of $V(q)$:

$$(1.11) \qquad \phi(q + m) = \phi(q) \text{ for all } q \in R^3 \text{ and } m \in Z^3$$

Conditions (1.10), (1.11) are equivalent to the property

$$(1.12) \qquad \psi(q + m) = e^{2\pi i\, p\cdot m}\ \psi(q) \text{ for all } q \in R^3 \text{ and } m \in Z^3$$

Functions that satisfy (1.12) will be said to be p-periodic. This class of solutions of (1.9) was introduced by F. Bloch [2] in the quantum theory of electrons in crystals. In the theory the parameters p_j are interpreted as the covariant components of a momentum vector $\vec{p} = \Sigma_{j=1}^{3} p_j \vec{a}^j$ where $\vec{a}^1$, $\vec{a}^2$, $\vec{a}^3$ is the basis dual to the crystal lattice basis $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$. The two bases are related by $\vec{a}^j \cdot \vec{a}_k = 2\pi\ \delta^j_k$. It is clear from (1.12) that the p_j are only determined modulo Z and hence p may be restricted to the set Ω. This is equivalent to restricting $\vec{p}$ to the unit cell of the reciprocal lattice.

Condition (1.12) implies that each Bloch wave is determined by its values at the points $q \in \Omega$ and its momentum $p \in \Omega$. Moreover, the Bloch waves corresponding to each fixed p are the eigenfunctions of a p-dependent selfadjoint realization of H in $L_2(\Omega)$. To see how such an operator may be defined note that the six faces of the cube $\partial\Omega$ have the equations $q^j = \pm 1/2$ $(j = 1,2,3)$ and (1.12) implies

$$(1.13) \qquad \psi(q)\Big|_{q^j=\frac{1}{2}} = e^{2\pi i\, p_j}\ \psi(q)\Big|_{q^j=-\frac{1}{2}} \text{ for } j = 1,2,3$$

and

(1.14) $$\partial\psi(q)/\partial q^k \Big|_{q^j=\frac{1}{2}} = e^{2\pi i p_j}\, \partial\psi(q)/\partial q^k \Big|_{q^j=-\frac{1}{2}} \quad \text{for } j,k = 1,2,3$$

The last condition implies

(1.15) $$\partial\psi(q)/\partial\nu \Big|_{q^j=\frac{1}{2}} = -e^{2\pi i p_j}\, \partial\psi(q)/\partial\nu \Big|_{q^j=-\frac{1}{2}} \quad \text{for } j = 1,2,3$$

where $\partial/\partial\nu = \vec{\nu}\cdot\nabla$ and $\vec{\nu}(q)$ is an exterior unit normal to $\partial\Omega$ (and hence $\vec{\nu}(q)\Big|_{q^j=\frac{1}{2}} = -\vec{\nu}(q)\Big|_{q^j=-\frac{1}{2}}$). Moreover, conditions (1.13)-(1.15) are meaningful for all $\psi \in L_2^2(\Omega)$ by the trace theorem [13]. It will be shown that H, acting on the subset of $L_2^2(\Omega)$ defined by (1.13), (1.15), is a selfadjoint operator $H(p)$ in $L_2(\Omega)$. It will be convenient to consider first the operator $H_0(p)$ in $L_2(\Omega)$ defined by $H_0 = -\Delta$ acting on the same domain. Thus

(1.16) $$D(H_0(p)) = L_2^2(\Omega) \cap \{\psi\colon\ \psi \text{ satisfies (1.13) and (1.15)}\}$$

(1.17) $$H_0(p)\psi = -\Delta\psi \text{ for all } \psi \in D(H_0(p))$$

It is easy to verify by Fourier analysis that

(1.18) $$\psi_m^0(q,p) = e^{2\pi i p\cdot q}\, e^{-2\pi i m\cdot q}, \quad m \in Z^3$$

defines a complete orthonormal sequence of eigenfunctions for $H_0(p)$, with corresponding eigenvalues

(1.19) $$\lambda_m^0(p) = 4\pi^2 |p-m|^2 = 4\pi^2 \sum_{j,k=1}^{3} g^{jk}(p_j - m_j)(p_k - m_k),$$

and that $H_0(p)^* = H_0(p) \geq 0$. The following analogue of Lemma 1.1 is valid for $H_0(p)$.

Lemma 1.3. There exists a constant $C_0 > 0$ such that for all $\psi \in D(H_0(p))$, all $r \geq 1$ and all $p \in R^3$

(1.20) $$\|V\psi\|^2_{L_2(\Omega)} \le C_0\|V\|^2_{L_2(\Omega)}\ r^{-1/2}\ (\|H_0(p)\psi\|^2_{L_2(\Omega)} + r^2\|\psi\|^2_{L_2(\Omega)})$$

Lemma 1.3 and Kato's theorem [12, pp. 287-291] imply

Lemma 1.4. For all $p \in R^3$ the operator $H(p) = H_0(p) + V$ with domain $D(H(p)) = D(H_0(p))$ is selfadjoint in $L_2(\Omega)$. Moreover, $H(p)$ is uniformly bounded below; $H(p) \ge -\alpha$ for all $p \in R^3$.

Adding α to $V(q)$ produces a non-negative operator, as in the case of H; i.e.,

(1.21) $$H(p) \ge 0 \text{ for all } p \in R^3$$

In what follows it is assumed that (1.21) holds.

Lemma 1.4 and the compactness of the embedding of $L_2^2(\Omega)$ in $L_2(\Omega)$ (Rellich's selection theorem [16]) imply

Lemma 1.5. The resolvent operator $R_\zeta(H(p)) = (H(p) - \zeta)^{-1}$ is compact for every $p \in R^3$ and every ζ in the resolvent set of $H(p)$. Hence, in particular, $H(p)$ has a discrete spectrum $\sigma(H(p))$ for every $p \in R^3$.

The Bloch waves for the operator H and momentum p are by definition the eigenfunctions of $H(p)$. The remainder of the paper is devoted to the study of these functions and their eigenvalues. Note that since $H(p+m) = H(p)$ for all $p \in R^3$ and $m \in Z^3$ it is sufficient to study $H(p)$ for $p \in \overline{\Omega} = \{p: -\frac{1}{2} \le p_1, p_2, p_3 \le \frac{1}{2}\}$.

The eigenvalues of $H(p)$, enumerated by magnitude and repeated according to their finite multiplicities define a sequence $\{\lambda_n(p)\}$ such that (recall (1.8))

(1.22) $$0 \le \lambda_1(p) \le \lambda_2(p) \le \cdots \le \lambda_n(p) \le \cdots$$

Moreover, $\lambda_n(p) \to \infty$ for $n \to \infty$. In fact, the estimates of Eastham [8, p. 101] imply that there exists a constant $c > 0$ such that for every $p \in R^3$

$$\lambda_n(p) \sim c\, n^{2/3}, \quad n \to \infty \tag{1.23}$$

The continuity of the functions $\lambda_n \colon \bar{\Omega} \to R$ can be derived from perturbation theory [7, 8, 12]. Moreover, each $\lambda_n(p)$ is a holomorphic function of the individual coordinates p_j [12, p. 392]. However, perturbation theory is inadequate to prove that $\lambda_n(p)$ is a holomorphic function of all three variables [12, p. 117]. One goal of this paper is to prove that each $\lambda_n(p)$ is holomorphic for $p \in \bar{\Omega} - X_n$ where X_n is an analytic variety of degree ≤ 2 in R^3. In particular, X_n is a closed nullset in R^3. This result is proved by showing that the graphs of the $\lambda_n(p)$ are components of a real analytic variety in R^4. More precisely, the following result is proved in section 4.

Theorem 1. To each potential $V(q)$ that satisfies (1.4), (1.6) and each $\gamma > 0$ there corresponds a function $D(p,\lambda)$, holomorphic for $|\text{Im } p| \leq \gamma$ and $\lambda \in C$ and satisfying $D(p+m,\lambda) = D(p,\lambda)$, such that for each $p \in R^3$ the sequence $\{\lambda_n(p)\}$ is precisely the set of zeros of $D(p,\lambda)$, enumerated by magnitude and repeated according to their multiplicities.

The assertion that $D(p,\lambda)$ is holomorphic on the closed set defined by $|\text{Im } p| \leq \gamma$ means, as usual, that it is holomorphic on an open set containing this set. A construction of a function $D(p,\lambda)$ having the properties listed in Theorem 1 is given in section 4.

Lemma 1.5 implies that for each $p \in R^3$ there exist complete orthonormal sequences of eigenfunctions of $H(p)$. In the literature most authors, after defining $H(p)$, say "let $\{\psi_n(q,p)\}$ be a complete orthonormal sequence of eigenfunctions of $H(p)$" and proceed to talk about "the" eigenfunctions $\psi_n(q,p)$. This language and notation are misleading because the eigenfunctions are not unique. Indeed, even if the eigenvalues $\lambda_n(p)$ are simple for all

$p \in R^3$ the phase of each eigenfunction can be chosen to be an arbitrary function of p. If the $\lambda_n(p)$ are degenerate and their multiplicities vary with p the range of choices is much wider. The formal basis of the customary definition of the Bloch waves is evidently the axiom of choice applied to the uncountable set of all $p \in R^3$. It is clear that this approach cannot provide any information about the p-dependence of the Bloch waves. Even the existence of p-measurable families is in doubt. In section 5 of this paper an explicit construction of families of Bloch waves is given that implies the following theorem.

Theorem 2. There exist sequences of functions ψ_n: $\bar{\Omega} \times \bar{\Omega} \to C$ and closed nullsets $Z_n \subset \bar{\Omega}$ such that $p \to \psi_n(\cdot,p) \in C(\bar{\Omega})$ is holomorphic for $p \in \bar{\Omega} - Z_n$ and $\{\psi_n(\cdot,p)\}$ is a complete orthonormal sequence of eigenfunctions of H(p) for all $p \in \bar{\Omega} - Z$ where $Z = \bigcup_{n=1}^{\infty} Z_n$.

The mapping $p \to \psi_n(\cdot,p)$ is holomorphic as a function of p with values in the Banach space $C(\bar{\Omega})$ with the maximum norm (see [11] for definitions). Note that Z is a nullset.

A family $\{\psi_n(q,p)\}$ with the properties described in Theorem 2 will be called an "almost holomorphic family" of Bloch waves. The continuity assertion of Theorem 2 is close to the best possible. Indeed, continuous families of eigenvectors do not exist, in general, even when H(p) is a holomorphic family of selfadjoint operators on a finite dimensional space, as may be shown by simple examples.

2. A DISCUSSION OF RELATED LITERATURE

Following the publication of F. Bloch's paper [2] in 1928 the Bloch waves and their associated energy band functions became the central concepts in the theory of electronic states in crystals. An introduction to the large physical literature on these topics can be obtained from the books of J. M. Ziman [26] and A. P. Cracknell and K. C. Wong [6]. By contrast, the mathematical theory of Bloch waves has developed much more slowly. The first results on expansions in Bloch waves are due to I. M. Gelfand [9]. In this paper, published in 1950, a proof is outlined of the Parseval relation for Bloch waves in $L_2(R^3)$ (and $L_2(R^n)$). In the notation of section 1, Gelfand's theorem states that for every $f \in L_2(R^3)$ the limits

$$\hat{f}_n(p) = L_2(\Omega)\text{-}\lim_{M\to\infty} \int_{|q|\leq M} \overline{\psi_n(q,p)}\, f(q)\, dq \tag{2.1}$$

exist for $n = 1,2,3,\cdots$ and

$$\| f\|^2_{L_2(R^3)} = \sum_{n=1}^{\infty} \|\hat{f}_n\|^2_{L_2(\Omega)} \tag{2.2}$$

The book on eigenfunction expansions of E. C. Titchmarsh [21], published in 1958, contains a chapter on Schrödinger operators with periodic potentials. The Parseval relation for Bloch waves in dimensions $n > 1$ is not discussed in this book. However, V. B. Lidskii showed in 1961 that Titchmarsh's methods can be used to derive (2.1), (2.2). A proof along these lines is presented in the book of Eastham [8].

A more detailed discussion of Bloch waves was published in 1964 by F. Odeh and J. B. Keller [15]. This paper contains derivations of both the Parseval relation (2.1), (2.2) and the Bloch wave expansion of functions $f \in L_2(R^3)$. The latter takes the form

$$(2.3) \qquad f(q) = L_2(R^3)\text{-}\lim_{N\to\infty} \sum_{n=1}^{N} \int_{\Omega} \psi_n(q,p)\, \hat{f}_n(p)\, dp$$

in the notation of section 1. The paper also contains a discussion of the energy band functions $\lambda_n(p)$ and a derivation of the relation

$$(2.4) \qquad \sigma(H) = \bigcup_{n=1}^{\infty} \lambda_n(\bar{\Omega})$$

More recently these topics have been discussed by several other authors. In 1971 Eastham [7] gave another proof of (2.4), together with two other characterization of $\sigma(H)$. In 1973 L. E. Thomas [20] showed that H is spectrally absolutely continuous [12]. The proof was based on his theorem that the Fermi surfaces $\Omega_\lambda = \{p \in \Omega\colon \ \lambda_n(p) = \lambda \text{ for some } n = 1,2,3,\cdots\}$ have Lebesgue measure zero in R^3 for every $\lambda \in R$.

None of the literature cited above contains a constructive definition of a family of Bloch waves. In each case appeal is made, explicitly or tacitly, to the "axiom of choice definition" of section 1 which provides no information about the p-dependence. Hence, the proofs of the expansion theorem (2.1)-(2.3) presented in these papers must be regarded as incomplete, or valid only under additional (unspecified) hypotheses concerning the measurability and integrability properties of the Bloch waves.

The Odeh-Keller paper contains a discussion, based on Rellich's perturbation theory, of the p-dependence of Bloch eigenfunctions and eigenvalues. The assertion [15, p. 1504, remark (iii)] that the eigenfunctions $\psi_n(q,p)$

have the same analyticity properties in p as the eigenvalues is incorrect. This statement is true of the projection operators onto the eigenspaces [12] but it is not clear how these can be used to construct families of linearly independent eigenvectors with the same regularity. As remarked at the end of section 1, piecewise holomorphy is the most that can be proved by general methods. This result could perhaps be proved by perturbation theory when the eigenvalues are all simple. No general criteria for this case are known but it is presumably rare. It is known that, for many classes of crystals, the eigenvalues $\lambda_n(p)$ have "intrinsic" degeneracies for certain values of p which are imposed by the symmetry group of the crystal and are independent of the precise form of the potential within its symmetry class [6, p. 33].

3. AN INTEGRAL EQUATION FOR BLOCH WAVES

In this section the Bloch waves are characterized as the eigenfunctions of a holomorphic family of Fredholm operators K(p) acting in $L_2(\Omega)$. The principal steps in the construction of K(p) are formulated here as a series of lemmas whose proofs are given in section 6. The construction begins with the resolvent of $H_0(p)$ evaluated at a point $-\gamma_0^2$ of the resolvent set. The notation

$$R_0(p) = (H_0(p) + \gamma_0^2)^{-1}, \quad \gamma_0 > 0, \quad p \in R^3 \tag{3.1}$$

will be used. $R_0(p)$ is an integral operator in $L_2(\Omega)$ of the form

$$R_0(p)\, f(q) = \int_\Omega G_0(q - q', p)\, f(q')\, dq', \quad f \in L_2(\Omega) \tag{3.2}$$

where $G_0(q,p)$ is a periodic function of $p \in R^3$ with the Fourier expansion

$$G_0(q,p) = \sum_{m \in Z^3} \frac{e^{-\gamma_0 |q-m|}}{4\pi |q-m|}\, e^{2\pi i\, p \cdot m}, \quad q \notin Z^3 \tag{3.3}$$

The function $G_0(q,p)$ is needed for $q \in 2\bar{\Omega} = \{q = 2q' : q' \in \bar{\Omega}\}$ to define the difference kernel of an operator (3.2) in $L_2(\Omega)$. Actually, the series in (3.3) converges and defines $G_0(q,p)$ for all $q \in R^3 - Z^3$ and all complex $p \in C^3$ such that $|\mathrm{Im}\, p| < \gamma_0/2\pi$. More precisely, one has

Lemma 3.1. The series in (3.3) converges for $(q,p) \in (R^3 - Z^3) \times \{p \in C^3 : |\mathrm{Im}\, p| < \gamma_0/2\pi\}$ and the convergence is uniform on compact subsets. Moreover, if $G_0'(q,p)$ is defined by

(3.4) $$G_0(q,p) = \sum_{m\in N} \Gamma(q-m)\, e^{2\pi i p\cdot m} + G_0'(q,p)$$

where $\Gamma(q) = e^{-\gamma_0 |q|}/4\pi|q|$ and $N = Z^3 \cap \{m: |m| \le \sqrt{3}\}$ then $G_0'(\cdot,p) \in C(2\bar{\Omega})$ and the mapping $p \to G_0'(\cdot,p) \in C(2\bar{\Omega})$ is holomorphic for $|\mathrm{Im}\ p| < \gamma_0/2\pi$.

<u>Lemma 3.2</u>. For each $p \in C^3$ with $|\mathrm{Im}\ p| < \gamma_0/2\pi$ the kernel $G_0(q-q',p) \in L_2(\Omega\times\Omega)$ and (3.2) holds. In particular, $R_0(p) \in \mathcal{B}_2(L_2(\Omega))$, the class of Hilbert-Schmidt operators in $L_2(\Omega)$, and $p \to R_0(p) \in \mathcal{B}_2(L_2(\Omega))$ is holomorphic for $|\mathrm{Im}\ p| < \gamma_0/2\pi$.

In the last statement the Hilbert space topology in $\mathcal{B}_2(L_2(\Omega))$ defined by the Hilbert-Schmidt norm is understood [12].

<u>Lemma 3.3</u>. If $V(q) \in L_2(\Omega)$ then for all $p \in C^3$ with $|\mathrm{Im}\ p| < \gamma_0/2\pi$ the operator $R_0(p)V$ is densely defined and closable as an operator in $L_2(\Omega)$. Moreover, the closure of $R_0(p)V$, denoted by $L_0(p)$, is in $\mathcal{B}_2(L_2(\Omega))$ with kernel

(3.5) $$L_0(q,q',p) = G_0(q-q',p)V(q') \in L_2(\Omega\times\Omega)$$

and the mapping $p \to L_0(p) \in \mathcal{B}_2(L_2(\Omega))$ is holomorphic for $|\mathrm{Im}\ p| < \gamma_0/2\pi$.

<u>Lemma 3.4</u>. To each $V(q) \in L_2(\Omega)$ and each $\gamma > 0$ there corresponds a constant $M = M(V,\gamma) > 2\pi\gamma$ such that $\gamma_0 \ge M$ implies

(3.6) $$\|L_0(p)\|_{HS} \le 1/2 \text{ for } |\mathrm{Im}\ p| \le \gamma$$

where $\|\cdot\|_{HS}$ denotes the Hilbert-Schmidt norm for $\mathcal{B}_2(L_2(\Omega))$.

Lemma 3.4 implies that

(3.7) $$(1+L_0(p))^{-1} = \sum_{n=0}^{\infty} (-1)^n L_0(p)^n, \quad |\mathrm{Im}\ p| \le \gamma$$

and the remainder in the Neumann series tends to zero in $\mathcal{B}_2(L_2(\Omega))$.

Lemma 3.5. Let $V(q) \in L_2(\Omega)$, $\gamma > 0$ and $\gamma_0 \geq M(V,\gamma)$. Then

$$(3.8) \qquad L(p) = (1 + L_0(p))^{-1} R_0(p) \in \mathcal{B}_2(L_2(\Omega)) \text{ for } |\mathrm{Im}\ p| \leq \gamma$$

and has the representation

$$(3.9) \qquad L(p) = \sum_{n=0}^{\infty} (-1)^n R_0(p)[V R_0(p)]^n \text{ for } |\mathrm{Im}\ p| \leq \gamma$$

in the sense of convergence in $\mathcal{B}_2(L_2(\Omega))$. The mapping $p \to L(p) \in \mathcal{B}_2(L_2(\Omega))$ is holomorphic for $|\mathrm{Im}\ p| \leq \gamma$ and $L(p)$ has the properties

$$(3.10) \qquad L(p + m) = L(p) \text{ for } |\mathrm{Im}\ p| \leq \gamma \text{ and } m \in Z^3$$

and

$$(3.11) \qquad L(p)^* = L(p) \text{ for all } p \in R^3$$

The relationship of $L(p)$ to the Bloch waves is described by

Lemma 3.6. For all $p \in R^3$ and $\gamma_0^2 \geq M(V,\gamma)$, $L(p) = (H(p) + \gamma_0^2)^{-1}$. Hence $\psi \in L_2(\Omega)$ is an eigenfunction of $H(p)$ and $H(p)\psi = \lambda\psi$ if and only if ψ is an eigenfunction of $L(p)$ with singular value $\mu = \lambda + \gamma_0^2$; i.e.,

$$(3.12) \qquad \mu\, L(p)\, \psi = \psi$$

Lemma 3.6 implies that the Bloch waves can be constructed by means of the Fredholm determinant theory for Hilbert-Schmidt operators as developed by T. Carleman [4], F. Smithies [19] and R. Sikorski [17, 18]. However, a simpler approach is made possible by

Lemma 3.7. Under the hypotheses of Lemma 3.5, the operator $K(p) = L(p)^2$ has the property that its kernel $K(q,q',p) \in C(\overline{\Omega} \times \overline{\Omega})$ and the mapping $p \to K(q,q',p) \in C(\overline{\Omega} \times \overline{\Omega})$ is holomorphic for $|\mathrm{Im}\ p| \leq \gamma$. Moreover, $\psi \in L_2(\Omega)$

is an eigenfunction of H(p) and H(p) $\psi = \lambda\psi$ if and only if ψ is an eigenfunction of K(p) with singular value $\nu = (\lambda + \gamma_0^2)^2$; i.e.

$$\nu\, K(p)\, \psi = \psi \tag{3.13}$$

4. A CONSTRUCTION OF THE ENERGY BAND FUNCTIONS

The purpose of this section is to construct the holomorphic function $D(p,\lambda)$ of Theorem 1 and to use it to derive the basic properties of the energy band functions $\lambda_n(p)$. The construction of $D(p,\lambda)$ is based on the classical Fredholm theory [10, 17] applied to $K(p)$.

The Fredholm determinant of $K(p)$ is the function $D_0(p,\nu)$ defined by the power series

$$D_0(p,\nu) = \sum_{\ell=0}^{\infty} D_{0,\ell}(p)\, \nu^\ell \tag{4.1}$$

where $D_{0,0}(p) \equiv 1$ and the remaining coefficients are defined by

$$D_{0,\ell}(p) = \frac{(-1)^\ell}{\ell!} \int_\Omega \cdots \int_\Omega K(q_1,\cdots,q_\ell;q_1',\cdots,q_\ell',p)\,dq_1\cdots dq_\ell, \quad \ell \geq 1 \tag{4.2}$$

where

$$K(q_1,\cdots,q_\ell;q_1',\cdots,q_\ell',p) = \begin{vmatrix} K(q_1,q_1',p) & \cdots & K(q_1,q_\ell',p) \\ \vdots & & \\ K(q_\ell,q_1',p) & \cdots & K(q_\ell,q_\ell',p) \end{vmatrix} \tag{4.3}$$

Lemma 3.7 implies

<u>Lemma 4.1</u>. For each $p \in C^3$ with $|\mathrm{Im}\ p| \leq \gamma$, $K(q_1,\cdots,q_\ell;q_1',\cdots,q_\ell',p) \in C(\bar{\Omega}^{2\ell})$ and $p \to K(\cdot,\cdots,\cdot,p) \in C(\bar{\Omega}^{2\ell})$ is holomorphic for $|\mathrm{Im}\ p| \leq \gamma$.

It follows that each $D_{0,\ell}(p)$ is holomorphic for $|\mathrm{Im}\ p| \leq \gamma$. Moreover, the classical Hadamard inequality applied to (4.3) implies

$$|D_{0,\ell}(p)| \leq \kappa^\ell\, \ell^{\ell/2}/\ell! \quad \text{for } |\mathrm{Im}\ p| \leq \gamma \tag{4.4}$$

where $\kappa = \kappa(V,\gamma) = \text{Max } |K(q,q',p)|$ and the maximum is taken over the compact set of $q \in \bar{\Omega}$, $q' \in \bar{\Omega}$, Re $p \in \bar{\Omega}$ and $|\text{Im } p| \leq \gamma$. This implies

Lemma 4.2. The series in (4.1) converges for all $p \in C^3$ with $|\text{Im } p| \leq \gamma$ and all $\nu \in C$. The convergence is uniform on compact subsets and hence $D_0(p,\nu)$ is holomorphic for $|\text{Im } p| \leq \gamma$, $\nu \in C$.

The function $D(p,\lambda)$ may now be defined by

$$D(p,\lambda) = D_0(p,(\lambda+\gamma_0^2)^2) \tag{4.5}$$

and one has the following lemmas.

Lemma 4.3. $D(p,\lambda)$ is holomorphic for $|\text{Im } p| \leq \gamma$ and $\lambda \in C$. Moreover, $D(p,\lambda)$ is real-valued for $p \in R^3$, $\gamma \in R$ and is a periodic function of p; $D(p+m,\lambda) = D(p,\lambda)$ for $|\text{Im } p| \leq \gamma$, $m \in Z^3$ and $\lambda \in C$.

Lemma 4.4. For all $p \in R^3$, $\lambda \in \sigma(H(p))$ if and only if $D(p,\lambda) = 0$. Moreover, the multiplicity of λ as an eigenvalue of $H(p)$ equals its multiplicity as a zero of $D(p,\lambda)$. Hence, the sequence $\{\lambda_n(p)\}$ defined in section 1 is precisely the sequence of zeros of $D(p,\lambda)$, arranged by magnitude and repeated according to multiplicity.

Lemma 4.4 implies that the variation with $p \in R^3$ of the energy band functions $\lambda_n(p)$ is described by the set

$$E = \{(p,\lambda) \in R^4\colon\ D(p,\lambda) = 0\} \tag{4.6}$$

E is a real C-analytic variety in R^4 [5]; i.e., the real part of a complex analytic variety. It is known that $E = E' \cup E''$ where E', the set of regular points of E, is a real C-analytic manifold of dimension 3 and E'', the set of singular points of E, is a real C-analytic variety of dimension ≤ 2 [5, 23]. A different decomposition of E will be used to discuss the properties of the functions $\lambda_n(p)$. It is based on the observation that for each

$(p_0,\lambda_0) \in E$ there exists an integer $m = m(p_0,\lambda_0) \geq 1$ with the property that there is a neighborhood $N(p_0,\lambda_0)$ of (p_0,λ_0) in R^4 such that

$$(4.7) \qquad \partial^j D(p,\lambda)/\partial\lambda^j = 0 \text{ in } E \cap N(p_0,\lambda_0)$$

for $j = 0,1,\cdots,m-1$ but there is no neighborhood $N(p_0,\lambda_0)$ such that (4.7) holds with $j = m$. This suggests the definition

$$(4.8) \qquad E^r = E \cap \{(p_0,\lambda_0): \ \partial^m D(p_0,\lambda_0)/\partial\lambda^m \neq 0, \ m = m(p_0,\lambda_0)\}$$

Its utility is based on

Lemma 4.5. $E = E^r \cup E^s$ where $E^r \subset E'$ and $E^s = E'' \cup (E' - E^r)$. Moreover, E^r is a real C-analytic manifold of dimension 3 and E^s is a real C-analytic subvariety of E of dimension ≤ 2.

E is unbounded in the positive λ-direction because $\lambda_n(p) \to \infty$ when $n \to \infty$. It will be convenient to define the compact subsets

$$(4.9) \qquad E_n = \bigcup_{\ell=1}^{n} \{(p,\lambda_\ell(p)): \ p \in \overline{\Omega}\} \subset E, \ n = 1,2,\cdots$$

and the sets

$$(4.10) \qquad E_n^r = E_n \cap E^r, \ E_n^s = E_n \cap E^s$$

and

$$(4.11) \qquad X_n = \{p \in \overline{\Omega}: \ (p,\lambda) \in E_n^s \text{ for some } \lambda\} \subset \overline{\Omega}$$

With this notation one has

Lemma 4.6. For each $n = 1,2,\cdots$ the set X_n is a real C-analytic variety in $\overline{\Omega}$ of dimension ≤ 2. In particular, X_n is a closed nullset. Moreover, the relatively open set $\overline{\Omega} - X_n$ has a finite number of topological components; say

$$(4.12)\qquad \bar{\Omega} - X_n = \Omega_{n,1} \cup \Omega_{n,2} \cup \cdots \cup \Omega_{n,N},\ N = N(n)$$

Lemma 4.7. For $\ell = 1,2,\cdots,n$ each of the functions $\lambda_\ell(p)$ is holomorphic on $\bar{\Omega} - X_n$ and has constant multiplicity $m = m(n,j,\ell)$ on the component $\Omega_{n,j}$, $j = 1,2,\cdots,N(n)$. Moreover, $(p,\lambda_\ell(p)) \in E_n^r$ for $p \in \Omega_{n,j}$, $\ell = 1,2,\cdots,n$ and $m(n,j,\ell) = m(p,\lambda_\ell(p))$ is the integer of the definition (4.8) of E^r.

5. A CONSTRUCTION OF ALMOST HOLOMORPHIC FAMILIES OF BLOCH WAVES

The purpose of this section is to prove Theorem 2 by giving a construction of the closed nullsets Z_n and Bloch waves $\psi_n(q,p)$. The construction is based on the classical theory of Fredholm minors applied to the operator $K(p)$.

The Fredholm minor of $K(p)$ of order $k \geq 1$ is the function $D_k(q_1,\cdots,q_k;q_1',\cdots,q_k',p,\nu)$ defined by the power series

$$(5.1)\qquad D_k(q_1,\cdots,q_k;q_1',\cdots,q_k',p,\nu) = \sum_{\ell=0}^{\infty} D_{k,\ell}(q_1,\cdots,q_k;q_1',\cdots,q_k',p)\nu^{\ell}$$

where $D_{k,0}(q_1,\cdots,q_k;q_1',\cdots,q_k',p) = K(q_1,\cdots,q_k;q_1',\cdots,q_k',p)$ is defined by (4.3) and for $\ell \geq 1$

$$(5.2)\qquad \begin{aligned} &D_{k,\ell}(q_1,\cdots,q_k;q_1',\cdots,q_k',p) \\ &= \frac{(-1)^{\ell}}{\ell!}\int_{\Omega}\cdots\int_{\Omega} K(q_1,\cdots,q_k,r_1,\cdots,r_{\ell};q_1',\cdots,q_k',r_1,\cdots,r_{\ell},p)dr_1\cdots dr_{\ell} \end{aligned}$$

Lemma 3.7 implies

<u>Lemma 5.1</u>. For each $p \in C^3$ with $|\mathrm{Im}\ p| \leq \gamma$, the coefficients defined by (5.2) are in $C(\bar{\Omega}^{2k})$ and $p \to D_{k,\ell}(q_1,\cdots,q_k;q_1',\cdots,q_k',p) \in C(\bar{\Omega}^{2k})$ is holomorphic for $|\mathrm{Im}\ p| \leq \gamma$.

Moreover, Hadamard's inequality implies

$$(5.3)\qquad |D_{k,\ell}(q_1,\cdots,q_k;q_1',\cdots,q_k',p)| \leq \kappa^{k+\ell}(k+\ell)^{(k+\ell)/2}/\ell! \text{ for } |\mathrm{Im}\ p| \leq \gamma$$

and all $(q_1,\cdots,q_k') \in \bar{\Omega}^{2k}$. This implies

<u>Lemma 5.2</u>. The series in (5.1) converges for all $(q_1,\cdots,q_k') \in \bar{\Omega}^{2k}$, all $p \in C^3$ with $|\text{Im } p| \leq \gamma$ and all $\nu \in C$. The convergence is uniform on compact subsets and hence $(p,\nu) \to D_k(\cdot,\cdots,\cdot,p,\nu) \in C(\bar{\Omega}^{2k})$ is holomorphic for $|\text{Im } p| \leq \gamma$, $\nu \in C$.

The results of section 4 imply that the singular values of $K(p)$ are the roots ν of $D_0(p,\nu)$ and the sequence defined by

$$\nu_\ell(p) = (\lambda_\ell(p) + \gamma_0^2)^2, \quad p \in R^3, \quad \ell = 1,2,\cdots \tag{5.4}$$

is an enumeration of these singular values arranged in increasing order and repeated according to their multiplicities. Moreover, the eigenspace of $K(p)$ for $\nu_\ell(p)$ coincides with the eigenspace of $H(p)$ for $\lambda_\ell(p)$. The construction of a basis for this space will be based on the classical result of Fredholm that, for each fixed p and singular value $\nu_\ell(p)$, there is an integer $m \geq 1$ such that the minors of orders $k \leq m - 1$ are identically zero as functions of $(q_1,\cdots,q_k') \in \bar{\Omega}^{2k}$ while the minor of order $k = m$ is not identically zero. With this choice of m there exist points $(a_1,\cdots,a_m') \in \bar{\Omega}^{2m}$ such that $D_m(a_1,\cdots,a_m',p,\nu_\ell(p)) \neq 0$ and then

$$\begin{cases} \tilde{\psi}_1(q,p) = D_m(q,a_2,\cdots,a_m;a_1',\cdots,a_m',p,\nu_\ell(p)) \\ \tilde{\psi}_2(q,p) = D_m(a_1,q,\cdots,a_m;a_1',\cdots,a_m',p,\nu_\ell(p)) \\ \\ \tilde{\psi}_m(q,p) = D_m(a_1,a_2,\cdots,q;a_1',\cdots,a_m',p,\nu_\ell(p)) \end{cases} \tag{5.5}$$

is a basis of linearly independent eigenfunctions for $\nu_\ell(p)$. A corresponding orthonormal set can then be constructed by the Gram-Schmidt method. Of course, m and $(a_1,\cdots,a_m')$ will vary with p. Theorem 2 is proved below by choosing m and $(a_1,\cdots,a_m')$ to be suitable functions of $p \in \bar{\Omega}$.

The eigenvalues $\nu_\ell(p)$ ($\ell = 1,2,\cdots,n$) are holomorphic and have constant multiplicities $m(n,j,\ell)$ on the components $\Omega_{n,j}$ of $\bar{\Omega} - X_n$, by Lemma 4.7. Moreover, the integer m of (5.5) is the dimension of the eigenspace for $\nu_\ell(p)$ and hence coincides with $m(n,j,\ell)$ for $p \in \Omega_{n,j}$. It follows that for fixed $(a_1,\cdots,a_m')$ the functions (5.5) are holomorphic for $p \in \Omega_{n,j}$. Moreover, if $D_m(a_1,\cdots,a_m',p,\nu_\ell(p)) \neq 0$ for $p = p_0 \in \Omega_{n,j}$ then by continuity the inequality holds in a neighborhood $B(p_0,r_0) = \{p: |p-p_0| \leq r_0\}$ and hence (5.5) defines a basis for the eigenspace for $\lambda_\ell(p)$ for all $p \in B(p_0,r_0)$.

Note that if $n_1 = \operatorname{Min}_j m(1,j,1) \geq 1$ then by (4.9) $E_1 = E_2 = \cdots = E_{n_1} \subsetneqq E_{n_1+1}$. Similarly, there is a sequence of integers $\{n_k\}$ such that $1 \leq n_1 < n_2 < n_3 < \cdots$ and for $k = 1,2,3,\cdots$

$$(5.6) \qquad \cdots = E_{n_k} \subsetneqq E_{n_k+1} = \cdots = E_{n_{k+1}} \subsetneqq E_{n_{k+1}+1} = \cdots$$

It will be convenient to define the almost holomorphic Bloch waves $\psi_j(q,p)$ in groups, starting with $\psi_1,\cdots,\psi_{n_1}$.

<u>Definition of $\psi_1,\cdots,\psi_{n_1}$.</u> Consider the components $\Omega_{n_1,j}$ $(j = 1,2,\cdots,N(n_1))$. On each of them the multiplicity $m(1,j,1) = m(n_1,j,n_j) \equiv m_{1,j}$ is constant and $\geq n_1$. Thus for each $p_0 \in \Omega_{n_1,j}$ there exist neighborhoods $B(p_0,r_0) \subset \Omega_{n_1,j}$ and points $(a_1,\cdots,a'_{m_{1,j}}) \in \bar{\Omega}^{2m_{1,j}}$ such that (5.5) with $m = m_{1,j}$ defines a holomorphic basis for the eigenspace for $\lambda_1(p) = \cdots = \lambda_{m_{1,j}}(p)$ in $B(p_0,r_0)$. The Gram-Schmidt algorithm then gives a holomorphic orthonormal basis $\psi_1(q,p),\cdots,\psi_{m_{1,j}}(q,p)$ in $B(p_0,r_0)$.

To every $p \in \Omega_{n_1,j}$ there correspond neighborhoods $B(p_0,r_0)$ and holomorphic orthonormal bases of eigenfunctions. Almost holomorphic orthonormal bases $\psi_1(q,p),\cdots,\psi_{m_{1,j}}(q,p)$ in $\Omega_{n_1,j}$ may now be constructed by a procedure defined in [25, pp. 17-18]. The exceptional set $Z(n_1,j) \subset \Omega_{n_1,j}$ on which $\psi_1(\cdot,p),\cdots,\psi_{m_{1,j}}(\cdot,p)$ are discontinuous is a union of portions of spheres

$S(p_0, r_0) = \{p: |p - p_0| = r_0\}$ whose limit points all lie in the compact set X_{n_1}. Hence, $Z(n_1, j) \cup X_n$ is a closed nullset. Finally, the definition of $\psi_1(q,p), \cdots, \psi_{n_1}(q,p)$ for $p \in \overline{\Omega}$ is completed by setting $\psi_j(q,p) = 0$ for $q \in \overline{\Omega}$ and $p \in Z_j$ where

$$(5.7) \qquad Z_1 = \cdots = Z_{n_1} = X_{n_1} \cup \left(\bigcup_{j=1}^{N(n_1)} Z(n_1, j) \right)$$

is a closed nullset.

<u>Definition of $\psi_{n_1+1}, \cdots, \psi_{n_2}$.</u> Consider the components $\Omega_{n_2, j}$ $(j = 1, 2, \cdots, N(n_2))$ and let $m(n_1+1, j, n_1+1) = m(n_2, j, n_2) \equiv m_{2,j}$. To define ψ_j for $j = n_1+1, \cdots, n_2$ note that if $m_{1,j} > n_1$ then $m_{1,j} \geq n_2$, $\nu_{n_2}(p) = \nu_{n_1}(p)$ on $\Omega_{n_2,j}$ $(= \Omega_{n_1,j'}$, for some $j')$ and hence ψ_j and $Z(n_2, j) = Z(n_1, j')$ have already been defined. If $m_{1,j} = n_1$ then $\nu_{n_2}(p) > \nu_{n_1}(p)$ and $\psi_{n_1+1}, \cdots, \psi_{n_2}$ can be defined by the procedure explained in the preceding paragraph.

The definition of $\psi_{n_k+1}, \cdots, \psi_{n_{k+1}}$ can be completed by induction on k. The basic inductive step is the construction described above. It is clear from the construction that the resulting sequence $\{\psi_n(q,p)\}$ has the properties stated in Theorem 2.

6. PROOFS OF THE LEMMAS

This section contains proofs of the lemmas that were formulated in the preceding sections. For brevity the proofs are based as directly as possible on results in the literature.

Proof of Lemma 1.1. The starting point is an inequality of S. L. Sobolev and S. Agmon [1, p. 32] which states that for each domain $G \subset R^3$ that has the ordinary cone property [1, p. 11] there is a constant $\gamma = \gamma(G)$ such that for all $u \in L_2^2(G)$, $q \in G$ and $r \geq 1$

$$|u(q)|^2 \leq \gamma^2 r^{-1/2} (\|u\|_{2,G} + r^2 \|u\|_{0,G}) \tag{6.1}$$

where $\|u\|_{2,G}$ is the norm in $L_2^2(G)$ and $\|u\|_{0,G}$ is the norm in $L_2(G)$. Applying this to the domain $\Omega_m = \{q = q' + m: q' \in \Omega\}$, where $m \in Z^3$, then multiplying by $|V(q)|^2$ and integrating over Ω_m gives (since $\|V\|_{0,\Omega_m} = \|V_u\|_{0,\Omega}$ by (1.4))

$$\|Vu\|^2_{0,\Omega_m} \leq \gamma^2 \|V\|^2_{0,\Omega} r^{-1/2} (\|u\|^2_{2,\Omega_m} + r^2 \|u\|^2_{0,\Omega_m}) \tag{6.2}$$

Then summing over $m \in Z^3$ gives, for all $u \in L_2^2(R^3)$,

$$\|Vu\|^2_{0,R^3} \leq \gamma^2 \|V\|^2_{0,\Omega} r^{-1/2} (\|u\|^2_{2,R^3} + r^2 \|u\|^2_{0,R^3}) \tag{6.3}$$

This proves that $L_2^2(R^3) \subset D(V)$. To prove (1.7) one may use the elementary inequality [24, Lemma 3.3]

$$\|u\|^2_{2,R^3} \leq \gamma_0^2 (\|\Delta u\|^2_{0,R^3} + \|u\|^2_{0,R^3}) \text{ for all } u \in L_2^2(R^3) \tag{6.4}$$

Combining (6.3) and (6.4) gives (1.7) with a suitable choice of C.

Proof of Lemma 1.3. The proof is similar to the preceding one. The analogue of (6.4) for $H_0(p)$ is

$$\|u\|^2_{2,\Omega} \leq \gamma_1^2 \left(\|H_0(p)u\|^2_{0,\Omega} + \|u\|^2_{0,\Omega}\right) \text{ for all } u \in D(H_0(p)) \tag{6.5}$$

where γ_1 is independent of p. (6.5) can be proved by Fourier analysis. Combining it with the Sobolev-Agmon result (6.1) for $G = \Omega$ gives (1.20), as in the proof of Lemma 1.1.

Proof of Lemma 3.1. Let $K \subset R^3$ be compact and let $N(K) = Z^3 \cap K$, a finite set. Let $\mu = \text{Max}\,\{|q|: q \in K\}$ so that $|q - m| \geq |m| - \mu$ for all $q \in K$ and $m \in Z^3$. It will be shown that

$$\sum_{m \in Z^3 - N(K)} \Gamma(q-m)\, e^{2\pi i\, p\cdot m} \tag{6.6}$$

converges uniformly for $q \in K$, $|\text{Im } p| \leq \gamma < \gamma_0/2\pi$. Note that

$$\begin{aligned} 2\pi \text{ Im } p \cdot m + \gamma_0 \,|q-m| &\geq (\gamma_0 - 2\pi\,|\text{Im } p|)|m| - \gamma_0\mu \\ &\geq (\gamma_0 - 2\pi\gamma)|m| - \gamma_0\mu \end{aligned} \tag{6.7}$$

whence

$$|\Gamma(q-m)\, e^{2\pi i\, p\cdot m}| \leq e^{\gamma_0\mu}\, e^{-(\gamma_0 - 2\pi\gamma)|m|}/4\pi|q-m| \tag{6.8}$$

for all $q \in K$ and $m \in Z^3 - N(K)$. The uniform convergence of (6.6) for $q \in K$, $|\text{Im } p| \leq \gamma < \gamma_0/2\pi$ follows. Applying this with $K = 2\overline{\Omega}$ gives

$$G_0'(q,p) = \sum_{m \in Z^3 - N(2\overline{\Omega})} \Gamma(q-m)\, e^{2\pi i\, p\cdot m} \tag{6.9}$$

and the uniform convergence implies that $G_0'(\cdot,p) \in C(2\overline{\Omega})$ and that $p \to G_0'(\cdot,p) \in C(2\overline{\Omega})$ is holomorphic for $|\text{Im } p| < \gamma_0/2\pi$.

Proof of Lemma 3.2. Note that $\Gamma(q - q' - m) \in L_2(\Omega\times\Omega)$ and $G_0'(q-q',p) \in C(\overline{\Omega}\times\overline{\Omega}) \subset L_2(\Omega\times\Omega)$. Hence (3.4) implies $G_0(q-q',p) \in L_2(\Omega\times\Omega)$ for each p such that $|\text{Im } p| < \gamma_0/2\pi$. To prove (3.2) note that $(-\Delta + \gamma_0^2)\ \Gamma(q - m) = \delta(q - m)$. Moreover, (6.8) implies that (3.3) can be differentiated termwise and $(-\Delta + \gamma_0^2)\ G_0(q - q', p) = \delta(q - q')$ all q, $q' \in \Omega$. Note that to prove (3.2) it suffices to verify it for $f \in C_0^\infty(\Omega)$. For such functions the differential equation for G_0 implies that $(-\Delta + \gamma_0^2)\ R_0(p)\ f(q) = f(q)$ for all $q \in \Omega$. Finally the form of the series in (3.3) implies that $R_0(p)\ f \in D(H_0(p))$ which completes the proof of (3.2). The holomorphy of $p \to R_0(p) \in \mathcal{B}_2(L_2(\Omega))$ is equivalent to that of $p \to G_0(q - q', p) \in L_2(\Omega \times \Omega)$ which follows from Lemma 3.1.

Proof of Lemma 3.3. A simple geometric argument implies that

$$\int_\Omega |G_0(q - q', p)|^2\, dq \leq \int_{2\Omega} |G_0(q, p)|^2\, dq \text{ for all } q' \in \Omega \tag{6.10}$$

This result and Fubini's theorem imply that $G_0(q - q', p)\ V(q') \in L_2(\Omega \times \Omega)$ for $|\text{Im } p| < \gamma_0/2\pi$. Moreover, for all $f \in D(V) = D(R_0(p)V)$

$$R_0(p)\ V\ f(q) = \int_\Omega G_0(q - q', p)\ V(q')\ f(q')\ dq' \tag{6.11}$$

by Lemma 3.2. This implies that $R_0(p)V$ is densely defined and closable with closure in $\mathcal{B}_2(L_2(\Omega))$ whose kernel is (3.5). The holomorphy of $p \to L_0(p) \in \mathcal{B}_2(L_2(\Omega))$ follows from Lemma 3.1.

Proof of Lemma 3.4. Note that (6.10) implies

$$\begin{aligned} \|L_0(p)\|_{HS}^2 &= \int_\Omega |V(q')|^2 \int_\Omega |G_0(q - q', p)|^2\, dq\, dq' \\ &\leq \|V\|_{L_2(\Omega)}^2 \int_{2\Omega} |G_0(q, p)|^2\, dq \end{aligned} \tag{6.12}$$

Hence it is enough to show that the last integral tends to 0 when $\gamma_0 \to \infty$, uniformly for $|\text{Im } p| \leq \gamma$. Moreover, for any fixed $m \in Z^3$

$$(6.13)\qquad \int_{2\Omega} |\Gamma(q-m)|^2 dq = \int_{2\Omega} \left\{e^{-\gamma_0|q-m|}/4\pi|q-m|^2\right\} dq \to 0 \text{ when } \gamma_0 \to \infty$$

by Lebesgue's dominated convergence theorem. Thus it is enough to prove that $G_0'(q,p) \to 0$ when $\gamma_0 \to \infty$, uniformly for $q \in 2\bar{\Omega}$ and $|\text{Im } p| \le \gamma$. To show this note that $|q-m| \ge |m| - |q|$, $|q| \le \sqrt{3}$ for $q \in 2\bar{\Omega}$ and $|m| \ge 2$ for $m \in Z^3 - N(2\bar{\Omega})$. Thus if ε, γ_0 satisfy $0 < \varepsilon < 1 - \sqrt{3}/2$, $\gamma_0 > (2\pi\gamma+1)/\varepsilon$ and $|\text{Im } p| \le \gamma$ then

$$(6.14)\qquad \begin{aligned} 2\pi \text{ Im } p \cdot m + \gamma_0|q-m| &\ge (\gamma_0 - 2\pi\gamma)\ |m| - \sqrt{3}\ \gamma_0 \\ &= |m| + (\gamma_0 - 2\pi\gamma - 1)\ |m| - \sqrt{3}\ \gamma_0 \\ &\ge |m| + (\varepsilon\gamma_0 - 2\pi\gamma - 1)|m| + ((1-\varepsilon)|m| - \sqrt{3})\gamma_0 \\ &\ge |m| + \delta\gamma_0 \end{aligned}$$

where $\delta = 2(1-\varepsilon) - \sqrt{3} > 0$. It follows from (6.9) and (6.14) that for all $q \in 2\bar{\Omega}$ and $|\text{Im } p| \le \gamma$

$$(6.15)\qquad |G_0'(q,p)| \le \sum_{|m|\ge 2} e^{-2\pi \text{ Im } p\cdot m - \gamma_0|q-m|}/4\pi|q-m| \le C\ e^{-\delta\gamma_0}$$

where C is a finite constant. This completes the proof.

Proof of Lemma 3.5. (3.8) follows from (3.6), the Neumann series for $(1 + L_0(p))^{-1}$ and the completeness of the Hilbert space $\mathcal{B}_2(L_2(\Omega))$. Moreover the range of $R_0(p)$ is $D(H_0(p)) \subset D(V)$ and hence for $n = 1,2,\cdots$

$$(6.16)\qquad L_0(p)^n\ R_0(p) = (R_0(p)\ V)^n\ R_0(p) = R_0(p)(V\ R_0(p))^n$$

which proves (3.9). The uniform convergence of the series in (3.9) on compact subsets of $|\text{Im } p| \le \gamma$ implies that $p \to L(p) \in \mathcal{B}_2(L_2(\Omega))$ is holomorphic there. Finally, (3.10) follows from $R_0(p+m) = R_0(p)$ and (3.11) follows from the selfadjointness of $R_0(p)[V\, R_0(p)]^n$ for all $p \in R^3$.

Proof of Lemma 3.6. Note that $u = (H(p) + \gamma_0^2)^{-1} f$ if and only if $u \in D(H(p)) = D(H_0(p))$ and $(H(p) + \gamma_0^2)u = f$. Since $H(p) = H_0(p) + V$ this may be written $(H_0(p) + \gamma_0^2)u = f - Vu$ or $u = R_0(p)f - R_0(p)\, Vu$ or $(1 + R_0(p)\, V)u = R_0(p)\, f$. Thus finally $u = L(p)\, f$ by Lemmas 3.3-3.5.

Proof of Lemma 3.7. If $A \in \mathcal{B}_2(L_2(\Omega))$ the corresponding kernel in $L_2(\Omega\times\Omega)$ will be denoted by $A(q,q')$. Similarly, if $A(p) \in \mathcal{B}_2(L_2(\Omega))$ for $|\mathrm{Im}\, p| \le \gamma$ then $A(q,q',p) \in L_2(\Omega\times\Omega)$ for $|\mathrm{Im}\, p| \le \gamma$. The notation $A(p) \sim 0$ will be used to mean that $A(q,q',p) \in C(\bar{\Omega}\times\bar{\Omega})$ and $p \to A(q,q',p) \in C(\bar{\Omega}\times\bar{\Omega})$ is holomorphic for $|\mathrm{Im}\, p| \le \gamma$. Thus Lemma 3.7 states that $K(p) = L(p)^2 \sim 0$. The notation $A(p) \sim B(p)$, meaning $A(p) - B(p) \sim 0$, will also be used. It is an equivalence relation.

By Lemma 3.5

$$L(p) = \sum_{n=0}^{\infty} (-1)^n\, L_n(p) \text{ in } \mathcal{B}_2(L_2(\Omega)) \tag{6.17}$$

where

$$L_0(p) = R_0(p), \quad L_n(p) = R_0(p)\, V\, L_{n-1}(p), \quad n = 1,2,\cdots \tag{6.18}$$

Moreover, by Lemma 3.1

$$L_0(p) = R_0(p) \sim \sum_{m\in N} \Gamma_m\, e^{2\pi i\, p\cdot m} \tag{6.19}$$

where Γ_m has kernel $\Gamma(q-q'-m)$. It will be shown first that

$$L_1(p) \sim \sum_{m+m'\in N} \Gamma_m\, V\, \Gamma_{m'}\, e^{2\pi i\, p\cdot(m+m')} \tag{6.20}$$

To prove this it is enough to show that $R_0'(p)\, V\, R_0'(p) \sim 0$, $\Gamma_m V\, R_0'(p) \sim 0$, $R_0'(p)\, V\, \Gamma_m \sim 0$ and $\Gamma_m V\, \Gamma_{m'} \sim 0$ for $m+m' \notin N$. Now $R_0'(p)\, V\, R_0'(p)$ has kernel

$$\text{(6.21)} \qquad \int_{\Omega} G_0'(q-q'',p)\ V(q'')\ G_0'(q''-q',p)\ dq''$$

The result $R_0'(p)\,V\,R_0'(p) \sim 0$ follows from the observation that $q' \to V(q'')\ G_0'(q''-q',p) \in L_2(\Omega)$ is continuous for $q' \in \overline{\Omega}$ and $p \to V(q'')\ G_0'(q''-q',p) \in C(\overline{\Omega},L_2(\Omega))$ is holomorphic for $|\mathrm{Im}\ p| \leq \gamma$. The remaining terms may be treated similarly.

Next it will be shown that $\Gamma_m V \Gamma_{m'}(q,q')$ is continuous for $q-q' \neq m+m'$ and

$$\text{(6.22)} \qquad \Gamma_m V \Gamma_{m'}(q,q') = \mathcal{O}(|q-q'-m-m'|^{-1/2}),\ q \to q' + m + m'$$

To show this note that

$$\text{(6.23)} \qquad \Gamma_m V \Gamma_{m'}(q,q') = \int_{\Omega} \Gamma(q-q''-m)\ V\ (q'')\ \Gamma(q''-q'-m')\ dq''$$

If $q-q' \neq m+m'$ then the singularities of the integrand at $q'' = q-m$ and $q'' = q'+m'$ are distinct and the continuity can be proved by the argument of the preceding paragraph. The result (6.22) is proved by applying Schwarz's inequality to (6.23):

$$\text{(6.24)} \qquad |\Gamma_m V \Gamma_{m'}(q,q')|^2 \leq \|V\|^2_{L_2(\Omega)} \int_{\Omega} |\Gamma(q-q''-m)\ \Gamma(q''-q'-m')|^2\ dq''$$

and estimating the singularity of the last integral at $q = q'+m+m'$ by a method of classical potential theory [14, p. 59].

Passing to $L_2(p)$, the method of the preceding paragraph can be used to prove

$$\text{(6.25)} \qquad L_2(p) \sim \sum_{m+m'+m'' \in N} \Gamma_m V \Gamma_{m'} V \Gamma_{m''}\ e^{2\pi i\, p\cdot(m+m'+m'')}$$

Moreover, $\Gamma_m V \Gamma_{m'} V \Gamma_{m''}(q,q')$ is continuous for $q-q' \neq m+m'+m''$ and

(6.26) $$\Gamma_m V \Gamma_{m'} V \Gamma_{m''}(q,q') = \mathcal{O}(|\ell n\ |q - q' - m - m' - m''||^{1/2})$$

Finally, the same arguments imply that $L_n(p) \sim 0$ for $n = 3,4,5,\cdots$ and

$$L(p) \sim L_0(p) - L_1(p) + L_2(p)$$

(6.27) $$\sim \sum_{m \in N} \Gamma_m e^{2\pi i p \cdot m} - \sum_{m+m' \in N} \Gamma_m V \Gamma_{m'} e^{2\pi i p \cdot (m+m')} + \sum_{m+m'+m'' \in N} \Gamma_m V \Gamma_{m'} V \Gamma_{m''} e^{2\pi i p \cdot (m+m'+m'')}$$

The last sum is a trigonometric polynomial in p. Hence, to complete the proof of $L(p)^2 \sim 0$ it is sufficient to show that the product of any pair of the operators Γ_m, $\Gamma_m V \Gamma_{m'}$ and $\Gamma_m V \Gamma_{m'} V \Gamma_{m''}$ has a kernel in $C(\bar{\Omega} \times \bar{\Omega})$. This follows from $\Gamma_m(q,q') = e^{-\gamma_0|q-q'-m|}/4\pi|q-q'-m|$, (6.22) and (6.26) by the argument following (6.21) (continuity of $q \to \Gamma_m(q,q') \in L_2(\Omega)$, etc.).

Proof of Lemma 4.3. The holomorphy follows from Lemma 4.2. To see that $D(p,\lambda) \in R$ for $p \in R^3$, $\lambda \in R$ note that $G_0(q,p) \in R$ for $p \in R^3$ by (3.3). Hence (3.9) implies that L(p) has a real-valued kernel, because V is real-valued, and therefore $K(q,q',p) \in R$ for $p \in R^3$. Thus (4.1) - (4.4) imply that $D(p,\lambda) \in R$. The property $D(p+m,\lambda) = D(p,\lambda)$ follows from (3.10).

Proof of Lemma 4.4. By Lemma 3.7, $\lambda \in \sigma(H(p))$ if and only if $\nu = (\lambda + \gamma_0^2)^2$ is a singular value of K(p). Hence Lemma 4.4 follows from classical Fredholm theory [10, 17]. In the general theory the multiplicity of an eigenvalue can be less than the multiplicity of the corresponding zero of $D_0(p,\nu)$. However, for selfadjoint operators the two multiplicities coincide.

Proof of Lemma 4.5. Let $(p_0,\lambda_0) \in E^r$. Then there is an $m = m(p_0,\lambda_0) \geq 1$ and a neighborhood $N(p_0,\lambda_0) \subset R^4$ such that

$$(6.28)\quad \begin{cases} F(p,\lambda) \equiv \partial^{m-1} D(p,\lambda)/\partial\lambda^{m-1} = 0 & \text{for } (p,\lambda) \in E \cap N(p_0,\lambda_0) \\ \partial F(p,\lambda)/\partial\lambda \equiv \partial^{m} D(p,\lambda)/\partial\lambda^{m} \neq 0 & \text{for } (p,\lambda) \in E \cap N(p_0,\lambda_0) \end{cases}$$

It follows by the implicit function theorem for analytic functions [3] that $E \cap N(p_0,\lambda_0) \subset E'$. In particular, $E^r \subset E'$ is a real C-analytic manifold of dimension 3. Next consider a point $(p_0,\lambda_0) \in E^S = E - E^r$. The definition of E^r implies that there is an integer $m = m(p_0,\lambda_0) \geq 1$ and a neighborhood $N(p_0,\lambda_0) \subset R^4$ such that

$$(6.29)\quad \begin{cases} F(p,\lambda) \equiv \partial^{m-1} D(p,\lambda)/\partial\lambda^{m-1} = 0 \text{ for } (p,\lambda) \in E \cap N(p_0,\lambda_0) \\ G(p,\lambda) \equiv \partial^{m} D(p,\lambda)/\partial\lambda^{m} \not\equiv 0 \quad \text{for } (p,\lambda) \in E \cap N(p_0,\lambda_0) \\ G(p_0,\lambda_0) = 0 \end{cases}$$

Thus $(p_0,\lambda_0) \in E \cap \{(p,\lambda)\colon\ G(p,\lambda) = 0\}$, a variety of dimension ≤ 2.

<u>Proof of Lemma 4.6</u>. The set $E_n^S \subset R^4$ is a real C-analytic variety of dimension ≤ 2. Hence X_n, its projection onto the hyperplane $\lambda = 0$ has the same property. The important property that $\overline{\Omega} - X_n$ has a finite number of topological components was proved by H. Whitney [22, 23].

<u>Proof of Lemma 4.7</u>. Let $p_0 \in \overline{\Omega} - X_n$ and let $1 \leq \ell \leq n$. Then $(p_0,\lambda_\ell(p_0)) \in E_n^r \subset E^r$ and hence there exists a neighborhood $N(p_0)$ in which $\lambda_\ell(p)$ is the unique holomorphic solution of $F(p,\lambda) = 0$ guaranteed by (6.28). To show that $\lambda_\ell(p)$ has constant multiplicity on each component of $\overline{\Omega} - X_n$, let $p_0 \in \Omega_{n,j}$ have multiplicity $m_0 = m(p_0,\lambda_\ell(p_0))$ (notation of (4.8)). Then $\lambda_\ell(p)$ has multiplicity m_0 throughout a neighborhood of p_0, by the definition of E^r and continuity of $\partial^{m_0} D(p,\lambda)/\partial\lambda^{m_0}$. Thus the set $\Omega_{n,j}^0 = \{p \in \Omega_{n,j}\colon$ $\lambda_\ell(p)$ has multiplicity $m_0\}$ is open and not empty in $\Omega_{n,j}$. Moreover, if

$p_1 \in \Omega_{n,j}$ is a limit point of $\Omega^0_{n,j}$ then $m(p_1,\lambda_\ell(p_1)) = m_0$ because $m(p,\lambda_\ell(p))$ is constant in a neighborhood of p_1. Thus $\Omega^0_{n,j}$ is both open and closed in $\Omega_{n,j}$ and therefore $\Omega^0_{n,j} = \Omega_{n,j}$ because $\Omega_{n,j}$ is connected.

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13. ABSTRACT

The Bloch waves of the one-electron theory of electronic states in crystals are the eigenfunctions of a family of unbounded selfadjoint operators H(p) that depend holomorphically on the wave momentum $p = (p_1,p_2,p_3) \in R^3$. H(p) has a discrete spectrum, with corresponding complete orthonormal sequences of eigenfunctions, and it is customary to denote such a sequence by $\{\psi_n(p)\}$ and speak of "the" Bloch waves. However, the eigenfunctions are not unique and a separate choice is required for each p. The customary definition therefore rests on the axiom of choice and can provide no information about the p-dependence of the Bloch waves. Some information is essential for applications. A minimal requirement is p-measurability. In this paper the operators $K(p) = (H(p) + \gamma_0^2)^{-2}$ are shown to form a family of Fredholm integral operators that is holomorphic for $p \in C^3$, $|\mathrm{Im}\, p| < \gamma_0$. The classical theory of Fredholm minors is then used to construct families of Bloch waves $\psi_n(p)$ which are holomorphic on the complement of a closed null-set.

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