Notice that the error $E_n(V) - (n\pi)^2 - \int_0^1 V(x)\,dx$ is the sum of two terms, one of which is $O(n^{-1})$ and the other of which is Re $\tilde{V}(2n)$. For smooth V's, this term is also at least $O(n^{-1})$ but, in general, $\sup_{n \geq m} \tilde{V}(2n)$ can go to zero arbitrarily slowly. The above results depend critically on the one-dimensional nature of the problem, for it is only in one dimension that the distance between eigenvalues of H_0 diverges as n goes to infinity.

XIII.16 Schrödinger operators with periodic potentials

In this section we study Schrödinger operators $-\Delta + V$ where V is a periodic function. That is, we assume that for some basis $\{\mathbf{a}_i\}_{i=1}^n \in \mathbb{R}^n$, V satisfies

$$V(\mathbf{x} + \mathbf{a}_i) = V(\mathbf{x}) \tag{135}$$

As we shall discuss, these operators are important in solid state physics.

We have already seen that the spectral properties of Schrödinger operators are highly dependent on the behavior of V at infinity. Basically, we have studied three distinct classes of Schrödinger operators. The class whose spectral properties were easiest to establish were those with $V(x) \to \infty$ as $x \to \infty$; this class had empty essential spectrum (Theorem XIII.16). The next simplest class consisted of the "one-body Schrödinger operators" where $V(x) \to 0$ as $x \to \infty$, at least in some "average sense" (such as $V(x) \in L^p(\mathbb{R}^n, dx)$ for some $p < \infty$); under fairly general hypotheses these operators have $\sigma_{\text{ess}} = [0, \infty)$ (see Theorem XIII.15) and empty singular continuous spectrum (Theorem XIII.33). The third class is made up of the "N-body Schrödinger operators" for which $V(x) \to 0$ as $x \to \infty$ in "most" directions (i.e., those directions in which all "coordinate" differences $|\mathbf{r}_i - \mathbf{r}_j| \to \infty$) but for which V did not have a limit in tubes about those spatial directions where $\mathbf{r}_i = \mathbf{r}_j$ (some i, j). These operators were much harder to analyze; we saw that under fairly general circumstances $\sigma_{\text{ess}} = [\Sigma, \infty)$ where Σ was a "computable" number (Theorem XIII.17) but were only able to prove $\sigma_{\text{sing}} = \emptyset$ under specialized hypotheses (Theorems XIII.27, XIII.29, and XIII.36). We see therefore that spectral properties are very sensitive to the behavior of V at infinity. Since V's obeying (135) do not have a limit as $x \to \infty$ in any direction one might expect the analysis of periodic Schrödinger operators to be difficult.

The property that allows one to analyze $H = -\Delta + V$ when V is periodic is that H has a large symmetry group. For letting

$$(U(\mathbf{t})\psi)(\mathbf{x}) = \psi(\mathbf{x} + \sum_{i=1}^{n} t_i \mathbf{a}_i)$$

where $t \in \mathbb{Z}^n$, we see that (formally)

$$U(t)H = HU(t) \tag{136}$$

One can in fact prove that $U(t)e^{-iHs} = e^{-iHs}U(t)$ (Problem 135). A part of the analysis of H is then a special case of general symmetry arguments which are the subject of Chapter XVI. In this sense our discussion here is premature. We emphasize to the reader that the constant fiber direct integrals described below are an example of a construction from Chapter XVI (with most of the essential features) and that the fact that periodic Schrödinger operators have a direct integral decomposition is a direct consequence of (136). We remark that historically the essentials of the decomposition were discovered both by mathematicians (Floquet) and physicists (Bloch) who did not realize they were speaking group theory. We too shall not explicitly use the connection with the symmetry group here but will develop the theory directly.

Let $\mathscr{H}'$ be a separable Hilbert space and $\langle M, \mu \rangle$ a σ-finite measure space. In Section II.1, we constructed the Hilbert space $L^2(M, d\mu; \mathscr{H}')$ of square integrable $\mathscr{H}'$-valued functions. Notice that if μ is a sum of point measures at a finite set of points $m_1, \ldots, m_k$, then any $f \in L^2(M, d\mu; \mathscr{H}')$ is determined by the k-tuple $\langle f(m_1), \ldots, f(m_k) \rangle$ so $L^2(M, d\mu; \mathscr{H}')$ is isomorphic to the direct sum $\bigoplus_{i=1}^{m} \mathscr{H}'$. In some sense then, $L^2(M, d\mu; \mathscr{H}')$ for more general μ is a kind of "continuous direct sum" but with identical summands. We shall thus call $\mathscr{H} \equiv L^2(M, d\mu; \mathscr{H}')$ a **constant fiber direct integral** and write

$$\mathscr{H} = \int_M^{\oplus} \mathscr{H}' \, d\mu$$

It may seem silly to give an old familiar object a strange new name, but the new name is intended to convey a new emphasis on the "fibers" $\mathscr{H}'$ rather than the points of M. A particular class of operators on $\mathscr{H}$ will concern us. A function $A(\cdot)$ from M to $\mathscr{L}(\mathscr{H}')$ is called measurable if and only if for each $\varphi, \psi \in \mathscr{H}'$, $(\varphi, A(\cdot)\psi)$ is measurable. $L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}'))$ denotes the space of (equivalence class of a.e. equal) measurable functions from M to $\mathscr{L}(\mathscr{H}')$ with

$$\|A\|_\infty \equiv \text{ess sup} \|A(m)\|_{\mathscr{L}(\mathscr{H}')} < \infty$$

Definition A bounded operator A on $\mathscr{H} = \int_M^\oplus \mathscr{H}' \, d\mu$ is said to be **decomposed** by the direct integral decomposition if and only if there is a function $A(\cdot)$ in $L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}'))$ so that for all $\psi \in \mathscr{H}$,

$$(A\psi)(m) = A(m)\psi(m) \tag{137}$$

We then call A **decomposable** and write

$$A = \int_M^\oplus A(m) \, d\mu(m)$$

The $A(m)$ are called the **fibers** of A.

We first note that every $A(\cdot)$ in $L^\infty(M, d\mu; \mathscr{H}')$ is associated with some decomposable operator:

Theorem XIII.83 If $A(\cdot) \in L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}'))$, then there is a unique decomposable operator $A \in \mathscr{L}(\mathscr{H})$ so that (137) holds. Moreover $\|A\|_{\mathscr{L}(\mathscr{H})} = \|A(\cdot)\|_\infty$.

Proof Uniqueness is obvious. We must only show that (137) takes measurable square integrable $\mathscr{H}'$-valued functions ψ into measurable square integrable $\mathscr{H}'$-valued functions and that the operator A so defined is bounded with norm $\|A(\cdot)\|_\infty$. Let $\psi \in L^2(M, d\mu; \mathscr{H}')$. Let $\{\eta_k\}_{k=1}^\infty$ be an orthonormal basis for $\mathscr{H}'$. Then $A(m)\psi(m) = \sum_{k=1}^\infty (\eta_k, \psi(m))A(m)\eta_k$, a.e. in m since $A(\cdot)$ is a.e. a bounded operator. Now, by definition of measurability for $A(\cdot)$, $A(m)\eta_k$ is weakly measurable, so for any $N < \infty$, $\varphi_N(m) \equiv \sum_{k=1}^N (\eta_k, \psi(m))A(m)\eta_k$ is strongly measurable (Theorem IV.22). Moreover,

$$\begin{aligned}\int \|\varphi_N(m)\|^2 \, d\mu &= \int \left\| A(m) \sum_{k=1}^N (\eta_k, \psi(m))\eta_k \right\|^2 d\mu \\ &\le \|A(\cdot)\|_\infty^2 \int \left\| \sum_{k=1}^N (\eta_k, \psi(m))\eta_k \right\|^2 d\mu \\ &\le \|A(\cdot)\|_\infty^2 \|\psi\|^2 \end{aligned} \tag{138}$$

A similar computation shows that that φ_N is Cauchy in $\mathscr{H}$. Thus it has a limit $\varphi \in L^2(M, d\mu; \mathscr{H}')$. But for almost all $m \in M$, $\varphi_N(m)$ converges to $A(m)\psi(m)$ in $\mathscr{H}'$. It follows that $A(\cdot)\psi(\cdot) \in L^2(M, d\mu; \mathscr{H}')$. By (138)

$$\|A(\cdot)\psi(\cdot)\| \le \|A\|_\infty \|\psi\|$$

so A is bounded and $\|A\|_{\mathscr{L}(\mathscr{H})} \le \|A(\cdot)\|_\infty$.

To prove the converse inequality, let $\{\beta_k\}_{k=1}^{\infty}$ be a dense subset of the unit ball in $\mathscr{H}'$ and let $f \in L^1(M, d\mu)$. We may decompose f as $f = gh$, with $g, h \in L^2$ and $\|g\|_2^2 = \|h\|_2^2 = \|f\|_1$. Fix k, ℓ and let $\psi = \bar{g}\beta_k$ and $\varphi = h\beta_\ell$. Then

$$\left|\int f(m)(\beta_k, A(m)\beta_\ell)\, d\mu\right| = |(\psi, A\varphi)| \le \|A\|\, \|\psi\|\, \|\varphi\|$$

$$= \|A\|\, \|\beta_k\|\, \|\beta_\ell\| \int |f(m)|\, d\mu$$

Since $L^\infty(M)$ is the dual of $L^1(M)$, it follows that

$$|(\beta_k, A(m)\beta_\ell)| \le \|\beta_k\|\, \|\beta_\ell\|\, \|A\|_{\mathscr{L}(\mathscr{H})}$$

a.e. in m. It follows that $\|A(\cdot)\|_\infty \le \|A\|_{\mathscr{L}(\mathscr{H})}$. ∎

The above theorem sets up an isometric isomorphism of $L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}'))$ and the decomposable operators on $\int_M^\oplus \mathscr{H}'\, d\mu$. Both these spaces are algebras in a natural way, and it is easy to see that the algebraic structure is preserved. $L^\infty(M, d\mu; \mathbb{C})$ is the natural subalgebra of $L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}'))$ corresponding to those decomposable operators whose fibers are all multiples of the identity.

Theorem XIII.84 Let $\mathscr{H} = \int_M^\oplus \mathscr{H}'\, d\mu$ where $\langle M, \mu\rangle$ is a separable σ-finite measure space and $\mathscr{H}'$ is separable. Let $\mathscr{A}$ be the algebra of decomposable operators whose fibers are all multiples of the identity. Then $A \in \mathscr{L}(\mathscr{H})$ is decomposable if and only if A commutes with each operator in $\mathscr{A}$.

Proof It is obvious that any decomposable A commutes with all the operators in $\mathscr{A}$, so we need only prove the converse. Since μ is σ-finite, we can find a strictly positive $F \in L^1$ so that $d\nu = F\, d\mu$ has unit mass. Let $\tilde{\mathscr{H}} = \int_M^\oplus \mathscr{H}'\, d\nu$. Then the map $U: \mathscr{H} \to \tilde{\mathscr{H}}$ by $Ug = F^{-1/2}g$ is unitary and $U\mathscr{A}U^{-1} = \tilde{\mathscr{A}}$. Moreover, A is decomposable if and only if UAU^{-1} is decomposable. As a result, we suppose without loss that $\int d\mu = 1$.

Suppose that A in $\mathscr{L}(\mathscr{H})$ commutes with any operator in $\mathscr{A}$. Choose an orthonormal basis $\{\eta_k\}_{k=1}^{\infty}$ for $\mathscr{H}'$ and let F_k be the element of $\mathscr{H}$ with $F_k(x) = \eta_k$ for all x. The F_k are orthonormal since $\int d\mu = 1$. Moreover, any $\psi \in \mathscr{H}$ has an expansion $\psi = \sum_{k=1}^{\infty} f_k(x)F_k$ with each $f_k \in L^2(M, d\mu; \mathbb{C})$ and $\|\psi\|^2 = \sum_k \|f_k\|^2$ (see Problem 12 of Chapter II). Define functions $a_{km}(x)$ by $AF_k = \sum_{m=1}^{\infty} a_{km}(x)F_m$. Choose a countable dense set D in $\mathscr{H}'$ of vectors of the form $\sum_{k=1}^{N} \alpha_k \eta_k = \varphi$ and set $A(x)\varphi = \sum_{k,m} \alpha_k a_{km}(x)\eta_m$. Then, for any $f \in L^\infty(M, d\mu; \mathbb{C})$,

$$A(f\varphi) = f(A\varphi) = \sum_{k}^{N} f\alpha_k AF_k$$
$$= \sum_{k,m} f\alpha_k a_{km}(\cdot)F_m$$

since $f\mathbb{1} \in \mathscr{A}$. Thus

$$\int |f(x)|^2 \sum_m \left| \sum_k \alpha_k a_{km}(x) \right|^2 d\mu(x) \le \|A\|^2 \left(\int |f(x)|^2 \right) \sum_k |\alpha_k|^2$$

It follows that, for almost all x and all $\varphi \in D$,

$$\|A(x)\varphi\| \le \|A\| \, \|\varphi\|$$

so $A(x)$ can be extended to an operator on $\mathscr{L}(\mathscr{H}')$ and $A(\cdot) \in L^\infty$. Let B be the corresponding decomposable operator. Let $\psi \in \mathscr{H}$ have the form $\psi = \sum_{k=1}^{N} f_k(x)F_k$ with each $f_k \in L^\infty$. Then

$$(A\psi)(x) = \sum_{k=1}^{N} f_k(x)(AF_k(x)) = \sum_{k=1}^{N} f_k(x)(A(x)\eta_k) = A(x)\sum_{k=1}^{N} f_k(x)\eta_k$$
$$= (B\psi)(x)$$

Since such ψ's are dense, $A = B$. ∎

The construction we use below depends basically on the fact that the $U(t)$ generate an algebra that is isomorphic to the algebra $\mathscr{A}$ for a suitable constant fiber direct integral decomposition of $\mathscr{H} = L^2(\mathbb{R}^n, dx)$.

Since $-\Delta + V$ is unbounded, we need to discuss unbounded decomposable self-adjoint operators.

Definition A function $A(\cdot)$ from a measure space M to the (not necessarily bounded) self-adjoint operators on a Hilbert space $\mathscr{H}'$ is called **measurable** if and only if the function $(A(\cdot) + i)^{-1}$ is measurable. Given such a function, we define an operator A on $\mathscr{H} = \int_M^\oplus \mathscr{H}'$ with domain

$$D(A) = \left\{ \psi \in \mathscr{H} \;\middle|\; \psi(m) \in D(A(m)) \text{ a.e.}; \int_M \|A(m)\psi(m)\|_{\mathscr{H}'}^2 \, d\mu(m) < \infty \right\}$$

by

$$(A\psi)(m) = A(m)\psi(m)$$

We write $A = \int_M^\oplus A(m)\, d\mu$.

The properties of such operators are summarized by:

Theorem XIII.85 Let $A = \int_M^\oplus A(m)\, d\mu$ where $A(\cdot)$ is measurable and $A(m)$ is self-adjoint for each m. Then:

(a) The operator A is self-adjoint.
(b) A self-adjoint operator A on $\mathscr{H}$ has the form $\int_M^\oplus A(m)\, d\mu$ if and only if $(A+i)^{-1}$ is a bounded decomposable operator.
(c) For any bounded Borel function F on $\mathbb{R}$,

$$F(A) = \int_M^\oplus F(A(m))\, d\mu \tag{139}$$

(d) $\lambda \in \sigma(A)$ if and only if for all $\varepsilon > 0$,

$$\mu(\{m \mid \sigma(A(m)) \cap (\lambda - \varepsilon, \lambda + \varepsilon) \neq \varnothing\}) > 0$$

(e) λ is an eigenvalue of A if and only if

$$\mu(\{m \mid \lambda \text{ is an eigenvalue of } A(m)\}) > 0$$

(f) If each $A(m)$ has purely absolutely continuous spectrum, then so does A.
(g) Suppose that $B = \int_M^\oplus B(m)\, d\mu(m)$ with each $B(m)$ self-adjoint. If B is A-bounded with A-bound a, then a.e. $B(m)$ is $A(m)$-bounded with $A(m)$-bound $a(m) \le a$. If $a < 1$, then

$$A + B = \int_M^\oplus (A(m) + B(m))\, d\mu \tag{140}$$

is self-adjoint on $D(A)$.

Proof (a) We first note that A is symmetric, so by the fundamental criterion, we need only prove that $\operatorname{Ran}(A \pm i) = \mathscr{H}$. Let $C(m) = (A(m) + i)^{-1}$. By hypothesis, $C(m)$ is measurable and $\|C(m)\| \le 1$, so we can define $C = \int_M^\oplus C(m)\, d\mu$. Let $\psi = C\eta$ for $\eta \in \mathscr{H}$. Then, a.e., $\psi(m) \in \operatorname{Ran} C(m) = D(A(m))$ and

$$\|A(m)\psi(m)\| = \|A(m)C(m)\eta(m)\| \le \|\eta(m)\| \in L^2(d\mu)$$

so $\psi \in D(A)$. Moreover $(A + i)\psi = \eta$ so $\operatorname{Ran}(A + i) = \mathscr{H}$. Similarly, since $(A(m) - i)^{-1} = C(m)^*$ is weakly measurable, $\operatorname{Ran}(A - i) = \mathscr{H}$.

(b) We leave this to the reader (Problem 136).

(c) Let us sketch the argument leaving the details to the reader (Problem 136). By the argument in (a), for any λ with $\operatorname{Im}\lambda \neq 0$,

$$(A-\lambda)^{-1} = \int_M^{\oplus} (A(m)-\lambda)^{-1}\, d\mu(m)$$

Since $e^{iAt} = \lim_{n\to\infty} (1-(itA/n))^{-n}$ (by the functional calculus), one sees, employing the dominated convergence theorem, that

$$e^{iAt} = \int_M^{\oplus} e^{itA(m)}\, d\mu$$

If $F \in \mathscr{S}(\mathbb{R})$, (139) follows by use of the Fourier transform. By a suitable limiting argument, (139) holds for arbitrary F.

(d) A particular case of (139) is

$$P_{(a,b)}(A) = \int_M^{\oplus} P_{(a,b)}(A(m))\, d\mu$$

Now (d) follows by noting that $\lambda \in \sigma(A)$ if and only if $P_{(\lambda-\varepsilon,\lambda+\varepsilon)}(A) \neq 0$ for all $\varepsilon > 0$ and that $\int_M^{\oplus} T(m)\, d\mu = 0$ if and only if $T(m) = 0$ a.e.

(e) The proof is similar to (d) using

$$P_{\{\lambda\}}(A) = \int_M^{\oplus} P_{\{\lambda\}}(A(m))\, d\mu$$

(f) Let $\psi \in \mathscr{H}$ and let $d\nu$ be the spectral measure for A associated to ψ. Let $d\nu_m$ be the spectral measure for $A(m)$ associated to $\psi(m)$. Then

$$d\nu = \int_M (d\nu_m)\, d\mu(m)$$

in the sense that

$$\int_{\mathbb{R}} F(x)\, d\nu = \int_M \left(\int_{\mathbb{R}} F(x)\, d\nu_m\right) d\mu(m) \tag{141}$$

(141) follows immediately from (139). Now, if each $A(m)$ has purely absolutely continuous spectrum, then

$$d\nu_m(x) = g_m(x)\, dx$$

for some $g_m \in L^1(\mathbb{R}, dx)$ with $\int g_m(x)\, dx = \|\psi(m)\|^2_{\mathscr{H}'}$. Thus

$$g(x) = \int g_m(x)\, d\mu(m)$$

is in $L^1(\mathbb{R}, dx)$ and, by (141),

$$d\nu = g(x)\, dx$$

It follows that $\psi \in \mathscr{H}_{\text{ac}}$ for A, so that A has purely absolutely continuous spectrum.

(g) If $\|B\psi\| \le a\|A\psi\| + b\|\psi\|$, then $\|B(A + ik)^{-1}\| \le a + bk^{-1}$ for any positive integer k. Therefore,

$$\|B(m)(A(m) + ik)^{-1}\| \le a + bk^{-1}$$

a.e. so $B(m)$ is $A(m)$-bounded with bound $a(m) \le a$. (140) is immediate. ∎

Part (f) of this last theorem says that a sufficient condition for $A = \int_M^\oplus A(m)\, d\mu(m)$ to have purely absolutely continuous spectrum is that each $A(m)$ have purely absolutely continuous spectrum. But this is certainly not necessary. In fact, A can have purely absolutely continuous spectrum even though each $A(m)$ has purely discrete spectrum! The following theorem illustrates the phenomenon.

Theorem XIII.86 Let $\langle M, d\mu\rangle$ be $[0, 1]$ with Lebesgue measure. Let $\mathscr{H}'$ be a fixed separable infinite-dimensional space and let $A = \int_{[0,1]}^\oplus A(m)\, d\mu(m)$ with each $A(m)$ self-adjoint. Suppose we are given $\mathscr{H}'$-valued functions $\{\psi_n(\cdot)\}_{n=1}^\infty$ on $[0, 1]$, real analytic on $(0, 1)$, continuous on $[0, 1]$, and complex-valued functions $E_n(\cdot)$, analytic in a neighborhood of $[0, 1]$, so that:

(i) No $E_n(\cdot)$ is constant.
(ii) $A(m)\psi_n(m) = E_n(m)\psi_n(m)$ for all $m \in [0, 1]$; $n = 1, 2, \ldots$.
(iii) For each m, the set $\{\psi_n(m)\}_{n=1}^\infty$ is a complete orthonormal basis for $\mathscr{H}'$.

Then A has purely absolutely continuous spectrum.

Proof Let

$$\mathscr{H}_n = \{\psi \in \mathscr{H} \mid \psi(m) = f(m)\psi_n(m); f \in L^2(M; d\mu)\}$$

Then the $\mathscr{H}_n$ are closed subspaces that are mutually orthogonal and $\mathscr{H} = \bigoplus \mathscr{H}_n$ since any $\psi \in \mathscr{H}$ has an expansion (Problem 134):

$$\psi = \sum_{n=1}^{\infty} (\psi_n(m), \psi(m))\psi_n(m)$$

Moreover, each $\mathscr{H}_n$ lies in $D(A)$ with $A[\mathscr{H}_n] \subset \mathscr{H}_n$. Consider the unitary map U_n: $\mathscr{H}_n \to L^2([0, 1], dx)$, given by $U_n(f(m)\psi_n(m)) = f(m)$. Then $A_n \equiv U_n A U_n^{-1}$ is given by

$$(A_n f)(m) = E_n(m) f(m) \tag{142}$$

We need only show that each A_n has purely absolutely continuous spectrum. Since $E_n(\cdot)$ is analytic in a neighborhood of $[0, 1]$ and nonconstant, dE_n/dm has only finitely many zeros in $(0, 1)$, say at $m_1, \ldots, m_{k-1}$. Let $m_0 = 0$ and $m_k = 1$. Then

$$L^2([0, 1], dx) = \bigoplus_{j=1}^{k} L^2((m_{j-1}, m_j), dx)$$

A_n leaves each summand invariant and acts on the summand by (142). On each interval (m_{j-1}, m_j), $E_n(\cdot)$ is strictly monotone, either increasing or decreasing. Consider the case where it is increasing. Define α: $(E_n(m_{j-1}), E_n(m_j)) \to (m_{j-1}, m_j)$ by $E_n(\alpha(\lambda)) = \lambda$. Then α is differentiable and the Stieltjes measure $d\alpha$ is absolutely continuous with respect to dx. In fact,

$$d\alpha = \left[\left(\frac{dE}{dm}\right)\bigg|_{m=\alpha(\lambda)}\right]^{-1} d\lambda$$

Let U be the unitary operator from $L^2((m_{j-1}, m_j), dx)$ to $L^2((E_n(m_{j-1}), E_n(m_j)), d\lambda)$ given by

$$(Uf)(\lambda) = \left(\frac{d\alpha}{d\lambda}\right)^{+1/2} f(\alpha(\lambda))$$

Then

$$(UA_nU^{-1})g(\lambda) = \lambda g(\lambda)$$

We have thus explicitly constructed a spectral representation for $A_n \restriction L^2([m_{j-1}, m_j], dx)$ for which the spectral measure $d\alpha$ is Lebesgue measure. It follows that each A_n, and thus A, has purely absolutely continuous spectrum. ∎

We turn now to an analysis of Schrödinger operators with periodic potentials. We first consider the case of one dimension with V piecewise continuous where differential equation methods are available and then the case of higher dimension and more general V.

To motivate our analysis, suppose that $V \in C_0^\infty(\mathbb{R})$ with bounded derivatives so that $-d^2/dx^2 + V$ takes $\mathscr{S}(\mathbb{R})$ into itself. If $f \in \mathscr{S}(\mathbb{R})$, then

$$\left[\left(-\frac{d^2}{dx^2} + V\right)f\right]^\wedge(p) = p^2\hat{f}(p) + (2\pi)^{-1/2}\int \hat{V}(p - p')\hat{f}(p')\,dp' \quad (143)$$

where the integral in (143) is a formal symbol for the convolution of the distribution $\hat{V}$ and the function $\hat{f}$. Now, let us suppose that V has period 2π. Then V has a uniformly convergent Fourier series (see Theorem II.8):

$$V(x) = \sum_{n=-\infty}^{\infty} \tilde{V}_n e^{inx} \tag{144}$$

where

$$\tilde{V}_n = \int_{-\pi}^{\pi} \tilde{V}(x) e^{-inx} \frac{dx}{2\pi}$$

(144) suggests that

$$(2\pi)^{-\frac{1}{2}} \hat{V}(p) = \sum_{n=-\infty}^{\infty} \tilde{V}_n \delta(p-n) \tag{145}$$

since putting (145) formally into the Fourier inversion formula yields (144). In fact, one can prove (145) as follows: If $f \in \mathscr{S}(\mathbb{R})$, then the uniform convergence of (144) implies that

$$\int f(x) V(x)\, dx = (2\pi)^{1/2} \sum_{n=-\infty}^{\infty} \tilde{V}_n \hat{f}(n)$$

from which (145) follows if the sum is viewed as convergent in the weak ($\sigma(\mathscr{S}', \mathscr{S})$) topology on $\mathscr{S}'$.

Now that we have analyzed Fourier transforms of periodic tempered distributions, we can use this analysis to rewrite (143) as

$$\left[\left(-\frac{d^2}{dx^2} + V\right) f\right]^{\wedge}(p) = p^2 \hat{f}(p) + \sum_{n=-\infty}^{\infty} \tilde{V}_n \hat{f}(p-n)$$

Thus, if $H = -d^2/dx^2 + V$, then $\widehat{Hf}(p)$ depends only on the values $\hat{f}(p-n)$; $n \in \mathbb{Z}$. We have therefore proven:

Theorem XIII.87 (direct integral decomposition of periodic Schrödinger operators—p-space version in one dimension) Let $\mathscr{H}' = \ell_2$ and let $\mathscr{H} = \int_{(-1/2, 1/2]}^{\oplus} \mathscr{H}'\, dx$. For $q \in (-\frac{1}{2}, \frac{1}{2}]$, let

$$(H(q)g)_j = (q+j)^2 g_j + \sum_{n=-\infty}^{\infty} \tilde{V}_n g_{j-n}$$

where $\tilde{V}_n$ are the Fourier series coefficients of some $V \in C^\infty(\mathbb{R})$ with period 2π. Map $L^2(\mathbb{R}, dx)$ to $\mathscr{H}$ by

$$[(Uf)(q)]_j = \hat{f}(q + j)$$

Let $H = -d^2/dx^2 + V$ on $L^2(\mathbb{R})$. Then,

$$UHU^{-1} = \int_{(-1/2, 1/2]}^{\oplus} H(q)\, dq$$

One can get quite far in the analysis of H by using this p-space version of the direct integral decomposition. In fact, this will be our main tool in the multidimensional case. However, in the one-dimensional case, the x-space translation of Theorem XIII.87 gives a little more information. While we could use Theorem XIII.87 directly to write down the x-space version, we shall give an independent proof, using Theorem XIII.87 merely for the following motivation. In case $V = 0$ the operator $H(q)$ has eigenvalues $(q + j)^2$ and eigenfunctions that are basically the Fourier transforms of the functions $e^{i(q+j)x}$. This suggests that somehow $H(q)$ is related to the operator $-d^2/dx^2$ on $L^2([0, 2\pi], dx)$ but with the boundary conditions

$$\psi(2\pi) = e^{2\pi i q}\psi(0), \qquad \psi'(2\pi) = e^{2\pi i q}\psi'(0)$$

Lemma Let $\mathscr{H}' = L^2([0, 2\pi], dx)$. Let

$$\mathscr{H} = \int_{[0, 2\pi)}^{\oplus} \mathscr{H}' \frac{d\theta}{2\pi} \tag{146}$$

Then $U: L^2(\mathbb{R}, dx) \to \mathscr{H}$ given by

$$(Uf)_\theta(x) = \sum_{n=-\infty}^{\infty} e^{-i\theta n} f(x + 2\pi n) \tag{147}$$

for θ and x in $[0, 2\pi)$, is well defined for $f \in \mathscr{S}(\mathbb{R})$ and uniquely extendable to a unitary operator. Moreover,

$$U\left(-\frac{d^2}{dx^2}\right)U^{-1} = \int_{[0, 2\pi)}^{\oplus} \left(-\frac{d^2}{dx^2}\right)_\theta \frac{d\theta}{2\pi} \tag{148}$$

where $(-d^2/dx^2)_\theta$ is the operator $-d^2/dx^2$ on $L^2([0, 2\pi])$ with the boundary conditions

$$\psi(2\pi) = e^{i\theta}\psi(0), \qquad \psi'(2\pi) = e^{i\theta}\psi'(0)$$

Proof For $f \in \mathcal{S}$, the sum (147) is clearly convergent. To prove that Uf is in $\mathcal{H}$, we compute that for $f \in \mathcal{S}$,

$$\int_0^{2\pi} \left(\int_0^{2\pi} \left| \sum_{n=-\infty}^{\infty} e^{-in\theta} f(x + 2\pi n) \right|^2 dx \right) \frac{d\theta}{2\pi}$$
$$= \int_0^{2\pi} \left[\left(\sum_{n=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \overline{f(x + 2\pi n)} f(x + 2\pi j) \right) \int_0^{2\pi} e^{-i(j-n)\theta} \frac{d\theta}{2\pi} \right] dx$$
$$= \int_0^{2\pi} \left(\sum_{n=-\infty}^{\infty} |f(x + 2\pi n)|^2 \right) dx = \int_{-\infty}^{\infty} |f(x)|^2 \, dx$$

where we have used the Fubini and Plancherel theorems. Thus we see that U is well defined and has a unique extension to an isometry. To see that U is onto $\mathcal{H}$, we compute U^*. For $g \in \mathcal{H}$, we define, for $0 \le x \le 2\pi$, $n \in \mathbb{Z}$,

$$(U^*g)(x + 2\pi n) = \int_0^{2\pi} e^{in\theta} g_\theta(x) \frac{d\theta}{2\pi} \tag{149}$$

A direct computation shows that this is indeed the formula for the adjoint of U. Moreover,

$$\|U^*g\|_2^2 = \int_{-\infty}^{\infty} |(U^*g)(y)|^2 \, dy$$
$$= \int_0^{2\pi} \left(\sum_{n=-\infty}^{\infty} |(U^*g)(2\pi n + x)|^2 \right) dx$$
$$= \int_0^{2\pi} \left(\sum_{n=-\infty}^{\infty} \left| \int e^{in\theta} g_\theta(x) \frac{d\theta}{2\pi} \right|^2 \right) dx$$
$$= \int_0^{2\pi} \left(\int_0^{2\pi} |g_\theta(x)|^2 \frac{d\theta}{2\pi} \right) dx$$
$$= \|g\|^2$$

In the next to the last step we have used the Parseval relation for Fourier series.

To verify (148), let A be the operator on the right-hand side of (148). We shall show that if $f \in \mathcal{S}(\mathbb{R})$, then $Uf \in D(A)$ and $U(-f'') = A(Uf)$. Since $-d^2/dx^2$ is essentially self-adjoint on $\mathcal{S}$ and A is self-adjoint, (148) will follow. So, suppose $f \in \mathcal{S}(\mathbb{R}^n)$. Then Uf is given by the convergent sum (147) so that Uf is C^∞ on $(0, 2\pi)$ with $(Uf)'_\theta(x) = (Uf')_\theta(x)$ and similarly for higher derivatives. Moreover, it is clear that

$$(Uf)_\theta(2\pi) = \sum_{n=-\infty}^{\infty} e^{-i\theta n} f(2\pi(n+1))$$

$$= \sum_{n=-\infty}^{\infty} e^{-i\theta(n-1)} f(2\pi n) = e^{i\theta}(Uf)_\theta(0)$$

Similarly, $(Uf)'_\theta(2\pi) = e^{i\theta}(Uf_\theta)'(0)$. Thus, for each θ, $(Uf)_\theta \in D((-d^2/dx^2)_\theta)$ and

$$\left(-\frac{d^2}{dx^2}\right)_\theta (Uf) = U(-f'')_\theta$$

We conclude that $Uf \in D(A)$ and $A(Uf) = U(-f'')$. This proves (148). ∎

Theorem XIII.88 (direct integral decomposition of periodic Schrödinger operators—x-space version in one dimension) Let V be a bounded measurable function on $\mathbb{R}$ with period 2π. For $\theta \in [0, 2\pi)$, let

$$H(\theta) = \left(-\frac{d^2}{dx^2}\right)_\theta + V(x)$$

as an operator on $L^2[0, 2\pi]$. Let U be given by (147). Then, under the decomposition (146),

$$U\left(-\frac{d^2}{dx^2} + V\right)U^{-1} = \int_{[0,2\pi)}^{\oplus} H(\theta)\frac{d\theta}{2\pi} \tag{150}$$

Proof Let V be the θ-independent operator acting on the fiber $\mathscr{H}' = L^2([0, 2\pi), dx)$ by

$$(V_\theta f)(x) = V(x)f(x), \qquad 0 \le x \le 2\pi$$

(150) follows from Theorem XIII.85g and the lemma if we can prove that

$$UVU^{-1} = \int_{[0,2\pi)}^{\oplus} V_\theta \frac{d\theta}{2\pi} \tag{151}$$

By (147), for $f \in \mathscr{S}$,

$$(UVf)_\theta(x) = \sum_{n=-\infty}^{\infty} e^{-in\theta} V(x+2\pi n) f(x+2\pi n)$$

$$= V(x) \sum_{n=-\infty}^{\infty} e^{-in\theta} f(x+2\pi n)$$

$$= V_\theta(Uf)_\theta(x)$$

since V is periodic. This proves (151) and so (150). ∎

As a result, to analyze $-d^2/dx^2 + V$ with V periodic, we need only analyze $(-d^2/dx^2)_\theta + V$ for each θ. As a preliminary, we note:

Lemma

(a) For each $\theta \in [0, 2\pi)$, $(-d^2/dx^2)_\theta$ has compact resolvent.
(b) For $\theta = 0$, $\exp(-t(-d^2/dx^2)_{\theta=0})$ is a positivity improving semigroup (see Section 12).
(c) $[(-d^2/dx^2)_\theta + 1]^{-1}$ is an analytic operator-valued function of θ in a neighborhood of $[0, 2\pi)$.

Proof We shall later prove the analogue of this lemma in the multidimensional case by using general arguments that could be used here. However, it is easy to obtain explicit formulas for $K_\theta \equiv [(-d^2/dx^2)_\theta + 1]^{-1}$. Let $f \in C_0^\infty(0, 2\pi)$. Let K be the inverse of $-d^2/dx^2 + 1$ defined on all of $L^2(\mathbb{R})$. Let $g = Kf$. By our arguments in Section IX.7, K is an integral operator with kernel $G(x-y)$ where $\hat{G}(p) = (2\pi)^{-1/2}(p^2+1)^{-1}$. A direct computation of G is possible (Problem 137) and one finds

$$g(x) \equiv Kf(x) = \tfrac{1}{2}\int e^{-|x-y|}f(y)\,dy \tag{152}$$

Now, both Kf and $K_\theta f$ solve the differential equation $-u''(x) + u(x) = f(x)$ on $(0, 2\pi)$. It follows that their difference $v = K_\theta f - Kf$ obeys $-v'' + v = 0$ so that

$$(K_\theta f)(x) = g(x) + ae^x + be^{-x}$$

Since $K_\theta f \in D((-d/dx^2)_\theta)$, a and b must be chosen so that $K_\theta f$ obeys the boundary conditions

$$u(2\pi) = e^{i\theta}u(0), \qquad u'(2\pi) = e^{i\theta}u'(0) \tag{153}$$

Direct computation using (152) shows that

$$(K_\theta f)(x) = \int_0^{2\pi} G_\theta(x, y)f(y)\,dy$$

$$G_\theta(x, y) = \tfrac{1}{2}e^{-|x-y|} + \alpha(\theta)e^{x-y} + \beta(\theta)e^{y-x} \tag{154}$$

$$\alpha(\theta) = \tfrac{1}{2}(e^{2\pi - i\theta} - 1)^{-1}$$

$$\beta(\theta) = \tfrac{1}{2}(e^{2\pi + i\theta} - 1)^{-1}$$

One can read the properties claimed for $(-d^2/dx^2)_\theta$ directly from (154). Since $G_\theta(x, y)$ is bounded in x, y for each fixed θ,

$$\int_0^{2\pi}\int_0^{2\pi} |G_\theta(x, y)|^2\, dx\, dy < \infty$$

so K_θ is Hilbert–Schmidt and so compact, proving (a). By direct examination, the kernel $G_{\theta=0}(x, y)$ is strictly positive. A similar computation proves that $[(-d^2/dx^2)_{\theta=0} + a]^{-1}$ has a strictly positive kernel for any $a > 0$ and so by Theorem XIII.44 and the preceding proposition, $\exp(-t(-d^2/dx^2)_{\theta=0})$ is a positivity improving semigroup. Finally, to prove (c), we note that the formulas (154) allow us to define a Hilbert–Schmidt operator K_θ for any θ with $|\text{Im}\,\theta| < 2\pi$ and that $\theta \to K_\theta$ is clearly analytic in θ. ∎

It may seem striking at first sight that $K_\theta - K_{\theta'}$ is a rank two operator for any θ, θ', but, in fact, this is just a reflection of the fact that $-d^2/dx^2 \restriction C_0^\infty(0, 2\pi)$ has deficiency indices $\langle 2, 2\rangle$ so that K_θ is completely determined in a θ-independent way on the closure of the space $(-d^2/dx^2 + 1)[C_0^\infty(0, 2\pi)]$ which has codimension 2.

An analysis similar to that above shows that $((-d^2/dx^2)_\theta + a)^{-1}$ is analytic in the region $|\text{Im}\,\theta| < 2\pi\sqrt{a}$ so that the map $\theta \mapsto (-d^2/dx^2)_\theta$ can be extended to an entire analytic family. This family is neither type (A) nor type (B).

Armed with the lemma, we are prepared for a complete analysis of the operators

$$H(\theta) = \left(-\frac{d^2}{dx^2}\right)_\theta + V \tag{155}$$

Theorem XIII.89 Suppose that V is piecewise continuous and periodic of period 2π. Then:

(a) $H(\theta)$ has purely discrete spectrum and is real analytic in θ.

(b) $H(\theta)$ and $H(2\pi - \theta)$ are antiunitarily equivalent under ordinary complex conjugation. In particular, their eigenvalues are identical and their eigenfunctions are complex conjugates.

(c) For $\theta \in (0, \pi)$, or in $(\pi, 2\pi)$, $H(\theta)$ has only nondegenerate eigenvalues.

(d) Let $E_n(\theta)$ $(n = 1, 2, \ldots; 0 \le \theta \le \pi)$ denote the nth eigenvalue of $H(\theta)$. Then each $E_n(\cdot)$ is analytic in $(0, \pi)$ and continuous at $\theta = 0$ and π.

(e) For n odd (respectively, even) $E_n(\theta)$ is strictly monotone increasing (respectively, decreasing) as θ increases from 0 to π. In particular,

$$E_1(0) < E_1(\pi) \le E_2(\pi) < E_2(0) \le \cdots \le E_{2n-1}(0) < E_{2n-1}(\pi) \le E_{2n}(\pi) < E_{2n}(0) \le \cdots$$

See Figure XIII.13.

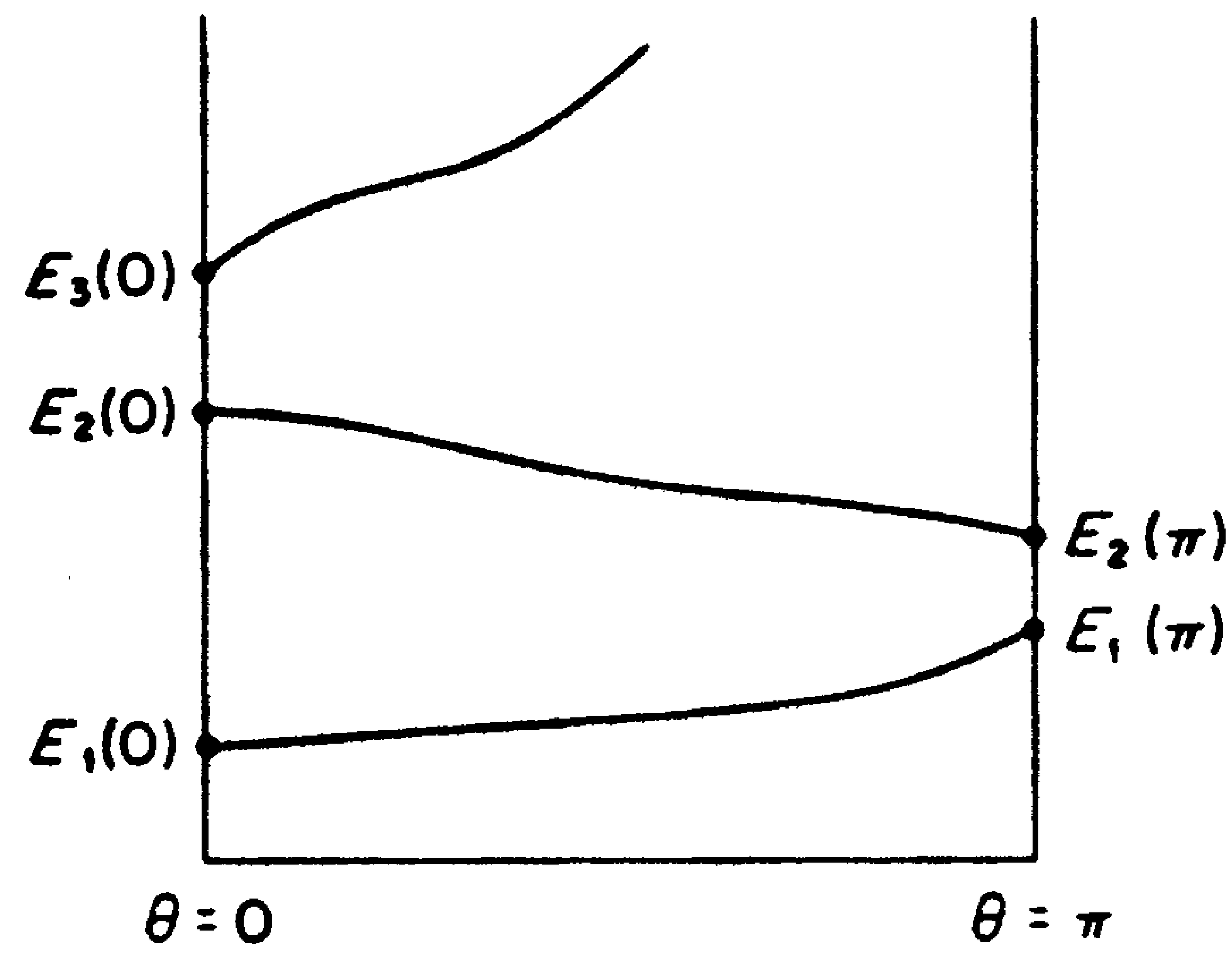


FIGURE XIII.13 Bands in one-dimensional Schrödinger operators.

(f) One can choose the eigenvectors $\psi_n(\theta)$ so that they are analytic in θ for $\theta \in (0, \pi) \cup (\pi, 2\pi)$, continuous at π and 0 (with $\psi_n(0) = \psi_n(2\pi)$).

Proof (a) This follows directly from the lemma and the basic perturbation Theorems XII.11 and XIII.64.

(b) When $V = 0$, this is a simple consequence of the definition of $(-d^2/dx^2)_\theta$. Since $\overline{V\psi} = V\bar{\psi}$, the results hold for general V.

(c) If E is an eigenvalue of $H(\theta)$, $\theta \in (0, \pi)$, then $-u'' + Vu = Eu$ has a solution obeying the boundary condition (153). So $\bar{u}$ is a solution obeying a distinct boundary condition. Since $-u'' + Vu = Eu$ has only two linearly independent solutions and not all of them obey (153), at most one can.

(d) Consider $E_1(0)$. This is a simple eigenvalue of $H(0)$ since $H(0)$ generates a positivity preserving semigroup. Since $H(\theta)$ is analytic near $\theta = 0$, we can find $\tilde{f}_1(\theta)$ an eigenvalue of $H(\theta)$ for $\theta \in [0, \varepsilon)$ analytic in $[0, \varepsilon)$ with $\tilde{f}_1(0) = E_1(0)$. Let $\varepsilon < \pi$. The only thing that can prevent one from analytically continuing past $\theta = \varepsilon$ is if $\tilde{f}_1(\theta) \to \infty$ as $\theta \uparrow \varepsilon$. For since $H(\theta) \ge -\|V\|_\infty$, if $\tilde{f}_1(\theta)$ does not approach ∞, then there is a sequence $\theta_n \to \varepsilon$ such that $\tilde{f}_1(\theta_n) \to \tilde{E}$. But then one sees that $\tilde{E}$ is an eigenvalue of $H(\varepsilon)$. By (c), it is a simple eigenvalue, so for $|\theta - \varepsilon| < \delta$, there is a unique eigenvalue $g(\theta)$ of $H(\theta)$ near $\tilde{E}$ and g is analytic for $|\theta - \varepsilon| < \delta$. In particular, for n large $g(\theta_n) = \tilde{f}_1(\theta_n)$ so g provides an analytic continuation for $\tilde{f}_1$ past ε. Thus to prove that $\tilde{f}_1$ can be analytically continued to all of $[0, \pi)$, we need only show that $\tilde{f}_1(\theta)$ remains finite as θ varies. We first show that $H(\theta)$

has no eigenvalue smaller than $\tilde{f}_1(\theta)$ if $\theta \in [0, \varepsilon)$. If it did, we could continue that back to $\theta = 0$; this continuation could not go to infinity as we decreased θ since it is always strictly less than $\tilde{f}_1(\theta)$ by the simplicity of eigenvalues and the argument above. Continuing back to $\theta = 0$, we would find an eigenvalue less than E_1. Since $\tilde{f}_1(\theta)$ is the smallest eigenvalue of $H(\theta)$ it cannot go to infinity as $\theta \to \varepsilon$. Thus, $\tilde{f}_1(\theta)$ has a continuation to $[0, \pi]$ and this continuation is the smallest eigenvalue of $H(\theta)$, i.e., it is $E_1(\theta)$.

Now look at $E_2(0)$. This may be doubly degenerate; for example it is when $V = 0$. If it is though, the degeneracy must be broken for $\theta \neq 0$ since the spectrum of $H(\theta)$, $\theta \neq 0$ is simple. By degenerate perturbation theory, the eigenvalue (or eigenvalues if $E_2(0)$ is degenerate) near $E_2(0)$ is given by analytic function(s). Let $\tilde{f}_2(\theta)$ be this function if $E_2(0)$ is simple, and the smaller of the functions if $E_2(0)$ is degenerate. Then by mimicking the argument above, $\tilde{f}_2(\theta)$ can be continued throughout $[0, \pi]$ and is the second eigenvalue $E_2(\theta)$. By repeating this argument, we can handle all the eigenvalues.

(e) This is the deepest part of the theorem, so we shall give a detailed proof. As a preliminary, we prove that $E_1(0) \leq E_1(\theta)$ for all θ. Since $e^{-tH(0)}$ is positivity improving, the eigenvector $\psi_1(0)$ associated to $E_1(0)$ is strictly positive and by the boundary condition, it has a periodic extension to all of $\mathbb{R}$. Fix k, an integer, and consider $H^{(k)}(0)$ the operator $-d^2/dx^2 + V$ on $L^2(-2\pi k, 2\pi k)$ with periodic boundary conditions. Then $\psi_1(0)$ periodically extended is a strictly positive eigenvector of $H^{(k)}(0)$ and so $E_1(0) = \inf \sigma(H^k(0))$ (see Section XIII.12). It follows that if $f \in C_0^\infty(-2\pi k, 2\pi k)$, then $(f, (-d^2/dx^2 + V)f) = (f, H^k(0)f) \geq E_1(f, f)$, and thus the operator $-d^2/dx^2 + V$ on $L^2(\mathbb{R})$ obeys $-d^2/dx^2 + V \geq E_1$. By the direct integral decomposition, $H(\theta) \geq E_1(0)$, a.e. in θ so $E_1(\theta) \geq E_1(0)$, a.e. in θ. Since $E_1(\theta)$ is continuous $E_1(\theta) \geq E_1(0)$ for all $\theta \in (0, 2\pi)$.

Now we introduce an important function, $D(E)$, associated to the differential equation

$$-u'' + Vu = Eu \tag{156}$$

Let $u_1(E, x)$ be the solution of (156) with $u_1(0) = 1$, $u_1'(0) = 0$, and let $u_2(E, x)$ be the solution of (156) with $u_2(0) = 0$, $u_2'(0) = 1$. Then $u_i(x, E)$ is analytic in E for each x by the standard theory of ordinary differential equations. Let $M(E)$ be the analytic two by two matrix

$$M(E) = \begin{bmatrix} u_1(E, 2\pi) & u_2(E, 2\pi) \\ u_1'(E, 2\pi) & u_2'(E, 2\pi) \end{bmatrix} \tag{157}$$

The **discriminant** of $-u'' + Vu$ is the function

$$D(E) \equiv \mathrm{Tr}(M(E)) = u_1(E, 2\pi) + u_2'(E, 2\pi)$$

$M(E)$ is a natural object, for if v satisfies (156), then

$$\begin{bmatrix} v(2\pi) \\ v'(2\pi) \end{bmatrix} = M(E) \begin{bmatrix} v(0) \\ v'(0) \end{bmatrix}$$

In particular, the equation $H(\theta)\psi = E\psi$ has a nonzero solution if and only if $M(E)$ has an eigenvalue $e^{i\theta}$. Now $M(E)$ has determinant 1 since $W(x) = u_1(E, x)u_2'(E, x) - u_1'(E, x)u_2(E, x)$ is a constant. Thus its eigenvalues are λ and λ^{-1} and $D(E) = \lambda + \lambda^{-1}$. We conclude that *$E$ is an eigenvalue of $H(\theta)$ if and only if $D(E) = 2\cos\theta$.* What we will prove is that $D(E)$ has a graph somewhat like the one in Figure XIII.14.

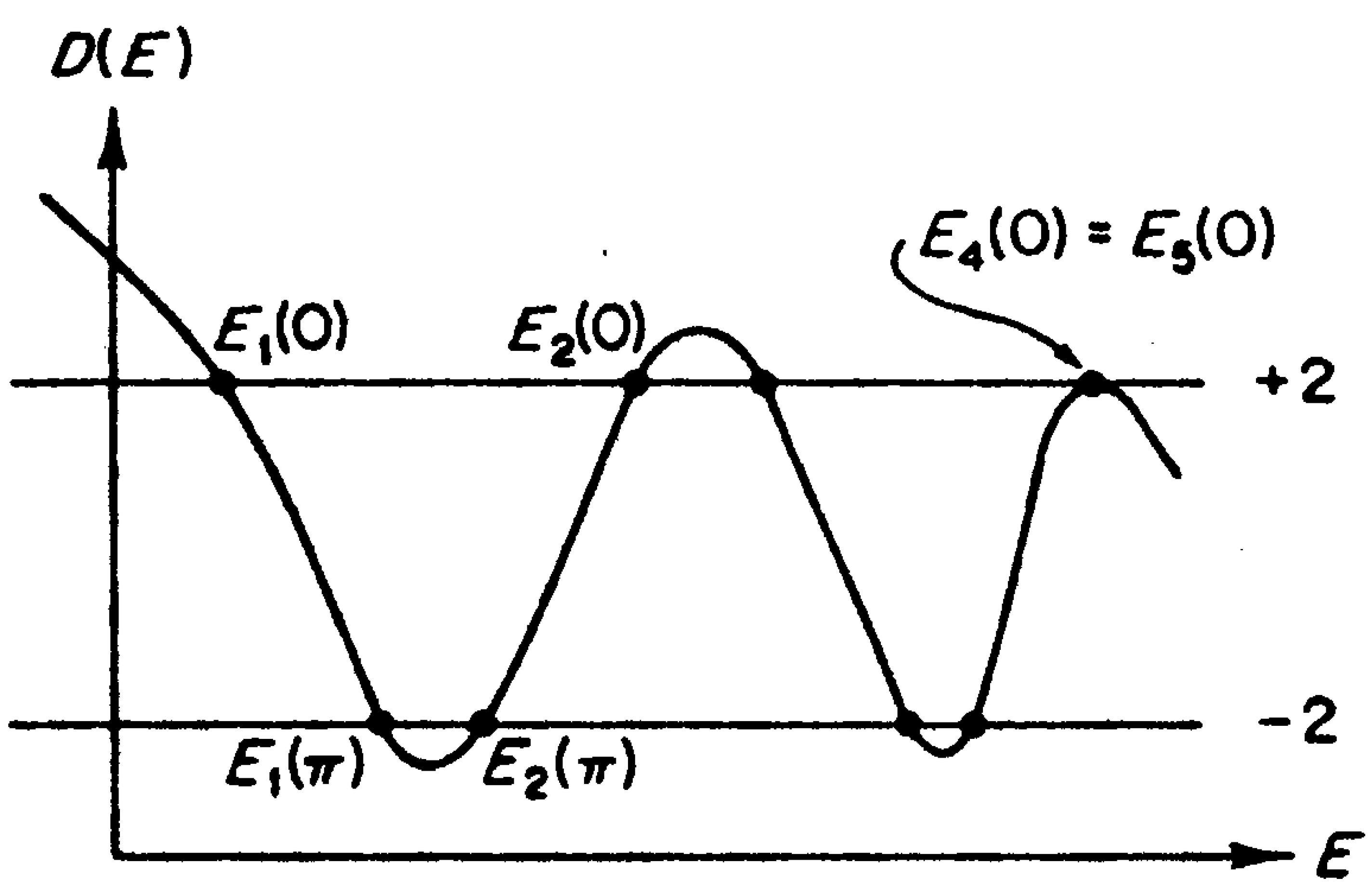
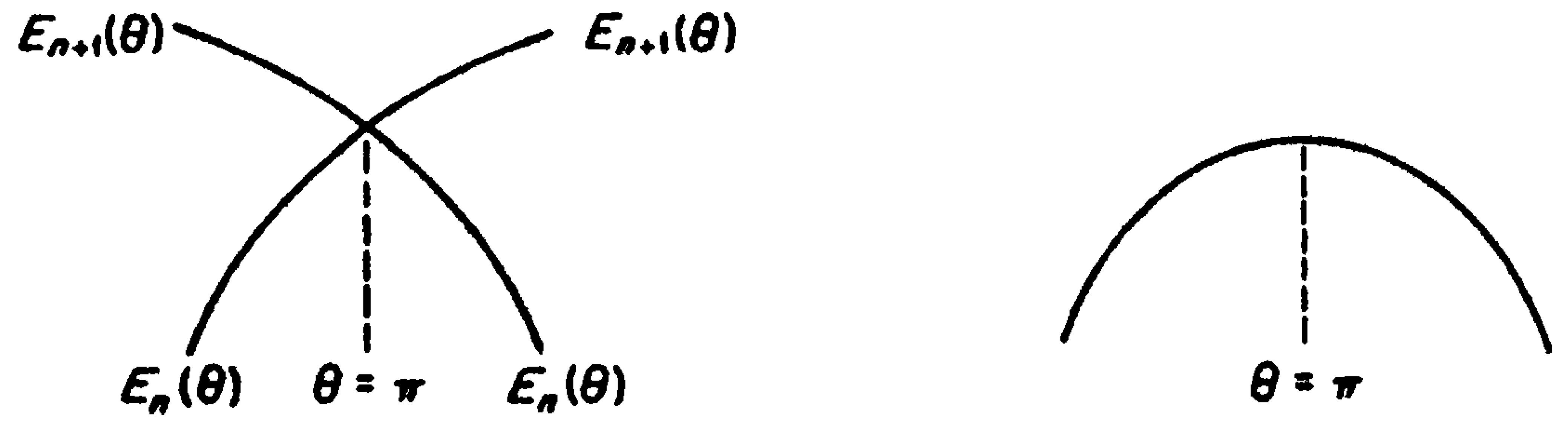


FIGURE XIII.14 A typical discriminant.

We have proven that $E_1(0) \leq E_1(\theta)$ for all θ, so $D(E)$ cannot have any value in $[-2, 2]$ for $E < E_1(0)$. Now $D(E) = 2$ for $E = E_1(0)$. As θ varies from 0 to π, $D(E_1(\theta))$ varies from 2 to -2. E_1 must therefore be strictly monotone increasing since it has an inverse function Arc cos $\frac{1}{2}D(E_1(\theta)) = \theta$. We have $D(E_1(\pi)) = -2$. D must eventually turn around (since $H(\pi)$ has additional eigenvalues) so the next value of $D(\theta)$ in $[-2, 2]$ to occur must be -2. This occurs at $E_2(\pi)$ and then D runs from -2 to 2 as θ goes from π to 0. Thus we have the picture in Figure XIII.14. The only subtlety is that we must show that if D has a turning point at $+2$ or -2, then $H(0)$ or $H(\pi)$ has a double eigenvalue. But if $D(E)$ has a turning point at $E = E_0$ with $D(E) = +2$, then for θ near 0, $H(\theta)$ has two eigenvalues near E_0 corresponding to the fact that $D(E) = 2\cos\theta$ has two solutions near $E = E_0$. By analytic perturbation theory E_0 must be a double eigenvalue of $H(0)$.

(f) This follows from the analytic perturbation theory of Section XII.2. ▌

The reader may have noticed that while we have been careful to avoid saying that $E_n(\theta)$ is analytic near $\theta = \pi$ or 0, it clearly is. However, if $E_n(\theta)$ is continued through $\theta = \pi$, the continuation may be $E_{n+1}(\theta)$ or $E_{n-1}(\theta)$ if $E_n(\pi)$ is a doubly degenerate eigenvalue (see Figure XIII.15). A similar phenomenon can occur at $\theta = 0$ if we identify θ and $\theta - 2\pi$.



(a) $E_n(\pi)$ degenerate (b) $E_n(\pi)$ nondegenerate

FIGURE XIII.15 Crossed bands.

We can now combine Theorems XIII.85, 86, 88, and 89 to conclude:

Theorem XIII.90 Let V be a piecewise continuous function of period 2π. Let $H = -d^2/dx^2 + V$ on $L^2(\mathbb{R}, dx)$. Let $E_1(0), E_2(0), \ldots$ be the eigenvalues of the corresponding operator on $(0, 2\pi)$ with periodic boundary conditions and let $E_1(\pi), \ldots$ be the eigenvalues with antiperiodic boundary conditions. Let

$$\alpha_n = \begin{cases} E_n(0), & n \text{ odd} \\ E_n(\pi), & n \text{ even} \end{cases} \qquad \beta_n = \begin{cases} E_n(\pi), & n \text{ odd} \\ E_n(0), & n \text{ even} \end{cases}$$

Then:

(a) $\sigma(H) = \bigcup_{n=1}^{\infty} [\alpha_n, \beta_n]$.
(b) H has no eigenvalues.
(c) H has purely absolutely continuous spectrum.

Proof (a) Since the $E_n(\theta)$ are continuous, if θ_0 and ε are given, then for some δ,

$$\{\theta \,|\, |\theta - \theta_0| < \delta\} \subset \{\theta \,|\, |E_n(\theta) - E_n(\theta_0)| < \varepsilon\}$$

so by Theorem XIII.85, $\sigma(H) = \bigcup_n [\alpha_n, \beta_n]$.

(b) No function E_n is constant since the E_n are strictly monotone. Thus for each E_0, $\{\theta \,|\, E_n(\theta) = E_0\}$ is a set with at most two points. Such a set has measure zero, so by Theorem XIII.86, E_0 is not an eigenvalue.

(c) follows by Theorems XIII.86 and 89. ▮

We remark that $-d^2/dx^2 + V$ has a simple eigenfunction expansion, but since we shall give the general n-dimensional result below, we do not pause to give the details now.

The most striking feature of Theorem XIII.90 is that $\sigma(H)$ has gaps $(\beta_1, \alpha_2), \ldots, (\beta_n, \alpha_{n+1}), \ldots$. Of course, all we know is that $\beta_n \leq \alpha_{n+1}$, so that some of the "gaps" listed may be empty. In fact, if $V = 0$, then there are no gaps, so it is necessary to impose some condition on V for any given gap to be nonempty. The beautiful feature of this analysis is that the occurrence of any gap is reduced to a question about the degeneracy of some eigenvalue.

Example 1 (the Mathieu equation) Let

$$V(x) = \mu \cos x$$

with $\mu \neq 0$. We claim that for all n, $\alpha_{n+1} \neq \beta_n$, i.e., every gap occurs. Let H_0^{P} (respectively, H_0^{A}) be $-d^2/dx^2$ on $L^2(0, 2\pi)$ with periodic (respectively, antiperiodic) boundary conditions. We need only show that $H_0^{\mathrm{P}} + V$ and $H_0^{\mathrm{A}} + V$ have no double eigenvalues. We give the proof for $H_0^{\mathrm{P}} + V$; the proof is similar for $H_0^{\mathrm{A}} + V$. Consider the functions $\varphi_n = (2\pi)^{-1/2} e^{inx}$. Then $\varphi_n \in D(H_0^{\mathrm{P}})$ and $H_0^{\mathrm{P}} \varphi_n = n^2 \varphi_n$. If ψ solves $(H_0^{\mathrm{P}} + V)\psi = E\psi$ and $a_n = (\varphi_n, \psi)$, then

$$(n^2 - E)a_n + \tfrac{1}{2}\mu(a_{n+1} + a_{n-1}) = 0 \tag{158a}$$

If η also solves $(H_0^{\mathrm{P}} + V)\eta = E\eta$ and $b_n = (\varphi_n, \eta)$, then

$$(n^2 - E)b_n + \tfrac{1}{2}\mu(b_{n+1} + b_{n-1}) = 0 \tag{158b}$$

Eliminating the $n^2 - E$ term from (158) and using $\mu \neq 0$, we have $b_n a_{n+1} - a_n b_{n+1} = a_n b_{n-1} - b_n a_{n-1}$ so $b_n a_{n+1} - a_n b_{n+1} = c$, where c is some constant. Since $\eta, \psi \in L^2$, $\sum a_n^2 < \infty$, $\sum b_n^2 < \infty$, so $a_n \to 0$ and $b_n \to 0$ as $n \to \infty$. Therefore c must be zero, and thus

$$a_n b_{n+1} = b_n a_{n+1} \tag{159}$$

By (158a), if any two successive a_j are zero, all the a_j are zero so for any n, either $a_n \neq 0$ or $a_{n+1} \neq 0$. A similar result holds for the b_n. Now suppose that E is a doubly degenerate eigenfunction. Since $\cos x$ is even under $x \to -x$, we can choose ψ to be the even solution of $-\psi'' + V\psi = E\psi$ and η to be the odd solution since all solutions are periodic if $H_0^{\mathrm{P}} + V$ has E as a degenerate eigenvalue. Since η is odd, $b_0 = \int_{-\pi}^{\pi} \eta(x)\, dx = 0$. Thus, by our remark above, $b_1 \neq 0$. Since ψ is even, $a_n = a_{-n}$ and so, in particular, by (158a)

$$-Ea_0 + \mu a_1 = 0$$

It follows that $a_0 \neq 0$ since if it were zero, a_1 would be zero, violating the remark above. Thus $a_0 b_1 \neq 0$ but $a_1 b_0 = 0$. This violates (159). We conclude that $H_0^{\mathrm{P}} + V$ has no degenerate eigenvalues.

There is another example in Problem 139 where one can obtain an asymptotic formula for $\ell_n = \alpha_{n+1} - \beta_n$ as $n \to \infty$, which proves that at least for large n (where $\ell_n \neq 0$), there are lots of gaps. There are also the following general results whose proofs can be found in the references in the Notes.

Theorem XIII.91 Let V be periodic of period 2π. Then:

(a) If no gaps are present, V is a constant.
(b) If precisely one gap occurs, then V is a Weierstrass elliptic function.
(c) If all the odd gaps are absent (i.e., if $H_0^{\mathrm{A}} + V$ has only degenerate eigenvalues), then V has period π. More generally, if, for fixed n, all gaps (β_k, α_{k+1}) are absent for $k \neq 2^n m$ $(m = 1, 2, \ldots)$, then V has period $2^{-n}(2\pi)$ and the converse relation is true.
(d) If only finitely many gaps are present, then V is real analytic as a function on $\mathbb{R}$.
(e) Topologize Y, the space of all C^∞ functions on $\mathbb{R}$ with period 2π, with the seminorms $\|f\|_n = \|D^n f\|_\infty$, $n = 0, 1, \ldots$. Then the set of potentials in V for which *all* gaps are nonzero is a dense G_δ set of Y. (See the discussion of "Baire almost every" in the notes to Section III.5.)

There are some general results about when two potentials V and W produce the same energy bands.

Theorem XIII.92 Let V and W be two potentials of period 2π so that $-d^2/dx^2 + V$ and $-d^2/dx^2 + W$, on $[0, 2\pi]$ with periodic boundary conditions, have the same eigenvalues. Then their energy bands are the same.

Proof We shall sketch the main ideas. Fuller details can be found in the reference in the notes. Let $D_V(E)$ and $D_W(E)$ be the respective discriminants. By the analysis used in the proof of Theorem XIII.89, it suffices to prove that the discriminants are equal. We claim that

$$|D_V(E)| + |D_W(E)| \leq C_1 \exp(C_2 |E|^{1/2}) \tag{160}$$

$$D_V(E)/2\cos(2\pi\sqrt{E}) \to 1 \quad \text{as} \quad E \to i\infty \tag{161}$$

$$D_W(E)/2\cos(2\pi\sqrt{E}) \to 1 \quad \text{as} \quad E \to i\infty \tag{162}$$

Deferring the proofs of (160)–(162), let us complete the proof that $D_V = D_W$. By (160) and the Hadamard factorization theorem of complex analysis,

$$2 - D_V(E) = C_V \prod_{j=1}^{\infty} (1 - E_j(V)^{-1}E)$$

$$2 - D_W(E) = C_W \prod_{j=1}^{\infty} (1 - E_j(W)^{-1}E)$$

where $E_j(V)$ are the zeros of $D_V(E) - 2$. By hypothesis, the zeros of $2 - D_V$ and $2 - D_W$ are the same. By (161) and (162), $(2 - D_V)/(2 - D_W) \to 1$ as $E \to i\infty$, so $D_V = D_W$.

(160)–(162) follow by a detailed analysis of the solutions $u_j(x, E)$. One shows that they solve integral equations, for example,

$$u_1(x, E) = \cos(x\sqrt{E}) + \frac{1}{\sqrt{E}} \int_0^x \sin((x - y)\sqrt{E})V(y)u_1(y, E)\, dy$$

By iterating these equations, one proves (160)–(162). ∎

At first sight, one might think that there are not many pairs V, W with $D_V = D_W$. Quite the contrary: In the Notes, the reader can find references for the following two theorems:

Theorem XIII.93 Let $V(x, t)$ solve the partial differential equation

$$\frac{\partial V}{\partial t} = 3V\frac{\partial V}{\partial x} - \frac{1}{2}\frac{\partial^3 V}{\partial x^3} \tag{163}$$

with $V(x, 0)$ periodic of period 2π. Then for each fixed t, $V(x, t)$ is periodic of period 2π and has energy bands independent of t.

Equation (163) is called the **Korteweg–de Vries equation.**

Theorem XIII.94 Topologize the C^∞ functions on $\mathbb{R}$ with period 2π by the seminorms $\|D^\alpha f\|_\infty$. Fix V and suppose that the spectrum of $-d^2/dx^2 + V$ has n gaps (n may be infinite). Then $\{W \mid D_V = D_W\}$ is homeomorphic to an n-dimensional torus.

In the one-dimensional case one can also say quite a lot about global analytic properties of $E_n(\theta)$.

Theorem XIII.95 (Kohn's theorem) Suppose that all the gaps in a one-dimensional problem are nonzero. Then the energy band functions $E_n(\theta)$ are the branches of a single multisheeted function that has no singularities other than square root branch points on the lines $\text{Im}\,\theta = m\pi$, $m = 0, \pm 1, \ldots$. Explicitly, there exist positive numbers $\alpha_1, \alpha_2, \ldots$ so that the Riemann surface of $E(\theta)$ can be described as follows. E is equal to $E_n(\theta)$ on the nth sheet which is cut in $\bigcup_m [(2m+1)\pi] \pm i(\alpha_n, \infty)$ and $\bigcup_m (2m\pi) \pm i(\alpha_{n-1}, \infty)$ for n odd; and $\bigcup_m [2m\pi] \pm i(\alpha_n, \infty)$ and $\bigcup_m [(2m+1)\pi] \pm i(\alpha_{n-1}, \infty)$ for n even. The nth and $(n+1)$th sheet are joined by crossing the cuts $2m\pi \pm i(\alpha_n, \infty)$ (n even) and $(2m+1)\pi \pm i(\alpha_n, \infty)$ (n odd); see Figure XIII.16.

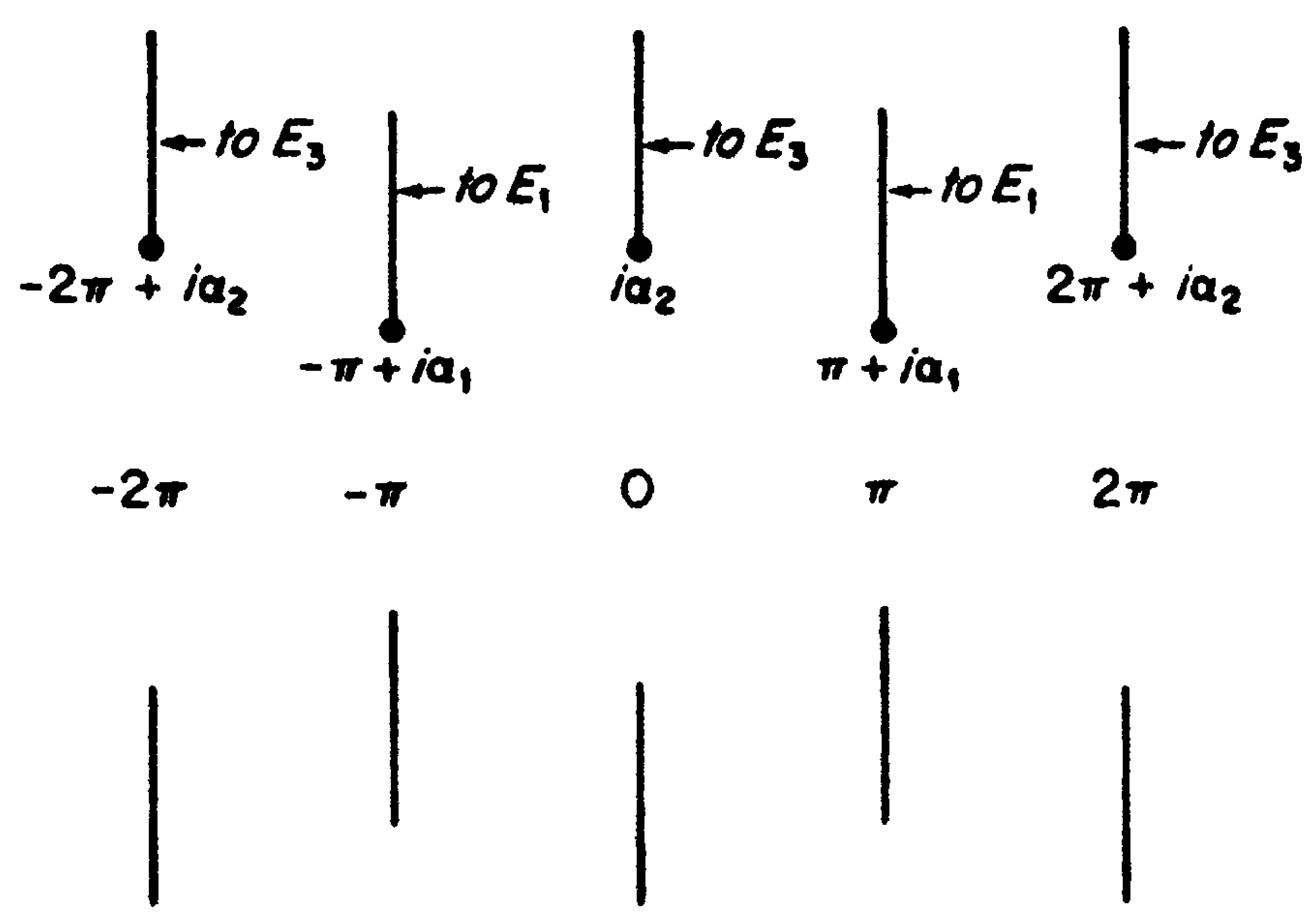


FIGURE XIII.16 The Riemann surfaces of an energy band; $n = 2$.

For a proof of this theorem, see the references in the Notes.

Now we turn to the general n-dimensional case. The direct integral decomposition in both the x-space and p-space versions will go through without significant change. The main difficulty will be in extending the analysis of the fibers of H (Theorem XIII.89). For that analysis depended critically on the simplicity of the eigenvalues of $H(\theta)$, which fails in the multidimensional case. An additional complication is that in the multivariable case, eigenvalues are not necessarily analytic (in a single-valued sense) at degeneracy points: See the example in the Notes to Section XII.1. It will turn out to be easier to analyze the fibers of the direct integral decomposition in the p-space version.

We want to allow for the possibility of local singularities in V in our discussion of the general n-dimensional case. The perturbation criteria, as stated in Section X.2, are not applicable if V is unbounded since such a periodic V cannot be in any $L^p + L^\infty$ with $p < \infty$; but if V is L^p over all bounded sets and periodic, then it will be uniformly locally L^p where:

Definition A measurable function V on $\mathbb{R}^n$ is called **uniformly locally L^p** if and only if

$$\int_C |V(x)|^p \, d^n x \le A$$

for any unit cube C and some C-independent constant A.

The perturbation theory of Section X.2 extends to uniformly locally L^p perturbations (for suitable p) by the following localization method.

Theorem XIII.96 Let $p = 2$ if $n \le 3$, $p > 2$ if $n = 4$ and $p > n/2$ if $n \ge 5$. Then any real-valued function on $\mathbb{R}^n$ that is uniformly locally L^p is a $-\Delta$-bounded operator with relative bound zero.

Proof Let q be such that $p^{-1} + q^{-1} = \frac{1}{2}$. We proved in Section X.2 that for any ε, there is an A_ε so that

$$\|\varphi\|_q^2 \le \varepsilon \|\Delta\varphi\|_2^2 + A_\varepsilon \|\varphi\|_2^2 \tag{164}$$

For any cube C, let

$$\|\varphi\|_{r;C}^r \equiv \int_C |\varphi(x)|^r \, d^n x$$

Let C be a unit cube and let C' be the cube with side 3 and the same center as C. Let η be a C^∞ function with support in C' that is identically 1 on C. Now, by (164),

$$\begin{aligned} \|\varphi\|_{q,C}^2 &\le \|\eta\varphi\|_q^2 \\ &\le \varepsilon \|\Delta(\eta\varphi)\|_2^2 + A_\varepsilon \|\eta\varphi\|_2^2 \\ &\le 3\varepsilon \|\Delta\varphi\|_{2;C'}^2 + B\|\nabla\varphi\|_{2;C'}^2 + D\|\varphi\|_{2;C'}^2 \end{aligned} \tag{165}$$

where we have used $\Delta(\eta\varphi) = \varphi \, \Delta\eta + \eta \, \Delta\varphi + 2 \, \nabla\eta \cdot \nabla\varphi$, the triangle inequality, the fact that $(a + b + c)^2 \le 3(a^2 + b^2 + c^2)$, and the fact that η, $\nabla\eta$, and $\Delta\eta$ are bounded functions with support in C'. Notice that since the various $\|D^\alpha\eta\|_\infty$ can be chosen independently of C, (165) holds with constants that are independent of C. For $\alpha \in \mathbb{Z}^n$, let C_α be the unit cube with center α and C'_α the corresponding C'. Then, since V is uniformly locally L^p,

$$|||V|||^2 \equiv \sup_\alpha \|V\|_{p,C_\alpha}^2 < \infty$$

Thus,

$$\begin{aligned}
\|V\varphi\|_2^2 &= \sum_\alpha \|V\varphi\|_{2;C_\alpha}^2 \\
&\le \sum_\alpha \|V\|_{p;C_\alpha}^2 \|\varphi\|_{q;C_\alpha}^2 \\
&\le |||V|||^2 \sum_\alpha (3\varepsilon\|\Delta\varphi\|_{2;C_{\alpha'}}^2 + B\|\nabla\varphi\|_{2;C_{\alpha'}}^2 + D\|\varphi\|_{2;C_{\alpha'}}^2) \\
&= |||V|||^2 3^n(3\varepsilon\|\Delta\varphi\|_2^2 + B\|\nabla\varphi\|_2^2 + D\|\varphi\|_2^2) \\
&\le |||V|||^2 3^n(4\varepsilon\|\Delta\varphi\|_2^2 + (D + \tfrac{1}{4}\varepsilon^{-1}B)\|\varphi\|_2^2)
\end{aligned}$$

In the next to the last step, we have used the fact that each $x \in \mathbb{R}^n$ not on the boundary of some C_α lies in precisely 3^n of the C'_α. Then, in the last step we used,

$$\|\nabla\varphi\|_2^2 \le \delta\|\Delta\varphi\|_2^2 + \tfrac{1}{4}\delta^{-1}\|\varphi\|_2^2$$

which via the Plancherel theorem follows by the numerical inequality $a \le \delta a^2 + \frac{1}{4}\delta^{-1}$. ∎

Notice that if V is uniformly locally L^p for some $p > n/2$ then it is automatically uniformly locally $L^{n/2}$ so we stated $p = n/2$ rather than $p \ge n/2$ in the above theorem.

Given the above criterion, the following theorem has a proof that differs only in notation from the corresponding one-dimensional result (Theorem XIII.88).

Theorem XIII.97 Let $\mathbf{a}_1, \ldots, \mathbf{a}_n$ be n independent vectors in $\mathbb{R}^n$. Let V be a real-valued function on $\mathbb{R}^n$ obeying:

(i) $V(\mathbf{x} + \mathbf{a}_i) = V(\mathbf{x})$, $i = 1, \ldots, n$.
(ii) $\int_Q |V(\mathbf{x})|^p \, d^n x < \infty$ where Q is a **basic period cell**

$$Q = \left\{\mathbf{x} \,\middle|\, \mathbf{x} = \sum_{i=1}^n t_i \mathbf{a}_i;\ 0 \le t_i < 1\right\}$$

and $p = 2$ if $n \le 3$, $p > 2$ if $n = 4$; $p = n/2$ if $n \ge 5$.

For each $\boldsymbol{\theta} \in [0, 2\pi)^n$, let $H^{(0)}(\boldsymbol{\theta})$ be the operator $-\Delta$ on $L^2(Q, d^n x) \equiv \mathscr{H}$ with the boundary conditions

$$\varphi(\mathbf{x} + \mathbf{a}_j) = e^{i\theta_j}\varphi(\mathbf{x}), \qquad \frac{\partial\varphi}{\partial y_j}(\mathbf{x} + \mathbf{a}_j) = e^{i\theta_j}\frac{\partial\varphi}{\partial y_j}(\mathbf{x}) \tag{166}$$

for all x with $\mathbf{x}, \mathbf{x} + \mathbf{a}_j \in \bar{Q}$ (i.e., for x on suitable faces of ∂Q where y_j is the coordinate given by $\mathbf{x} = \sum y_i \mathbf{a}_i$. Let

$$\mathscr{H} = \int_{[0, 2\pi)^n}^{\oplus} \mathscr{H}' \frac{d^n\theta}{(2\pi)^n}$$

and let $U: L^2(\mathbb{R}^n, d^n x) \to \mathscr{H}$ by defining U on $\mathscr{S}$ by

$$(Uf)_{\boldsymbol{\theta}}(\mathbf{x}) = \sum_{m \in Z^n} e^{-i\boldsymbol{\theta} \cdot \mathbf{m}} f(\mathbf{x} + \sum m_i \mathbf{a}_i)$$

and extended as a unitary operator to L^2.

Then:

(a) For almost all $\boldsymbol{\theta} \in [0, 2\pi)^n$, V is an $H^{(0)}(\boldsymbol{\theta})$-bounded multiplication operator on $L^2(Q, d^n x)$ with relative bound zero.

(b) $U(-\Delta + V)U^{-1} = \int_{[0, 2\pi)^n}^{\oplus} H(\boldsymbol{\theta})\, d^n\theta/(2\pi)^n$ where $H(\boldsymbol{\theta}) = H^{(0)}(\boldsymbol{\theta}) + V$.

We remark that it is possible to prove that V is everywhere, and not just almost everywhere, $H^{(0)}(\boldsymbol{\theta})$-bounded with relative bound zero. This follows, for example, from analyticity arguments.

One consequence of this theorem is the existence of an eigenfunction expansion for H in the sense of Section XI.6:

Theorem XIII.98 Each $H(\boldsymbol{\theta})$ has a complete set of eigenfunctions $\psi_m(\boldsymbol{\theta}; x)$ with eigenvalues $E_m(\boldsymbol{\theta})$. Extend $\psi_m(\boldsymbol{\theta}; x)$ to all of $\mathbb{R}^n$ by using the boundary condition (166). For $\varphi \in \mathscr{S}(\mathbb{R}^n)$, let

$$\tilde{\varphi}(m; \boldsymbol{\theta}) = \int_{\mathbb{R}^n} \overline{\psi_m(\boldsymbol{\theta}; x)}\, \varphi(x)\, d^n x$$

Then:

(a)
$$\int_{\mathbb{R}^n} |\varphi(x)|^2\, d^n x = \sum_m \int_{[0, 2\pi)^n} |\tilde{\varphi}(m; \boldsymbol{\theta})|^2 \frac{d^n\theta}{(2\pi)^n}$$

(b)
$$\varphi(x) = \frac{1}{(2\pi)^n} \sum_m \int_{[0, 2\pi)^n} \tilde{\varphi}(m; \boldsymbol{\theta}) \psi_m(\boldsymbol{\theta}; x)\, d^n\theta$$

(c) Extend $\tilde{}$ to $L^2(\mathbb{R}^n)$ by continuity. Then $H = -\Delta + V$ obeys

$$\widetilde{H\varphi}(m; \boldsymbol{\theta}) = E_m(\boldsymbol{\theta}) \tilde{\varphi}(m; \boldsymbol{\theta})$$

for all $\varphi \in D(H)$.

(d) $\tilde{}$ maps $L^2(\mathbb{R}^n, d^n x)$ *onto* $\bigoplus_m L^2([0, 2\pi)^n, d^n\theta)$.

Proof It is possible to find a complete set of eigenvectors for $H^{(0)}(\boldsymbol{\theta})$ explicitly; namely,

$$\psi_{\mathbf{k}}^{(0)}(\boldsymbol{\theta}; x) = (2\pi)^{-n/2} \exp\left[i \sum_{j=1}^{n} (\theta_j + 2\pi k_j) y_j\right]$$

for $k_j \in \mathbb{Z}^n$, where y_j is defined by $\mathbf{x} = \sum_{i=1}^{n} y_i \mathbf{a}_i$. The corresponding eigenvalues tend toward infinity as $|\mathbf{k}| \to \infty$ so $H^{(0)}(\boldsymbol{\theta})$ has compact resolvent. It follows that $H(\boldsymbol{\theta})$ has compact resolvent by Theorem XIII.68. Thus it has discrete eigenvalues $\{E_m(\boldsymbol{\theta})\}_{m=1}^{\infty}$ and a corresponding complete set of eigenfunctions. By the min–max principle, one can prove that the functions $E_m(\boldsymbol{\theta})$ are measurable and that the corresponding eigenfunctions can be chosen measurably (Problem 140). Since, for $\boldsymbol{\theta}$ fixed, the $\psi_m(\boldsymbol{\theta})$ are an orthonormal basis in $\mathscr{H}'$ of eigenfunctions for $H(\boldsymbol{\theta})$, we have for $\eta \in \mathscr{H} = \int_{[0,2\pi)^n}^{\oplus} \mathscr{H}' \, d^n\theta/(2\pi)^n$,

$$(\eta, \eta)_{\mathscr{H}} = \sum_m \int |(\eta_{\boldsymbol{\theta}}, \psi_m(\boldsymbol{\theta}))_{\mathscr{H}'}|^2 \frac{d^n\theta}{(2\pi)^n}$$

$$\eta_{\boldsymbol{\theta}} = \sum_m (\psi_m(\boldsymbol{\theta}), \eta_{\boldsymbol{\theta}})_{\mathscr{H}'} \psi_m(\boldsymbol{\theta})$$

$$(\psi_m(\boldsymbol{\theta}), (A\eta)_{\boldsymbol{\theta}}) = E_m(\boldsymbol{\theta})(\psi_m(\boldsymbol{\theta}), \eta_{\boldsymbol{\theta}})$$

where

$$A = \int_{[0,2\pi)^n}^{\oplus} H(\boldsymbol{\theta}) \frac{d^n\theta}{(2\pi)^n}$$

(a)–(c) now follow using the definition of U and the way we have extended $\psi_m(\boldsymbol{\theta})$. (d) has a similar proof. ▮

To give the p-space analysis, we need a definition that differs by a factor of 2π from the more common one.

Definition Let $\mathbf{a}_1, \ldots, \mathbf{a}_n$ be a basis for $\mathbb{R}^n$. The **dual basis** $\mathbf{K}_1, \ldots, \mathbf{K}_n$ is defined by

$$(\mathbf{K}_i, \mathbf{a}_j) = (2\pi)\delta_{ij}$$

Theorem XIII.99 Let V be a function on $\mathbb{R}^n$ with $V(\mathbf{x} + \mathbf{a}_j) = V(\mathbf{x})$ $(j = 1, \ldots, n)$ where $\{\mathbf{a}_j\}_{j=1}^{n}$ is a basis for $\mathbb{R}^n$. Let Q be the basic period cell for the basis $\{\mathbf{a}_i\}$ and let $\tilde{Q}$ be the basic period cell for the dual basis $\{\mathbf{K}_i\}$, i.e.,

$$\tilde{Q} = \left\{ \sum_{i=1}^{n} t_i \mathbf{K}_i \,\middle|\, 0 \le t_i < 1 \right\}$$

Let $\mathscr{H}' = \ell_2(\mathbb{Z}^n)$ and $\mathscr{H} = \int_{\tilde{Q}}^{\oplus} \mathscr{H}' \, d^n k$. Suppose that V is uniformly locally L^p (with $p = 2$ if $n \le 3$, $p > 2$ if $n = 4$, $p = n/2$ if $n \ge 5$) and let $\tilde{V}_{\mathbf{m}}$ be the Fourier coefficients for V as a function on Q; i.e., for $\mathbf{m} \in \mathbb{Z}^n$,

$$\tilde{V}_{\mathbf{m}} = (\text{vol } Q)^{-1} \int_Q \exp\left(-i \sum_{j=1}^{n} m_j \mathbf{K}_j \cdot \mathbf{x}\right) V(\mathbf{x}) \, d^n x \tag{167}$$

For $\mathbf{k} \in \tilde{Q}$, define the operator $H(\mathbf{k})$ on $\mathscr{H}'$ by

$$(H(\mathbf{k})g)_{\mathbf{m}} = (\mathbf{k} + \sum m_j \mathbf{K}_j)^2 g_{\mathbf{m}} + \sum_{\alpha \in \mathbb{Z}^n} \tilde{V}_\alpha g_{\mathbf{m}-\alpha} \tag{168}$$

with domain

$$D_0 = \{g \in \mathscr{H}' \mid \sum \mathbf{m}^2 |g_{\mathbf{m}}|^2 < \infty\}$$

Finally, let $U: L^2(\mathbb{R}^n) \to \mathscr{H}$ by

$$[(Uf)(\mathbf{k})]_{\mathbf{m}} = \hat{f}(\mathbf{k} + \sum m_j \mathbf{K}_j)$$

Then U is unitary and

$$U(-\Delta + V)U^{-1} = \int_{\tilde{Q}}^{\oplus} H(\mathbf{k}) \, d^n k$$

Proof That U is unitary is just the Plancherel theorem. Moreover, it is clear that

$$[(U(-\Delta)U^{-1})g](\mathbf{k})_{\mathbf{m}} = (\mathbf{k} + \sum m_j \mathbf{K}_j)^2 g(\mathbf{k})_{\mathbf{m}}$$

since $-\widehat{\Delta f}(\ell) = \ell^2 \hat{f}(\ell)$. Because V is $-\Delta$-bounded with relative bound zero, we need only prove that

$$[(UVU^{-1}g)(\mathbf{k})]_{\mathbf{m}} = \sum_{\alpha \in \mathbb{Z}^n} V_\alpha g_{\mathbf{m}-\alpha}(\mathbf{k})$$

and this follows if we prove that, for $f \in \mathscr{S}(\mathbb{R}^n)$,

$$\widehat{Vf}(k) = \sum_{\alpha \in \mathbb{Z}^n} \tilde{V}_\alpha \hat{f}\left(\mathbf{k} - \sum_{j=1}^{n} \alpha_j \mathbf{K}_j\right) \tag{169}$$

To prove (169) we need only show that, as a tempered distribution, V has the Fourier transform

$$\hat{V}(\mathbf{k}) = (2\pi)^{n/2} \sum_{\alpha \in \mathbb{Z}^n} \tilde{V}_\alpha \, \delta\left(\mathbf{k} - \sum_{j=1}^{n} \alpha_j \mathbf{K}_j\right)$$

As in the one-dimensional case, this is true because the Fourier series

$$V(\mathbf{x}) = \sum_{\alpha \in \mathbb{Z}^n} \tilde{V}_\alpha \exp\left(i \sum_{j=1}^{n} \alpha_j \mathbf{K}_j \cdot \mathbf{x}\right)$$

is locally L^2 convergent since V is locally uniformly L^2. ∎

One advantage of the k-space decomposition in the form we have presented it is that the operators $H(\mathbf{k})$ have a fixed domain D_0. In fact, we can use (168) to define $H(\mathbf{k})$ for any $\mathbf{k} \in \mathbb{C}^n$ and $H(\mathbf{k})$ so defined is an entire analytic family of type (A). The easiest way of seeing this is to let

$$(\mathbf{P}g)_{\mathbf{m}} = \left(\sum_{j=1}^{n} m_j \mathbf{K}_j\right) g_{\mathbf{m}}$$

so that $\mathbf{P}$ is $H(\mathbf{0})$-bounded with relative bound zero and

$$H(\mathbf{k}) = H(\mathbf{0}) + 2\mathbf{k} \cdot \mathbf{P} + \sum_{j=1}^{n} k_j^2 \tag{170}$$

$H(\mathbf{k})$ depends on n parameters; but it is useful to fix $n-1$ of them for two reasons. First, we avoid the nonanalyticity that can occur in real multiparameter eigenvalue variations. The second reason is more subtle. Let $\mathbf{a}$ and $\mathbf{b}$ be fixed vectors in $\mathbb{R}^n$. Let $z = \lambda + iy$ and define

$$E_{\mathbf{m}}(z) = (\mathbf{a} + z\mathbf{b} + \sum m_j \mathbf{K}_j)^2$$

Of course $H(\mathbf{k}) = H_0(\mathbf{k}) + V$ where $H_0(\mathbf{a} + z\mathbf{b})$ has a complete orthogonal set of eigenvectors with eigenvalues $E_{\mathbf{m}}(z)$. Now

$$\operatorname{Im} E_{\mathbf{m}}(z) = 2y[\mathbf{b} \cdot (\mathbf{a} + \lambda\mathbf{b} + \sum m_j \mathbf{K}_j)]$$

is especially simple if the numbers $\mathbf{b} \cdot \mathbf{K}_j$ are rationally dependent for in that case the number in square brackets will not get arbitrarily small as $\mathbf{m}$ varies. It is thus convenient to pick $\mathbf{b}$ as the first vector in the x-space lattice, i.e.,

$$\mathbf{b} \cdot \mathbf{K}_j = 2\pi\delta_{j1} \tag{171}$$

and λ by

$$\mathbf{b} \cdot (\mathbf{a} + \lambda\mathbf{b}) = \pi \tag{172}$$

In that case, $\operatorname{Im} E_{\mathbf{m}}(z) = 2\pi y(2m_1 + 1)$, so

$$|\operatorname{Im} E_{\mathbf{m}}(z)| \geq \pi|y|(1 + |m_1|) \tag{173a}$$

Moreover, it is easy to see that (Problem 141a)

$$|\operatorname{Re}(E_{\mathbf{m}}(z) + 1)| \geq c_1|\mathbf{m}|^2 \qquad \text{if} \quad |\mathbf{m}| \geq c_2(1 + |y|) \tag{173b}$$

for suitable c_1 and c_2 (which will depend on $\mathbf{a}$ through the choice of λ in (172)). From (173), one deduces that (Problem 141):

Lemma 1 Let $n \geq 2$. Let $\mathbf{b}$ be given by (171) and λ by (172). Then

(a) If $\alpha > \frac{1}{2}n$ and $\alpha \geq n - 1$,

$$f_\alpha(y) \equiv \sum_{\mathbf{m}} |E_{\mathbf{m}}(\lambda + iy) + 1|^{-\alpha}$$

is convergent and bounded for $|y| \geq 1$.

(b) If moreover $\alpha > n - 1$, then $\lim_{y \to \pm\infty} f_\alpha(y) = 0$.

The point of Lemma 1 is that it will allow us to control $\|V(H_0(\lambda + iy) + 1)^{-1}\|$ as $y \to \infty$ for suitable V's.

Lemma 2 Let $n \geq 2$. Let V be a periodic potential whose Fourier coefficients (167) obey

$$\sum_{\mathbf{m}} |\tilde{V}_{\mathbf{m}}|^\beta < \infty \tag{174}$$

where $\beta < (n-1)/(n-2)$ if $n \geq 3$ and $\beta = 2$ if $n = 2$. Fix $\mathbf{a} \in \mathbb{R}^n$ and let $\mathbf{b}$ obey (171). Let

$$A(t) = H(\mathbf{a} + \mathbf{b}t)$$

for $t \in \mathbb{R}$. Then:

(a) Each $A(t)$ has compact resolvent.

(b) There are real analytic functions $\{E_j(t)\}$ and corresponding analytic vector-valued functions $\psi_j(t)$ so that $\psi_j(t)$ is a basis for $\mathscr{H}' = \ell^2(\mathbb{Z}^n)$ and, for each t,

$$A(t)\psi(t) = E_j(t)\psi_j(t)$$

(c) No $E_j(t)$ is constant.

Proof (a) Since $\beta \leq 2$, (174) and the Hausdorff–Young inequality imply that V is in $L^\alpha(Q)$ where $\alpha < n - 1$ if $n \geq 3$ and $\alpha = 2$ if $n = 2$. Thus V is $H_0(\mathbf{k})$ relatively bounded so it suffices to prove that $H_0(\mathbf{k})$ has compact resolvent. This follows from the fact that $H_0(\mathbf{k})$ has a complete set of eigenvectors with eigenvalues going to infinity.

(b) Let $E_j(0)$ be the eigenvalues of $A(t = 0)$, ordered so that $E_1(0) \leq E_2(0) \leq \cdots$. Now, we can continue the eigenvalues and eigenvectors using, if necessary, degenerate perturbation theory. As in the one-dimensional case, we need only show that $E_j(t)$ does not go to infinity at some finite t to conclude that a continuation is possible for all t. By (170)

$$\frac{dA(t)}{dt} = 2(\mathbf{b} \cdot \mathbf{P} + \mathbf{b} \cdot (\mathbf{a} + t\mathbf{b}))$$

so, by first-order perturbation theory, and the fact that $\mathbf{P}$ is $H_0(\mathbf{k})$-bounded,

$$\left|\frac{dE_j(t)}{dt}\right| \le c(|E_j(t)| + |t| + 1)$$

from which it follows that $E_j(t)$ cannot blow up at finite *real* t.

(c) By Lemma 1, the hypothesis on V, Hölder's inequality and Young's inequality,

$$\lim_{y\to\infty} \|(A_0(\lambda + iy) + 1)^{-1}\| = 0$$

$$\lim_{y\to\infty} \|V[A_0(\lambda + iy) + 1]^{-1}\| = 0$$

where λ is chosen so that (172) holds. From these results and standard perturbation arguments we see that for $|y| \ge Y_0$, $(A(\lambda + iy) + 1)^{-1}$ exists and

$$\lim_{y\to\infty} \|[A(\lambda + iy) + 1]^{-1}\| = 0 \tag{175}$$

Now suppose that some $E_j(t)$ is a constant C for all t. Since $A(t)$ has compact resolvent for all real t, it has a compact resolvent for all $t \in \mathbb{C}$ so that C is always an eigenvalue of $A(t)$. It follows that $(C + 1)^{-1}$ is always an eigenvalue of $(A(t) + 1)^{-1}$ so that

$$\|(A(t) + 1)^{-1}\| \ge (C + 1)^{-1}$$

This violates (175), so no $E_j(t)$ can be constant. ▮

We are now able to give a complete analysis of the spectral properties of Schrödinger operators with periodic potentials:

Theorem XIII.100 Let V be a periodic potential whose Fourier *series* coefficients are in ℓ_β where $\beta < (n-1)/(n-2)$ if $n \ge 3$, $\beta = 2$ if $n = 2, 3$. Then $-\Delta + V$ has purely absolutely continuous spectrum.

Proof $\mathbf{b}, \mathbf{K}_2, \ldots, \mathbf{K}_n$ form a basis for $\mathbb{R}^n$, so we can write the interior of $\tilde{Q}$ in terms of a decomposition $\mathbf{k} = s_1\mathbf{b} + \cdots + s_n\mathbf{K}_n$ as $\{\langle s_1, s_\perp\rangle | s_1 \in M(s_\perp), s_\perp \in N\}$ where for every $s_\perp \in N$, $M(s_\perp)$ is an open connected set (Figure XIII.17). We can write

$$H = \int_{s_\perp \in N} \int_{s_1 \in M(s_\perp)} H(s_1\mathbf{b} + \cdots + s_n\mathbf{K}_n)\, ds_1\, d^{n-1}s$$

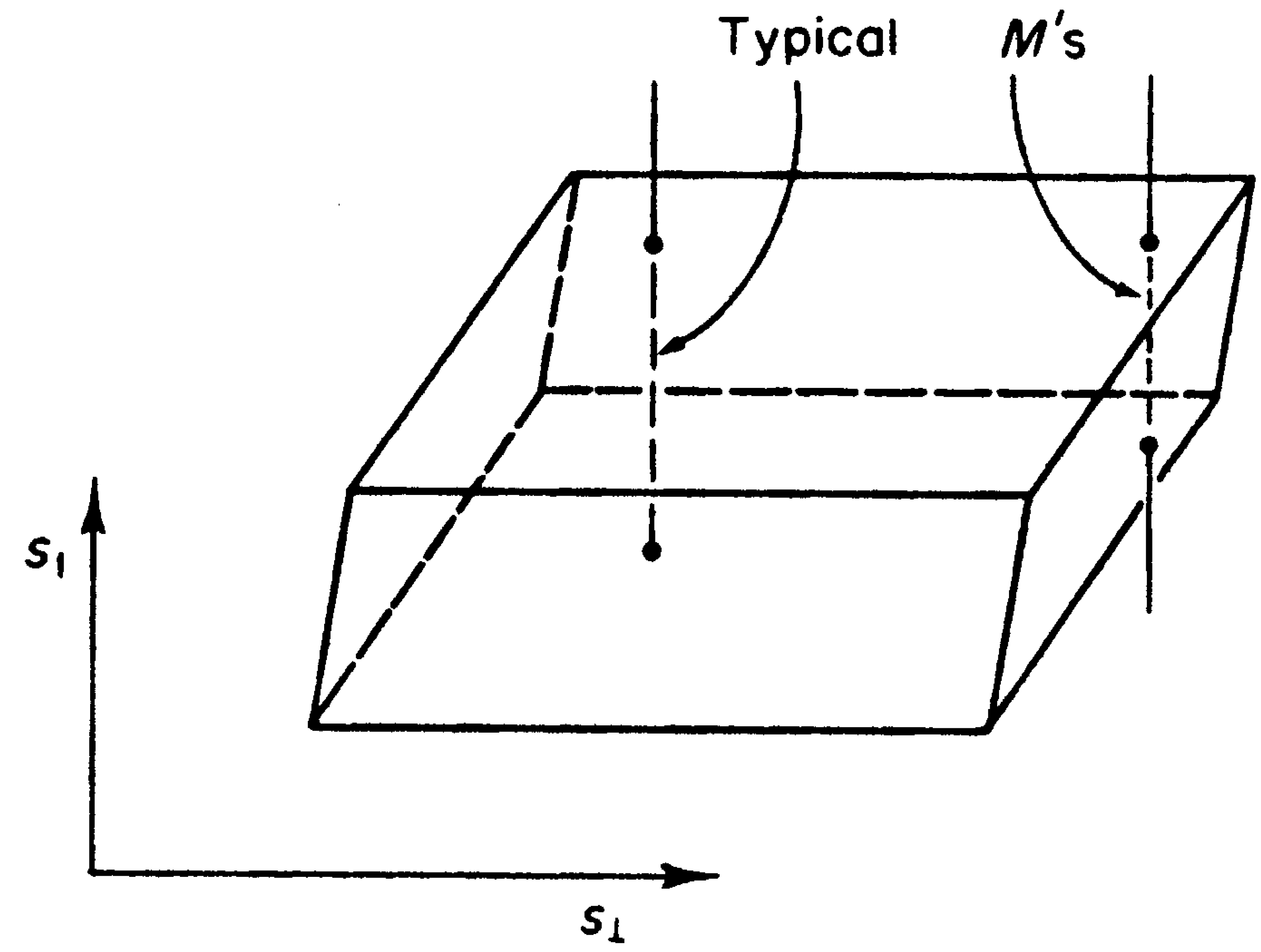


FIGURE XIII.17 The s decomposition of $\tilde{Q}$.

in a suitable direct integral decomposition. By Lemma 2 and Theorem XIII.86, the s_1 direct integral has purely absolutely continuous spectrum for each $s_\perp \in N$ and thus, by Theorem XIII.85f, H has purely absolutely continuous spectrum. ▮

We note that as in the one-dimensional case, the spectrum of H breaks up into "bands," but there are two big differences. First, due to degeneracy there may be some ambiguity in definition at singularities in the many-variable functions. Secondly, bands can "overlap" unlike the one-dimensional case.

Before discussing some of the connections between the ideas above and a simple model of solid state physics, we want to mention an arbitrariness in choice of $\mathbf{a}_1, \ldots, \mathbf{a}_n$. Given V, what is determined without any choice is

$$\mathscr{L}_V = \{\mathbf{a} \mid V(\mathbf{x} + \mathbf{a}) = V(\mathbf{x}), \text{ a.e. in } \mathbf{x}\}$$

For periodic potentials, $\mathscr{L}_V$ is always a lattice where:

Definition A **lattice** is a subset $\mathscr{L}$ of $\mathbb{R}^n$ obeying:

(i) $\mathscr{L}$ is discrete, i.e., it has no finite limit points.
(ii) $\mathscr{L}$ is a subgroup of the additive group of $\mathbb{R}^n$.
(iii) No proper vector subspace of $\mathbb{R}^n$ contains $\mathscr{L}$.

Any such $\mathscr{L}$ has a **basis**, i.e., a set $\mathbf{a}_1, \ldots, \mathbf{a}_n \in \mathscr{L}$, so that any $\mathbf{a} \in \mathscr{L}$ is uniquely of the form $\mathbf{a} = \sum_{i=1}^n m_i \mathbf{a}_i$ with $m_i \in \mathbb{Z}$. Such bases are not unique and the corresponding basic period cell Q is not unique; for example, see Figure XIII.18. What all basic cells have in common is the property that $\mathbb{R}^n = \bigcup_{\mathbf{a} \in \mathscr{L}} \overline{\tau_\mathbf{a} Q}$, where $\tau_\mathbf{a} S = \{\mathbf{x} + \mathbf{a} \mid \mathbf{x} \in S\}$, with $\tau_\mathbf{a} Q^{\text{int}} \cap \tau_\mathbf{b} Q^{\text{int}} = \emptyset$, if

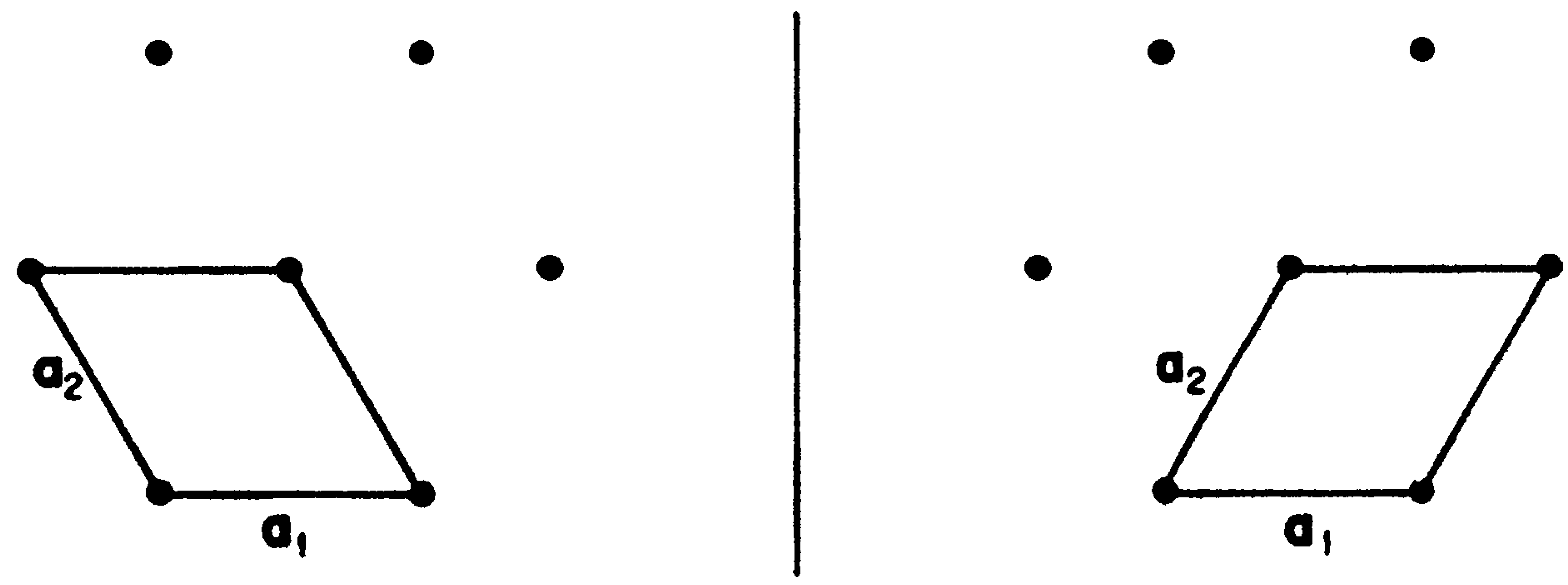


FIGURE XIII.18 Two choices of basis and basic cell.

$\mathbf{a} \neq \mathbf{b}$. There is another "basic cell," C with this property, although it is not associated to any basis. This is the **Wigner–Seitz cell for** $\mathscr{L}$ defined by

$$C = \{x \in \mathbb{R}^n \mid x \text{ is closer to 0 than any other point of } \mathscr{L}\}$$

Two examples of Wigner–Seitz cells are shown in Figure XIII.19. One can

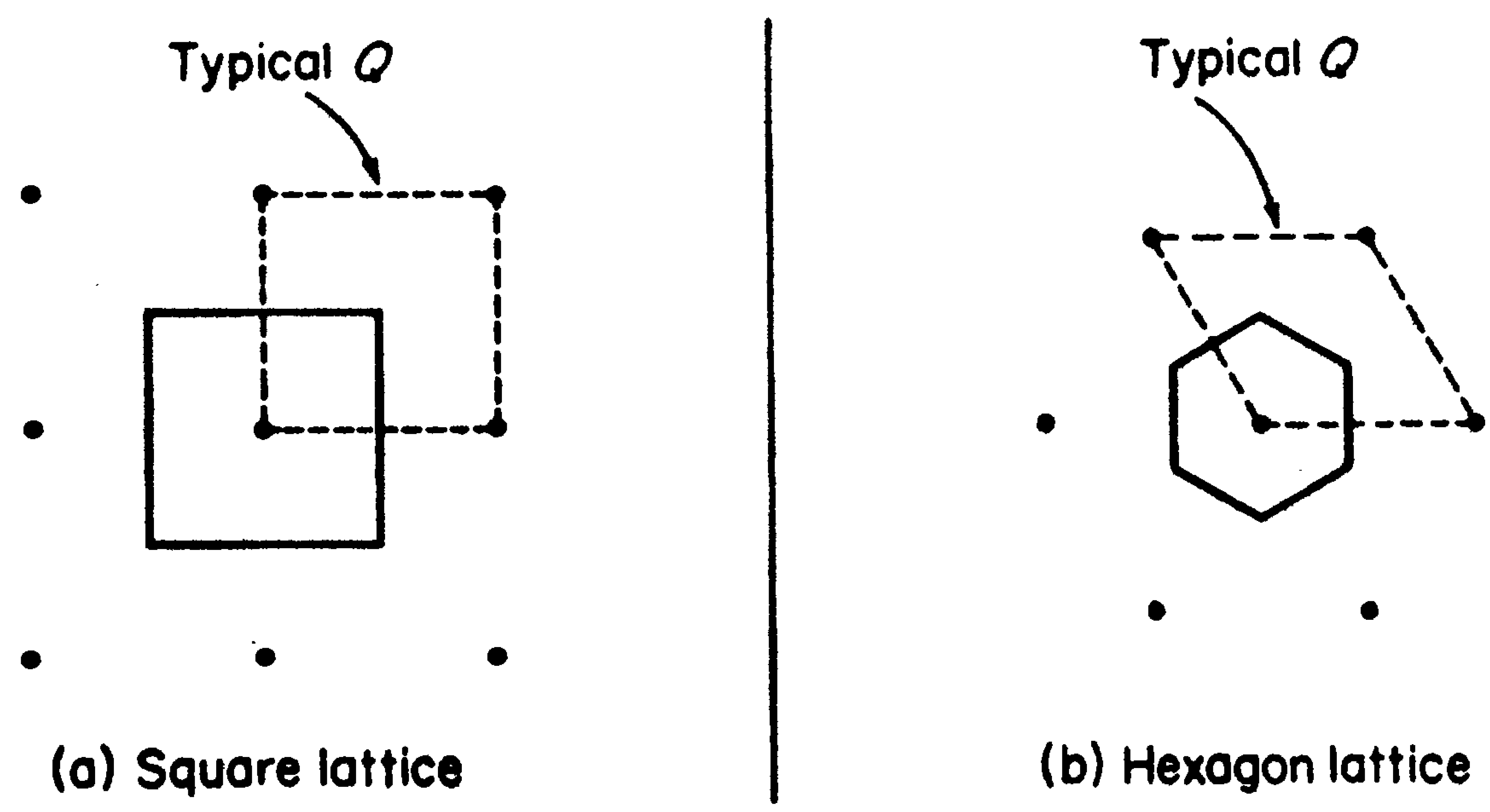


FIGURE XIII.19 Two Wigner–Seitz cells.

show (Problem 143) that any Wigner–Seitz cell is a polyhedron, i.e., the intersection of finitely many slabs $\{x \mid a \leq \ell(x) \leq b\}$, ℓ a linear functional. The Wigner–Seitz cell is unique.

Similarly, the dual basis depends on the choice of basis for $\mathscr{L}_V$; but the dual lattice $\mathscr{L}'_V = \{\mathbf{k} \in \mathbb{R}^n \mid \mathbf{k} \cdot \mathbf{a} \in 2\pi\mathbb{Z} \text{ for all } \mathbf{a} \in \mathscr{L}\}$ and its Wigner–Seitz cell, called the **Brillouin zone** B, are independent of the basis chosen.

We mention the above terminology for the following reason. One can make an x-space direct integral decomposition with Q replaced by C and a p-space decomposition with $\tilde{Q}$ replaced by B. The study of solids in the physics literature usually begins with a construction that is a disguised form of the p-space direct integral decomposition over the Brillouin zone.

We now turn to applications of our analysis to solid state physics. To the mathematical physicist who is used to looking at atomic physics or even quantum field theory, the bewildering array of approximations known as solid state theory often appears to be more an art than a science. While there is some truth in this attitude, we would like to emphasize that the difference between atomic physics and solid state physics is really one of degree, for the "standard" purely Coulomb atomic Hamiltonian is an approximation to "real" atoms. In the first place, relativistic corrections to the kinetic energy are not included nor is spin–orbit coupling. In addition, experiments on atoms are not done with isolated atoms but with aggregates, so it is an approximation to discuss a simple atomic model and then compare it with experiment. Finally, there are the couplings to the radiation field (quantum electrodynamics) which are certainly not understood at a fundamental level. The big difference between atomic and solid state physics is that in atomic physics one model describes the most basic physical phenomena, while in solid state physics the model as described below explains qualitatively only a limited range of phenomena. Many phenomena require one to take into account lattice vibrations ("phonons") and interactions between electrons and of the electrons with the phonons. In the end, the mathematical physicist is presented with a well-defined model (or several well-defined models) to study and this is all that he or she can reasonably demand.

It is an observed phenomenon that the nuclei in a solid lie more or less in regular arrays (crystals), i.e., there is a lattice in $\mathbb{R}^n$ so that the nuclei more or less lie at the lattice points. No one has given an explanation from first principles of why crystals form; i.e., no one has proven that a large number of heavy nuclei with enough electrons to produce neutrality, interacting via Coulomb potentials, have a ground state that is approximately a crystal. We thus postulate in our model that there is a *fixed* nucleus with a number of core electrons at each site of a lattice. To obtain simplicity we replace a large solid by one filling all of $\mathbb{R}^n$. Thus if we ignore electron–electron interactions, we have electrons moving under a Hamiltonian $-\Delta + V$ with V periodic. This model is known as the **one-electron model of solids**. We want to use our analysis of periodic Schrödinger operators to describe two things:

(1) the notion of density of states and the qualitative explanation of the difference between metals and insulators;
(2) impurity scattering in the one electron model.

For simplicity of notation we suppose that space is three dimensional.

Definition Let $\tilde{Q}$ be a basic period cell in the dual lattice and let $E_n(\mathbf{k})$ be the energy levels of $H(\mathbf{k})$ (ordered by $E_1 \le E_2 \le \cdots$). The **density of states measure** ρ is the measure on $\mathbb{R}$ defined by

$$\rho(-\infty, E] = \frac{2}{|\tilde{Q}|} \sum_n \left| \{\mathbf{k} \in \tilde{Q} \,|\, E_n(\mathbf{k}) \le E\} \right| \tag{176}$$

where $|\tilde{Q}|$ is the Lebesgue measure of $\tilde{Q}$ and $|\{\cdots\}|$ is the Lebesgue measure of $\{\cdots\}$.

We note that since $E_n(\mathbf{k}) \to \infty$ uniformly in $\mathbf{k}$ as $n \to \infty$ (Problem 144), the number $\rho(-\infty, E]$ is finite. Moreover, one can show easily (Problem 145) from our general analysis that ρ is absolutely continuous with respect to dE, Lebesgue measure on $\mathbb{R}$. The Radon–Nikodym derivative $d\rho/dE$ is usually called the **density of states**. To explain the importance of ρ to an analysis of solids, we introduce another notion. Let Q be the basic x-space cell and, given $m \in \mathbb{Z}$, let $Q^{(m)}$ be the set of volume $m^3|Q|$ obtained by stacking up an $m \times m \times m$ set of Q's. Let H_m be the operator $-\Delta_{\mathrm{P}} + V$ on $L^2(Q^{(m)})$ where $-\Delta_{\mathrm{P}}$ denotes periodic boundary conditions. Let $P_m(\Omega)$ be the spectral projections for H_m and define

$$\rho_m(-\infty, E] = 2 \dim P_m(-\infty, E]/m^3$$

Then:

Theorem XIII.101 As $m \to \infty$, $\rho_m \to \rho$ in the sense that $\rho_m(-\infty, E] \to \rho(-\infty, E]$ for every E.

Proof We sketch the main ideas, leaving the details to the reader (Problem 147). The key point is that H_m has a direct *sum* decomposition described as follows. Parametrize $\tilde{Q}$ as $\{\sum_{i=1}^{3} t_i \mathbf{K}_i \,|\, 0 \le t_i < 1\}$. Then

$$L^2(Q^{(m)}) \cong \bigoplus_{\alpha_1, \alpha_2, \alpha_3 = 0}^{m-1} \ell^2(\mathbb{Z}^3)$$

in such a way that H_m becomes

$$\bigoplus_{\alpha_1, \alpha_2, \alpha_3 = 0}^{m-1} H\left(\frac{\alpha_1}{m}\mathbf{K}_1 + \frac{\alpha_2}{m}\mathbf{K}_2 + \frac{\alpha_3}{m}\mathbf{K}_3\right)$$

where $H(\mathbf{k})$ are the fibers of the infinite volume operator H. The reason that this decomposition holds is that one shows that any φ periodic on $Q^{(m)}$ is a sum of φ's with $\varphi(\mathbf{x} + \mathbf{a}_j) = e^{2\pi\alpha_j i/m}\varphi(\mathbf{x})$. As a result of this decomposition,

$$\rho_m(-\infty, E] = 2m^{-3}\, \#\{n; \alpha_i \in \{0, 1, \ldots, m-1\} \,|\, E_n(m^{-1} \textstyle\sum (\alpha_j \mathbf{K}_j)) \le E\}$$

and, since $E(\cdot)$ is continuous, this expression is an approximation for $\rho(-\infty, E]$. ∎

Now we return to our model of solids. Suppose that each nucleus in free space is surrounded by ℓ electrons. Then in our model we wish to have ℓ electrons per unit cell. While we ignore interactions between the electrons, we cannot ignore the Pauli principle which asserts for noninteracting electrons that each eigenvalue of H can contain at most two electrons. How do we take this into account when H does not have eigenfunctions and when there are infinitely many electrons (in our infinite crystal lattice!)? We claim that a reasonable way of taking the Pauli principle into account is to say that in the ground state, the electrons fill up the continuum eigenstates up to that energy E where $\rho(-\infty, E] = \ell$. For if we have a large but finite $m \times m \times m$ crystal with periodic boundary conditions, there are $m^3\ell$ electrons, and in the ground state these fill up the eigenstates of H_m to an energy E_m determined by $\rho_m(-\infty, E_m) = \ell$. The smallest number E with $\rho(-\infty, E] = \ell$ is called the **Fermi energy,** E_F. The set of $\mathbf{k} \in B$, the Brillouin zone, with $E_n(\mathbf{k}) = E_F$ for some n is called the **Fermi surface.** This picture is similar to the elementary discussion of the periodic table based on the hydrogen atom but with the complication of continuum states.

We are now in a position to explain why electron conduction is hard in some solids (insulators) and easy in others (metals). In the ground state one can use complex conjugation symmetry to prove that there is no net movement of electrons. To get flow of electrons one must excite some of the electrons. We have seen that typically a periodic Schrödinger operator has gaps in its spectrum. There is a qualitative difference if E_F occurs at the bottom of a gap or not. If E_F is at the bottom of a gap, then H has no spectrum in $(E_F, E_F + \varepsilon)$ and there is a discrete amount of energy needed to

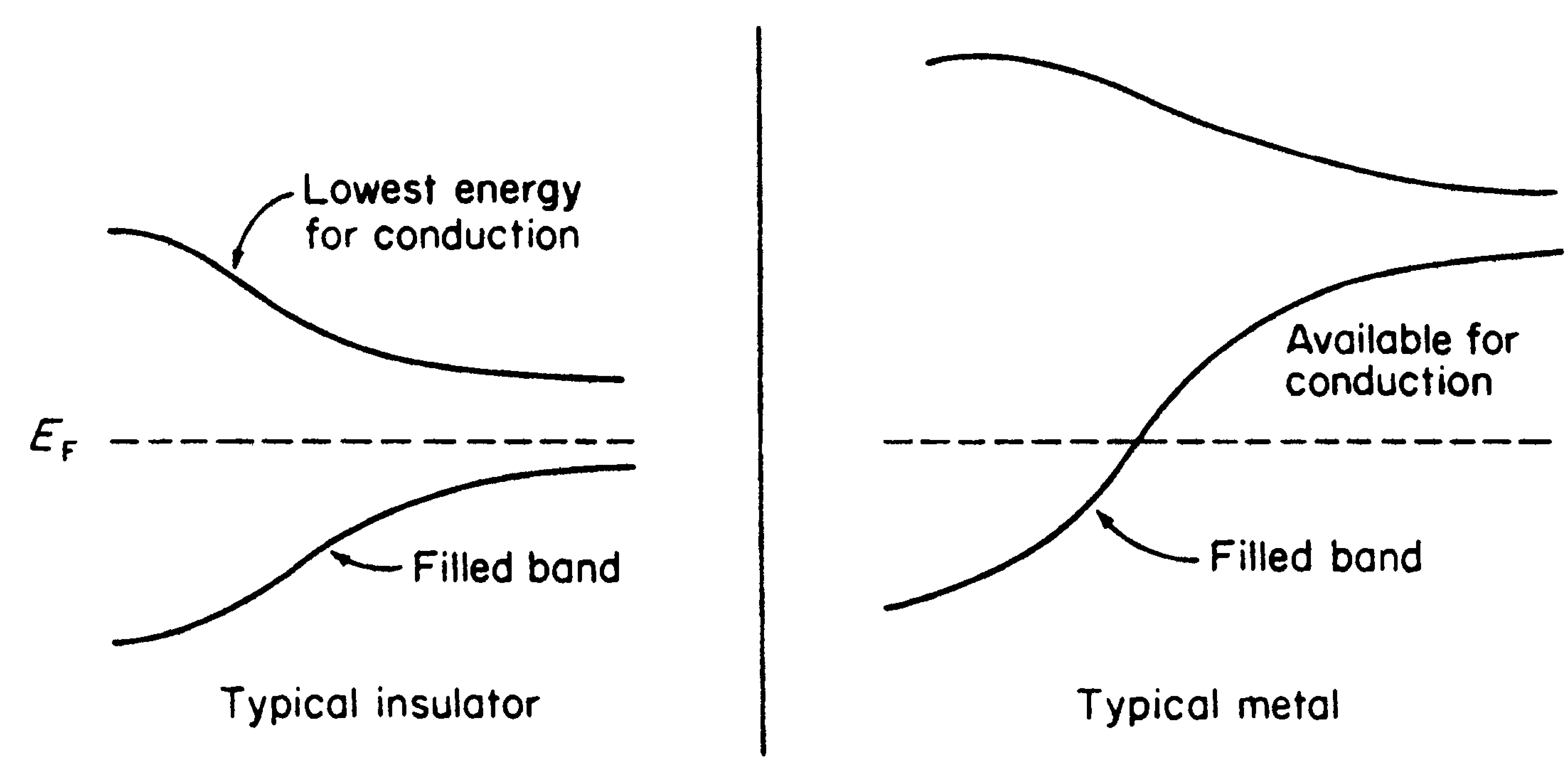


FIGURE XIII.20 Energy bands in conductors and insulators.

set up a current (see Figure XIII.20). In this case one has an insulator. If E_F is not at the bottom of a gap, one has a metal! Of course, if E_F is at the bottom of a small gap (ε small) or if E_F is not at the bottom of a gap but is fairly close to the bottom of a gap, then one has an intermediate case where the metal/insulator distinction is not sharp (semimetals, semiconductors) and in dealing with real solids one must take into account the fact that the solid is not in the ground state but rather in a finite temperature state determined by statistical mechanics. Notice that the gaps in the spectrum are crucial for this theory of insulators versus metals.

As a final topic in the one-electron theory of solids, we mention impurity scattering. Suppose that one of the lattice points has an impurity atom instead of the kind of atom at all the other sites. An electron in this crystal experiences a potential $V + W$ where V is periodic and W, which represents the difference of the potential of the impurity and what it replaces, is short range. One expects electrons in such a crystal to scatter from the impurity according to the usual scattering theory formalism.

Theorem XIII.102 Let V be a periodic potential on $\mathbb{R}^3$ that is square integrable over a basic cell. Let W be a potential in $L^1 \cap L^2(\mathbb{R}^3)$. Then

$$\Omega^{\pm} = \operatorname*{s-lim}_{t \to \mp\infty} \exp[+it(H_0 + V + W)] \exp[-it(H_0 + V)]$$

exist and have identical ranges and, in particular, the S matrix is unitary.

Proof Since $H_0 + V$ has purely absolutely continuous spectrum (Theorem XIII.100), we can prove the theorem by showing that $(-\Delta + V + W + c)^{-1} - (-\Delta + V + c)^{-1}$ is trace class for some c, for then we can apply the Kato–Birman theory (Theorem XI.9). Choose c so that $-\Delta + V + W \geq -c + 1$, $-\Delta + V \geq -c + 1$. Since V and W are $-\Delta$-bounded with relative bound zero,

$$\begin{aligned}
&(-\Delta + V + W + c)^{-1} - (-\Delta + V + c)^{-1} \\
&\quad = -(-\Delta + V + W + c)^{-1} W(-\Delta + V + c)^{-1} \\
&\quad = -[(-\Delta + V + W + c)^{-1}(-\Delta + 1)][(-\Delta + 1)^{-1} W(-\Delta + 1)^{-1}] \\
&\qquad \times [(-\Delta + 1)(-\Delta + V + c)^{-1}]
\end{aligned}$$

The first and third factors are bounded operators by the relative boundedness and since $W \in L^1 \cap L^2$, the middle factor is trace class (see Theorem XI.20). Thus the difference of resolvents is trace class. ∎