Periodic Schrödinger Operators

Let $\Gamma$ be a lattice of static ions that generate an electric potential $V(x)$ that is periodic with respect to $\Gamma$.

\[
H = -\frac{1}{2m} \Delta + V(x)
\]

Then the Hamiltonian for a single electron moving in this lattice is

This Hamiltonian commutes with all of the translation operators

\[
(T_{\gamma} \phi)(x) = \phi(x + \gamma) \quad \gamma \in \Gamma
\]
Simultaneous eigenfunctions for these operators obey

\[ H\phi_\alpha = e_\alpha \phi_\alpha \]

\[ T_\gamma \phi_\alpha = \lambda_{\alpha,\gamma} \phi_\alpha \quad \forall \gamma \in \Gamma \]

\( T_\gamma \) is unitary \( \Rightarrow \)

\[ |\lambda_{\alpha,\gamma}| = 1 \Rightarrow \lambda_{\alpha,\gamma} = e^{i\beta_{\alpha,\gamma}} \]

\[ T_\gamma T_{\gamma'} \phi_\alpha = T_{\gamma+\gamma'} \phi_\alpha \Rightarrow \]

\[ \Rightarrow \lambda_{\alpha,\gamma} \lambda_{\alpha,\gamma'} \phi_\alpha = \lambda_{\alpha,\gamma+\gamma'} \phi_\alpha \]

\[ \Rightarrow \beta_{\alpha,\gamma} + \beta_{\alpha,\gamma'} = \beta_{\alpha,\gamma+\gamma'} \mod 2\pi \quad \forall \gamma, \gamma' \in \Gamma \]

Write

\[ \Gamma = \{ n_1 \gamma_1 + \cdots + n_d \gamma_d \mid n_1, \cdots, n_d \in \mathbb{Z} \} \]

For each \( \alpha \), all \( \beta_{\alpha,\gamma}, \gamma \in \Gamma \) are determined, mod \( 2\pi \), by \( \beta_{\alpha,\gamma_i}, 1 \leq i \leq d \). Given any \( d \) numbers \( \beta_1, \cdots, \beta_d \) the system of linear equations (with unknowns \( k_1, \cdots, k_d \))

\[ \gamma_i \cdot k = \beta_i \quad 1 \leq i \leq d \]

that is \( \sum_{j=1}^{d} \gamma_{i,j} k_j = \beta_i \quad 1 \leq i \leq d \)
(where $\gamma_{i,j}$ is the $j^{th}$ component of $\gamma_i$) has a unique solution. So, for each $\alpha$, there exists a $k_{\alpha} \in \mathbb{R}^d$ such that $k_{\alpha} \cdot \gamma_i = \beta_{\alpha,\gamma_i}$ for all $1 \leq i \leq d$ and hence

$$\beta_{\alpha,\gamma} = k_{\alpha} \cdot \gamma \mod 2\pi \quad \forall \gamma \in \Gamma$$

Notice that, for each $\alpha$, $k_{\alpha}$ is not uniquely determined. Indeed

$$\beta_{\alpha,\gamma} = k_{\alpha} \cdot \gamma \mod 2\pi, \quad \beta_{\alpha,\gamma} = k'_{\alpha} \cdot \gamma \mod 2\pi \quad \forall \gamma \in \Gamma$$

$$\iff (k_{\alpha} - k'_{\alpha}) \cdot \gamma \in 2\pi \mathbb{Z} \quad \forall \gamma \in \Gamma$$

$$\iff k_{\alpha} - k'_{\alpha} \in \Gamma^\#$$

where the dual lattice, $\Gamma^\#$, of $\Gamma$ is

$$\Gamma^\# = \{ \ b \in \mathbb{R}^d \mid b \cdot \gamma \in 2\pi \mathbb{Z} \quad \text{for all} \ \gamma \in \Gamma \ \}$$

Relabel, replacing the index $\alpha$ by the corresponding value of $k \in \mathbb{R}^d/\Gamma^\#$ and another index $n$. Under the new labeling the eigenvalue/eigenvector equations are

$$H\phi_{n,k} = e_n(k, V)\phi_{n,k}$$

$$T_{\gamma}\phi_{n,k} = e^{ik \cdot \gamma}\phi_{n,k} \quad \forall \gamma \in \Gamma$$

i.e.

$$\phi_{n,k}(x + \gamma) = e^{ik \cdot \gamma}\phi_{n,k}(x) \quad \forall \gamma \in \Gamma$$
or equivalently, with $\phi_{n,k}(x) = e^{ik \cdot x} \psi_{n,k}(x)$,

$$
\frac{1}{2m} (i \nabla - k)^2 \psi_{n,k} + V \psi_{n,k} = e_n(k, V) \psi_{n,k}
$$

$$
\psi_{n,k}(x + \gamma) = \psi_{n,k}(x)
$$

Denote by $\mathbb{N}_k$ the set of values of $n$ that appear in pairs $\alpha = (k, n)$ and define

$$
\mathcal{H}_k = \text{span} \left\{ \phi_{n,k} \mid n \in \mathbb{N}_k \right\}
$$

$$
\tilde{\mathcal{H}}_k = \text{span} \left\{ \psi_{n,k} \mid n \in \mathbb{N}_k \right\}
$$

Then, formally, and in particular ignoring that $k$ runs over an uncountable set,

$$
L^2(\mathbb{R}^d) = \text{span} \left\{ \phi_{n,k} \mid k \in \mathbb{R}^d/\Gamma^#, \ n \in \mathbb{N}_k \right\}
$$

$$
= \bigoplus_{k \in \mathbb{R}^d/\Gamma^#} \mathcal{H}_k
$$

unitary

$$
\cong \bigoplus_{k \in \mathbb{R}^d/\Gamma^#} \tilde{\mathcal{H}}_k
$$

The restriction of the Schrödinger operator $H$ to $\tilde{\mathcal{H}}_k$ is

$$
\frac{1}{2m} (i \nabla - k)^2 + V \text{ applied to functions that are periodic with respect to } \Gamma.
$$
So what have we gained? At least formally, we now know that to find the spectrum of

\[ H = \frac{1}{2m} (i\nabla)^2 + V(x) \]

acting on \( L^2(\mathbb{R}^d) \), it suffices to find, for each \( k \in \mathbb{R}^d / \Gamma^\# \), the spectrum of

\[ H_k = \frac{1}{2m} (i\nabla - k)^2 + V(x) \]

acting on \( L^2(\mathbb{R}^d / \Gamma) \). Unlike \( H \), \( H_k \) has compact resolvent. So, the spectrum of \( H_k \) necessarily consists of a sequence of eigenvalues \( e_n(k) \) converging to \( \infty \). The functions \( e_n(k) \) are continuous in \( k \) and periodic with respect to \( \Gamma^\# \) and the spectrum of \( H \) is precisely

\[ \{ e_n(k) \mid n \in \mathbb{N}, \ k \in \mathbb{R}^d / \Gamma^\# \} \]
Rigorousification

$$\bigoplus_{k \in \mathbb{R}^d/\Gamma^\#} \tilde{H}_k = \bigoplus_{k \in \mathbb{R}^d/\Gamma^\#} \text{span} \{ \psi_{n,k} \mid n \in \mathbb{N}_k \}$$

is implemented using

$$\mathcal{S}(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma)$$

$$= \left\{ \psi \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d) \mid \psi(k, x + \gamma) = \psi(k, x) \quad \forall \gamma \in \Gamma \right. \left. e^{i b \cdot x} \psi(k + b, x) = \psi(k, x) \quad \forall b \in \Gamma^\# \right\}$$

with inner product

$$\langle \psi, \phi \rangle_\Gamma = \frac{1}{|\Gamma^\#|} \int_{\mathbb{R}^d/\Gamma^\#} dk \int_{\mathbb{R}^d/\Gamma} dx \bar{\psi}(k, x) \phi(k, x)$$

and completion

$$L^2(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma)$$

Also define

$$\mathcal{S}(\mathbb{R}^d) = \left\{ f \in C^\infty(\mathbb{R}^d) \mid \right. \left. \sup_x \left| (1 + x^{2n}) \left( \prod_{j=1}^d \frac{\partial^{i_j} f(x)}{\partial x_{j}^{i_j}} \right) \right| < \infty \right.$$ \left. \forall n, i_1, \ldots, i_d \in \mathbb{N} \right\}$$

Its completion is $$L^2(\mathbb{R}^d)$$. 
Set
\[
(u\psi)(x) = \frac{1}{|\Gamma|} \int_{\mathbb{R}^d/\Gamma} d^d k \ e^{i k \cdot x} \psi(k, x)
\]
\[
(\tilde{u}f)(k, x) = \sum_{\gamma \in \Gamma} e^{-i k \cdot (x + \gamma)} f(x + \gamma)
\]

Let \( V \in C^\infty_{\mathbb{R}}(\mathbb{R}^d/\Gamma) \) and set
\[
h = (i \nabla)^2 + V(x) \quad D_h = \mathcal{S}(\mathbb{R}^d)
\]
\[
\kappa = (i \nabla_x - k)^2 + V(x) \quad D_\kappa = \mathcal{S}(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma)
\]

**Proposition S.3, S.5** There is a unitary map \( U \) such that \( U \) extends \( u \), \( U^* = U^{-1} \) extends \( \tilde{u} \) and
\[
\mathcal{S}(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma) \xrightarrow{\text{dense}} \mathcal{S}(\mathbb{R}^d)
\]
\[
\left\{ \begin{array}{c}
L^2(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma) \\
\text{dense}
\end{array} \right\} \xrightarrow{\text{dense}} L^2(\mathbb{R}^d)
\]

Furthermore, \( h \) and \( \kappa \) have unique self-adjoint extensions, \( H \) and \( K \), and
\[
\tilde{u}hu = \kappa \quad U^*HU = K
\]
Now fix any $k \in \mathbb{R}^d$ and $V \in C^\infty(\mathbb{R}^d/\Gamma)$ and set
\[
h_k = (i \nabla_x - k)^2 + V(x) \quad D_{h_k} = C^\infty(\mathbb{R}^d/\Gamma)
\]

**Lemma S.7, S.8**

a) The operator $h_k$ has a unique self–adjoint extension, $H_k$, in $L^2(\mathbb{R}^d/\Gamma)$.

b) If $\Im \lambda \neq 0$ or $\lambda < -\sup_x |V(x)|$, then $\lambda$ is not in the spectrum of $H_k$. If $\lambda$ is not in the spectrum of $H_k$, the resolvent $[H_k - \lambda \mathbb{1}]^{-1}$ is compact.

c) Let $R > 0$ and $\lambda < -\sup_x |V(x)|$. There is a constant $C'$ such that
\[
\left\| [H_k - \lambda \mathbb{1}]^{-1} - [H_{k'} - \lambda \mathbb{1}]^{-1} \right\| \leq C' |k - k'|
\]
for all $k, k' \in \mathbb{R}^d$ with $|k|, |k'| \leq R$.

d) Let $c \in \Gamma^\#$ and define $\mathcal{U}_c$ to be the multiplication operator $e^{ic \cdot x}$ on $L^2(\mathbb{R}^d/\Gamma)$. Then $\mathcal{U}_b$ is unitary and
\[
\mathcal{U}_c^* H_k \mathcal{U}_c = H_{k+c}
\]
Idea of Proof: $H_k$ is a bounded perturbation of $(i
abla_x - k)^2$, acting on $L^2(\mathbb{R}^d/\Gamma)$. The latter is diagonalized by the Fourier transform. It’s spectrum is

$$\{ (b - k)^2 \mid b \in \Gamma^\# \}$$

**Proposition S.9** The spectrum of $H_k$ consists of a sequence of eigenvalues

$$e_1(k) \leq e_2(k) \leq e_3(k) \leq \cdots$$

with, for each $n$, $e_n(k)$ continuous in $k$ and periodic with respect to $\Gamma^\#$ and $\lim_{n \to \infty} e_n(k) = \infty$. The limit is uniform in $k$.

**Theorem S.10** The spectrum of $H$ is

$$\{ e_n(k) \mid k \in \mathbb{R}^d/\Gamma^\#, \ n \in \mathbb{N} \}$$