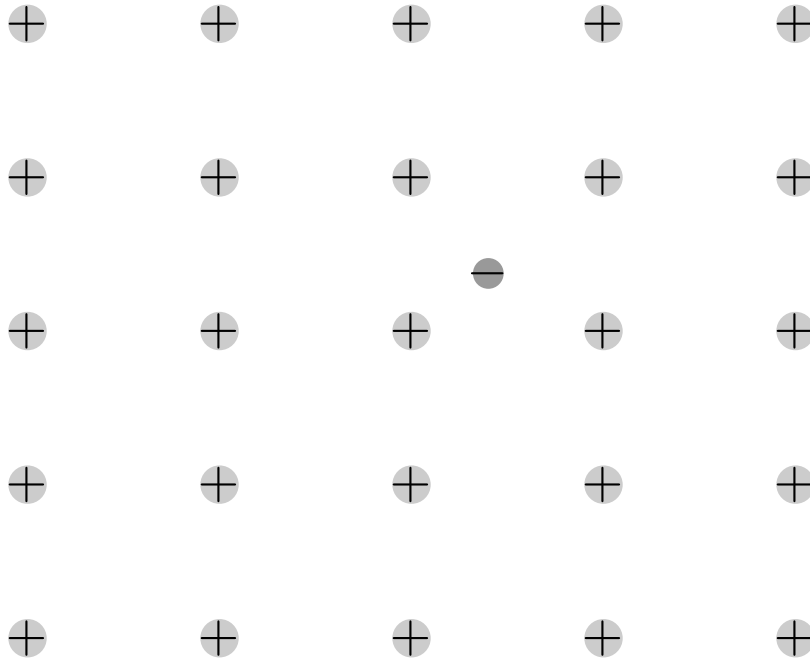


Periodic Schrödinger Operators

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



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

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

This Hamiltonian commutes with all of the translation operators

$$(T_{\boldsymbol{\gamma}}\phi)(\mathbf{x}) = \phi(\mathbf{x} + \boldsymbol{\gamma}) \quad \boldsymbol{\gamma} \in \Gamma$$

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_γ is unitary \Rightarrow

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

$$T_\gamma T_{\gamma'}\phi_\alpha = T_{\gamma+\gamma'}\phi_\alpha \Rightarrow$$

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

$$\Rightarrow \beta_{\alpha,\gamma} + \beta_{\alpha,\gamma'} = \beta_{\alpha,\gamma+\gamma'} \pmod{2\pi} \quad \forall \gamma, \gamma' \in \Gamma$$

Write

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

For each α , all $\beta_{\alpha,\gamma}$, $\gamma \in \Gamma$ are determined, mod 2π , by β_{α,γ_i} , $1 \leq i \leq d$. Given any d numbers β_1, \dots, β_d the system of linear equations (with unknowns k_1, \dots, k_d)

$$\gamma_i \cdot \mathbf{k} = \beta_i \quad 1 \leq i \leq d$$

$$\text{that is } \sum_{j=1}^d \gamma_{i,j} k_j = \beta_i \quad 1 \leq i \leq d$$

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

$$\beta_{\alpha,\gamma} = \mathbf{k}_\alpha \cdot \gamma \pmod{2\pi} \quad \forall \gamma \in \Gamma$$

Notice that, for each α , \mathbf{k}_α is not uniquely determined.

Indeed

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

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

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

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

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

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

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

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

$$\text{i.e. } \phi_{n,\mathbf{k}}(\mathbf{x} + \gamma) = e^{i\mathbf{k}\cdot\gamma}\phi_{n,\mathbf{k}}(\mathbf{x}) \quad \forall \gamma \in \Gamma$$

or equivalently, with $\phi_{n,\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\psi_{n,\mathbf{k}}(\mathbf{x})$,

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

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

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

$$\mathcal{H}_{\mathbf{k}} = \text{span} \{ \phi_{n,\mathbf{k}} \mid n \in \mathbb{N}_{\mathbf{k}} \}$$

$$\tilde{\mathcal{H}}_{\mathbf{k}} = \text{span} \{ \psi_{n,\mathbf{k}} \mid n \in \mathbb{N}_{\mathbf{k}} \}$$

Then, formally, and in particular ignoring that \mathbf{k} runs over an uncountable set,

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

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

$$\stackrel{\text{unitary}}{\cong} \bigoplus_{\mathbf{k} \in \mathbb{R}^d/\Gamma^\#} \tilde{\mathcal{H}}_{\mathbf{k}}$$

The restriction of the Schrödinger operator H to $\tilde{\mathcal{H}}_{\mathbf{k}}$ is $\frac{1}{2m} (i\nabla - \mathbf{k})^2 + V$ applied to functions that are periodic with respect to Γ .

So what have we gained? At least formally, we now know that to find the spectrum of

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

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

$$H_{\mathbf{k}} = \frac{1}{2m} (i\nabla - \mathbf{k})^2 + V(\mathbf{x})$$

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

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

Rigorousification

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

is implemented using

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

$$= \left\{ \psi \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d) \mid \right.$$

$$\psi(\mathbf{k}, \mathbf{x} + \boldsymbol{\gamma}) = \psi(\mathbf{k}, \mathbf{x}) \quad \forall \boldsymbol{\gamma} \in \Gamma$$

$$\left. e^{i\mathbf{b} \cdot \mathbf{x}} \psi(\mathbf{k} + \mathbf{b}, \mathbf{x}) = \psi(\mathbf{k}, \mathbf{x}) \quad \forall \mathbf{b} \in \Gamma^\# \right\}$$

with inner product

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

and completion

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

Also define

$$\mathcal{S}(\mathbb{R}^d) = \left\{ f \in C^\infty(\mathbb{R}^d) \mid \right.$$

$$\sup_{\mathbf{x}} \left| (1 + \mathbf{x}^{2n}) \left(\prod_{j=1}^d \frac{\partial^{i_j}}{\partial x_j^{i_j}} f(\mathbf{x}) \right) \right| < \infty$$

$$\left. \forall n, i_1, \dots, i_d \in \mathbb{N} \right\}$$

Its completion is $L^2(\mathbb{R}^d)$.

Set

$$(u\psi)(\mathbf{x}) = \frac{1}{|\Gamma^\#|} \int_{\mathbb{R}^d/\Gamma^\#} d^d\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{x}} \psi(\mathbf{k}, \mathbf{x})$$

$$(\tilde{u}f)(\mathbf{k}, \mathbf{x}) = \sum_{\boldsymbol{\gamma} \in \Gamma} e^{-i\mathbf{k}\cdot(\mathbf{x}+\boldsymbol{\gamma})} f(\mathbf{x} + \boldsymbol{\gamma})$$

Let $V \in C_{\mathbb{R}}^\infty(\mathbb{R}^d/\Gamma)$ and set

$$h = (i\nabla)^2 + V(\mathbf{x}) \quad \mathcal{D}_h = \mathcal{S}(\mathbb{R}^d)$$

$$\kappa = (i\nabla_{\mathbf{x}} - \mathbf{k})^2 + V(\mathbf{x}) \quad \mathcal{D}_\kappa = \mathcal{S}(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma)$$

Proposition S.3, S.5 *There is a unitary map U such that U extends u , $U^* = U^{-1}$ extends \tilde{u} and*

$$\begin{array}{ccc} \mathcal{S}(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma) & \begin{array}{c} \xrightarrow{u} \\ \xleftarrow{\tilde{u}} \end{array} & \mathcal{S}(\mathbb{R}^d) \\ \text{dense} \bigcap & & \bigcap \text{dense} \\ L^2(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma) & \begin{array}{c} \xrightarrow{U} \\ \xleftarrow{U^*} \end{array} & L^2(\mathbb{R}^d) \end{array}$$

Furthermore, h and κ have unique self-adjoint extensions, H and K , and

$$\tilde{u}hu = \kappa \quad U^*HU = K$$

Now fix any $\mathbf{k} \in \mathbb{R}^d$ and $V \in C_{\mathbb{R}}^{\infty}(\mathbb{R}^d/\Gamma)$ and set

$$h_{\mathbf{k}} = (i\nabla_{\mathbf{x}} - \mathbf{k})^2 + V(\mathbf{x}) \quad \mathcal{D}_{h_{\mathbf{k}}} = C^{\infty}(\mathbb{R}^d/\Gamma)$$

Lemma S.7,S.8

a) The operator $h_{\mathbf{k}}$ has a unique self-adjoint extension, $H_{\mathbf{k}}$, in $L^2(\mathbb{R}^d/\Gamma)$.

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

c) Let $R > 0$ and $\lambda < -\sup_{\mathbf{x}} |V(\mathbf{x})|$. There is a constant C' such that

$$\left\| [H_{\mathbf{k}} - \lambda\mathbb{1}]^{-1} - [H_{\mathbf{k}'} - \lambda\mathbb{1}]^{-1} \right\| \leq C' |\mathbf{k} - \mathbf{k}'|$$

for all $\mathbf{k}, \mathbf{k}' \in \mathbb{R}^d$ with $|\mathbf{k}|, |\mathbf{k}'| \leq R$.

d) Let $\mathbf{c} \in \Gamma^{\#}$ and define $\mathfrak{U}_{\mathbf{c}}$ to be the multiplication operator $e^{i\mathbf{c}\cdot\mathbf{x}}$ on $L^2(\mathbb{R}^d/\Gamma)$. Then $\mathfrak{U}_{\mathbf{b}}$ is unitary and

$$\mathfrak{U}_{\mathbf{c}}^* H_{\mathbf{k}} \mathfrak{U}_{\mathbf{c}} = H_{\mathbf{k}+\mathbf{c}}$$

Idea of Proof: $H_{\mathbf{k}}$ is a bounded perturbation of $(i\nabla_{\mathbf{x}} - \mathbf{k})^2$, acting on $L^2(\mathbb{R}^d/\Gamma)$. The latter is diagonalized by the Fourier transform. It's spectrum is

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

Proposition S.9 *The spectrum of $H_{\mathbf{k}}$ consists of a sequence of eigenvalues*

$$e_1(\mathbf{k}) \leq e_2(\mathbf{k}) \leq e_3(\mathbf{k}) \leq \dots$$

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

Theorem S.10 *The spectrum of H is*

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