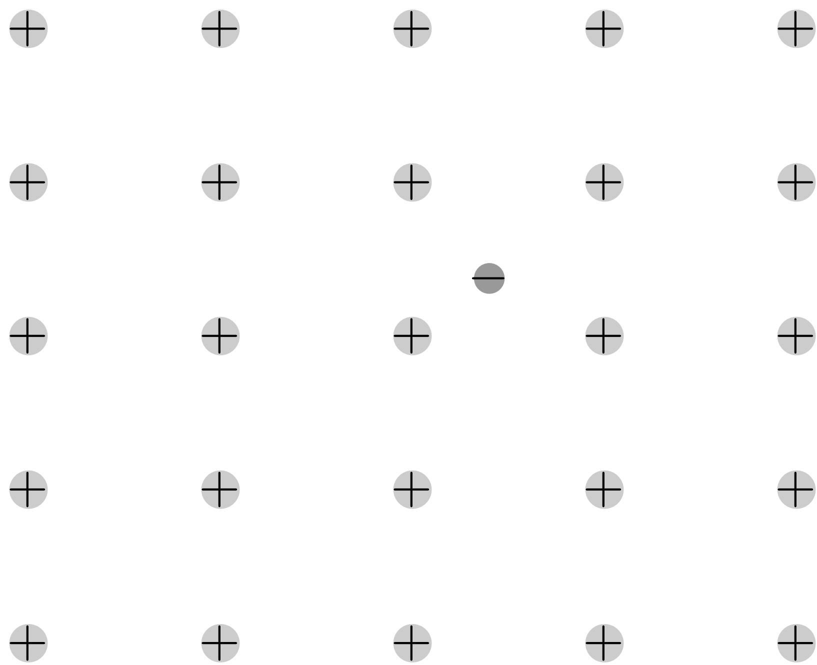
Periodic Schrödinger Operators

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

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

This Hamiltonian commutes with all of the translation operators

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

Simultaneous eigenfunctions for these operators obey

$$H\phi_\alpha = e_\alpha \phi_\alpha$$

$$T_{\boldsymbol{\gamma}}\phi_\alpha = \lambda_{\alpha,\boldsymbol{\gamma}}\phi_\alpha \qquad\qquad \forall \boldsymbol{\gamma} \in \Gamma$$

$T_{\boldsymbol{\gamma}}$ is unitary $\Rightarrow$

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

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

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

$$\Rightarrow\ \beta_{\alpha,\boldsymbol{\gamma}} + \beta_{\alpha,\boldsymbol{\gamma}'} = \beta_{\alpha,\boldsymbol{\gamma}+\boldsymbol{\gamma}'} \bmod 2\pi \qquad\qquad \forall \boldsymbol{\gamma},\boldsymbol{\gamma}' \in \Gamma$$

Write

$$\Gamma = \left\{\ n_1\boldsymbol{\gamma}_1 + \cdots n_d\boldsymbol{\gamma}_d \ \middle|\ n_1,\cdots,n_d \in \mathbb{Z}\ \right\}$$

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

$$\boldsymbol{\gamma}_i \cdot \mathbf{k} = \beta_i \qquad\qquad 1 \le i \le d$$

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

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

$$\beta_{\alpha,\boldsymbol{\gamma}} = \mathbf{k}_\alpha \cdot \boldsymbol{\gamma} \bmod 2\pi \qquad\qquad \forall \boldsymbol{\gamma} \in \Gamma$$

Notice that, for each α, $\mathbf{k}_\alpha$ is not uniquely determined. Indeed

$$\begin{aligned} &\beta_{\alpha,\boldsymbol{\gamma}} = \mathbf{k}_\alpha \cdot \boldsymbol{\gamma} \bmod 2\pi,\ \ \beta_{\alpha,\boldsymbol{\gamma}} = \mathbf{k}'_\alpha \cdot \boldsymbol{\gamma} \bmod 2\pi \quad \forall \boldsymbol{\gamma} \in \Gamma \\ &\iff (\mathbf{k}_\alpha - \mathbf{k}'_\alpha) \cdot \boldsymbol{\gamma} \in 2\pi\mathbb{Z} \qquad\qquad \forall \boldsymbol{\gamma} \in \Gamma \\ &\iff \mathbf{k}_\alpha - \mathbf{k}'_\alpha \in \Gamma^\# \end{aligned}$$

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

$$\Gamma^\# = \left\{\ \mathbf{b} \in \mathbb{R}^d\ \middle|\ \mathbf{b} \cdot \boldsymbol{\gamma} \in 2\pi\mathbb{Z} \text{ for all } \boldsymbol{\gamma} \in \Gamma\ \right\}$$

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

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

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

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

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

$$\tfrac{1}{2m}\big(i\boldsymbol{\nabla} - \mathbf{k}\big)^2\psi_{n,\mathbf{k}} + V\psi_{n,\mathbf{k}} = e_n(\mathbf{k},V)\psi_{n,\mathbf{k}}$$
$$\psi_{n,\mathbf{k}}(\mathbf{x}+\boldsymbol{\gamma}) = \psi_{n,\mathbf{k}}(\mathbf{x})$$

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

$$\mathcal{H}_{\mathbf{k}} = \operatorname{span}\left\{ \ \phi_{n,\mathbf{k}} \ \middle| \ n \in \mathbb{N}_{\mathbf{k}} \ \right\}$$
$$\tilde{\mathcal{H}}_{\mathbf{k}} = \operatorname{span}\left\{ \ \psi_{n,\mathbf{k}} \ \middle| \ n \in \mathbb{N}_{\mathbf{k}} \ \right\}$$

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

$$\begin{aligned} L^2(\mathbb{R}^d) &= \operatorname{span}\left\{ \ \phi_{n,\mathbf{k}} \ \middle| \ \mathbf{k} \in \mathbb{R}^d/\Gamma^\#, \ n \in \mathbb{N}_{\mathbf{k}} \ \right\} \\ &= \oplus_{\mathbf{k}\in\mathbb{R}^d/\Gamma^\#}\mathcal{H}_{\mathbf{k}} \\ &\overset{\text{unitary}}{\cong} \ \oplus_{\mathbf{k}\in\mathbb{R}^d/\Gamma^\#}\tilde{\mathcal{H}}_{\mathbf{k}} \end{aligned}$$

The restriction of the Schrödinger operator H to $\tilde{\mathcal{H}}_{\mathbf{k}}$ is $\tfrac{1}{2m}\big(i\boldsymbol{\nabla} - \mathbf{k}\big)^2 + V$ 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

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

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

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

acting on $L^2\big(\mathbb{R}^d/\Gamma\big)$. 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

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

Rigorousification

$$\oplus_{\mathbf{k}\in\mathbb{R}^d/\Gamma^\#}\tilde{\mathcal{H}}_{\mathbf{k}} = \oplus_{\mathbf{k}\in\mathbb{R}^d/\Gamma^\#}\mathrm{span}\left\{\ \psi_{n,\mathbf{k}}\ \middle|\ n\in\mathbb{N}_{\mathbf{k}}\ \right\}$$

is implemented using

$$\mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$$
$$= \Big\{\ \psi\in C^\infty\big(\mathbb{R}^d\times\mathbb{R}^d\big)\ \Big|$$
$$\psi(\mathbf{k},\mathbf{x}+\boldsymbol{\gamma}) = \psi(\mathbf{k},\mathbf{x}) \quad \forall\boldsymbol{\gamma}\in\Gamma$$
$$e^{i\mathbf{b}\cdot\mathbf{x}}\psi(\mathbf{k}+\mathbf{b},\mathbf{x}) = \psi(\mathbf{k},\mathbf{x}) \quad \forall\mathbf{b}\in\Gamma^\#\ \Big\}$$

with inner product

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

and completion

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

Also define

$$\mathcal{S}\big(\mathbb{R}^d\big) = \Big\{\ f\in C^\infty\big(\mathbb{R}^d\big)\ \Big|$$
$$\sup_{\mathbf{x}}\Big|(1+\mathbf{x}^{2n})\Big(\prod_{j=1}^{d}\tfrac{\partial^{i_j}}{\partial x_j^{i_j}}f(\mathbf{x})\Big)\Big| < \infty$$
$$\forall n, i_1,\cdots i_d\in\mathbb{N}\Big\}$$

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

Set

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

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

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

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

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

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

$$\begin{array}{ccc} \mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big) & \underset{\tilde{u}}{\overset{u}{\rightleftarrows}} & \mathcal{S}\big(\mathbb{R}^d\big) \\ \textit{dense}\bigcap & & \bigcap\textit{dense} \\ L^2\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big) & \underset{U^*}{\overset{U}{\rightleftarrows}} & L^2\big(\mathbb{R}^d\big) \end{array}$$

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

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

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

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

Lemma S.7,S.8

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

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 $\big[H_{\mathbf{k}} - \lambda\mathbb{1}\big]^{-1}$ is compact.

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

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

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 $\left(i\nabla_{\mathbf{x}} - \mathbf{k}\right)^2$, acting on $L^2\left(\mathbb{R}^d/\Gamma\right)$. The latter is diagonalized by the Fourier transform. It's spectrum is

$$\left\{\ (\mathbf{b}-\mathbf{k})^2\ \middle|\ \mathbf{b} \in \Gamma^{\#}\ \right\}$$

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

$$e_1(\mathbf{k}) \le e_2(\mathbf{k}) \le e_3(\mathbf{k}) \le \cdots$$

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

Theorem S.10 *The spectrum of H is*

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