The Spectrum of Periodic Schrödinger Operators

§I The Main Idea

Let Γ be a lattice of static ions in $\mathbb{R}^d$. Suppose that the ions 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

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

This Hamiltonian commutes with all of the translation operators

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

Problem S.1 Prove that

i) $T_{\boldsymbol{\gamma}}$ is a unitary operator on $L^2(\mathbb{R}^d)$ for all $\boldsymbol{\gamma}\in\mathbb{R}^d$.

ii) $T_{\boldsymbol{\gamma}}T_{\boldsymbol{\gamma}'} = T_{\boldsymbol{\gamma}+\boldsymbol{\gamma}'}$ for all $\boldsymbol{\gamma},\boldsymbol{\gamma}'\in\mathbb{R}^d$

Problem S.2 Prove that

i) $T_{\boldsymbol{\gamma}}\frac{\partial\varphi}{\partial x_i} = \frac{\partial T_{\boldsymbol{\gamma}}\varphi}{\partial x_i}$ for all differentiable functions φ on $\mathbb{R}^d$, $1\le i\le d$ and $\boldsymbol{\gamma}\in\mathbb{R}^d$

ii) $T_{\boldsymbol{\gamma}}V\varphi = VT_{\boldsymbol{\gamma}}\varphi$ for all $\boldsymbol{\gamma}\in\Gamma$, all functions V that are periodic with respect to Γ and all functions φ on $\mathbb{R}^d$.

Pretend, for the rest of §I, that H and the $T_{\boldsymbol{\gamma}}$'s are matrices. We'll give a rigorous version of this argument later. We know that for each family of commuting normal matrices, like $\{H,\ T_{\boldsymbol{\gamma}},\ \boldsymbol{\gamma}\in\Gamma\}$, there is an orthonormal basis of simultaneous eigenvectors. These eigenvectors obey

$$\begin{aligned} H\phi_\alpha &= e_\alpha\phi_\alpha \\ T_{\boldsymbol{\gamma}}\phi_\alpha &= \lambda_{\alpha,\boldsymbol{\gamma}}\phi_\alpha \qquad \forall\boldsymbol{\gamma}\in\Gamma \end{aligned}$$

for some numbers e_α and $\lambda_{\alpha,\boldsymbol{\gamma}}$.

As $T_{\boldsymbol{\gamma}}$ is unitary, all its eigenvalues must be complex numbers of modulus one. So there must exist real numbers $\beta_{\alpha,\boldsymbol{\gamma}}$ such that $\lambda_{\alpha,\boldsymbol{\gamma}} = e^{i\beta_{\alpha,\boldsymbol{\gamma}}}$. By Problem S.1.ii,

$$\begin{aligned} T_{\boldsymbol{\gamma}}T_{\boldsymbol{\gamma}'}\varphi_\alpha = T_{\boldsymbol{\gamma}+\boldsymbol{\gamma}'}\varphi_\alpha &\qquad = e^{i\beta_{\alpha,\boldsymbol{\gamma}+\boldsymbol{\gamma}'}}\varphi_\alpha \\ = T_{\boldsymbol{\gamma}}e^{i\beta_{\alpha,\boldsymbol{\gamma}'}}\varphi_\alpha = e^{i\beta_{\alpha,\boldsymbol{\gamma}}}e^{i\beta_{\alpha,\boldsymbol{\gamma}'}}\varphi_\alpha &= e^{i(\beta_{\alpha,\boldsymbol{\gamma}}+\beta_{\alpha,\boldsymbol{\gamma}'})}\varphi_\alpha \end{aligned}$$

which forces

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

Thus, 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 $k_1,\cdots,k_d$)

$$\begin{aligned} \boldsymbol{\gamma}_i\cdot\mathbf{k} &= \beta_i \qquad & 1\le i\le d \\ \text{that is} \quad \sum_{j=1}^d \gamma_{i,j}k_j &= \beta_i \qquad & 1\le i\le d \end{aligned}$$

(where $\gamma_{i,j}$ is the $j^{\rm th}$ component of $\boldsymbol{\gamma}_i$) has a unique solution because the linear independence of $\boldsymbol{\gamma}_1,\cdots,\boldsymbol{\gamma}_d$ implies that the matrix $\big[\gamma_{i,j}\big]_{1\le i,j\le d}$ is invertible. 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

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

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

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

Now relabel the eigenvalues and eigenvectors, replacing the index α by the corresponding value of $\mathbf{k}\in\mathbb{R}^d/\Gamma^\#$ and another index n. The index n is needed because many $\mathbf{k}_\alpha$'s with different values of α can be equal. Under the new labelling the eigenvalue/eigenvector equations are

$$\begin{aligned} H\phi_{n,\mathbf{k}} &= e_n(\mathbf{k})\phi_{n,\mathbf{k}} \\ T_{\boldsymbol{\gamma}}\phi_{n,\mathbf{k}} &= e^{i\mathbf{k}\cdot\boldsymbol{\gamma}}\phi_{n,\mathbf{k}} \qquad \forall\boldsymbol{\gamma}\in\Gamma \end{aligned} \tag{S.1}$$

The H–eigenvalue is denoted $e_n(\mathbf{k})$ rather than $e_{n,\mathbf{k}}$ because, while $\mathbf{k}$ runs over the continuous set $\mathbb{R}^d/\Gamma^\#$, n will turn out to run over a countable set. Now fix any $\mathbf{k}$ and observe that "$T_{\boldsymbol{\gamma}}\phi_{n,\mathbf{k}} = e^{i\mathbf{k}\cdot\boldsymbol{\gamma}}\phi_{n,\mathbf{k}}$ for all $\boldsymbol{\gamma}\in\Gamma$" means that

$$\phi_{n,\mathbf{k}}(\mathbf{x}+\boldsymbol{\gamma}) = e^{i\mathbf{k}\cdot\boldsymbol{\gamma}}\phi_{n,\mathbf{k}}(\mathbf{x})$$

for all $\mathbf{x}\in\mathbb{R}^d$ and $\boldsymbol{\gamma}\in\Gamma$. If the $e^{i\mathbf{k}\cdot\boldsymbol{\gamma}}$ were not there, this would just say that $\phi_{n,\mathbf{k}}$ is periodic with respect to Γ. We can make a simple change of variables that eliminates the $e^{i\mathbf{k}\cdot\boldsymbol{\gamma}}$. Define

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

Then subbing $\phi_{n,\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\psi_{n,\mathbf{k}}(\mathbf{x})$ into (S.1) gives

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

Problem S.3 Prove that, for all $\psi(\mathbf{x})$ in the obvious domains

i) $(i\boldsymbol{\nabla})\big(e^{i\mathbf{k}\cdot\mathbf{x}}\psi_{n,\mathbf{k}}(\mathbf{x})\big) = e^{i\mathbf{k}\cdot\mathbf{x}}(i\boldsymbol{\nabla} - \mathbf{k})\psi_{n,\mathbf{k}}(\mathbf{x})$

ii) $(i\boldsymbol{\nabla})^2\big(e^{i\mathbf{k}\cdot\mathbf{x}}\psi_{n,\mathbf{k}}(\mathbf{x})\big) = e^{i\mathbf{k}\cdot\mathbf{x}}(i\boldsymbol{\nabla} - \mathbf{k})^2\psi_{n,\mathbf{k}}(\mathbf{x})$

iii) $V(\mathbf{x})\big(e^{i\mathbf{k}\cdot\mathbf{x}}\psi_{n,\mathbf{k}}(\mathbf{x})\big) = e^{i\mathbf{k}\cdot\mathbf{x}}V(\mathbf{x})\psi_{n,\mathbf{k}}(\mathbf{x})$

iv) $T_{\boldsymbol{\gamma}}\big(e^{i\mathbf{k}\cdot\mathbf{x}}\psi_{n,\mathbf{k}}(\mathbf{x})\big) = e^{i\mathbf{k}\cdot\mathbf{x}}e^{i\mathbf{k}\cdot\boldsymbol{\gamma}}T_{\boldsymbol{\gamma}}\psi_{n,\mathbf{k}}(\mathbf{x})$

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

$$\mathcal{H}_{\mathbf{k}} = \operatorname{span}\big\{\ \phi_{n,\mathbf{k}}\ \big|\ n \in \mathbb{N}_{\mathbf{k}}\ \big\}$$

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

$$L^2(\mathbb{R}^d) = \operatorname{span}\big\{\ \phi_{n,\mathbf{k}}\ \big|\ \mathbf{k} \in \mathbb{R}^d/\Gamma^{\#},\ n \in \mathbb{N}_{\mathbf{k}}\ \big\} = \oplus_{\mathbf{k}\in\mathbb{R}^d/\Gamma^{\#}}\mathcal{H}_{\mathbf{k}}$$

Set

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

As multiplication by $e^{-i\mathbf{k}\cdot\mathbf{x}}$ is a unitary operator, $\mathcal{H}_{\mathbf{k}}$ is unitarily equivalent to $\tilde{\mathcal{H}}_{\mathbf{k}}$ and $L^2(\mathbb{R}^d)$ is unitarily equivalent to $\oplus_{\mathbf{k}\in\mathbb{R}^d/\Gamma^{\#}}\tilde{\mathcal{H}}_{\mathbf{k}}$. The restriction of the Schrödinger operator H to $\tilde{\mathcal{H}}_{\mathbf{k}}$ is $\frac{1}{2m}\big(i\boldsymbol{\nabla} - \mathbf{k}\big)^2 + V$ 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 $H = \frac{1}{2m}\big(i\boldsymbol{\nabla}\big)^2 + V(\mathbf{x})$, 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 $H_{\mathbf{k}} = \frac{1}{2m}\big(i\boldsymbol{\nabla} - \mathbf{k}\big)^2 + V(\mathbf{x})$ acting on $L^2\big(\mathbb{R}^d/\Gamma\big)$. We shall shortly prove that, unlike H, $H_{\mathbf{k}}$ has compact resolvent. So, unlike H (which we shall see has continuous spectrum), the spectrum of $H_{\mathbf{k}}$ necessarily consists of a sequence of eigenvalues $e_n(\mathbf{k})$ converging to ∞. We shall also prove that the functions $e_n(\mathbf{k})$ are continuous in $\mathbf{k}$ and periodic with respect to $\Gamma^{\#}$ and that the spectrum of H is precisely $\big\{\ e_n(\mathbf{k})\ \big|\ n \in \mathbb{N},\ \mathbf{k} \in \mathbb{R}^d/\Gamma^{\#}\ \big\}$.

Our next steps are to really prove that the spectrum of H is determined by the spectra of the $H_{\mathbf{k}}$'s and then that the $H_{\mathbf{k}}$'s have compact resolvent.

§II The Reduction from H to the $H_{\mathbf{k}}$'s

We now rigorously express H as a "sum" (technically a direct integral) of $H_{\mathbf{k}}$'s. Because we are working in a rather concrete setting, we will never have to define what a direct integral is. We shall make "$L^2(\mathbb{R}^d)$ is unitarily equivalent to $\oplus_{\mathbf{k}\in\mathbb{R}^d/\Gamma^\#}\tilde{\mathcal{H}}_{\mathbf{k}}$" rigorous by constructing a unitary operator U from the space of L^2 functions $f(\mathbf{x}), \mathbf{x}\in\mathbb{R}^d$ to the space of L^2 functions $\psi(\mathbf{k},\mathbf{x}),\ \mathbf{k}\in\mathbb{R}^d/\Gamma^\#,\ \mathbf{x}\in\mathbb{R}^d/\Gamma$ with the property that

$$(UHU^*\psi)(\mathbf{k},\mathbf{x}) = H_{\mathbf{k}}\psi(\mathbf{k},\mathbf{x})$$

Define

$$\mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big) = \left\{ \psi\in C^\infty\big(\mathbb{R}^d\times\mathbb{R}^d\big) \;\middle|\; \begin{array}{rl} \psi(\mathbf{k},\mathbf{x}+\boldsymbol{\gamma}) = \psi(\mathbf{k},\mathbf{x}) & \forall\boldsymbol{\gamma}\in\Gamma \\ e^{i\mathbf{b}\cdot\mathbf{x}}\psi(\mathbf{k}+\mathbf{b},\mathbf{x}) = \psi(\mathbf{k},\mathbf{x}) & \forall\mathbf{b}\in\Gamma^\# \end{array} \right\}$$

Define an inner product on $\mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$ by

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

With this inner product $\mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$ is almost a Hilbert space. The only missing axiom is completeness. Call the completion $L^2\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$.

Remark S.1 The condition $\psi(\mathbf{k},\mathbf{x}+\boldsymbol{\gamma}) = \psi(\mathbf{k},\mathbf{x})\ \forall\boldsymbol{\gamma}\in\Gamma$ just says that ψ is periodic with respect to Γ in the argument $\mathbf{x}$. The condition $e^{i\mathbf{b}\cdot\mathbf{x}}\psi(\mathbf{k}+\mathbf{b},\mathbf{x}) = \psi(\mathbf{k},\mathbf{x})\ \forall\mathbf{b}\in\Gamma^\#$, or equivalently $e^{i(\mathbf{k}+\mathbf{b})\cdot\mathbf{x}}\psi(\mathbf{k}+\mathbf{b},\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\psi(\mathbf{k},\mathbf{x})\ \forall\mathbf{b}\in\Gamma^\#$, says that $e^{i\mathbf{k}\cdot\mathbf{x}}\psi(\mathbf{k},\mathbf{x})$ is periodic with respect to $\Gamma^\#$ in the argument $\mathbf{k}$. The extra factor $e^{i\mathbf{k}\cdot\mathbf{x}}$ means that $\psi(\mathbf{k},\mathbf{x})$ itself need not be periodic with respect to $\Gamma^\#$ in the argument $\mathbf{k}$. So $\psi(\mathbf{k},\mathbf{x})$ need not be continuous on the torus $\mathbb{R}^d/\Gamma^\#\times\mathbb{R}^d/\Gamma$ and my notation $\mathcal{S}\big(\mathbb{R}^d/\Gamma^\#\times\mathbb{R}^d/\Gamma\big)$ is not very technically correct. There is a fancy way of formulating the second condition as a continuity condition which leads to the statement "$\psi(\mathbf{k},\mathbf{x})$ is a smooth section of the line bundle ... over $\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma$".

Remark S.2 On the other hand, if both $\psi(\mathbf{k},\mathbf{x})$ and $\phi(\mathbf{k},\mathbf{x})$ are in $\mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$, then the integrand $\overline{\psi(\mathbf{k},\mathbf{x})}\ \phi(\mathbf{k},\mathbf{x})$ is periodic with respect to $\Gamma^\#$ in $\mathbf{k}$ and is periodic with respect to Γ in $\mathbf{x}$. Hence if D is any fundamental domain for Γ and $D^\#$ is any fundamental domain for $\Gamma^\#$

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

The value of the integral is independent of the choice of D and $D^{\#}$. Thus, you can always realize $L^2\big(\mathbb{R}^d/\Gamma^{\#}\times\mathbb{R}^d/\Gamma\big)$ as the conventional $L^2\big(D^{\#}\times D\big)$.

Also define

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

This is called "Schwartz space". A function $f(\mathbf{x})$ is in Schwartz space if and only all of its derivatives are continuous and decay, for large $|\mathbf{x}|$, faster than one over any polynomial. Think of $\mathcal{S}\big(\mathbb{R}^d\big)$ as a subset of $L^2(\mathbb{R}^d)$. Set

$$\begin{aligned}(u\psi)(\mathbf{x})&=\tfrac{1}{|\Gamma^{\#}|}\int_{\mathbb{R}^d/\Gamma^{\#}}d^d\mathbf{k}\ e^{i\mathbf{k}\cdot\mathbf{x}}\psi(\mathbf{k},\mathbf{x})\\(\tilde{u}f)(\mathbf{k},\mathbf{x})&=\sum_{\boldsymbol{\gamma}\in\Gamma}e^{-i\mathbf{k}\cdot(\mathbf{x}+\boldsymbol{\gamma})}f(\mathbf{x}+\boldsymbol{\gamma})\end{aligned}$$

Proposition S.3

i) $u:\mathcal{S}\big(\mathbb{R}^d/\Gamma^{\#}\times\mathbb{R}^d/\Gamma\big)\rightarrow\mathcal{S}\big(\mathbb{R}^d\big)$

ii) $\tilde{u}:\mathcal{S}\big(\mathbb{R}^d\big)\rightarrow\mathcal{S}\big(\mathbb{R}^d/\Gamma^{\#}\times\mathbb{R}^d/\Gamma\big)$

iii) $\tilde{u}u\psi=\psi$ *for all* $\psi\in\mathcal{S}\big(\mathbb{R}^d/\Gamma^{\#}\times\mathbb{R}^d/\Gamma\big)$

iv) $u\tilde{u}f=f$ *for all* $f\in\mathcal{S}\big(\mathbb{R}^d\big)$

v) $\langle\tilde{u}f,\tilde{u}g\rangle_\Gamma=\langle f,g\rangle$ *for all* $f,g\in\mathcal{S}\big(\mathbb{R}^d\big)$

vi) $\langle u\psi,u\phi\rangle=\langle\psi,\phi\rangle_\Gamma$ *for all* $\psi,\phi\in\mathcal{S}\big(\mathbb{R}^d/\Gamma^{\#}\times\mathbb{R}^d/\Gamma\big)$

vii) $\langle f,u\phi\rangle=\langle\tilde{u}f,\phi\rangle_\Gamma$ *for all* $f\in\mathcal{S}\big(\mathbb{R}^d\big)$, $\phi\in\mathcal{S}\big(\mathbb{R}^d/\Gamma^{\#}\times\mathbb{R}^d/\Gamma\big)$

Proof:

i) This is **Problem S.4** . It is the usual integration by parts game. Note that the integrand $e^{i\mathbf{k}\cdot\mathbf{x}}\psi(\mathbf{k},\mathbf{x})$ is periodic with respect to $\Gamma^{\#}$ in the integration variable $\mathbf{k}$.

ii) Fix $f\in\mathcal{S}\big(\mathbb{R}^d\big)$ and set

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

As $f(\mathbf{x})$ and all of its derivatives are bounded by $\frac{\text{const}}{1+|\mathbf{x}|^{d+1}}$ the series

$$\sum_{\boldsymbol{\gamma}\in\Gamma}\prod_{\ell=1}^{d}\frac{\partial^{i_\ell}}{\partial x_\ell^{i_\ell}}\frac{\partial^{j_\ell}}{\partial k_\ell^{j_\ell}}\; e^{-i\mathbf{k}\cdot(\mathbf{x}+\boldsymbol{\gamma})}f(\mathbf{x}+\boldsymbol{\gamma})$$

converges absolutely and uniformly in $\mathbf{k}$ and $\mathbf{x}$ (on any compact set) for all $i_1,\cdots,i_d,j_1,\cdots j_d$. Consequently $\psi(\mathbf{k},\mathbf{x})$ exists and is C^∞. We now verify the periodicity conditions. If $\boldsymbol{\gamma}\in\Gamma$,

$$\begin{aligned}\psi(\mathbf{k},\mathbf{x}+\boldsymbol{\gamma}) &= \sum_{\boldsymbol{\gamma}'\in\Gamma} e^{-i\mathbf{k}\cdot(\mathbf{x}+\boldsymbol{\gamma}+\boldsymbol{\gamma}')}f(\mathbf{x}+\boldsymbol{\gamma}+\boldsymbol{\gamma}')\\ &= \sum_{\boldsymbol{\gamma}''\in\Gamma} e^{-i\mathbf{k}\cdot(\mathbf{x}+\boldsymbol{\gamma}'')}f(\mathbf{x}+\boldsymbol{\gamma}'') \qquad \text{where } \boldsymbol{\gamma}''=\boldsymbol{\gamma}+\boldsymbol{\gamma}'\\ &= \psi(\mathbf{k},\mathbf{x})\end{aligned}$$

and, if $\mathbf{b}\in\Gamma^\#$,

$$\begin{aligned}e^{i(\mathbf{k}+\mathbf{b})\cdot\mathbf{x}}\psi(\mathbf{k}+\mathbf{b},\mathbf{x}) &= \sum_{\boldsymbol{\gamma}\in\Gamma} e^{i(\mathbf{k}+\mathbf{b})\cdot\mathbf{x}}e^{-i(\mathbf{k}+\mathbf{b})\cdot(\mathbf{x}+\boldsymbol{\gamma})}f(\mathbf{x}+\boldsymbol{\gamma}) = \sum_{\boldsymbol{\gamma}\in\Gamma} e^{-i(\mathbf{k}+\mathbf{b})\cdot\boldsymbol{\gamma}}f(\mathbf{x}+\boldsymbol{\gamma})\\ &= \sum_{\boldsymbol{\gamma}\in\Gamma} e^{-i\mathbf{k}\cdot\boldsymbol{\gamma}}f(\mathbf{x}+\boldsymbol{\gamma}) = e^{i\mathbf{k}\cdot\mathbf{x}}\sum_{\boldsymbol{\gamma}\in\Gamma} e^{-i\mathbf{k}\cdot(\mathbf{x}+\boldsymbol{\gamma})}f(\mathbf{x}+\boldsymbol{\gamma})\\ &= e^{i\mathbf{k}\cdot\mathbf{x}}\psi(\mathbf{k},\mathbf{x})\end{aligned}$$

iii) Let

$$\begin{aligned}f(\mathbf{x}) = (u\psi)(\mathbf{x}) \quad &= \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d^d\mathbf{k}\; e^{i\mathbf{k}\cdot\mathbf{x}}\psi(\mathbf{k},\mathbf{x})\\ \Psi(\mathbf{k},\mathbf{x}) = (\tilde{u}f)(\mathbf{k},\mathbf{x}) &= \sum_{\boldsymbol{\gamma}\in\Gamma} e^{-i\mathbf{k}\cdot(\mathbf{x}+\boldsymbol{\gamma})}f(\mathbf{x}+\boldsymbol{\gamma})\end{aligned}$$

Then

$$\Psi(\mathbf{k},\mathbf{x}) = \sum_{\boldsymbol{\gamma}\in\Gamma} e^{-i\mathbf{k}\cdot(\mathbf{x}+\boldsymbol{\gamma})}\tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d^d\mathbf{p}\; e^{i\mathbf{p}\cdot(\mathbf{x}+\boldsymbol{\gamma})}\psi(\mathbf{p},\mathbf{x}+\boldsymbol{\gamma})$$

so that, by the periodicity of ψ in $\boldsymbol{\gamma}$,

$$e^{i\mathbf{k}\cdot\mathbf{x}}\Psi(\mathbf{k},\mathbf{x}) = \sum_{\boldsymbol{\gamma}\in\Gamma} e^{-i\mathbf{k}\cdot\boldsymbol{\gamma}}\tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d^d\mathbf{p}\; e^{i\mathbf{p}\cdot(\mathbf{x}+\boldsymbol{\gamma})}\psi(\mathbf{p},\mathbf{x})$$

Fix any $\mathbf{x}$ and recall that $h(\mathbf{p}) = e^{i\mathbf{p}\cdot\mathbf{x}}\psi(\mathbf{p},\mathbf{x})$ is periodic in $\mathbf{p}$ with respect to $\Gamma^\#$. Hence by Theorem L.10, (all labels "L.*" refer to the notes "Lattices and Periodic Functions") with $\Gamma\to\Gamma^\#$, $\mathbf{b}\to-\boldsymbol{\gamma}$, $f\to h$, $\mathbf{x}\to\mathbf{p}$ in the integral and $\mathbf{x}\to\mathbf{k}$ in the sum

$$h(\mathbf{k}) = \tfrac{1}{|\Gamma^\#|}\sum_{\boldsymbol{\gamma}\in\Gamma} e^{-i\boldsymbol{\gamma}\cdot\mathbf{k}}\int_{\mathbb{R}^d/\Gamma^\#} d^d\mathbf{p}\; e^{i\boldsymbol{\gamma}\cdot\mathbf{p}}\,h(\mathbf{p})$$

Subbing in $h(\mathbf{p}) = e^{i\mathbf{p}\cdot\mathbf{x}}\psi(\mathbf{p},\mathbf{x})$

$$e^{i\mathbf{k}\cdot\mathbf{x}}\psi(\mathbf{k},\mathbf{x}) = \tfrac{1}{|\Gamma^\#|}\sum_{\boldsymbol{\gamma}\in\Gamma} e^{-i\boldsymbol{\gamma}\cdot\mathbf{k}} \int_{\mathbb{R}^d/\Gamma^\#} d^d\mathbf{p}\ e^{i\boldsymbol{\gamma}\cdot\mathbf{p}}\, e^{i\mathbf{p}\cdot\mathbf{x}}\psi(\mathbf{p},\mathbf{x})$$

so that $e^{i\mathbf{k}\cdot\mathbf{x}}\Psi(\mathbf{k},\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\psi(\mathbf{k},\mathbf{x})$ and $\Psi(\mathbf{k},\mathbf{x}) = \psi(\mathbf{k},\mathbf{x})$, as desired.

iv) Let

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

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

Then

$$\begin{aligned}
F(\mathbf{x}) &= \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d^d\mathbf{k} \sum_{\boldsymbol{\gamma}\in\Gamma} e^{-i\mathbf{k}\cdot\boldsymbol{\gamma}} f(\mathbf{x}+\boldsymbol{\gamma}) = \sum_{\boldsymbol{\gamma}\in\Gamma} f(\mathbf{x}+\boldsymbol{\gamma}) \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d^d\mathbf{k}\ e^{-i\mathbf{k}\cdot\boldsymbol{\gamma}} \\
&= \sum_{\boldsymbol{\gamma}\in\Gamma} f(\mathbf{x}+\boldsymbol{\gamma}) \begin{cases} 1 & \text{if } \gamma = 0 \\ 0 & \text{if } \gamma \neq 0 \end{cases} \\
&= f(\mathbf{x})
\end{aligned}$$

v) Let

$$[\boldsymbol{\gamma}_1, \cdots \boldsymbol{\gamma}_d] = \Big\{ \sum_{j=1}^d t_j\boldsymbol{\gamma}_j \ \Big|\ 0 \le t_j \le 1 \text{ for all } 1 \le j \le d \Big\}$$

be the parallelepiped with the $\boldsymbol{\gamma}_j$'s as edges.

$$\begin{aligned}
\langle \tilde{u}f, \tilde{u}g\rangle_\Gamma &= \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d\mathbf{k} \int_{\mathbb{R}^d/\Gamma} d\mathbf{x}\ \ \overline{(\tilde{u}f)(\mathbf{k},\mathbf{x})}\ (\tilde{u}g)(\mathbf{k},\mathbf{x}) \\
&= \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d\mathbf{k} \int_{[\boldsymbol{\gamma}_1,\cdots,\boldsymbol{\gamma}_d]} d\mathbf{x}\ \ \overline{(\tilde{u}f)(\mathbf{k},\mathbf{x})}\ (\tilde{u}g)(\mathbf{k},\mathbf{x}) \\
&= \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d\mathbf{k} \int_{[\boldsymbol{\gamma}_1,\cdots,\boldsymbol{\gamma}_d]} d\mathbf{x}\ \ \Big[\overline{\sum_{\boldsymbol{\gamma}\in\Gamma} e^{-i\mathbf{k}\cdot(\mathbf{x}+\boldsymbol{\gamma})} f(\mathbf{x}+\boldsymbol{\gamma})}\Big]\Big[\sum_{\boldsymbol{\gamma}'\in\Gamma} e^{-i\mathbf{k}\cdot(\mathbf{x}+\boldsymbol{\gamma}')} g(\mathbf{x}+\boldsymbol{\gamma}')\Big] \\
&= \int_{[\boldsymbol{\gamma}_1,\cdots,\boldsymbol{\gamma}_d]} d\mathbf{x} \sum_{\boldsymbol{\gamma},\boldsymbol{\gamma}'\in\Gamma} \overline{f(\mathbf{x}+\boldsymbol{\gamma})} g(\mathbf{x}+\boldsymbol{\gamma}')\ \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d\mathbf{k}\ \ e^{i\mathbf{k}\cdot(\boldsymbol{\gamma}-\boldsymbol{\gamma}')} \\
&= \int_{[\boldsymbol{\gamma}_1,\cdots,\boldsymbol{\gamma}_d]} d\mathbf{x} \sum_{\boldsymbol{\gamma}\in\Gamma} \overline{f(\mathbf{x}+\boldsymbol{\gamma})}\, g(\mathbf{x}+\boldsymbol{\gamma}) \\
&= \int_{\mathbb{R}^d} d\mathbf{x}\ \overline{f(\mathbf{x})}\, g(\mathbf{x})
\end{aligned}$$

vi) Set $f = u\psi$ and $g = u\phi$. Then, by part (iii), $\tilde{u}f = \psi$ and $\tilde{u}g = \phi$ so that, by part (v),

$$\langle u\psi, u\phi\rangle = \langle f, g\rangle = \langle \tilde{u}f, \tilde{u}g\rangle_\Gamma = \langle \psi, \phi\rangle_\Gamma$$

vii) Set $g = u\phi$. Then, by part (iii), $\tilde{u}g = \phi$ so that, by part (v),

$$\langle f, u\phi\rangle = \langle f, g\rangle = \langle \tilde{u}f, \tilde{u}g\rangle_\Gamma = \langle \tilde{u}f, \phi\rangle_\Gamma$$

■

The mass m plays no role, so we set it to $\frac{1}{2}$ from now on.

Proposition S.4 *Let V be a C^∞ function that is periodic with respect to Γ and set*

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

with domains $\mathcal{S}\big(\mathbb{R}^d\big)$ and $\mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$, respectively. Then,

$$(\tilde{u}Hu\,\psi)(\mathbf{k},\mathbf{x}) = (H_\mathbf{k}\psi)(\mathbf{k},\mathbf{x})$$

for all $\psi \in \mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$

Proof: Observe that

$$\big(i\boldsymbol{\nabla}_\mathbf{x}\big)\Big[e^{i\mathbf{k}\cdot\mathbf{x}}\psi(\mathbf{k},\mathbf{x})\Big] = -\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{x}}\psi(\mathbf{k},\mathbf{x}) + e^{i\mathbf{k}\cdot\mathbf{x}}\big(i\boldsymbol{\nabla}_\mathbf{x}\psi\big)(\mathbf{k},\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\big([i\boldsymbol{\nabla}_\mathbf{x} - \mathbf{k}]\psi\big)(\mathbf{k},\mathbf{x})$$

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

$$\begin{aligned}(Hu\psi)(\mathbf{x}) &= \big[\big(i\boldsymbol{\nabla}\big)^2 + V(\mathbf{x})\big]\tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d^d\mathbf{k}\ e^{i\mathbf{k}\cdot\mathbf{x}}\psi(\mathbf{k},\mathbf{x}) \\ &= \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d^d\mathbf{k}\ e^{i\mathbf{k}\cdot\mathbf{x}}\Big(\big([i\boldsymbol{\nabla}_\mathbf{x} - \mathbf{k}]^2\psi\big)(\mathbf{k},\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{k},\mathbf{x})\Big) \\ &= (uH_\mathbf{k}\psi)(\mathbf{x})\end{aligned}$$

Now apply $\tilde{u}$ to both sides and use Proposition S.3.iii. ■

Theorem S.5

i) The operators u and $\tilde{u}$ have unique bounded extensions $U : L^2\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big) \to L^2\big(\mathbb{R}^d\big)$ and $\tilde{U} : L^2\big(\mathbb{R}^d\big) \to L^2\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$ and

$$\tilde{U}U = \mathbb{1}_{L^2\left(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\right)} \qquad U\tilde{U} = \mathbb{1}_{L^2\left(\mathbb{R}^d\right)} \qquad \tilde{U} = U^* \qquad U = \tilde{U}^*$$

ii) The operators H (defined on $\mathcal{S}\big(\mathbb{R}^d\big)$) and $H_\mathbf{k}$ (defined on $\mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$) have unique self–adjoint extensions to $L^2\big(\mathbb{R}^d\big)$ and $L^2\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$. We also call the extensions H and $H_\mathbf{k}$. They obey

$$U^*HU = H_\mathbf{k}$$

Proof: i) $\tilde{u}$ and u are bounded by Proposition S.3 parts (v) and (vi) respectively. As $\mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$ is dense in $L^2\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$ and $\mathcal{S}\big(\mathbb{R}^d\big)$ is dense in $L^2\big(\mathbb{R}^d\big)$, $\tilde{u}$ and u have unique bounded extensions $\tilde{U}$ and U. The remaining claims now follow from Proposition S.3 parts (iii), (iv), (vii) and (vii) respectively, by continuity.

ii) Step 1: $\big(i\boldsymbol{\nabla}\big)^2$ *is essentially self–adjoint on the domain* $\mathcal{S}\big(\mathbb{R}^d\big)$

The Fourier transform is a unitary map from $L^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$, that maps $\mathcal{S}(\mathbb{R}^d)$ onto $\mathcal{S}(\mathbb{R}^d)$. Under this unitary map $-\Delta$, with domain $\mathcal{S}\big(\mathbb{R}^d\big)$, becomes the multiplication operator $M_{\mathbf{x}^2} : \mathcal{S}(\mathbb{R}^d) \subset L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ defined by $M_{\mathbf{x}^2}\varphi(\mathbf{x}) = \mathbf{x}^2\varphi(\mathbf{x})$. So it suffices to prove that the operator $M_{\mathbf{x}^2}$ is essentially self–adjoint on $\mathcal{S}(\mathbb{R}^d)$. But if $\varphi(\mathbf{x}) \in \mathcal{S}(\mathbb{R}^d)$, then $\frac{\varphi(\mathbf{x})}{\mathbf{x}^2 \pm i} \in \mathcal{S}(\mathbb{R}^d)$. Hence the range of $M_{\mathbf{x}^2} \pm i$ contains all of $\mathcal{S}(\mathbb{R}^d)$ and consequently is dense in $L^2(\mathbb{R}^d)$. Now just apply the Corollary of [Reed and Simon, volume I, Theorem VIII.3].

ii) Step 2: Prove Lemma S.6, below.

ii) Step 3: *Finish off the proof.*

In step 1, we saw that $\big(i\boldsymbol{\nabla}\big)^2$ is essentially self–adjoint on $\mathcal{S}\big(\mathbb{R}^d\big)$. The multiplication operator $V(\mathbf{x})$ is bounded and self–adjoint on $L^2\big(\mathbb{R}^d\big)$. Consequently, by step 2, their sum, H is essentially self–adjoint on $\mathcal{S}\big(\mathbb{R}^d\big)$ and has a unique self–adjoint extension in $L^2\big(\mathbb{R}^d\big)$. The unitary operator U provides a unitary equivalence with

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

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

$$H_{\mathbf{k}} \restriction \mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big) \leftrightarrow H \restriction \mathcal{S}\big(\mathbb{R}^d\big)$$

So $H_{\mathbf{k}}$ is essentially self–adjoint on $\mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$, has a unique self–adjoint extension in $L^2\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$ and the extensions obey $U^*HU = H_{\mathbf{k}}$. ■

Lemma S.6 *Let $\mathcal{H}$ be a Hilbert space and $\mathcal{D}$ a dense subspace of $\mathcal{H}$. Let $T : \mathcal{D} \to \mathcal{H}$ be essentially self-adjoint, with unique self–adjoint extension $\bar{T}$, and $V : \mathcal{H} \to \mathcal{H}$ be bounded and self–adjoint. Then $T + V : \mathcal{D} \to \mathcal{H}$ is essentially self–adjoint and the unique self–adjoint extension of $T + V$ is $\bar{T} + V$.*

Proof: As V is bounded,

$$\varphi = \lim_{n\to\infty} \varphi_n,\ \psi = \lim_{n\to\infty} T\varphi_n \qquad \Longleftrightarrow \qquad \varphi = \lim_{n\to\infty} \varphi_n,\ \psi + V\varphi = \lim_{n\to\infty} (T+V)\varphi_n$$

for any sequence $\varphi_1,\ \varphi_2,\ \cdots \in \mathcal{D}$. The left hand side defines "$\varphi \in D_{\overline{T}}$, $\overline{T}\varphi = \psi$" and the right hand side defines "$\varphi \in D_{\overline{T+V}}$, $\overline{T+V}\varphi = \psi + V\varphi$", so $T + V$ is closeable with closure $\overline{T+V} = \overline{T} + V$.

To prove that $\overline{T}+V$ is self–adjoint, it suffices to prove that, for any densely define operator A and any bounded operator V, $(A+V)^*=A^*+V^*$. But, as V is bounded and $D_{A+V}=D_A$,

$$\begin{aligned} f\in D_{A^*} &\iff \sup_{g\in D_A,\|g\|=1} \big|\langle Ag,f\rangle\big|<\infty \\ &\iff \sup_{g\in D_A,\|g\|=1} \big|\langle (A+V)g,f\rangle\big|<\infty \\ &\iff f\in D_{(A+V)^*} \end{aligned}$$

and, for all $g\in D_A=D_{A+V},\ f\in D_{A^*}=D_{(A+V)^*}$

$$\langle g,(A+V)^*f\rangle=\langle (A+V)g,f\rangle=\langle Ag,f\rangle+\langle Vg,f\rangle=\langle g,A^*f\rangle+\langle g,V^*f\rangle=\langle g,(A^*+V^*)f\rangle$$

■

§III Compactness of the Resolvent of $H_{\mathbf{k}}$, for each fixed $\mathbf{k}$

In this section we fix a lattice Γ in $\mathbb{R}^d$, a vector $\mathbf{k}\in\mathbb{R}^d$ and a smooth, real–valued, function $V(\mathbf{x})\in C^\infty(\mathbb{R}^d/\Gamma)$ and study the operator

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

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

We denote by

$$\begin{aligned} \big(\mathcal{F}f\big)(\mathbf{b}) &= \tfrac{1}{\sqrt{|\Gamma|}}\int_{\mathbb{R}^d/\Gamma} d^d\mathbf{x}\ e^{-i\mathbf{b}\cdot\mathbf{x}}f(\mathbf{x}) \\ \big(\mathcal{F}^{-1}\varphi\big)(\mathbf{x}) &= \tfrac{1}{\sqrt{|\Gamma|}}\sum_{\mathbf{b}\in\Gamma^\#} e^{i\mathbf{b}\cdot\mathbf{x}}\varphi(\mathbf{b}) \end{aligned} \tag{S.3}$$

the Fourier transform and its inverse, normalized so that they are unitary maps from $L^2\big(\mathbb{R}^d/\Gamma\big)$ to $\ell^2(\Gamma^\#)$ and from $\ell^2(\Gamma^\#)$ to $L^2\big(\mathbb{R}^d/\Gamma\big)$ respectively.

Lemma S.7

a) The operator $\big(i\boldsymbol{\nabla}-\mathbf{k}\big)^2$ is self–adjoint on the domain

$$\mathcal{D}=\big\{\ \mathcal{F}^{-1}\varphi\ \big|\ \varphi(\mathbf{b}),\ \mathbf{b}^2\varphi(\mathbf{b})\in\ell^2(\Gamma^\#)\ \big\}$$

and essentially self–adjoint on the domain

$$\mathcal{D}_0=\big\{\ \mathcal{F}^{-1}\varphi\ \big|\ \varphi(\mathbf{b})=0 \text{ for all but finitely many } \mathbf{b}\in\Gamma^\#\ \big\}$$

b) The spectrum of $\big(i\nabla - \mathbf{k}\big)^2 - \lambda\mathbb{1}$ *is*

$$\big\{\ (\mathbf{b}-\mathbf{k})^2 - \lambda\ \big|\ \mathbf{b}\in\Gamma^\#\ \big\}$$

c) If 0 *is not in* $\big\{\ (\mathbf{b}-\mathbf{k})^2 - \lambda\ \big|\ \mathbf{b}\in\Gamma^\#\ \big\}$, $\big[\big(i\nabla - \mathbf{k}\big)^2 - \lambda\mathbb{1}\big]^{-1}$ *exists and is a compact operator with norm*

$$\Big\|\big[\big(i\nabla - \mathbf{k}\big)^2 - \lambda\mathbb{1}\big]^{-1}\Big\| = \Big[\min_{\mathbf{b}\in\Gamma^\#} |(\mathbf{b}-\mathbf{k})^2 - \lambda|\Big]^{-1}$$

For $d < 4$*, it is Hilbert-Schmidt.*

Proof: a) Let

$$\begin{aligned}
\tilde{\mathcal{D}} &= \big\{\ \varphi\in\ell^2(\Gamma^\#)\ \big|\ \mathbf{b}^2\varphi(\mathbf{b})\in\ell^2(\Gamma^\#)\ \big\}\\
\tilde{\mathcal{D}}_0 &= \big\{\ \varphi\in\ell^2(\Gamma^\#)\ \big|\ \varphi(\mathbf{b}) = 0 \text{ for all but finitely many } \mathbf{b}\in\Gamma^\#\ \big\}\\
M &= \text{the operator of multiplication by } (\mathbf{b}-\mathbf{k})^2 \text{ on } \tilde{\mathcal{D}}\\
m &= \text{the operator of multiplication by } (\mathbf{b}-\mathbf{k})^2 \text{ on } \tilde{\mathcal{D}}_0
\end{aligned}$$

If $\varphi\in\tilde{\mathcal{D}}_0$ then $\frac{\varphi(\mathbf{b})}{(\mathbf{b}-\mathbf{k})^2\pm i}$ is also in $\tilde{\mathcal{D}}_0$ so that $\varphi = (m\pm i)\frac{\varphi}{(\mathbf{b}-\mathbf{k})^2\pm i}$ is in the range of $m\pm i$. Thus the range of $m\pm i$ is all of $\tilde{\mathcal{D}}_0$ and hence is dense in $\ell^2(\Gamma^\#)$. This proves that m is essentially self–adjoint.

Recall that, since $(\alpha-\beta)^2\ge 0$, we have $2\alpha\beta\le\alpha^2+\beta^2$ for all real α and β. Hence

$$\begin{aligned}
\mathbf{b}^2 = (\mathbf{b}-\mathbf{k}+\mathbf{k})^2 &= (\mathbf{b}-\mathbf{k})^2 + 2(\mathbf{b}-\mathbf{k})\cdot\mathbf{k} + \mathbf{k}^2 \le (\mathbf{b}-\mathbf{k})^2 + 2\|\mathbf{b}-\mathbf{k}\|\,\|\mathbf{k}\| + \mathbf{k}^2\\
&\le (\mathbf{b}-\mathbf{k})^2 + \|\mathbf{b}-\mathbf{k}\|^2 + \|\mathbf{k}\|^2 + \mathbf{k}^2 = 2(\mathbf{b}-\mathbf{k})^2 + 2\mathbf{k}^2
\end{aligned}$$

Consequently, if $\varphi\in\ell^2(\Gamma^\#)$, then $\frac{\varphi(\mathbf{b})}{(\mathbf{b}-\mathbf{k})^2\pm i}\in\tilde{\mathcal{D}}$ so that $\varphi = (M\pm i)\frac{\varphi}{(\mathbf{b}-\mathbf{k})^2\pm i}$ is in the range of $M\pm i$. Thus the range of $M\pm i$ is all of $\ell^2(\Gamma^\#)$. This proves that M is self–adjoint and hence is the unique self–adjoint extension of m.

The operator $\mathcal{F}\big(i\nabla-\mathbf{k}\big)^2\mathcal{F}^{-1}$ is the operator of multiplication by $(\mathbf{b}-\mathbf{k})^2$ on $\ell^2(\Gamma^\#)$. Hence $\big(i\nabla-\mathbf{k}\big)^2$ is self–adjoint on $\mathcal{F}^{-1}\tilde{\mathcal{D}} = \mathcal{D}$ and essentially self–adjoint on $\mathcal{F}^{-1}\tilde{\mathcal{D}}_0 = \mathcal{D}_0$.

b) The operator $\big(i\nabla-\mathbf{k}\big)^2 - \lambda\mathbb{1}$ is unitarily equivalent to the operator of multiplication by $(\mathbf{b}-\mathbf{k})^2-\lambda$ on $\ell^2(\Gamma^\#)$. The function $(\mathbf{b}-\mathbf{k})^2-\lambda$ takes the values $\big\{\ (\mathbf{b}-\mathbf{k})^2-\lambda\ \big|\ \mathbf{b}\in\Gamma^\#\ \big\}$. Each of these values is taken on a set of nonzero measure (with respect to the counting measure on $\Gamma^\#$). So the spectrum of $(\mathbf{b}-\mathbf{k})^2-\lambda$ contains $\big\{\ (\mathbf{b}-\mathbf{k})^2-\lambda\ \big|\ \mathbf{b}\in\Gamma^\#\ \big\}$.

In part c, below, we shall show that, if 0 is not in $\big\{\ (\mathbf{b}-\mathbf{k})^2-\lambda\ \big|\ \mathbf{b}\in\Gamma^\#\ \big\}$, then $\frac{1}{(\mathbf{b}-\mathbf{k})^2-\lambda}$ is bounded uniformly in $\mathbf{b}$. That is, 0 is not in the spectrum of multiplication by

$(\mathbf{b}-\mathbf{k})^2-\lambda$. This is all we need, because if μ is not in $\{\ (\mathbf{b}-\mathbf{k})^2-\lambda \ \big|\ \mathbf{b}\in\Gamma^\#\ \}$, then 0 is not in $\{\ (\mathbf{b}-\mathbf{k})^2-\lambda' \ \big|\ \mathbf{b}\in\Gamma^\#\ \}$, with $\lambda'=\lambda+\mu$, so that 0 is not in the spectrum of multiplication by $(\mathbf{b}-\mathbf{k})^2-\lambda'$ and μ is not in the spectrum of multiplication by $(\mathbf{b}-\mathbf{k})^2-\lambda$.

c) Fix any $\mathbf{k}$ and any $\lambda\in\mathbb{C}$ such that $(\mathbf{b}-\mathbf{k})^2-\lambda$ is nonzero for all $\mathbf{b}\in\Gamma^\#$. Set

$$C_r=\inf\left\{\ \big|(\mathbf{b}-\mathbf{k})^2-\lambda\big| \ \Big|\ \mathbf{b}\in\Gamma^\#,\ |\mathbf{b}|\ge r\ \right\}$$

Since $(\mathbf{b}-\mathbf{k})^2\ge\frac{1}{2}\mathbf{b}^2-\mathbf{k}^2$, $C_r\ge\frac{1}{2}r^2-\mathbf{k}^2-\lambda$ so that $\lim_{r\to\infty}C_r=\infty$ and

$$\sup_{\mathbf{b}\in\Gamma^\#}\left|\tfrac{1}{(\mathbf{b}-\mathbf{k})^2-\lambda}\right|=\Big[\inf_{\mathbf{b}\in\Gamma^\#}\big|(\mathbf{b}-\mathbf{k})^2-\lambda\big|\Big]^{-1}=\max\left\{\max_{|\mathbf{b}|<r}\left|\tfrac{1}{(\mathbf{b}-\mathbf{k})^2-\lambda}\right|,\tfrac{1}{C_r}\right\}<\infty$$

Let R and R_r be the operators on $\ell^2(\Gamma^\#)$ of multiplication by $\frac{1}{(\mathbf{b}-\mathbf{k})^2-\lambda}$ and

$$\tfrac{1}{(\mathbf{b}-\mathbf{k})^2-\lambda}\begin{cases}1 & \text{if } |\mathbf{b}|\le r\\ 0 & \text{if } |\mathbf{b}|>r\end{cases}$$

respectively. Then R is a bounded operator, with norm $\Big[\min_{\mathbf{b}\in\Gamma^\#}\big|(\mathbf{b}-\mathbf{k})^2-\lambda\big|\Big]^{-1}$, R_r is a finite rank operator and $\|R-R_r\|=\frac{1}{C_r}$ converges to zero as r tends to infinity. This proves that R is compact. As $\big(i\boldsymbol{\nabla}-\mathbf{k}\big)^2-\lambda\mathbb{1}$ is unitarily equivalent to the multiplication operator $(\mathbf{b}-\mathbf{k})^2-\lambda$, its inverse $\big[(i\boldsymbol{\nabla}-\mathbf{k})^2-\lambda\mathbb{1}\big]^{-1}$ is unitarily equivalent to R and is also compact, with the same operator norm as R.

Now restrict to $d<4$. The spectrum of R is $\left\{\ \frac{1}{(\mathbf{b}-\mathbf{k})^2-\lambda}\ \Big|\ \mathbf{b}\in\Gamma^\#\ \right\}$ and its set of singular values is $\left\{\ \frac{1}{|(\mathbf{b}-\mathbf{k})^2-\lambda|}\ \Big|\ \mathbf{b}\in\Gamma^\#\ \right\}$. To prove that R is Hilbert-Schmidt, we must prove that

$$\sum_{\mathbf{b}\in\Gamma^\#}\left|\tfrac{1}{(\mathbf{b}-\mathbf{k})^2-\lambda}\right|^2<\infty$$

Choose any $\mathbf{b}_1,\cdots,\mathbf{b}_d$ such that

$$\Gamma^\#=\left\{\ n_1\mathbf{b}_1+\cdots+n_d\mathbf{b}_d\ \big|\ n_1,\cdots,n_d\in\mathbb{Z}\ \right\}$$

Let B be the $d\times d$ matrix whose (i,j) matrix element is $\mathbf{b}_i\cdot\mathbf{b}_j$. For every nonzero $\mathbf{x}=(x_1,\cdots,x_d)\in\mathbb{C}^d$

$$\mathbf{x}\cdot B\mathbf{x}=|x_1\mathbf{b}_1+\cdots x_d\mathbf{b}_d|^2>0$$

since the $\mathbf{b}_i$, $1\le i\le d$ are independent. Consequently, all of the eigenvalues of B are strictly larger than zero. Let β be the smallest eigenvalue of B. Then

$$|x_1\mathbf{b}_1+\cdots x_d\mathbf{b}_d|^2=\mathbf{x}\cdot B\mathbf{x}\ge\beta|\mathbf{x}|^2$$

Hence if $\mathbf{b} = n_1\mathbf{b}_1 + \cdots + n_d\mathbf{b}_d$ and $\mathbf{n}^2 = \big|(n_1,\cdots,n_d)\big|^2 \ge \frac{4}{\beta}\big(\mathbf{k}^2 + |\lambda|\big)$

$$\big|(\mathbf{b}-\mathbf{k})^2 - \lambda\big| \ge \tfrac{1}{2}\mathbf{b}^2 - \mathbf{k}^2 - |\lambda| \ge \tfrac{\beta}{2}\mathbf{n}^2 - \mathbf{k}^2 - |\lambda| \ge \tfrac{\beta}{2}\mathbf{n}^2 - \tfrac{\beta}{4}\mathbf{n}^2 \ge \tfrac{\beta}{4}\mathbf{n}^2$$

so that

$$\begin{aligned}
\sum_{\mathbf{b}\in\Gamma^\#} \Big|\tfrac{1}{(\mathbf{b}-\mathbf{k})^2-\lambda}\Big|^2 &= \sum_{\mathbf{n}\in\mathbb{Z}^d} \Big|\tfrac{1}{(n_1\mathbf{b}_1+\cdots+n_d\mathbf{b}_d-\mathbf{k})^2-\lambda}\Big|^2 \\
&\le \sum_{\substack{\mathbf{n}\in\mathbb{Z}^d \\ \mathbf{n}^2\le\frac{4}{\beta}(\mathbf{k}^2+|\lambda|)}} \Big|\tfrac{1}{(n_1\mathbf{b}_1+\cdots+n_d\mathbf{b}_d-\mathbf{k})^2-\lambda}\Big|^2 + \sum_{\substack{\mathbf{n}\in\mathbb{Z}^d \\ \mathbf{n}^2>\frac{4}{\beta}(\mathbf{k}^2+|\lambda|)}} \Big|\tfrac{4}{\beta\mathbf{n}^2}\Big|^2 \\
&\le \#\big\{\ \mathbf{n}\in\mathbb{Z}^d\ \big|\ \mathbf{n}^2 \le \tfrac{4}{\beta}(\mathbf{k}^2+|\lambda|)\ \big\} \max_{\substack{\mathbf{n}\in\mathbb{Z}^d \\ \mathbf{n}^2\le\frac{4}{\beta}(\mathbf{k}^2+|\lambda|)}} \Big|\tfrac{1}{(n_1\mathbf{b}_1+\cdots+n_d\mathbf{b}_d-\mathbf{k})^2-\lambda}\Big|^2 \\
&\qquad + \tfrac{16}{\beta^2}\sum_{\substack{\mathbf{n}\in\mathbb{Z}^d \\ \mathbf{n}\ne 0}} \tfrac{1}{|\mathbf{n}|^4}
\end{aligned}$$

This is finite because $d < 4$ and we have assumed that $(\mathbf{b}-\mathbf{k})^2 - \lambda$ does not vanish for any $\mathbf{b}\in\Gamma^\#$. ■

Lemma S.8 *The following hold for all* $\mathbf{k}\in\mathbb{R}^d$.

a) The operator $H_\mathbf{k}$ *is self–adjoint on the domain*

$$\mathcal{D} = \big\{\ \mathcal{F}^{-1}\varphi\ \big|\ \varphi(\mathbf{b}),\ \mathbf{b}^2\varphi(\mathbf{b}) \in \ell^2(\Gamma^\#)\ \big\}$$

and essentially self–adjoint on the domain

$$\mathcal{D}_0 = \big\{\ \mathcal{F}^{-1}\varphi\ \big|\ \varphi(\mathbf{b}) = 0 \text{ for all but finitely many } \mathbf{b}\in\Gamma^\#\ \big\}$$

b) If λ *is not in the spectrum of* $H_\mathbf{k}$*, the resolvent* $\big[H_\mathbf{k} - \lambda\mathbb{1}\big]^{-1}$ *is compact. If* $d < 4$ *it is Hilbert-Schmidt. If* $\operatorname{Im}\lambda \ne 0$ *or* $\lambda < -\sup_\mathbf{x}|V(\mathbf{x})|$*, then* λ *is not in the spectrum of* $H_\mathbf{k}$.

c) Let $R > 0$*. There is a constant* C *such that*

$$\Big\|\big(H_\mathbf{k} - H_{\mathbf{k}'}\big)\tfrac{1}{1-\Delta}\Big\| \le C|\mathbf{k}-\mathbf{k}'|$$

for all $\mathbf{k},\mathbf{k}'\in\mathbb{R}^d$ *with* $|\mathbf{k}|, |\mathbf{k}'| \le R$*. The constant* C *depends on* V *and* R*, but is otherwise independent of* $\mathbf{k}$ *and* $\mathbf{k}'$.

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

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

for all $\mathbf{k}, \mathbf{k}' \in \mathbb{R}^d$ *with* $|\mathbf{k}|, |\mathbf{k}'| \le R$. *The constant* C' *depends on* V, λ *and* R, *but is otherwise independent of* $\mathbf{k}$ *and* $\mathbf{k}'$.

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

$$U_\mathbf{c}^* H_\mathbf{k} U_\mathbf{c} = H_{\mathbf{k}+\mathbf{c}}$$

Proof: a) $\big(i\nabla - \mathbf{k}\big)^2$ is self–adjoint on $\mathcal{D}$ and essentially self–adjoint on $\mathcal{D}_0$ and $V(\mathbf{x})$ is a bounded operator on $L^2\big(\mathbb{R}^d/\Gamma\big)$. Apply Lemma S.6.

b) If λ is not in the spectrum of $H_\mathbf{k}$, the resolvent $\big[H_\mathbf{k} - \lambda 1\!\!1\big]^{-1}$ exists and is bounded. This is just the definition of "spectrum". As $H_\mathbf{k}$ is self–adjoint, its spectrum is a subset of $\mathbb{R}$. Now consider $\lambda < -\sup_\mathbf{x}|V(\mathbf{x})|$. As $\big[\big(i\nabla - \mathbf{k}\big)^2 - \lambda 1\!\!1\big]^{-1}$ is unitarily equivalent to multiplication by $\frac{1}{(\mathbf{b}-\mathbf{k})^2 - \lambda 1\!\!1} \le \frac{1}{|\lambda|}$, it is a bounded operator with norm at most $\frac{1}{|\lambda|}$. As $\lambda < -\sup_\mathbf{x}|V(\mathbf{x})|$, $\big[\big(i\nabla - \mathbf{k}\big)^2 - \lambda 1\!\!1\big]^{-1} V$ has operator norm at most $\sup_\mathbf{x}|V(\mathbf{x})|/|\lambda| < 1$ and

$$\Big\|\frac{1}{H_\mathbf{k} - \lambda 1\!\!1}\Big\| = \Big\|\frac{1}{1\!\!1 + \frac{1}{(i\nabla-\mathbf{k})^2 - \lambda 1\!\!1}V}\,\frac{1}{\big(i\nabla - \mathbf{k}\big)^2 - \lambda 1\!\!1}\Big\| \le \frac{1}{1 - \frac{\sup_\mathbf{x}|V(\mathbf{x})|}{|\lambda|}}\,\frac{1}{|\lambda|} = \frac{1}{|\lambda| - \sup_\mathbf{x}|V(\mathbf{x})|}$$

Hence the spectrum of $H_\mathbf{k}$ is a subset of $[-\sup_\mathbf{x}|V(\mathbf{x})|, \infty)$.

By the resolvent identity

$$\begin{aligned}\big[H_\mathbf{k} - \lambda 1\!\!1\big]^{-1} &= \big[\big(i\nabla - \mathbf{k}\big)^2 + 1\!\!1\big]^{-1} - \big[H_\mathbf{k} - \lambda 1\!\!1\big]^{-1}[V - (1+\lambda)1\!\!1)]\big[\big(i\nabla - \mathbf{k}\big)^2 + 1\!\!1\big]^{-1} \\ &= \Big\{1\!\!1 - \big[H_\mathbf{k} - \lambda 1\!\!1\big]^{-1}[V - (1+\lambda)1\!\!1)]\Big\}\big[\big(i\nabla - \mathbf{k}\big)^2 + 1\!\!1\big]^{-1}\end{aligned}$$

The left factor $\Big\{1\!\!1 - \big[H_\mathbf{k} - \lambda 1\!\!1\big]^{-1}[V - (1+\lambda)1\!\!1)]\Big\}$ is a bounded operator and, by Lemma S.7, the right factor $\big[\big(i\nabla - \mathbf{k}\big)^2 + 1\!\!1\big]^{-1}$ is compact (Hilbert-Schmidt for $d < 4$), so the product is compact (Hilbert-Schmidt for $d < 4$).

c) First observe that, by Problem S.6 below, $\frac{1}{1\!\!1-\Delta}$ maps all of $L^2(\mathbb{R}^d/\Gamma)$ into $\mathcal{D}$ so that $H_\mathbf{k}\frac{1}{1-\Delta}$ and $H_{\mathbf{k}'}\frac{1}{1-\Delta}$ are both defined on all of $L^2\big(\mathbb{R}^d/\Gamma\big)$. Expanding gives

$$\big(H_\mathbf{k} - H_{\mathbf{k}'}\big)\tfrac{1}{1-\Delta} = \big[\big(i\nabla - \mathbf{k}\big)^2 - \big(i\nabla - \mathbf{k}'\big)^2\big]\tfrac{1}{1-\Delta} = \big[-2i(\mathbf{k} - \mathbf{k}')\cdot\nabla + \mathbf{k}^2 - \mathbf{k}'^2\big]\tfrac{1}{1-\Delta}$$

Hence $\mathcal{F}\big(H_\mathbf{k} - H_{\mathbf{k}'}\big)\frac{1}{1-\Delta}\mathcal{F}^{-1}$ is the multiplication operator

$$\tfrac{2(\mathbf{k}-\mathbf{k}')\cdot\mathbf{b} + \mathbf{k}^2 - \mathbf{k}'^2}{1+\mathbf{b}^2} = (\mathbf{k} - \mathbf{k}')\cdot\tfrac{2\mathbf{b}+\mathbf{k}+\mathbf{k}'}{1+\mathbf{b}^2}$$

The claim then follows from

$$\Big|\tfrac{2\mathbf{b}+\mathbf{k}+\mathbf{k}'}{1+\mathbf{b}^2}\Big| \le \tfrac{2|\mathbf{b}|+2R}{1+\mathbf{b}^2} \le \tfrac{1+\mathbf{b}^2+2R}{1+\mathbf{b}^2} \le 1 + 2R$$

d) By the resolvent identity

$$\begin{aligned}\frac{1}{H_{\mathbf{k}}-\lambda\mathbb{1}}-\frac{1}{H_{\mathbf{k}'}-\lambda\mathbb{1}}&=\frac{1}{H_{\mathbf{k}}-\lambda\mathbb{1}}\big[H_{\mathbf{k}'}-H_{\mathbf{k}}\big]\frac{1}{H_{\mathbf{k}'}-\lambda\mathbb{1}}\\&=\frac{1}{H_{\mathbf{k}}-\lambda\mathbb{1}}\big[H_{\mathbf{k}'}-H_{\mathbf{k}}\big]\frac{1}{1-\Delta}\,\frac{1-\Delta}{(i\nabla-\mathbf{k}')^2-\lambda\mathbb{1}}\,\frac{1}{\mathbb{1}+V\frac{1}{(i\nabla-\mathbf{k}')^2-\lambda\mathbb{1}}}\end{aligned}$$

By part c and the bound on the resolvent in part b,

$$\Big\|\tfrac{1}{H_{\mathbf{k}}-\lambda\mathbb{1}}-\tfrac{1}{H_{\mathbf{k}'}-\lambda\mathbb{1}}\Big\|\le\tfrac{1}{|\lambda|-\sup_{\mathbf{x}}|V(\mathbf{x})|}C|\mathbf{k}-\mathbf{k}'|\Big\|\tfrac{1-\Delta}{(i\nabla-\mathbf{k}')^2-\lambda\mathbb{1}}\Big\|\tfrac{|\lambda|}{|\lambda|-\sup_{\mathbf{x}}|V(\mathbf{x})|}$$

As $\frac{1-\Delta}{(i\nabla-\mathbf{k}')^2-\lambda\mathbb{1}}$ is unitarily equivalent to multiplication by $\frac{1+\mathbf{b}^2}{(\mathbf{b}-\mathbf{k}')^2-\lambda}$, $\big\|\frac{1-\Delta}{(i\nabla-\mathbf{k}')^2-\lambda\mathbb{1}}\big\|$ is bounded uniformly on $|\mathbf{k}'|<R$.

e) Since multiplication operators commute, $U_{\mathbf{c}}^*VU_{\mathbf{c}}=U_{\mathbf{c}}^*U_{\mathbf{c}}V=V$ and the claim follows immediately from Problem S.5, below.

■

Problem S.5 Let $\mathbf{c}\in\Gamma^{\#}$ and $U_{\mathbf{c}}$ be the multiplication operator $e^{i\mathbf{c}\cdot\mathbf{x}}$ on $L^2(\mathbb{R}^d/\Gamma)$. Let $\mathcal{F}$ be the Fourier transform operator of (S.3).

a) Fill in the formulae

$$\begin{aligned}\big(\mathcal{F}U_{\mathbf{c}}\mathcal{F}^{-1}\varphi\big)(\mathbf{b})&=\qquad\varphi(\mathbf{b}\qquad)\\\big(\mathcal{F}U_{\mathbf{c}}^*\mathcal{F}^{-1}\varphi\big)(\mathbf{b})&=\qquad\varphi(\mathbf{b}\qquad)\end{aligned}$$

b) Prove that $U_{\mathbf{c}}$ and $U_{\mathbf{c}}^*$ both leave the domain $\mathcal{D}$ invariant.

c) Prove that

$$U_{\mathbf{c}}^*\big(i\nabla-\mathbf{k}\big)^2U_{\mathbf{c}}=\big(i\nabla-\mathbf{k}-\mathbf{c}\big)^2$$

Problem S.6 Prove that $\frac{1}{\mathbb{1}-\Delta}$ maps all of $L^2(\mathbb{R}^d/\Gamma)$ into $\mathcal{D}$.

§IV The spectrum of H

We have just proven that the spectrum of the operator $H_{\mathbf{k}}$ (acting on $L^2(\mathbb{R}^d/\Gamma)$) is contained in the half of the real line to the right of $-\sup_{\mathbf{x}}|V(\mathbf{x})|$. We have also just proven that the resolvent of $H_{\mathbf{k}}$ is compact. Hence the spectrum of $\big[H_{\mathbf{k}}-\lambda\mathbb{1}\big]^{-1}$ (for any fixed suitable λ) is a sequence of eigenvalues converging to zero, so that the spectrum of $H_{\mathbf{k}}$ consists of a sequence of eigenvalues converging to $+\infty$. Denote the eigenvalues of $H_{\mathbf{k}}$ by

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

Proposition S.9

a) For each n, $e_n(\mathbf{k})$ is continuous in $\mathbf{k}$ and periodic with respect to $\Gamma^\#$.

b) $\lim_{n\to\infty} e_n(\mathbf{k}) = \infty$, with the limit uniform in $\mathbf{k}$.

c) Denote by V_d the volume of a sphere of radius one in $\mathbb{R}^d$. Let $\mathbf{b}_1, \cdots, \mathbf{b}_d$ be any set of generators for $\Gamma^\#$ and $B = \big\{ \sum_{j=1}^d t_j \mathbf{b}_j \ \big|\ -\frac{1}{2} \le t_j < \frac{1}{2} \text{ for all } 1 \le j \le d \big\}$ be the parallelepiped, centered on the origin, with the $\mathbf{b}_j$'s as edges. Denote by D the diameter of B. For each $\mathbf{k} \in \mathbb{R}^d$ and each $R > 0$

$$\#\big\{ \ n \in \mathbb{N} \ \big|\ e_n(\mathbf{k}) < R \ \big\} \le \tfrac{V_d}{|\Gamma^\#|}\big(\sqrt{R + \|V\|} + \tfrac{1}{2}D\big)^d = \tfrac{V_d}{|\Gamma^\#|} R^{d/2} + O\big(R^{\frac{d-1}{2}}\big)$$

For each $\mathbf{k} \in \mathbb{R}^d$ and each $R > \frac{1}{4}D^2 + \|V\|$

$$\#\big\{ \ n \in \mathbb{N} \ \big|\ e_n(\mathbf{k}) < R \ \big\} \ge \tfrac{V_d}{|\Gamma^\#|}\big(\sqrt{R - \|V\|} - \tfrac{1}{2}D\big)^d = \tfrac{V_d}{|\Gamma^\#|} R^{d/2} + O\big(R^{\frac{d-1}{2}}\big)$$

This more detailed result concerning the rate at which $e_n(\mathbf{k})$ tends to infinity with n is not used in these notes and so may be safely skipped.

Proof: b) Denote, in increasing order, the eigenvalues of $\big(i\boldsymbol{\nabla} - \mathbf{k}\big)^2$

$$\hat{e}_1(\mathbf{k}) \le \hat{e}_2(\mathbf{k}) \le \hat{e}_3(\mathbf{k}) \le \cdots$$

Each $\hat{e}_n(\mathbf{k})$ is $(\mathbf{b} - \mathbf{k})^2$, for some $\mathbf{b} \in \Gamma^\#$. Furthermore, by Lemma S.7, the spectrum of $\big(i\boldsymbol{\nabla} - \mathbf{k}\big)^2$ is periodic in $\mathbf{k}$, so that each $\hat{e}_n(\mathbf{k})$ is periodic in $\mathbf{k}$. We have already observed that $(\mathbf{b} - \mathbf{k})^2 \ge \frac{1}{2}\mathbf{b}^2 - \mathbf{k}^2$, so that, as n tends to infinity, $\hat{e}_n(\mathbf{k})$ tends to infinity, uniformly in $\mathbf{k}$.

By the min-max principle

$$\begin{aligned}
e_n(\mathbf{k}) &= \sup_{\varphi_1,\cdots,\varphi_{n-1}} \ \inf_{\substack{\psi\in\mathcal{D},\ \|\psi\|=1 \\ \psi\perp\varphi_1,\cdots,\varphi_{n-1}}} \ \langle \psi, H_{\mathbf{k}}\psi\rangle \\
&= \sup_{\varphi_1,\cdots,\varphi_{n-1}} \ \inf_{\substack{\psi\in\mathcal{D},\ \|\psi\|=1 \\ \psi\perp\varphi_1,\cdots,\varphi_{n-1}}} \ \Big(\big\langle \psi, (\mathbf{b}-\mathbf{k})^2\psi\big\rangle + \langle \psi, V\psi\rangle \Big) \\
\hat{e}_n(\mathbf{k}) &= \sup_{\varphi_1,\cdots,\varphi_{n-1}} \ \inf_{\substack{\psi\in\mathcal{D},\ \|\psi\|=1 \\ \psi\perp\varphi_1,\cdots,\varphi_{n-1}}} \ \big\langle \psi, (\mathbf{b}-\mathbf{k})^2\psi\big\rangle
\end{aligned}$$

For any unit vector ψ, $\big|\, \langle \psi, V\psi\rangle \,\big| \le \sup_{\mathbf{x}} |V(\mathbf{x})|$, so

$$\big|e_n(\mathbf{k}) - \hat{e}_n(\mathbf{k})\big| \le \sup_{\mathbf{x}} |V(\mathbf{x})|$$

and, as n tends to infinity, $e_n(\mathbf{k})$ tends to infinity, uniformly in $\mathbf{k}$.

a) Fix any $\lambda < -\sup_{\mathbf{x}} |V(\mathbf{x})|$. Denote, in increasing order, the eigenvalues of $-[H_{\mathbf{k}} - \lambda\mathbb{1}]^{-1}$

$$\tilde{e}_1(\mathbf{k}) \le \tilde{e}_2(\mathbf{k}) \le \tilde{e}_3(\mathbf{k}) \le \cdots$$

As

$$\begin{aligned}\big(\varphi, [H_{\mathbf{k}} - \lambda\mathbb{1}]\varphi\big) &= \big(\varphi, \big(i\nabla - \mathbf{k}\big)^2\varphi\big) + \big(\varphi, [V - \lambda\mathbb{1}]\varphi\big)\\ &\ge \int_{\mathbb{R}^d/\Gamma} [V(\mathbf{x}) - \lambda]\big|\varphi(\mathbf{x})\big|^2\, d\mathbf{x}\\ &\ge \big[|\lambda| - \sup_{\mathbf{x}} |V(\mathbf{x})|\big]\,(\varphi,\varphi)\end{aligned}$$

for all $\varphi \in \mathcal{D}$, $\tilde{e}_n(\mathbf{k}) < 0$ and

$$e_n(\mathbf{k}) = -\tfrac{1}{\tilde{e}_n(\mathbf{k})} + \lambda$$

for all n. Pick any $R > 0$. By Lemma S.8.d, for all unit vectors φ and all $\mathbf{k}, \mathbf{k}'$ with $|\mathbf{k}|, |\mathbf{k}'| < R$,

$$\Big|\Big\langle \varphi, \big[\tfrac{1}{H_{\mathbf{k}} - \lambda\mathbb{1}} - \tfrac{1}{H_{\mathbf{k}'} - \lambda\mathbb{1}}\big]\varphi\Big\rangle\Big| \le C'|\mathbf{k} - \mathbf{k}'|$$

Consequently, by the min-max principle, applied to $A = -\frac{1}{H_{\mathbf{k}} - \lambda\mathbb{1}}$ and $B = -\frac{1}{H_{\mathbf{k}'} - \lambda\mathbb{1}}$

$$\big|\tilde{e}_n(\mathbf{k}) - \tilde{e}_n(\mathbf{k}')\big| \le C'|\mathbf{k} - \mathbf{k}'|$$

Hence, each $\tilde{e}_n(\mathbf{k})$, and consequently each $e_n(\mathbf{k})$, is continuous.

c) By Lemma S.7, the spectrum of $\big(i\nabla - \mathbf{k}\big)^2$ is $\big\{\ (\mathbf{b} - \mathbf{k})^2 \ \big|\ \mathbf{b} \in \Gamma^{\#}\ \big\}$. Label these eigenvalues, in order, $f_1(\mathbf{k}) \le f_2(\mathbf{k}) \le f_3(\mathbf{k}) \le \cdots$. Observe that $H_{\mathbf{k}}$ and $\big(i\nabla - \mathbf{k}\big)^2$ both have domain $\mathcal{D}$ and that, for every $\varphi \in \mathcal{D}$,

$$\Big|\Big\langle \varphi, \big[H_{\mathbf{k}} - \big(i\nabla - \mathbf{k}\big)^2\big]\varphi\Big\rangle\Big| = \big|\,\langle \varphi, V\varphi\rangle\,\big| \le \|V\|\,\|\varphi\|^2$$

Hence, by the min-max principle,

$$\big|e_n(\mathbf{k}) - f_n(\mathbf{k})\big| \le \|V\|$$

for all n and $\mathbf{k}$ so that, for all $R > 0$,

$$\begin{aligned}\#\big\{\ n \in \mathbb{N}\ \big|\ e_n(\mathbf{k}) < R\ \big\} &\le \#\big\{\ n \in \mathbb{N}\ \big|\ f_n(\mathbf{k}) < R + \|V\|\ \big\}\\ \#\big\{\ n \in \mathbb{N}\ \big|\ f_n(\mathbf{k}) < R\ \big\} &\le \#\big\{\ n \in \mathbb{N}\ \big|\ e_n(\mathbf{k}) < R + \|V\|\ \big\}\end{aligned} \tag{S.4}$$

Let $\mathbf{b} + B$ be the half open parallelepiped, centered on $\mathbf{b}$, with edges parallel to the $\mathbf{b}_j$'s. Then $\big\{\ \mathbf{b} + B\ \big|\ \mathbf{b} \in \Gamma^{\#}\ \big\}$ is a paving of $\mathbb{R}^d$. This means that $(\mathbf{b} + B) \cap (\mathbf{b}' + B) = \emptyset$ unless $\mathbf{b} = \mathbf{b}'$ and every point in $\mathbb{R}^d$ is in some $\mathbf{b} + B$. So, for each $r > 0$

$$\begin{aligned}\#\big\{\ n \in \mathbb{N}\ \big|\ f_n(\mathbf{k}) < r\ \big\} &= \#\big\{\ \mathbf{b} \in \Gamma^{\#}\ \big|\ |\mathbf{b} - \mathbf{k}| < \sqrt{r}\ \big\}\\ &= \tfrac{1}{|\Gamma^{\#}|}\mathrm{Volume}\Big(\cup_{b \in S_r}\ \mathbf{b} + B\Big)\end{aligned} \tag{S.5}$$

where $S_r = \{\ \mathbf{b}\in\Gamma^\# \bigm| |\mathbf{b}-\mathbf{k}| < \sqrt{r}\ \}$.

Every point of $\mathbf{b}+B$ lies within distance of $\frac{1}{2}D$ of $\mathbf{b}$, so every point of $\cup_{b\in S_r}\mathbf{b}+B$ lies within a distance $\sqrt{r}+\frac{1}{2}D$ of $\mathbf{k}$. On the other hand, if $\mathbf{p}\in\mathbb{R}^d$ lies within a distance $\sqrt{r}-\frac{1}{2}D$ of $\mathbf{k}$, then $\mathbf{p}$ lies in precisely one $\mathbf{b}+B$ and that $\mathbf{b}$ obeys $|\mathbf{p}-\mathbf{b}|\le\frac{1}{2}D$ and hence $|\mathbf{b}-\mathbf{k}|\le\sqrt{r}-\frac{1}{2}D+\frac{1}{2}D\le\sqrt{r}$. Thus

$$V_d\big(\sqrt{r}-\tfrac{1}{2}D\big)^d \le \mathrm{Volume}\Big(\cup_{b\in S_r}\,\mathbf{b}+B\Big) \le V_d\big(\sqrt{r}+\tfrac{1}{2}D\big)^d \tag{S.6}$$

Subbing (S.6) in (S.5) gives

$$\tfrac{V_d}{|\Gamma^\#|}\big(\sqrt{r}-\tfrac{1}{2}D\big)^d \le \#\{\ n\in\mathbb{N} \bigm| f_n(\mathbf{k})<r\ \} \le \tfrac{V_d}{|\Gamma^\#|}\big(\sqrt{r}+\tfrac{1}{2}D\big)^d$$

and subbing this into (S.4) gives the desired bounds.

■

Problem S.7 Let $\mathbf{b}_1,\cdots,\mathbf{b}_d$ be any set of generators for $\Gamma^\#$ and

$$B = \Big\{\ \sum_{j=1}^d t_j\mathbf{b}_j \Bigm| -\tfrac{1}{2}\le t_j<\tfrac{1}{2} \text{ for all } 1\le j\le d\ \Big\}$$

Prove that $\{\ \mathbf{b}+B \bigm| \mathbf{b}\in\Gamma^\#\ \}$ is a paving of $\mathbb{R}^d$.

Theorem S.10 *Let V be a C^∞ function of $\mathbb{R}^d$ that is periodic with respect to the lattice Γ and $H=\big(i\boldsymbol{\nabla}\big)^2+V(\mathbf{x})$ the self–adjoint operator of Theorem S.5. The spectrum of H is*

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

Proof: Denote by Σ_H the spectrum of H and by

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

the set of all eigenvalues of all the $H_{\mathbf{k}}$'s.

Proof that $S\subset\Sigma_H$: Fix any $\mathbf{p}\in\mathbb{R}^d$ and any $n\in\mathbb{N}$. We shall construct, for each $\varepsilon>0$, a vector $\psi_\varepsilon\in\mathcal{S}\big(\mathbb{R}^d/\Gamma^\#\times\mathbb{R}^d/\Gamma\big)$ obeying

$$\big\|\big(\tilde{u}Hu-e_n(\mathbf{p})\mathbb{1}\big)\psi_\varepsilon\big\| \le \varepsilon\|\psi\|$$

This will prove that $\big[\tilde u H u - e_n(\mathbf{p})\mathbb{1}\big]^{-1}$ and hence $\big[H - e_n(\mathbf{p})\mathbb{1}\big]^{-1}$ cannot be a bounded operator with norm at most $\frac{1}{\varepsilon}$, for any $\varepsilon > 0$; hence that $\big[H - e_n(\mathbf{p})\mathbb{1}\big]^{-1}$ cannot be a bounded operator and hence that $e_n(\mathbf{p}) \in \Sigma_H$.

By hypothesis, $e_n(\mathbf{p})$ is an eigenvalue of $H_{\mathbf{p}}$. So there is a nonzero vector $\tilde\varphi(\mathbf{x}) \in \mathcal{D}$ such that $\big[H_{\mathbf{p}} - e_n(\mathbf{p})\big]\tilde\varphi = 0$. As $H_{\mathbf{p}}$ is essentially self–adjoint on $\mathcal{D}_0$, there is a sequence of functions $\varphi_m(\mathbf{x}) \in \mathcal{D}_0$ obeying

$$\begin{array}{lll} & \lim\limits_{m\to\infty} \varphi_m = \tilde\varphi & \lim\limits_{m\to\infty} H_{\mathbf{p}}\varphi_m = H_{\mathbf{p}}\tilde\varphi \\ \Longrightarrow & \lim\limits_{m\to\infty} \|\varphi_m\| = \|\tilde\varphi\| \ne 0 & \lim\limits_{m\to\infty} \big\|\big(H_{\mathbf{p}} - e_n(\mathbf{p})\mathbb{1}\big)\varphi_m\big\| = 0 \end{array}$$

Hence there is a member of that sequence, call it $\varphi_\varepsilon(\mathbf{x})$, for which

$$\big\|\big(H_{\mathbf{p}} - e_n(\mathbf{p})\mathbb{1}\big)\varphi_\varepsilon\big\| \le \tfrac{\varepsilon}{2}\|\varphi_\varepsilon\|$$

Let $f(\mathbf{k})$ be any nonnegative C^∞ function that is supported in $\big\{\ \mathbf{k} \in \mathbb{R}^d\ \big|\ |\mathbf{k}| < 1\ \big\}$ and whose square has integral one. Define, for each $\delta > 0$,

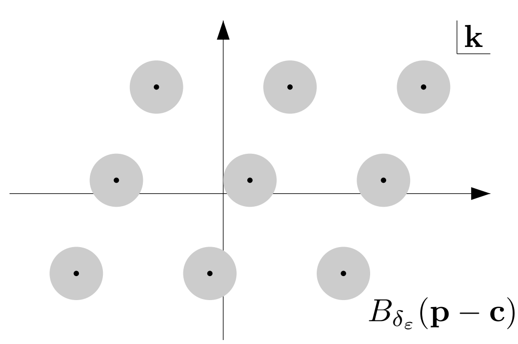
$$f_\delta(\mathbf{k}) = \tfrac{1}{\delta^{d/2}} f\big(\tfrac{\mathbf{k}}{\delta}\big)$$

Observe that $f_\delta(\mathbf{k})$ is a nonnegative C^∞ function that is supported in $\big\{\ \mathbf{k} \in \mathbb{R}^d\ \big|\ |\mathbf{k}| < \delta\ \big\}$ and whose square has integral one. Set

$$\psi_\varepsilon(\mathbf{k},\mathbf{x}) = \sum_{\mathbf{c}\in\Gamma^\#} e^{i\mathbf{c}\cdot\mathbf{x}} f_{\delta_\varepsilon}(\mathbf{k} - \mathbf{p} + \mathbf{c})\varphi_\varepsilon(\mathbf{x})$$

We shall choose δ_ε later. The function $\psi_\varepsilon(\mathbf{k},\mathbf{x})$ is in $\mathcal{S}\big(\mathbb{R}^d/\Gamma^\# \times \mathbb{R}^d/\Gamma\big)$ because

- the term $f_{\delta_\varepsilon}(\mathbf{k} - \mathbf{p} + \mathbf{c})\varphi_\varepsilon(\mathbf{x})$ vanishes unless $\mathbf{k}$ is within a distance δ_ε of $\mathbf{p} - \mathbf{c}$. Hence ψ_ε vanishes unless $\mathbf{k} \in B_{\delta_\varepsilon}(\mathbf{p} - \mathbf{c})$, the ball of radius δ_ε centered on $\mathbf{p} - \mathbf{c}$, for some $\mathbf{c} \in \Gamma^\#$. There is a nonzero lower bound on the distance between points of $\Gamma^\#$. We will choose δ_ε to be strictly smaller than half that lower bound. Then the balls $B_{\delta_\varepsilon}(\mathbf{p} - \mathbf{c}),\ \mathbf{c} \in \Gamma^\#$ are disjoint. For $\mathbf{k}$ outside their union $\psi_\varepsilon(\mathbf{k},\mathbf{x})$ vanishes. For $\mathbf{k}$ in $B_{\delta_\varepsilon}(\mathbf{p} - \mathbf{c}_0)$ the only term in the sum that does not vanish is that with $\mathbf{c} = \mathbf{c}_0$. Consequently $\psi_\varepsilon(\mathbf{k},\mathbf{x})$ is C^∞.



- $\psi_\varepsilon(\mathbf{k},\mathbf{x})$ is periodic in $\mathbf{x}$ with respect to Γ because $\varphi_\varepsilon(\mathbf{x})$ is.
- $$\begin{aligned}\psi_\varepsilon(\mathbf{k}+\mathbf{b},\mathbf{x}) &= \sum_{\mathbf{c}\in\Gamma^\#} e^{i\mathbf{c}\cdot\mathbf{x}} f_{\delta_\varepsilon}(\mathbf{k}+\mathbf{b}-\mathbf{p}+\mathbf{c})\varphi_\varepsilon(\mathbf{x})\\ &= \sum_{\mathbf{c}'\in\Gamma^\#} e^{i(\mathbf{c}'-\mathbf{b})\cdot\mathbf{x}} f_{\delta_\varepsilon}(\mathbf{k}-\mathbf{p}+\mathbf{c}')\varphi_\varepsilon(\mathbf{x})\\ &= e^{-i\mathbf{b}\cdot\mathbf{x}}\psi_\varepsilon(\mathbf{k},\mathbf{x})\end{aligned}$$

  so $\psi_\varepsilon(\mathbf{k},\mathbf{x})$ has the required "twisted" periodicity in $\mathbf{k}$.

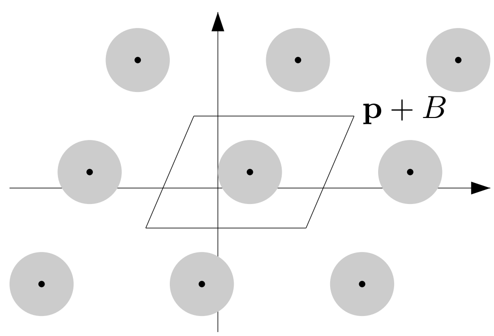
The square of the norm

$$\big\|\big(\tilde u H u - e_n(\mathbf{p})\mathbb{1}\big)\psi_\varepsilon\big\|^2 = \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d\mathbf{k} \int_{\mathbb{R}^d/\Gamma} d\mathbf{x}\ \ \big|\big((\tilde u H u - e_n(\mathbf{p})\mathbb{1})\psi_\varepsilon\big)(\mathbf{k},\mathbf{x})\big|^2$$

By Problem L.4 of the notes "Lattices and Periodic Functions", we may choose

$$\mathbf{p}+B = \mathbf{p}+\Big\{\ \sum_{j=1}^d t_j\mathbf{b}_j\ \Big|\ -\tfrac12\le t_j<\tfrac12 \text{ for all } 1\le j\le d\ \Big\}$$

as the domain of integration in $\mathbf{k}$. This domain contains the ball $B_{\delta_\varepsilon}(\mathbf{p}-\mathbf{c})$ with $\mathbf{c}=\mathbf{0}$ and does not intersect $B_{\delta_\varepsilon}(\mathbf{p}-\mathbf{c})$ for any $\mathbf{c}\in\Gamma^\#\setminus\{\mathbf{0}\}$ (again assuming that δ_ε has been chosen



sufficiently small). On $\mathbf{p}+B$, $\psi_\varepsilon(\mathbf{k},\mathbf{x}) = f_{\delta_\varepsilon}(\mathbf{k}-\mathbf{p})\varphi_\varepsilon(\mathbf{x})$ and

$$\big((\tilde u H u - e_n(\mathbf{p})\mathbb{1})\psi_\varepsilon\big)(\mathbf{k},\mathbf{x}) = f_{\delta_\varepsilon}(\mathbf{k}-\mathbf{p})\big(H_\mathbf{k}-e_n(\mathbf{p})\mathbb{1})\varphi_\varepsilon\big)(\mathbf{x})$$

so that

$$\begin{aligned}\big\|\big(\tilde u H u - e_n(\mathbf{p})\mathbb{1}\big)\psi_\varepsilon\big\|^2 &= \tfrac{1}{|\Gamma^\#|}\int d\mathbf{k}\int_{\mathbb{R}^d/\Gamma} d\mathbf{x}\quad f_{\delta_\varepsilon}(\mathbf{k}-\mathbf{p})^2\ \big|\big(H_\mathbf{k}-e_n(\mathbf{p})\mathbb{1})\varphi_\varepsilon\big)(\mathbf{x})\big|^2\\ &= \tfrac{1}{|\Gamma^\#|}\int d\mathbf{k}\ f_{\delta_\varepsilon}(\mathbf{k}-\mathbf{p})^2\big\|\big(H_\mathbf{k}-e_n(\mathbf{p})\mathbb{1}\big)\varphi_\varepsilon\big\|^2_{L^2(\mathbb{R}^d/\Gamma,d\mathbf{x})}\end{aligned}$$

The norm

$$\begin{aligned}\big\|\big(H_\mathbf{k}-e_n(\mathbf{p})\mathbb{1}\big)\varphi_\varepsilon\big\| &\le \big\|\big(H_\mathbf{p}-e_n(\mathbf{p})\mathbb{1}\big)\varphi_\varepsilon\big\| + \big\|\big(H_\mathbf{k}-H_\mathbf{p}\big)\varphi_\varepsilon\big\|\\ &\le \tfrac{\varepsilon}{2}\big\|\varphi_\varepsilon\big\| + \big\|\big(H_\mathbf{k}-H_\mathbf{p}\big)\tfrac{1}{\mathbb{1}-\Delta}\big\|\,\|(\mathbb{1}-\Delta)\varphi_\varepsilon\|\\ &\le \tfrac{\varepsilon}{2}\big\|\varphi_\varepsilon\big\| + C|\mathbf{k}-\mathbf{p}|\,\|(\mathbb{1}-\Delta)\varphi_\varepsilon\|\\ &\le \tfrac{\varepsilon}{2}\big\|\varphi_\varepsilon\big\| + C\delta_\varepsilon\,\|(\mathbb{1}-\Delta)\varphi_\varepsilon\|\end{aligned}$$

for $\mathbf{k}$ in the support of $f_{\delta_\varepsilon}(\mathbf{k}-\mathbf{p})$. Now choose

$$\delta_\varepsilon = \tfrac{\varepsilon}{2C}\tfrac{\|\varphi_\varepsilon\|}{\max\{1,\|(\mathbb{1}-\Delta)\varphi_\varepsilon\|\}}$$

With this choice of δ_ε, $\big\|\big(H_{\mathbf{k}}-e_n(\mathbf{p})\mathbb{1}\big)\varphi_\varepsilon\big\|_{L^2(\mathbb{R}^d/\Gamma,d\mathbf{x})} \le \varepsilon\big\|\varphi_\varepsilon\big\|_{L^2(\mathbb{R}^d/\Gamma,d\mathbf{x})}$ so that

$$\big\|\big(\tilde{u}Hu-e_n(\mathbf{p})\mathbb{1}\big)\psi_\varepsilon\big\|^2 \le \tfrac{\varepsilon^2}{|\Gamma^\#|}\int d\mathbf{k}\ f_{\delta_\varepsilon}(\mathbf{k}-\mathbf{p})^2\|\varphi_\varepsilon\|^2_{L^2(\mathbb{R}^d/\Gamma,d\mathbf{x})} = \varepsilon^2\|\psi_\varepsilon\|^2$$

as desired.

Proof that $\Sigma_H \subset S$: Fix any $\lambda \notin S$. We must show that $\lambda \notin \Sigma_H$. As, for each fixed n, $e_n(\mathbf{k})$ is periodic and continuous in $\mathbf{k}$,

$$\inf_{\mathbf{k}}\big|e_n(\mathbf{k})-\lambda\big| > 0$$

By Lemma S.9.b,

$$\lim_{n\to\infty}\inf_{\mathbf{k}} e_n(\mathbf{k}) = \infty$$

Hence

$$D = \inf_{\substack{\mathbf{k}\in\mathbb{R}^d\\ n\in\mathbb{N}}}\big|e_n(\mathbf{k})-\lambda\big| > 0$$

By the spectral theorem

$$\big\|\big(H_{\mathbf{k}}-\lambda\mathbb{1}\big)\varphi\big\|_{L^2(\mathbb{R}^d/\Gamma,d\mathbf{x})} \ge D\big\|\varphi\big\|_{L^2(\mathbb{R}^d/\Gamma,d\mathbf{x})}$$

for all φ in the domain, $\mathcal{D}$, of $H_{\mathbf{k}}$ and in particular for all $\varphi\in C^\infty\big(\mathbb{R}^d/\Gamma\big)$. Consequently, for all $\psi(\mathbf{k},\mathbf{x})\in\mathcal{S}\big(\mathbb{R}^d/\Gamma^\#\times\mathbb{R}^d/\Gamma\big)$

$$\begin{aligned}
\big\|\big(\tilde{u}Hu-\lambda\mathbb{1}\big)\psi\big\|^2 &= \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d\mathbf{k}\int_{\mathbb{R}^d/\Gamma} d\mathbf{x}\ \ \big|\big((\tilde{u}Hu-\lambda\mathbb{1})\psi\big)(\mathbf{k},\mathbf{x})\big|^2\\
&= \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d\mathbf{k}\int_{\mathbb{R}^d/\Gamma} d\mathbf{x}\ \ \big|\big((H_{\mathbf{k}}-\lambda\mathbb{1})\psi\big)(\mathbf{k},\mathbf{x})\big|^2\\
&= \tfrac{1}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d\mathbf{k}\ \ \big\|(H_{\mathbf{k}}-\lambda\mathbb{1})\psi(\mathbf{k},\,\cdot\,)\big\|^2_{L^2(\mathbb{R}^d/\Gamma,d\mathbf{x})}\\
&\ge \tfrac{D^2}{|\Gamma^\#|}\int_{\mathbb{R}^d/\Gamma^\#} d\mathbf{k}\ \ \big\|\psi(\mathbf{k},\,\cdot\,)\big\|^2_{L^2(\mathbb{R}^d/\Gamma,d\mathbf{x})}\\
&= D^2\|\psi\|^2
\end{aligned}$$

Recall that u is a unitary map from $\mathcal{S}\big(\mathbb{R}^d/\Gamma^\#\times\mathbb{R}^d/\Gamma\big)$ onto $\mathcal{S}(\mathbb{R}^d)$. Hence

$$\big\|(H-\lambda\mathbb{1})f\big\| \ge D\|f\| \tag{S.7}$$

for all $f\in\mathcal{S}(\mathbb{R}^d)$. By Theorem S.5, H is essentially self–adjoint on $\mathcal{S}(\mathbb{R}^d)$, so (S.7) applies for all f in the domain of H and $\big[H-\lambda\mathbb{1}\big]^{-1}$ is a bounded operator with norm at most $\frac{1}{D}$. Hence λ is not in the spectrum of H. ■

§V A Nontrivial Example – the Lamé Equation

Fix two real numbers $\beta, \gamma > 0$. The Weierstrass function with primitive periods γ and $i\beta$ is the function $\wp : \mathbb{C} \to \mathbb{C}$ defined by

$$\wp(z) = \frac{1}{z^2} + \sum_{\substack{\omega \in \gamma\mathbb{Z} \oplus i\beta\mathbb{Z} \\ \omega \neq 0}} \frac{1}{(z-\omega)^2} - \frac{1}{\omega^2}$$

It is an elliptic function, which means that it is a meromorphic function that is doubly periodic. It is analytic everywhere except for a double pole at each point of $\gamma\mathbb{Z} \oplus i\beta\mathbb{Z}$ and it has periods γ and $i\beta$. The Weierstrass function is discussed in the notes "An Elliptic Function – The Weierstrass Function". The labels "W.*" refer to those notes. Two functions closely related to $\wp$ are

$$\sigma(z) = z \prod_{\substack{\omega \in \gamma\mathbb{Z} \oplus i\beta\mathbb{Z} \\ \omega \neq 0}} \left(1 - \tfrac{z}{\omega}\right) e^{\frac{z}{\omega} + \frac{1}{2}\frac{z^2}{\omega^2}}$$

$$\zeta(z) = \tfrac{\sigma'(z)}{\sigma(z)} = \tfrac{1}{z} + \sum_{\substack{\omega \in \gamma\mathbb{Z} \oplus i\beta\mathbb{Z} \\ \omega \neq 0}} \tfrac{1}{z-\omega} + \tfrac{1}{\omega} + \tfrac{z}{\omega^2}$$

As $\zeta'(z) = -\wp(z)$, ζ is an antiderivative of $-\wp$ and consequently is, except for some constants of integration, periodic too. Similarly, σ is the exponential of an antiderivative of ζ and it is not hard to determine how $\sigma(z+\gamma)$ and $\sigma(z+i\beta)$ are related to $\sigma(z)$.

Lemma W.4 *There are constants* $\eta_1 \in \mathbb{R}$ *and* $\eta_2 \in i\mathbb{R}$ *satisfying*

$$\eta_1 i\beta - \eta_2\gamma \ = \ 2\pi i$$

such that

$$\zeta(z+\gamma) = \zeta(z) + \eta_1 \qquad \zeta(z+i\beta) = \zeta(z) + \eta_2$$

$$\sigma(z+\gamma) = -\sigma(z)\ e^{\eta_1(z+\frac{\gamma}{2})} \qquad \sigma(z+i\beta) = -\sigma(z)\ e^{\eta_2(z+i\frac{\beta}{2})}$$

Now set, for $z \in \mathbb{C} \setminus \big(\gamma\mathbb{Z} \oplus i\beta\mathbb{Z}\big)$,

$$\varphi(z,x) \ = \ e^{\zeta(z)x}\ \frac{\sigma\big(z - x - i\frac{\beta}{2}\big)}{\sigma\big(x + i\frac{\beta}{2}\big)}$$

$$\lambda(z) = -\wp(z)$$

$$k(z) = -i\big(\zeta(z) - z\tfrac{\eta_1}{\gamma}\big)$$

$$\xi(z) \ = \ e^{\gamma i k(z)} \ = \ e^{\gamma\zeta(z) - z\eta_1}$$

Lemma S.11

a)

$$\varphi(z,x+\gamma) \;=\; \xi(z)\;\varphi(z,x)$$

b)

$$-\tfrac{d^2}{dx^2}\varphi(z,x) \;+\; 2\wp\big(x+i\tfrac{\beta}{2}\big)\varphi(z,x) \;=\; \lambda(z)\varphi(z,x)$$

c)

$$\xi(z+\gamma) \;=\; \xi(z) \qquad\qquad \xi(z+i\beta) \;=\; \xi(z)$$

Proof: a) By Problem W.3.d and Lemma W.4

$$\begin{aligned}
\varphi(z,x+\gamma) &= e^{\zeta(z)(x+\gamma)}\;\frac{\sigma\big(z-x-\gamma-i\frac{\beta}{2}\big)}{\sigma\big(x+\gamma+i\frac{\beta}{2}\big)}\\
&= -e^{\zeta(z)(x+\gamma)}\;\frac{\sigma\big(-z+x+\gamma+i\frac{\beta}{2}\big)}{\sigma\big(x+\gamma+i\frac{\beta}{2}\big)}\\
&= -e^{\zeta(z)(x+\gamma)}\;\frac{\sigma\big(-z+x+i\frac{\beta}{2}\big)e^{\eta_1(-z+x+i\frac{\beta}{2}+\frac{\gamma}{2})}}{\sigma\big(x+i\frac{\beta}{2}\big)e^{\eta_1(x+i\frac{\beta}{2}+\frac{\gamma}{2})}}\\
&= e^{\zeta(z)(x+\gamma)}e^{-\eta_1 z}\;\frac{\sigma\big(z-x-i\frac{\beta}{2}\big)}{\sigma\big(x+i\frac{\beta}{2}\big)}\\
&= e^{\zeta(z)\gamma-\eta_1 z}\;\varphi(z,x)
\end{aligned}$$

b) First observe that, since

$$\begin{aligned}
\frac{d}{dx}\frac{\sigma\big(z-x-i\frac{\beta}{2}\big)}{\sigma\big(x+i\frac{\beta}{2}\big)} &= -\Big[\frac{\sigma'\big(z-x-i\frac{\beta}{2}\big)}{\sigma\big(z-x-i\frac{\beta}{2}\big)}+\frac{\sigma'\big(x+i\frac{\beta}{2}\big)}{\sigma\big(x+i\frac{\beta}{2}\big)}\Big]\frac{\sigma\big(z-x-i\frac{\beta}{2}\big)}{\sigma\big(x+i\frac{\beta}{2}\big)}\\
&= -\Big[\zeta\big(z-x-i\tfrac{\beta}{2}\big)+\zeta\big(x+i\tfrac{\beta}{2}\big)\Big]\frac{\sigma\big(z-x-i\frac{\beta}{2}\big)}{\sigma\big(x+i\frac{\beta}{2}\big)}
\end{aligned}$$

we have

$$\tfrac{d}{dx}\varphi(z,x) = \Big(\zeta(z)-\zeta\big(z-x-i\tfrac{\beta}{2}\big)-\zeta\big(x+i\tfrac{\beta}{2}\big)\Big)\,\varphi(z,x)$$

Differentiate again

$$\begin{aligned}\tfrac{d^2}{dx^2}\varphi(z,x) &= \Big(\zeta'\big(z-x-i\tfrac{\beta}{2}\big)-\zeta'\big(x+i\tfrac{\beta}{2}\big)\Big)\varphi(z,x)\\ &\qquad +\big[\zeta(z)-\zeta\big(z-x-i\tfrac{\beta}{2}\big)-\zeta\big(x+i\tfrac{\beta}{2}\big)\big]^2\varphi(z,x)\\ &= -\Big(\wp\big(z-x-i\tfrac{\beta}{2}\big)-\wp\big(x+i\tfrac{\beta}{2}\big)\Big)\varphi(z,x)\\ &\qquad +\big[\zeta(z)-\zeta\big(z-x-i\tfrac{\beta}{2}\big)-\zeta\big(x+i\tfrac{\beta}{2}\big)\big]^2\varphi(z,x)\end{aligned}$$

Lemma W.5 says that

$$\big[\zeta(u+v)-\zeta(u)-\zeta(v)\big]^2=\wp(u+v)+\wp(u)+\wp(v)$$

for all $u,v\in\mathbb{C}$ such that none of u, v, $u+v$ are in $\gamma\mathbb{Z}\oplus i\beta\mathbb{Z}$ (basically because, for each fixed $v\in\mathbb{C}\setminus(\gamma\mathbb{Z}\oplus i\beta\mathbb{Z})$, both the left and right hand sides are periodic and have double poles, with the same singular part, at each $u\in\gamma\mathbb{Z}\oplus i\beta\mathbb{Z}$ and each $u\in -v+\gamma\mathbb{Z}\oplus i\beta\mathbb{Z}$). By this Lemma,

$$\begin{aligned}\tfrac{d^2}{dx^2}\varphi(z,x) &= -\Big(\wp\big(z-x-i\tfrac{\beta}{2}\big)-\wp\big(x+i\tfrac{\beta}{2}\big)\Big)\varphi(z,x)\\ &\qquad +\Big(\wp(z)+\wp\big(z-x-i\tfrac{\beta}{2}\big)+\wp\big(x+i\tfrac{\beta}{2}\big)\Big)\varphi(z,x)\\ &= \Big(\wp(z)+2\wp\big(x+i\tfrac{\beta}{2}\big)\Big)\varphi(z,x)\end{aligned}$$

c) By Lemma W.4,

$$\begin{aligned}\xi(z+\gamma) &= e^{\gamma\zeta(z+\gamma)-(z+\gamma)\eta_1} & \xi(z+i\beta) &= e^{\gamma\zeta(z+i\beta)-(z+i\beta)\eta_1}\\ &= e^{\gamma\zeta(z)-z\eta_1} & &= e^{\gamma\eta_2-i\beta\eta_1}e^{\gamma\zeta(z)-z\eta_1}\\ &= \xi(z) & &= \xi(z)\end{aligned}$$

■

Set $\Gamma=\gamma\mathbb{Z}$ and

$$\begin{aligned}V(x) &= 2\wp(x+i\tfrac{\beta}{2})\\ H &= \big(i\tfrac{d}{dx}\big)^2+V(x)\end{aligned}$$

By Problem W.1, parts (b), (c) and (f), $V\in C^\infty(\mathbb{R}/\Gamma)$ and is real valued. The Lamé equation is

$$-\tfrac{d^2}{dx^2}\phi+2\wp(x+i\tfrac{\beta}{2})\phi=\lambda\phi \qquad \text{i.e.}\quad H\phi=\lambda\phi \tag{S.8}$$

A solution $\phi(k,x)$ of (S.8) that satisfies

$$\phi(k,x+\gamma) \;=\; e^{i\gamma k}\phi(k,x) \tag{S.9}$$

is called a Bloch solution with energy λ and quasimomentum k.

Lemma S.11 says that, for each $z \in \mathbb{C} \setminus (\gamma\mathbb{Z} \oplus i\beta\mathbb{Z})$, $\varphi(z,x)$ is a Bloch solution of the Lamé equation with energy $\lambda = \lambda(z)$ and quasimomentum $k = k(z)$. I claim that the energy λ and multiplier $\xi = e^{\gamma ik}$ are fully parameterized by

$$\lambda(z) = -\wp(z) \qquad\qquad \xi(z) = e^{\gamma\zeta(z) - z\eta_1}$$

That is, the boundary value problem (S.8), (S.9) has a nontrivial solution if and only if $(\lambda, e^{i\gamma k}) = (\lambda(z), \xi(z))$, for some $z \in \mathbb{C} \setminus (\gamma\mathbb{Z} \oplus i\beta\mathbb{Z})$. The only if implication follows from the observation, which is an immediate consequence of Lemma S.12 below, that unless $2z \in \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}$ the functions $\varphi(z,x)$ and $\varphi(-z,x)$ are linearly independent solutions of (S.8) for $\lambda(z) = \lambda(-z)$. As a second order ordinary differential equation, (S.8) only has two linearly independent solutions for each fixed value of λ. For $z \in \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}$, $\lambda(z)$ is not finite. For $2z \in \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}$ with $z \notin \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}$, $\lambda'(z) = 0$, by Corollary W.3, and the second linearly independent solution is $\frac{\partial}{\partial z}\varphi(z,x)$.

Lemma S.12

a) Let $z_1, z_2 \in \mathbb{C} \setminus (\gamma\mathbb{Z} \oplus i\beta\mathbb{Z})$. If $z_1 - z_2 \notin \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}$, then $\varphi(z_1,x)$ and $\varphi(z_2,x)$ are linearly independent (as functions of x).

b) If $z \in \mathbb{C} \setminus (\gamma\mathbb{Z} \oplus i\beta\mathbb{Z})$, then $\varphi(z,x)$ and $\frac{\partial}{\partial z}\varphi(z,x)$ are linearly independent (as functions of x).

Proof: a) If $\varphi(z_1,x)$ and $\varphi(z_2,x)$ were linearly dependent, there would exist $a, b \in \mathbb{C}$, not both zero, such that $a\varphi(z_1,x) + b\varphi(z_2,x) = 0$ for all $x \in \mathbb{R}$. But

$$\varphi(z_1,x) = e^{\zeta(z_1)x}\,\frac{\sigma\big(z_1 - x - i\frac{\beta}{2}\big)}{\sigma\big(x + i\frac{\beta}{2}\big)} \qquad \text{and} \qquad \varphi(z_2,x) = e^{\zeta(z_2)x}\,\frac{\sigma\big(z_2 - x - i\frac{\beta}{2}\big)}{\sigma\big(x + i\frac{\beta}{2}\big)}$$

have analytic continuations to $x \in \mathbb{C} \setminus \big(-i\frac{\beta}{2} + \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}\big)$. These analytic continuations must obey $a\varphi(z_1,x) + b\varphi(z_2,x) = 0$ for all $x \in \mathbb{C} \setminus \big(-i\frac{\beta}{2} + \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}\big)$. In particular, the zero set of $\varphi(z_1,x)$, which is $z_1 - i\frac{\beta}{2} + \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}$, must coincide with the zero set of $\varphi(z_2,x)$, which is $z_2 - i\frac{\beta}{2} + \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}$. This is the case if and only if $z_1 - z_2 \in \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}$.

b) Fix any $z \in \mathbb{C} \setminus (\gamma\mathbb{Z} \oplus i\beta\mathbb{Z})$. As

$$\frac{\partial\varphi}{\partial z} = x\zeta'(x)\varphi(z,x) + e^{\zeta(z)x}\,\frac{\sigma'\big(z - x - i\frac{\beta}{2}\big)}{\sigma\big(x + i\frac{\beta}{2}\big)}$$

and σ has only simple zeroes, the zero set of $\frac{\partial\varphi}{\partial z}$ cannot coincide with that of φ. ■

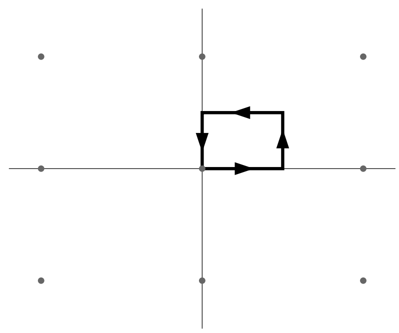
Theorem S.13 *Set*

$$\Lambda_1 = -\wp(\tfrac{\gamma}{2}) \qquad \Lambda_2 = -\wp(\tfrac{\gamma}{2} + i\tfrac{\beta}{2}) \qquad \Lambda_3 = -\wp(i\tfrac{\beta}{2})$$

Then $\Lambda_1, \Lambda_2, \Lambda_3$ *are real,* $\Lambda_1 < \Lambda_2 < \Lambda_3$ *and the spectrum of* H *is* $[\Lambda_1, \Lambda_2] \cup [\Lambda_3, \infty)$.

Proof: If, for given values of λ and k, the boundary value problem (S.8), (S.9) has a nontrivial solution and **if** k **is real** then λ is in the spectrum of H. We know that all such λ's are also real.

Imagine walking along the path in the z–plane that follows the four line segments from 0 to $\frac{\gamma}{2}$ to $\frac{\gamma}{2} + i\frac{\beta}{2}$ to $i\frac{\beta}{2}$ and back to 0. As $\overline{\wp(z)} = \wp(\bar{z})$, $\wp(-z) = \wp(z)$ and $\wp(z-\gamma) = \wp(z - i\beta) = \wp(z)$ (this is part of Problem W.1.f), $\lambda(z) = -\wp(z)$ remains real throughout the



entire excursion. Near $z = 0$,

$$\lambda(z) = -\wp(z) \approx -\tfrac{1}{z^2}$$

so λ starts out near $-\infty$ at the beginning of the walk and moves continuously to $+\infty$ at the end of the walk. Furthermore, by Corollary W.3, which states, in part,

$$\wp(z) = \wp(z') \textit{ if and only if } z - z' \in \gamma\mathbb{Z} \oplus i\beta\mathbb{Z} \textit{ or } z + z' \in \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}.$$

λ never takes the same value twice on the walk, because no two distinct points z, z' on the walk obey $z + z' \in \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}$ or $z - z' \in \gamma\mathbb{Z} \oplus i\beta\mathbb{Z}$.

- On the first quarter of the walk, from $z = 0$ to $z = \frac{\gamma}{2}$, $\lambda(z)$ increases from $-\infty$ to $\Lambda_1 = -\wp(\frac{\gamma}{2})$. But we cannot put these λ's into the spectrum of H because, by Problem W.5.e, $k(z)$ is pure imaginary on this part of the walk. You might worry that $k(z)$ might happen to be exactly zero at some points of this first quarter of the walk. This could only happen at isolated points, because $k(z)$ is a nonconstant analytic function. If this were to happen, the Lamé Schrödinger operator would have an isolated eigenvalue of finite multiplicity. We have already seen that no periodic Schrödinger operator can have such eigenvalues.

- On the second quarter of the walk, from $z = \frac{\gamma}{2}$ to $z = \frac{\gamma}{2} + i\frac{\beta}{2}$, $\lambda(z)$ increases from Λ_1 to $\Lambda_2 = -\wp(\frac{\gamma}{2} + i\frac{\beta}{2})$. By Problem W.5.d, $k(z)$ is pure real on this part of the walk, so these λ's are in the spectrum of H.
- On the third quarter of the walk, from $z = \frac{\gamma}{2} + i\frac{\beta}{2}$ to $z = i\frac{\beta}{2}$, $\lambda(z)$ increases from Λ_2 to $\Lambda_3 = -\wp(i\frac{\beta}{2})$. By Problem W.5.e, these λ's do not go into the spectrum of H.
- On the last quarter of the walk, from $z = i\frac{\beta}{2}$ back to zero, $\lambda(z)$ increases from Λ_3 to $+\infty$. By Problem W.5.d, these λ's are in the spectrum of H.

■

For more information on the Lamè equation, see

Edward Lindsay Ince, **Ordinary Differential Equations**, Dover Publications, 1956, section 15.62.

Edmund Taylor Whittaker and George Neville Watson, **A Course of Modern Analysis**, chapter XXIII.

