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The one Particle Theory of Periodic Point Interactions

Polymers, Monomolecular Layers, and Crystals

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Abstract. We solve explicitly and without approximation the problem of a quantum-mechanical particle in R^3 subjected to point interactions that are periodic in R^3 with periodicity of the type Z, Z^2, and Z^3. In the first case we get a model of an infinite straight polymer, in the second case we get a model of a monomolecular layer and in the third case we get a model of a crystal. In all three cases the unit cell of the Bravais lattice is allowed to contain any finite number of interaction sites (atomes), placed arbitrarily and with arbitrary interaction strength. In the case: one interaction site per unit cell we find explicit formulas for the resonance bands and energy bands and their corresponding wavefunctions.

Introduction

The one-electron theory of solids is based on the study of a Schrödinger particle in a periodic potential. This theory contains a large body of results that are obtained by perturbation methods or by symmetry arguments. However, it has not been possible up to now to check the perturbation results, which are necessarily only approximate, against an explicitly solvable three-dimensional model.

A class of non-separable two- and three-dimensional generalization of the Kronig-Penney model [1] has been solved in a recent paper by Sutherland [2]. The interactions in [2] are, however carried by lines (in two dimensions) or by planes (in three dimensions) which do not have a direct physical interpretation.

However it has been known for quite a while that there exists a Schrödinger operator with a point interaction in three dimensions. These operators and relatives of them have a history going back several decades. Their study started with Breit, Thomas, Wigner, and others as a model in nuclear physics for potential with short range interactions [3]. They observed that potential scattering converges in the low energy limit to scattering from a point interaction. In the late fifties, Huang, Yang, Lee, Luttinger, and Wu studied multiparticle operators with point interactions in low order perturbation theory [4].

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Beginning in the early sixties a series of papers by Danilov, Minlos and Faddeev was published concerning three-body operators with two-body point interactions [5]. The physical motivation was to compute the bound state of tritium. A survey article by Flamand [6], covers this part very well.

The many-center point interaction in three dimensions was first studied by Albeverio, Fenstad and Høegh-Krohn using methods of non standard analysis [7]. Further work on the many-center situation is to be found in [8] and [9].

As we see the point interactions has a long and venerable history. What we do in this article is to put the point interaction at work in the important field of solid state physics. We show that it is possible to use the point interactions to construct realistic models of solid states, models which may be built after specification. For instance in the crystal we may specify the lattice, the number and positions of atoms per lattice unite as well as their relative strength. With this input we construct the corresponding Hamiltonian and give explicit formulas for the resolvent kernel of the reduced Hamiltonian.

In Sect. 2 we give the general formula for a Hamiltonian with a potential with support on a discrete subset of R^2 and R^3. We call such Hamiltonians, Hamiltonians given by point interactions. It is worth mentioning that point interactions exist only in dimensions, 1, 2, and 3.

In Sect. 3 we apply the results of Sect. 2 to construct models of polymers, i.e. we consider point interactions in R^3 which are periodic with only one period. We compute the resolvent and scattering matrix explicitly up to the inversion of a $n \times n$ matrix where n is the number of atoms per polymer unit. In the case of one atom per polymer unite we get completely explicit formulas for the resonances and energy bands.

In Sect. 4 we consider monomolecular layers, i.e. point interactions in R^3 which are periodic with two independent periods. Again we compute the resolvent and the scattering matrix. The Bragg reflections come out of the scattering matrix in a very explicit manner.

In Sect. 5 we consider the crystals, i.e. point interactions with three independent periods. The resolvent kernel of the reduced Hamiltonian is given explicitely up to the inversion of an $n \times n$ matrix where n is the number of atoms per lattice unit. In the case of one atom per lattice unit we give the energy bands and corresponding wavefunctions explicitely.

In Sect. 6 we consider the case of the grating or the linear interferometer. Again we give explicit formulas for the energy bands and its corresponding wave functions. There are also formulas for the reduced resolvent kernel and the corresponding scattering matrix.

2. Point Interactions or Potentials with Discrete Support

Let Y be a discrete subset of R^3 such that the distance between any two points in Y is greater than a positive number d. We want to consider Hamiltonians of the form

$$-\Delta - \sum_{y \in Y} \lambda_y \delta(x-y). \tag{2.1}$$

In the Fourier transform representation (2.1) is given formally by the operator[1]

$$p^2 - \sum_{y\in Y} (2\pi)^{-3}\lambda_y e^{iy(p-q)}. \tag{2.2}$$

For finite subsets Y such Hamiltonians have been considered in [8]. The result of this discussion is that (2.2) makes sense in R^3 (and in R^2) if λ_y is chosen suitably infinitesimal. (For a discussion on this point see [7].) It is possible to extend these results to infinite discrete subsets in the following way.

Let first Y be a finite subset of R^3, then

$$H^\omega = p^2 - \sum_{y\in Y} |\psi_y^\omega\rangle\langle\psi_y^\omega|, \tag{2.3}$$

where

$$\psi_y^\omega(p) = (2\pi)^{-3/2}(\lambda_y(\omega))^{1/2}\chi_\omega(p)e^{iyp}, \tag{2.4}$$

$\chi_\omega(p)=1$ if $|p|\leqq\omega$ and zero if not, is a well defined self adjoint operator on $L_2(R^3)$, if we remark that $|\psi_y^\omega\rangle\langle\psi_y^\omega|f = (\psi_y^\omega, f)\psi_y^\omega$.

We consider H^ω to be an approximation to the formal expression (2.2). Hence the problem is to choose $\lambda_y(\omega)$ such that H^ω converges to some self adjoint operator as $\omega\to\infty$. Since

$$V^\omega = \sum_{y\in Y} |\psi_y^\omega\rangle\langle\psi_y^\omega| \tag{2.5}$$

is a bounded operator we have for complex E

$$(H^\omega - E)^{-1} = (p^2-E)^{-1/2}[1-(p^2-E)^{-1/2}V^\omega(p^2-E)^{-1/2}]^{-1}(p^2-E)^{-1/2}. \tag{2.6}$$

Using now the fact that V^ω is an operator of finite dimensional range we may compute (2.6) explicitely in the following way. Set

$$A = (p^2-E)^{-1/2}V^\omega(p^2-E)^{-1/2} \tag{2.7}$$

then

$$A^l = (p^2-E)^{-1/2}V^\omega(p^2-E)^{-1}\ \dots\ V^\omega(p^2-E)^{-1/2}. \tag{2.8}$$

Let

$$g_{xy}^\omega = (\psi_x^\omega, (p^2-E)^{-1}\psi_y^\omega) \tag{2.9}$$

then

$$\begin{aligned} g_{xy}^\omega &= \lambda_x^{1/2}(\omega)\lambda_y^{1/2}(\omega)(2\pi)^{-3}\int_{|p|\leqq\omega}\frac{e^{-i(x-y)p}}{p^2-E}dp \\ &= \lambda_x^{1/2}(\omega)\lambda_y^{1/2}(\omega)G_E^\omega(x-y). \end{aligned} \tag{2.10}$$

Let g^ω be the $n\times n$ matrix with elements $g_{x,y}^\omega$ $x,y\in Y$, $n=|Y|$. Then (2.8) takes the form

$$A^l = (p^2-E)^{-1/2}\left[\sum_{x,y\in Y}(g^{l-1})_{xy}|\psi_x^\omega\rangle\langle\psi_y^\omega|\right](p^2-E)^{-1/2}, \tag{2.11}$$

1 In (2.2) and in similar formulae we use a hybrid notation; p^2 is a multiplication operator, and $e^{i(p-q)}$ an integral kernel

where g^{l-1} is the $(l-1)^{\text{th}}$ power of the matrix g^{ω}_{xy}. From (2.11) we get that if 1 is not in the spectrum of A then

$$(1-A)^{-1}=1+(p^2-E)^{-1/2}\left[\sum_{x,y\in Y}[1-g^{\omega}]^{-1}_{xy}|\psi^{\omega}_x\rangle\langle\psi^{\omega}_y|\right](p^2-E)^{-1/2}. \quad (2.12)$$

Hence by (2.6)

$$(H^{\omega}-E)^{-1}=(p^2-E)^{-1}+(p^2-E)^{-1}\left[\sum_{x,y\in Y}[1-g^{\omega}]^{-1}_{xy}|\psi^{\omega}_x\rangle\langle\psi^{\omega}_y|\right](p^2-E)^{-1}, \quad (2.13)$$

where $[1-g]^{-1}_{xy}$ are the elements of the inverse $n\times n$ matrix of $1-g^{\omega}_{xy}\equiv\delta_{xy}-g^{\omega}_{xy}$.

Let now

$$\varphi^{\omega}_x(p)=(2\pi)^{-3/2}\chi_{\omega}(p)\frac{e^{ipx}}{p^2-E} \quad (2.14)$$

then

$$(H^{\omega}-E)^{-1}=(p^2-E)^{-1}+\sum_{x,y\in Y}[\delta_{xy}-\lambda^{1/2}_x(\omega)\lambda^{1/2}_y(\omega)G^{\omega}_E(x-y)]^{-1}\cdot\lambda^{1/2}_x(\omega)\lambda^{1/2}_y(\omega)|\varphi^{\omega}_x\rangle\langle\varphi^{\omega}_y|$$

hence

$$(H^{\omega}-E)^{-1}=(p^2-E)^{-1}+\sum_{x,y\in Y}[\lambda^{-1}_x(\omega)\delta_{xy}-G^{\omega}_E(x-y)]^{-1}|\varphi^{\omega}_x\rangle\langle\varphi^{\omega}_y|, \quad (2.15)$$

where $[\ ]^{-1}$ stands for the inverse $n\times n$ matrix.

Let now $\lambda_x(\omega)$ be given by

$$\lambda_x(\omega)^{-1}=(2\pi)^{-3}\int_{|p|\leqq\omega}\frac{dp}{p^2}+\alpha_x,$$

where α_x is independent of ω. Then

$$(H^{\omega}-E)^{-1}=(p^2-E)^{-1}+\sum_{x,y\in Y}\left[\left(\alpha_x-\frac{i\sqrt{E}}{4\pi}\right)\delta_{xy}-\tilde{G}^{\omega}_E(x-y)\right]^{-1}|\varphi^{\omega}_x\rangle\langle\varphi^{\omega}_y|, \quad (2.16)$$

where

$$\tilde{G}^{\omega}_E(x-y)=(2\pi)^{-3}\int_{|p|\leqq\omega}\frac{e^{-i(x-y)p}}{p^2-E}dp \quad \text{if} \quad x-y\neq 0 \quad (2.17)$$

and $\tilde{G}^{\omega}_E(0)=0$. Let

$$\tilde{G}_E(x-y)=(2\pi)^{-3}\int_{R^3}\frac{e^{-i(x-y)p}}{p^2-E}dp \quad \text{if} \quad x-y\neq 0 \quad (2.18)$$

and $\tilde{G}_E(0)=0$. Then we see that for complex E (2.16) converge strongly as $\omega\to\infty$ to

$$(H_{\alpha}-E)^{-1}=(p^2-E)^{-1}+\sum_{x,y\in Y}\left[\left(\alpha_x-\frac{i\sqrt{E}}{4\pi}\right)\delta_{xy}-\tilde{G}_E(x-y)\right]^{-1}\cdot(2\pi)^{-3}\frac{e^{i(px-qy)}}{(p^2-E)(q^2-E)}, \quad (2.19)$$

where α is a real function defined on Y such that $\alpha(y)=\alpha_y$, $y\in Y$, and $[\ ]^{-1}$ is the inverse $n\times n$ matrix $n=|Y|$.

The Fourier transform version of (2.19) is given by

$$(H_\alpha - E)^{-1}(x,y) = G_E(x-y) + \sum_{\tilde{x},\tilde{y}\in Y}\left[\left(\alpha_{\tilde{x}} - \frac{i\sqrt{E}}{4\pi}\right)\delta_{\tilde{x}\tilde{y}} - \tilde{G}_E(\tilde{x}-\tilde{y})\right]^{-1} \cdot G_E(x-\tilde{x})G_E(y-\tilde{y}), \tag{2.20}$$

where

$$G_E(x-y) = \frac{1}{4\pi}\frac{e^{i\sqrt{E}|x-y|}}{|x-y|}, \tag{2.21}$$

and

$$\tilde{G}_E(x) = G_E(x) \quad \text{for} \quad x \neq 0 \quad \text{and} \quad \tilde{G}(0)=0.$$

Let now X be a discrete set and $\alpha(x)$ is function on X which is bounded below.

Let $Y\subset X$ be a finite subset of X and α_Y the restriction of α to Y. Let now H_α^Y be the self adjoint operator, the resolvent of which is given by (2.19). Since

$$\lambda_x(\omega) = \left(\alpha_x + \frac{\omega}{2\pi^2}\right)^{-1} \tag{2.22}$$

is positive for ω large enough we see that

$$Y \to H_\alpha^Y$$

is a monotonically decreasing function from finite subsets of X into self adjoint operators, i.e.

$$Y_1 \subset Y_2 \Rightarrow H_\alpha^{Y_1} \geqq H_\alpha^{Y_2}. \tag{2.23}$$

This implies that the corresponding resolvents for large negative E are monotonically increasing, i.e. for $E<E'$ we have

$$Y_1 \subset Y_2 \Rightarrow (H_\alpha^{Y_1} - E)^{-1} \leqq (H_\alpha^{Y_2} - E)^{-1}. \tag{2.24}$$

Here E' depends on Y_2. We shall see however that it is possible to pick E' independent of Y_2.

From (2.21) we have that for $E<0$ we have that $\tilde{G}_E(x-y)$ is the kernel of a bounded operator on $l_2(X)$ which tends strongly to zero as $E\to\infty$. We use here the fact that X is discrete and the fact that $\tilde{G}_E(x)$ tends exponentially to zero in x. Since α_x is bounded below we see that

$$\left(\alpha_x - \frac{i\sqrt{E}}{4\pi}\right)\delta_{xy} - \tilde{G}_E(x-y) \tag{2.25}$$

is positive as a self adjoint operator on $l_2(X)$ for E large negative. Let now E_0 be the largest negative value of E such that (2.25) is still positive, or if there is no such largest negative value we set $E_0=0$. We observe that if (2.25) is positive as a kernel on $l_2(X)$ it is also positive as a kernel on $l_2(Y)$ for any subset $Y\subset X$.

Let now Y be a finite subset of X: then

$$(H_\alpha^Y - E)^{-1} = (p^2 - E)^{-1} + \sum_{x,y\in Y} \left[\left(\alpha_x - \frac{i\sqrt{E}}{4\pi}\right)\delta_{xy} - \tilde{G}_E(x-y)\right]_Y^{-1} \cdot (2\pi)^{-3} \frac{e^{i(px-qy)}}{(p^2-E)(q^2-E)}, \tag{2.26}$$

where $[\ ]_Y^{-1}$ is the inverse kernel in $l_2(Y)$. It follows from (2.26) that the spectrum of H_α^Y is the interval $(0, \infty)$ plus at most $n = |Y|$ negative eigenvalues E_n^Y where $E = E_n^Y$ are the points in $(-\infty, 0)$ where (2.25) as a kernel on $l_2(Y)$ has eigenvalue zero. From this we get that E_0 is a uniform lower bound on the spectrum of H_α^Y for all finite subsets X of Y. In particular, we get the uniform norm bound for $E < E_0$

$$\|(H_\alpha^Y - E)^{-1}\| \leqq |(E - E_0)^{-1}| \tag{2.27}$$

for all finite subsets $Y \subset X$. From this uniform bound and the monotonicity (2.24) we get that the strong limit

$$(H_\alpha^X - E)^{-1} = \operatorname*{strong\,lim}_{\substack{Y\subset X\\ |Y|<\infty}} (H_\alpha^Y - E)^{-1} \tag{2.28}$$

over the filter of all finite subsets $Y \subset X$ exists. Since the strong limit of resolvents is again a resolvent, (2.29) is the resolvent of a self adjoint operator H_α^X which is bounded below. From the strong convergence (2.28) and (2.26) it follows that the resolvent $(H_\alpha^X - E)^{-1}$ is given by

$$(H_\alpha^X - E)^{-1} = (p^2 - E)^{-1} + \sum_{x,y\in X} \left[\left(\alpha_x - \frac{i\sqrt{E}}{4\pi}\right)\delta_{xy} - \tilde{G}_E(x-y)\right]_X^{-1} \cdot (2\pi)^{-3} \frac{e^{i(px-qy)}}{(p^2-E)(q^2-E)}, \tag{2.29}$$

where $[\ ]_X^{-1}$ is the inverse as an operator on $l_2(X)$. The sum in (2.29) is absolutely convergent in the sense that if we integrate with respect to L_2-functions of p and q respectively, then the sum is absolutely convergent. Hence we have the following theorem.

Theorem 2.1. *Let Y be a finite subset of R^3 and let α_x be a function defined on Y. Let $\tilde{G}_E(x) = \frac{1}{4\pi|x|} e^{i\sqrt{E}|x|}$ for $x \neq 0$ and $\tilde{G}_E(0) = 0$. Let H^ω be the self adjoint operator in $L_2(R^3)$ given by*

$$(f, H^\omega f) = (f, p^2 f) - (2\pi)^{-3} \sum_{y\in Y} \lambda_y(\omega) \left| \int_{|p|\leqq\omega} f(p) e^{iyp} dp \right|^2 .$$

If $\lambda_y(\omega) = \left(\alpha_x + \frac{\omega}{2\pi^2}\right)^{-1}$ then H^ω converges in the strong resolvent sense, i.e. $(H^\omega - E)^{-1} \to (H_\alpha^Y - E)^{-1}$ strongly for complex E, where the limit operator is given by

$$(H_\alpha^Y - E)^{-1} = (p^2 - E)^{-1} - \sum_{x,y\in Y} \left[\left(\alpha_x - \frac{i\sqrt{E}}{4\pi}\right)\delta_{xy} - \tilde{G}_E(x-y)\right]_Y^{-1} \frac{(2\pi)^{-3} e^{i(px-qx)}}{(p^2-E)(q^2-E)},$$

where $[\ ]_Y^{-1}$ is the inverse as an operator in $l_2(Y)$.

Let X be a discrete subset of R^3 and α_x be a real function on X which is bounded below. Let $Y \subset X$ be a finite subset: then $Y \to (H_\alpha^Y - E)^{-1}$ is a monotonic function for $E \leqq E_0$ where E_0 is independent of Y. Moreover

$$(H_\alpha^X - E)^{-1} = \underset{\substack{Y \subset X \\ |Y| < \infty}}{\text{strong lim}} (H_\alpha^Y - E)^{-1}$$

exists and defines a self adjoint operator H_α^X bounded below. The corresponding resolvent is given by

$$(H_\alpha^X - E)^{-1} = (p^2 - E)^{-1} - \sum_{x, y \in X} \left[\left(\alpha_x - \frac{i\sqrt{E}}{4\pi}\right)\delta_{xy} - \tilde{G}_E(x-y)\right]_X^{-1} \frac{(2\pi)^{-3} e^{i(px - qy)}}{(p^2 - E)(q^2 - E)},$$

where $[\,]_X^{-1}$ is the inverse as an operator in $l_2(X)$. If we integrate with respect to L_2-functions in p and q the series is absolutely convergent.

There is an analog theorem in R^2, the proof of which is completely analogous to Theorem 1.1.

Theorem 1.2. *Let Y be a finite subset of R^2 and α_x be a function defined on Y. Let*

$$\tilde{G}_E(x) = (2\pi)^{-2} \int_{R^2} \frac{e^{ixp}}{p^2 - E} dp$$

for $x \neq 0$ and $\tilde{G}_E(0) = 0$. Let

$$\lambda_x(\omega) = \left(\frac{1}{4\pi} \ln(\omega^2 + 1) + \alpha_x\right)^{-1}$$

for $x \in Y$ and let

$$(f, H^\omega f) = (f, p^2 f) - (2\pi)^{-3} \sum_{y \in Y} \lambda_y(\omega) \left| \int_{|p| \leqq \omega} f(p) e^{iyp} dp \right|^2$$

define a self adjoint operator in $L_2(R^2)$. Then $(H^\omega - E)^{-1} \to (H_\alpha^Y - E)^{-1}$ strongly for complex E where the limit operator is given by

$$(H_\alpha^Y - E)^{-1} = (p^2 - E)^{-1} - \sum_{x, y \in Y} \left[\left(\alpha_x - \frac{\ln\sqrt{-E}}{2\pi}\right)\delta_{xy} - \tilde{G}_E(x-y)\right]_Y^{-1} \frac{(2\pi)^{-2} e^{i(px - qy)}}{(p^2 - E)(q^2 - E)}.$$

Let X be a discrete subset of R^2; then the analog statement of Theorem 1.1 holds.

3. Infinite Straight Polymers

Let $\Lambda_1 = \{an, n \in Z\}$, $a \in R^+$ be a discrete subgroup of R. We consider Λ_1 to be a discrete subgroup of R^3 by the injection $\Lambda_1 \subset R \hookrightarrow R^2 \times R$. If X is a finite subset of R^3 then $Y = \Lambda_1 + X$ is a discrete subset of R^3 invariant under the group Λ_1. If α is a real function on Y which is invariant under the action of Λ_1, i.e. $\alpha_{\lambda + x} = \alpha_x$ for $\lambda \in \Lambda_1$ and $x \in X$, then $H_\alpha \equiv H_\alpha^Y$ of Theorem 2.1 is invariant under the unitary group $\lambda \to U_\lambda$, $\lambda \in \Lambda_1$ where $(U_\lambda f)(x) = f(x - \lambda)$. We consider H_α to be the Hamiltonian for a model of an infinite straight polymer. The points y in Y are then the sites of the atoms in the polymer while α_y are the relative strengths of the interactions at the site y. α_y is actually the inverse scattering length of the atom at the site y. Since $U_\lambda H_\alpha U_\lambda^{-1} = H_\alpha$ we have that

$$H_\alpha = \int_{\hat{\Lambda}_1} H_\alpha(k) dk, \tag{3.1}$$

where $\tilde{\Lambda}_1$ is the dual group of Λ_1 and (3.1) is the direct integral over the spectrum of the unitary representation $\lambda \to U_\lambda$, $\lambda \in \Lambda_1$. $\hat{\Lambda}_1$ is the circle of radius a^{-1} or $\hat{\Lambda}_1 = R/\Gamma_1$ where $\Gamma_1 = \left\{\frac{2\pi}{a} n, n \in Z\right\}$. By Theorem 1.1 we have

$$(H_\alpha - E)^{-1} = (p^2 - E)^{-1} - (2\pi)^{-3} \sum_{x, y \in X} \sum_{\lambda, \lambda' \in \Lambda_1} \cdot \left[\left(\alpha_x - \frac{i\sqrt{E}}{4\pi}\right)\delta_{xy}\delta_{\lambda\lambda'} - \tilde{G}_E(x - y + \lambda - \lambda')\right]^{-1} \cdot \frac{e^{ipx} e^{ip\lambda}}{p^2 - E} \frac{e^{-iqy} e^{-iq\lambda'}}{q^2 - E}. \tag{3.2}$$

We may now utilize the fact that what is inside the square bracket above is translation invariant under $\lambda \in \Lambda_1$ to simplify the expression (3.2). We recall that $[\ ]^{-1}$ means the inverse kernel in

$$l_2(X \times \Lambda_1) = l_2(X) \otimes l_2(\Lambda_1),$$

and the method for simplification is to use Fourier analysis in $l_2(\Lambda_1)$. To compute the Fourier transform of the square bracket in (3.2) we first compute for $-\frac{\pi}{a} < k \leqq \frac{\pi}{a}$

$$h_E(x - y, k) = \sum_{\lambda \in \Lambda_1} \tilde{G}_E(x - y + \lambda) e^{-i\lambda k}, \tag{3.3}$$

where we have identified $\left(-\frac{\pi}{a}, \frac{\pi}{a}\right]$ with $\hat{\Lambda}_1$ by the mapping $k \to e^{i\lambda k}$. For $x - y \notin \Lambda_1$ we have by the Poisson summation formula

$$\begin{aligned} h_E(x - y, k) &= \sum_{\lambda \in \Lambda_1} \tilde{G}_E(x - y + \lambda) e^{-i\lambda k} \\ &= (2\pi)^{-3} \sum_{\lambda \in \Lambda_1} \int_{R^3} \frac{e^{ip(x-y)} e^{i(p_3 - k)\lambda}}{p^2 - E} dp \\ &= (2\pi)^{-2} \sum_{\gamma \in \Gamma_1} \int_{R^2} \frac{e^{ip_1(x_1 - y_1) + p_2(x_2 - y_2) + (\gamma + k)(x_3 - y_3)}}{p_1^2 + p_2^2 + (\gamma + k)^2 - E} dp_1 dp_2 . \end{aligned}$$

Hence for $x - y \notin \Lambda_1$ we have

$$h_E(x - y, k) = \sum_{\gamma \in \Gamma_1} K_0\left(\sqrt{(\gamma + k)^2 - E}\sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2}\right) e^{i(\gamma + k)(x_3 - y_3)}. \tag{3.4}$$

For $x-y=\lambda\in\Lambda_1$ we have that

$$h_E(\lambda,k)=e^{i\lambda k}h_E(0,k) \tag{3.5}$$

while

$$\begin{aligned}h_E(0,k)&=\sum_{\substack{\lambda\in\Lambda_1\\ \lambda\neq 0}} G_E(\lambda)e^{-i\lambda k}\\ &=\frac{1}{4\pi a}\sum_{n\neq 0}\frac{1}{|n|}e^{i\sqrt{E}a|n|}e^{-iank}\\ &=-\frac{1}{4\pi a}[\ln(1-e^{ia(\sqrt{E}-k)})+\ln(1-e^{ia(\sqrt{E}+k)})].\end{aligned}$$

Hence

$$h_E(0,k)=-\frac{1}{4\pi a}\ln[e^{2ia\sqrt{E}}-2\cos(ak)e^{ia\sqrt{E}}+1]. \tag{3.6}$$

In terms of $h_E(x-y,k)$ (3.2) now takes the form

$$\begin{aligned}(H_\alpha-E)^{-1}=(p^2-E)^{-1}-(2\pi)^{-3}\sum_{x,y\in X}\left[\left(\alpha_x-\frac{i\sqrt{E}}{4\pi}\right)\delta_{xy}-h_E(x-y),k)\right]^{-1}\\ \cdot\frac{e^{i(p_1x_1+p_2x_2+(\gamma+k)x_3)}e^{-i(q_1y_1+q_2y_2+(\gamma'+k')y_3)}}{q_1^2+q_2^2+(\gamma'+k')^2-E}\delta(k-k'),\end{aligned} \tag{3.7}$$

where $p_3=\gamma+k$, $q_3=\gamma'+k'$, with $\gamma,\gamma'\in\Gamma_1$ and $-\frac{\pi}{a}\leqq k,\ k'\leqq\frac{\pi}{a}$ and $[\ ]^{-1}$ is the inverse $n\times n$ matrix, $n=|X|$. Hence we get: the reduced Hamiltonian $H_\alpha(k)$ of (3.1) is given by its resolvent kernel on $L_2(R^2\times\Gamma)$ by the following theorem

Theorem 3.1. *Let $\Lambda_1=\{an, n\in Z\}$, $a\in R^+$, be a discrete subgroup of R considered as a discrete subgroup of R^3 by $\Lambda_1\equiv\{(0,0,an), n\in Z\}$. Let $\Gamma_1=\left\{\frac{2\pi}{a}n, n\in Z\right\}$ so that the dual group $\hat{\Lambda}_1=R/\Gamma_1$. By $k\to e^{ik\lambda}$, $\lambda\in\Lambda_1$, we identify $\hat{\Lambda}_1$ with the Brillouin zone $\left[-\frac{\pi}{a},\frac{\pi}{a}\right]$. Let X be a finite subset of R^3 and set $Y=X+\Lambda_1$, and let $\alpha_{x+\lambda}=\alpha_x$ be a Λ_1-invariant real function on Y. Then $H_\alpha\equiv H_\alpha^Y$ of Theorem 1.1 is invariant under Λ_1 so that*

$$H_\alpha=\int_{\hat{\Lambda}_1} H_\alpha(k)dk=\int_{-\pi/a}^{\pi/a} H_\alpha(k)dk,$$

where we have identified $\hat{\Lambda}_1$ with $\left[-\frac{\pi}{a},\frac{\pi}{a}\right]$. Let $h_E(x-y,k)$ be given by (3.4)–(3.6).

Then the reduced Hamiltonian $H_\alpha(k)$ is a self adjoint operator on the reduced Hilbert space $L_2(R^2 \times \Gamma_1)$ with resolvent kernel given by

$$(H_\alpha(k)-E)^{-1}=(p_1^2+p_2^2+(\gamma+k)^2-E)^{-1}$$

$$-(2\pi)^{-3}\sum_{x,y\in X}\left[\left(\alpha_x-\frac{i\sqrt{E}}{4\pi}\right)\delta_{xy}-h_E(x-y,k)\right]^{-1} \cdot\frac{e^{i(p_1x_1+p_2x_2+(\gamma+k)x_3)}}{p_1^2+p_2^2+(\gamma+k)^2-E}\cdot\frac{e^{-i(q_1y_1+q_2y_2+(\gamma'+k)y_3)}}{q_1^2+q_2^2+(\gamma'+k)^2-E},$$

where $[\ ]^{-1}$ stands for the inverse $n\times n$ matrix, $n=|X|$.

Let $H_\infty=p^2$ be the free Hamiltonian in $L_2(R^3)$; then

$$H_\infty=\int_{\hat{\Lambda}_1} H_\infty(k)dk \tag{3.8}$$

with

$$(H_\infty(k)-E)^{-1}=(p_1^2+p_2^2+(\gamma+k)^2-E)^{-1} \tag{3.9}$$

since H_∞ is invariant under the group of translation Λ_1. To prove that the wave operators

$$W_\pm(H_\alpha,H_\infty)=\underset{t\to\pm\infty}{\text{strong}\lim}\, e^{-itH_\alpha}e^{itH_\infty} \tag{3.10}$$

exist, it is enough to prove that the wave operators

$$W_\pm(H_\alpha(k),H_\infty(k))=\underset{t\to\pm\infty}{\text{strong}\lim}\, e^{-itH_\alpha(k)}e^{itH_\infty(k)} \tag{3.11}$$

exist for almost all k, since

$$W_\pm(H_\alpha,H_\infty)=\int_{\hat{\Lambda}_1} W_\pm(H_\alpha(k),H_\infty(k))dk. \tag{3.12}$$

Since the scattering matrix $S(H_\alpha,H_\infty)$ is given by

$$S(H_\alpha H_\infty)=W_+^*(H_\alpha,H_\infty)W_-(H_\alpha H_\infty) \tag{3.13}$$

we get in the same way that

$$S(H_\alpha,H_\infty)=\int_{\hat{\Lambda}_1} S(H_\alpha(k),H_\infty(k))dk, \tag{3.14}$$

so that the scattering matrix $S(H_\alpha(k),H_\infty(k))$ for the reduced pair $H_\alpha(k)$, $H_\infty(k)$ is actually the reduced scattering matrix and correspondingly for the wave operators.

From the formula for the resolvent kernel of $H_\alpha(k)$ in Theorem 3.1 we see that the kernel $(H_\alpha(k)-E)^{-1}$ is analytic in a neighborhood of the cut $[k^2,\infty)$ with smooth boundary values on the cut from above and from below. This implies by standard techniques that the reduced scattering matrix $S(H_\alpha(k),H_\infty(k))$ exists. Hence we have the following theorem

Theorem 3.2. *Let $H_\infty = p^2$ be the free Hamiltonian in $L_2(R^3)$, and let H_α be as given in Theorem 3.1. Then the wave operators*

$$W_\pm(H_\alpha, H_\infty) = \underset{t\to\pm\infty}{\text{strong}\lim}\, e^{-itH_\alpha} e^{itH_\infty}$$

exist. The corresponding scattering matrix $S_\alpha = W_+^* W_-$ is given by

$$S_\alpha(p_1 p_2 p_3, q_1 q_2 q_3) = \delta(p_1 - q_1)\delta(p_2 - q_2)\delta(p_3 - q_3)$$

$$- \sum_{x, y\in X} \left[\left(\alpha_x - \frac{i\sqrt{E}}{4\pi}\right)\delta_{xy} - h_{E+i0}(x-y, k)\right]^{-1}$$

$$\cdot\, e^{i[p_1 x_1 + p_2 x_2 + (\gamma + k)x_3]} \cdot e^{-i[q_1 y_1 + q_2 y_2 + (\gamma' + k)y_3]}$$

$$\cdot\, \delta(k - k')\delta(p_1^2 + p_2^2 + (\gamma + k)^2 - q_1^2 - q_2^2 - (\gamma' + k')^2),$$

where $E = p_1^2 + p_2^2 + p_3^2$, $p_3 = \gamma + k$, $q_3 = \gamma' + k'$ with $\gamma, \gamma' \in \Gamma_1$ and $k, k' \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$.

$h_{E+i0}(x-y, k) = h_E(x-y, k)$ is given by (3.4)–(3.6), while $h_{E-i0}(x-y, k)$ is the analytic continuation around the cut $[k^2, \infty)$. Hence for $x - y \notin \Lambda_1$

$$h_{E-i0}(x-y, k)$$

$$\sum_{|\gamma+k|<\sqrt{E}} K_0(-\sqrt{(\gamma+k)^2 - E}\cdot\sqrt{(x_1-y_1)^2 + (x_2-y_2)^2})e^{i(\gamma+k)(x_3-y_3)}$$

$$+ \sum_{|\gamma+k|>\sqrt{E}} K_0(\sqrt{(\gamma+k)^2 - E}\cdot\sqrt{(x_1-y_1)^2 + (x_2-y_2)^2})e^{i(\gamma+k)(x_3-y_3)}$$

and $h_{E-i0}(\lambda, k) = e^{-i\lambda k} h_{E-i0}(0, k)$ with

$$h_{E-i0}(0, k) = -\frac{1}{4\pi a}\ln\left[e^{-2ia\sqrt{E}} - 2\cos(ak)e^{-ia\sqrt{E}} + 1\right].$$

For a qualitative understanding of the reduced scattering matrix $S(H_\alpha(k), H_\infty(k))$ the resonances are important. We see from the formula of Theorem 3.1 that the reduced resolvent kernel $(H_\alpha(k) - E)^{-1}$ is a meromorphic function of $\sqrt{E}$ on some covering Riemann surface. The structure of this Riemann surface is quite complex and we see that there is actually a logarithmic branchcut along each of the halfline $[(\gamma + k), \infty)$; recall that $K_0(x)$ has a logarithmic singularity at zero. The resonances are the poles of this meromorphic function on its Riemann surface and the eigenvalues of $H_\alpha(k)$ are special cases of these poles for which the corresponding wavefunctions are square integrable.

Let now X consist of one point only and we may by translation invariance take $X = \{0\}$. In this case we have from Theorem 3.1 that

$$(H_\alpha(k) - E)^{-1} = (p_1^2 + p_2^2 + (\gamma + k)^2 - E)^{-1}\left(\alpha - \frac{i\sqrt{E}}{4\pi} - h_E(0, k)\right)^{-1} \tag{3.15}$$

$$\frac{1}{}\;\frac{1}{}$$

Hence $(H_\alpha(k)-E)^{-1}$ has the same Riemann surface and the same poles as

$$\left(\alpha-\frac{i\sqrt{E}}{4\pi}-h_E(0,k)\right)^{-1}. \tag{3.16}$$

In particular the resonances are given by the equation

$$\alpha-\frac{i\sqrt{E}}{4\pi}=-\frac{1}{4\pi a}\ln\left[e^{2ia\sqrt{E}}-2\cos(ak)e^{ia\sqrt{E}}+1\right] \tag{3.17}$$

which is equivalent to

$$e^{-4\pi a\alpha}\cdot e^{ia\sqrt{E}}=e^{2ia\sqrt{E}}-2\cos(ak)e^{ia\sqrt{E}}+1$$

or

$$e^{2ia\sqrt{E}}-(2\cos(ak)+e^{-4\pi a\alpha})e^{ia\sqrt{E}}+1=0. \tag{3.18}$$

Hence if $z_0(k)$ is a solution of

$$z^2-(2\cos(ak)+e^{-4\pi a\alpha})z+1=0 \tag{3.19}$$

then

$$\sqrt{E_n}=-\frac{i}{a}\ln(z_0(k))+\frac{2\pi}{a}n \tag{3.20}$$

are all the solution of (3.17). If z_0 is one solution of (3.19) then z_0^{-1} is the other, hence if $z_0(k)$ is the solution in the upper half plane then

$$E_n^{\pm}(k)=\frac{1}{a^2}(\pm i\cdot\ln(z_0(k))+2\pi n)^2, \qquad n=0,1,\ldots \tag{3.21}$$

are all the solutions of (3.17).

There are two different cases

(i) $$2\cos(ak)+e^{-4\pi a\alpha}>2 \tag{3.22}$$

then (3.19) has two real solutions $z_0(k)$ and $z_0(k)^{-1}$. Hence (3.21) is real only for $n=0$ and we find only one value

$$E_0(k)=-\frac{1}{a^2}(\ln(z_0(k)))^2. \tag{3.23}$$

From (3.15) we have that the corresponding eigenfunction is

$$\psi_0(p_1,p_2,\gamma;k)=\frac{1}{p_1^2+p_2^2+(\gamma+k)^2-E_0(k)} \tag{3.24}$$

which is square integrable. The other solutions

$$E_n^{\pm}(k)=\frac{1}{a^2}(\pm i\ln(z_0(k))+2\pi n)^2, \qquad n=1,2,\ldots \tag{3.25}$$

are complex resonances.

The other case is

(ii) $$|2\cos(ak)+e^{-4\pi a\alpha}|\leqq 2, \tag{3.26}$$

in which case (3.19) has a pair of complex conjugate solutions $z_0(k)$ and $\bar{z}_0(k)$ with $|z_0(k)|=|\bar{z}_0(k)|=1$. So that $\ln(z_0(k))$ is imaginary and (3.21) are all real solutions. If $\frac{1}{a}\cdot|\arg z_0(k)|=|i\ln(z_0(k))|<|k|$ then again

$$E_0(k)=\frac{1}{a^2}(\arg(z_0(k)))^2 \tag{3.27}$$

is an eigenvalue of $H_\alpha(k)$ with eigenfunction given by (3.24) if $\frac{1}{a}|\arg z_0(k)|>|k|$ then $E_0(k)$ is a resonance. $E_n^{\pm}(k)$, $n=1,2,\ldots$ given by (3.25) are all resonances imbedded in the continuous spectrum $[k^2,\infty)$ of $H_\alpha(k)$. Hence we have

Theorem 3.3. *Let $X=\{0\}$; then the essential spectrum of $H_\alpha(k)$ is absolutely continuous and is the half line $[k^2,\infty)$.*

In addition $H_\alpha(k)$ has at most one simple eigenvalue $E_0(k)$ which satisfies $E_0(k)<k^2$. Let z_0 be one of the solutions of

$$z^2-(2\cos(ak)+e^{-4\pi a\alpha})z+1=0.$$

Then

$$E_0(k)=-\frac{1}{a^2}(\ln(z_0(k)))^2$$

and the corresponding eigenfunction is

$$\psi_0(p_1,p_2,\gamma;k)=(p_1^2+p_2^2+(\gamma+k)^2-E_0(k))^{-1}.$$

If $E_0(k)\geqq k^2$ then $E_0(k)$ is a resonance imbedded in the continuous spectrum. The other resonances are given by

$$E_n^{\pm}(k)=\frac{1}{a^2}[\pm i\ln z_0(k)+2\pi n]^2, \qquad n=1,2,\ldots.$$

These resonances are complex if $2\cos(ak)+e^{-4\pi a\alpha}>2$ and they are all real and on the line $[k^2,\infty)$ if $|2\cos(ak)+e^{-4\pi a\alpha}|\leqq 2$.

We see that $2\cos(ak)+e^{-4\pi a\alpha}>2$ for all k if $e^{-4\pi a\alpha}>4$ or $-4\pi a\alpha>2\ln 2$. Hence if $\alpha<-\frac{1}{2\pi a}\ln 2$ we are in case (i) for all k. Hence we have

Theorem 3.4. *Let $X=\{0\}$, then the spectrum of H_α is absolutely continuous and if*

(i′) $\alpha\geqq-\frac{1}{2\pi a}\ln 2$ *then* $\operatorname{sp}H_\alpha=[e_0^-,\infty)$,

(ii) $\alpha<-\frac{1}{2\pi a}\ln 2$ *then* $\operatorname{sp}H_\alpha=[e_0^-,e_0^+]\cup[0,\infty)$,

where $e_0^{\pm}<0$ and

$$e_0^{\pm}=-\frac{1}{a^2}\left[\ln\left(\mp 1+\tfrac{1}{2}e^{-4\pi a\alpha}+\sqrt{(\mp 1+\tfrac{1}{2}e^{-4\pi a\alpha})^2-1}\right)\right]^2.$$

4. Monomolecular Layers

Let $\Lambda_2=\{n_1a_1+n_2a_2;(n_1,n_2)\in Z^2\}$ where $a_i\in R^2$, be a discrete subgroup of R^2. We shall identify Λ_2 as a discrete subgroup of R^3 by the standard injection of R^2 into R^3. Let X be a finite subset of R^3; then $Y=\Lambda_2+X$ is a discrete subset of R^3 invariant under the group Λ_2. Let α be a real function on Y which is invariant under the action of Λ_2 so that $\alpha_{\lambda+x}=\alpha_x$. Then H^Y_α of Theorem 1.1 is invariant under the unitary group $\lambda\to U_\lambda$, $\lambda\in\Lambda_2$, hence

$$H_\alpha=\int_{\hat{\Lambda}_2} H_\alpha(k)dk, \tag{4.1}$$

where the dual group $\hat{\Lambda}_2=R_2/\Gamma_2$ and Γ_2 is the reciprocal lattice i.e. $\Gamma_2=\{n_1b_1+n_2b_2,(n_1,n_2)\in Z^2\}$ and $(a_i,b_j)=2\pi\delta_{ij}$. Let B_2 be the corresponding Brillouin zone i.e.

$$B_2=\{s_1b_1+s_2b_2,\ -\tfrac{1}{2}\leqq s;\ \leqq\tfrac{1}{2},\ i=1,2\}. \tag{4.2}$$

As in Sect. 3 we start by computing

$$h_E(x-y,k)=\sum_{\lambda\in\Lambda_2}\tilde{G}_E(x-y+\lambda)e^{-i\lambda k}. \tag{4.3}$$

For $x-y\notin\Lambda_2$ we have

$$\begin{aligned}h_E(x-y,k)&=\sum_{\lambda\in\Lambda_2}G(x-y+\lambda)e^{-i\lambda k}\\&=(2\pi)^{-3}\sum_{\lambda\in\Lambda_2}\int_{R^3}\frac{e^{ip(x-y)}\cdot e^{i[(p_1-k_1)\lambda_1+(p_2-k_2)\lambda_2]}}{p^2-E}dp\\&=(2\pi)^{-1}\sum_{\lambda\in\Gamma_2}\int_R\\&\quad\cdot\frac{e^{i[(\gamma_1+k_1)(x_1-y_1)+(\gamma_2+k_2)(x_2-y_2)+p_3(x_3-y_3)]}}{p_3^2+(\gamma_1+k_1)^2+(\gamma_2+k_2)^2-E}dp_3.\end{aligned}$$

Hence for $x-y\notin\Lambda_2$ we have

$$h_E(x-y,k)=\sum_{\gamma\in\Gamma_2}\frac{e^{-\sqrt{(\gamma_1+k_1)^2(\gamma_2+k_2)^2-E}\cdot|x_3-y_3|}}{2\sqrt{(\gamma_1+k_1)^2+(\gamma_2+k_2)^2-E}}\cdot e^{i[(\gamma_1+k_1)(x_1-y_1)+(\gamma_2+k_2)(x_2-y_2)]}. \tag{4.4}$$

For

$$\lambda\in\Lambda_2\qquad h_E(\lambda,k)=e^{-i\lambda k}h_E(0,k) \tag{4.5}$$

and

$$h_E(0,k)=\sum_{\substack{\lambda\in\Lambda_2\\ \lambda\neq0}}G_E(\lambda)e^{-i\lambda k}.$$

Hence

$$h_E(0,k)=\lim_{\omega\to\infty}(2\pi)^{-3}\left[\sum_{\substack{|\gamma+k|\leqq\omega\\ \gamma\in\Gamma_2}}\tfrac{1}{2}[(\gamma_1+k_1)^2+(\gamma_2+k_2)^2-E]^{-1/2}-4\pi\omega\right]-\frac{i\sqrt{E}}{4\pi}.$$

Let now $g_E(x-y,k)=h_E(x-y,k)$ if $x-y\neq 0$ and

$$g_E(0,k)=\lim_{\omega\to\infty}(2\pi)^{-3}\left[\frac{1}{2}\sum_{\substack{|\gamma+k|\leq\omega\\ \gamma\in\Gamma_2}}[(\gamma_1+k_1)^2+(\gamma_2+k_2)^2-E]^{-1/2}-\frac{\omega}{2\pi^2}\right]. \quad (4.6)$$

Theorem 4.1. *Let $\Lambda_2=\{n_1a_1+n_2a_2;(n_1,n_2)\in Z^2\}$, where a_1 and a_2 are two independent vectors in R^2. We consider $\Lambda_2\subset R^2\subset R^3$ to be a discrete subgroup of R^3 by the standard injection of R^2 into R^3. Let X be a finite subset of R^3; then $Y=\Lambda_2+X$ is a discrete subset of R^3 invariant under Λ_2. Let α be a real function on Y which is invariant under the action of Λ_2 so that $\alpha_{\lambda+x}=\alpha_x$. Then H_α of Theorem 1.1 is invariant under Λ_2 so that*

$$H_\alpha=\int_{\hat{\Lambda}_2}H_\alpha(k)dk,$$

where $\hat{\Lambda}_2=R_2/\Gamma_2$, $\Gamma_2=\{n_1b_1+n_2b_2,(n_1,n_2)\in Z^2\}$, $(a_i,b_j)=2\pi\delta_{ij}$. Let $g_E(x-y,k)$ be given by (4.6)*; then the resolvent kernel of $H_\alpha(k)$ is*

$$(H_\alpha(k)-E)^{-1}=((\gamma_1+k_1)^2+(\gamma_2+k_2)^2+p_3^2-E)^{-1}-\sum_{x,y\in X}[\alpha_x\delta_{xy}-g_E(x-y,k)]^{-1}$$
$$\cdot\frac{e^{i[(\gamma_1+k_1)x_1+(\gamma_2+k_2)x_2+p_3x_3]}}{(\gamma_1+k_1)^2+(\gamma_2+k_2)^2+p_3^2-E}$$
$$\cdot\frac{e^{-i[(\gamma_1'+k_1)y_1+(\gamma_2'+k_2)y_2+q_3y_3]}}{(\gamma_1'+k_1)^2+(\gamma_2'+k_2)^2+q_3^2-E},$$

as a kernel on $L_2(\Gamma_2\times R)$, where $[\;]^{-1}$ is the inverse $n\times n$ matrix.

We may also compute the wave operators and the corresponding scattering matrix as in the previous section, and we get

Theorem 4.2. *Let $H_\infty=p^2$ be the free Hamiltonian in $L_2(R^3)$. and let H_α be given in Theorem 4.1; then the wave operators*

$$W_\pm(H_\alpha,H_\infty)=\text{strong}\lim_{t\to\pm\infty}e^{-itH_\alpha}e^{itH_\infty}$$

exist. The corresponding scattering matrix $S_\alpha=W_+^*W_-$ is given by

$$S_\alpha(p_1,p_2,p_3;q_1,q_2,q_3)=\delta(p_1-q_1)\delta(p_2-q_2)\delta(p_3-q_3)-\sum_{x,y\in X}$$
$$[\alpha_x\delta_{xy}-g_{E+i0}(x-y),k)]^{-1}$$
$$\cdot e^{i[(\gamma_1+k_1)x_1+(\gamma_2+k_2)x_2+p_3x_3]}\cdot e^{-i[(\gamma_1'+k_1')y_1+(\gamma_2'+k_2')y_2+q_3y_3]}$$
$$\cdot\delta(k_1-k_1')\delta(k_2-k_2')\delta((\gamma_1+k_1)^2+(\gamma_2+k_2)^2$$
$$+p_3^2-(\gamma_1'+k_1')^2-(\gamma_2'+k_2')^2-q_3^2),$$

where $E=p_1^2+p_2^2+p_3^2$, $p_1=\gamma_1+k_1$, $p_2=\gamma_2+k_2$, $q_1=\gamma_1'+k_1'$ and $q_2=\gamma_2'+k_2'$, $(\gamma_1,\gamma_2)\in\Gamma_2$ and $(k_1,k_2)\in B_2$. $g_{E-i0}(x-y,k)$ is defined by analytic continuation around the cut $[0,\infty]$.

Let now $X=\{0\}$; in this case eigenvalues and resonances are the solution of $\alpha=g_E(0,k)$, i.e.

$$\alpha=(2\pi)^{-3}\lim_{\omega\to\infty}\left[\frac{1}{2}\sum_{\substack{|\gamma+k|\leq\omega\\ \gamma\in\Gamma_2}}[(\gamma_1+k)^2+(\gamma_2+k)^2-E]^{-1/2}-4\pi\omega\right]. \tag{4.7}$$

Since $g_E(0,k)\to-\infty$ as $E\to-\infty$ and $g_E(0,k)\to+\infty$ as $E\to k^2$ we see that (4.7) as a unique solution $E_0(k)$ in the interval $(-\infty,k^2)$. $E_0(k)$ is obviously the bottom of the spectrum of $H_\alpha(k)$. $E_0(k)$ is the only real solution of (4.7) and it is an eigenvalue with corresponding eigenfunction in $L_2(\Gamma_2\times R)$

$$\psi_0(\gamma,p_3;k)=\frac{1}{(\gamma_1+k_1)^2+(\gamma_2+k_2)^2+p_3^2-E_0(k)}.$$

The resonances are the complex solutions of (4.7).

Theorem 4.3. *Let $X=\{0\}$ then the essential spectrum of $H_\alpha(k)$ is absolutely continuous and consists of the half line $[k^2,\infty)$. In addition $H_\alpha(k)$ has exactly one simple eigenvalue $E_0(k)<k^2$ with corresponding eigenfunction*

$$\psi_0(\gamma_1,\gamma_2,p_3;k_1,k_2)=\frac{1}{(\gamma_1+k_1)^2+(\gamma_2+k_2)^2+p_3^2-E_0(k)}.$$

5. Crystals

Let $\Lambda=\{n_1a_1+n_2a_2+n_3a_3;(n_1,n_2,n_3)\in Z^3\}$ where a_1,a_2,a_3 are three linearly independent vectors in R^3. Λ is then a discrete subgroup of R^3; let X be a finite subset of R^3. Then $Y=\Lambda+X$ is a discrete subset of R^3 invariant under the lattice group Λ. Let α be a real function on Y which is invariant under Λ, i.e. $\alpha_{x+\lambda}=\alpha_x$ for $\lambda\in\Lambda$ and $x\in X$. Then H_α of Theorem 1.1 is invariant under translations in Λ, i.e. $U_\lambda H_\alpha U_\lambda^{-1}=H_\alpha$, so that

$$H_\alpha=\int_{\hat\Lambda} H_\alpha(k)dk, \tag{5.1}$$

where $H_\alpha(k)$ is the reduced Hamiltonian for fixed lattice momentum $k\in\hat\Lambda=R^3/\Gamma$ where Γ is the reciprocal lattice, i.e.

$$\Gamma=\{n_1b_1+n_2b_2+n_3b_3;(n_1,n_2,n_3)\in Z^3\},$$

with $(a_i,b_j)=2\pi\delta_{ij}$. The projection $R^3\to R^3/\Gamma=\hat\Lambda$ is given by $k\to e^{ik\lambda}$. It is convenient to identify $\hat\Lambda$ with the Brillouin zone

$$B=\{s_1b_1+s_2b_2+s_3b_3;\ -\tfrac{1}{2}<s_i\leq\tfrac{1}{2}\}$$

by the identification $k\leftrightarrow e^{ik\lambda}$. From Theorem 1.1 we have that

$$(H_\alpha-E)^{-1}=(p^2-k^2)^{-1}-(2\pi)^{-3}\sum_{x,y\in X}\sum_{\lambda,\lambda'\in\Lambda}$$
$$\cdot\left[\left(\alpha_x-\frac{i\sqrt{E}}{4\pi}\right)\delta_{xy}\delta_{\lambda\lambda'}-\tilde G_E(x-y+\lambda-\lambda')\right]^{-1}\frac{e^{ipx}e^{ip\lambda}}{p^2-E}\frac{e^{-iqy}e^{-iq\lambda'}}{q^2-E},$$

where $\tilde{G}_E(x-y)=\dfrac{1}{4\pi|x-y|}e^{i\sqrt{E}|x-y|}$ if $x-y\neq 0$ and zero if not, and $[\ ]^{-1}$ is the inverse kernel as operator on $l_2(X\times\Lambda)=l_2(X)\otimes l_2(\Lambda)$. As in the two previous sections we compute

$$h_E(x-y,k)=\sum_{\lambda\in\Lambda}\tilde{G}_E(x-y+\lambda)e^{-ik\lambda}. \tag{5.3}$$

If $x-y\notin\Lambda$ we have that

$$\begin{aligned}h_E(x-y,k)&=\sum_{\lambda\in\Lambda}G_E(x-y+\lambda)e^{-i\lambda k}\\&=\sum_{\lambda\in\Lambda}(2\pi)^{-3}\int\frac{e^{ip(x-y)}e^{i(p-k)\lambda}}{p^2-E}dp\end{aligned}$$

which by the Poisson summation formula gives

$$h_E(x-y,k)=(2\pi)^{-3}\sum_{\gamma\in\Gamma}\frac{e^{i(\gamma+k)(x-y)}}{(\gamma+k)^2-E}\quad\text{for}\quad x-y\notin\Lambda. \tag{5.4}$$

For $x-y=\lambda\in\Lambda$ we have

$$h_E(\lambda,k)=e^{-i\lambda k}h_E(0,k) \tag{5.5}$$

while

$$\begin{aligned}h_E(0,k)&=\sum_{\substack{\lambda\in\Lambda\\ \lambda\neq 0}}G_E(\lambda)e^{-idk}\\&=\lim_{\omega\to\infty}(2\pi)^{-3}\left[\sum_{\substack{\gamma\in\Gamma\\ |\gamma+k|\leqq\omega}}\frac{1}{(\gamma+k)^2-E}-\int_{|p|\leqq\omega}\frac{dp}{p^2-E}\right],\end{aligned}$$

hence

$$h_E(0,k)=\lim_{\omega\to\infty}(2\pi)^{-3}\left[\sum_{\substack{\gamma\in\Gamma\\ |\gamma+k|\leqq\omega}}\frac{1}{(\gamma+k)^2-E}-4\pi\omega\right]-\frac{i\sqrt{E}}{4\pi}. \tag{5.6}$$

Let now

$$\begin{aligned}g_E(x-y,k)&=h_E(x-y,k)\quad\text{for}\quad x-y\neq 0\\ g_E(0,k)&=\lim_{\omega\to\infty}(2\pi)^{-3}\left[\sum_{\substack{\gamma\in\Gamma\\ |\gamma+k|\leqq\omega}}\frac{1}{|\gamma+k|^2-E}-4\pi\omega\right].\end{aligned} \tag{5.7}$$

Then

$$\sum_{\lambda}\left[\left(\alpha_x-\frac{i\sqrt{E}}{4\pi}\right)\delta_{0\lambda}\delta_{xy}-\tilde{G}_E(x-y+\lambda)\right]e^{i\lambda k}=\alpha_x\delta_{xy}-g_E(x-y,k) \tag{5.8}$$

which implies that (5.2) takes the form

$$\begin{aligned}(H_\alpha-E)^{-1}&=((\gamma+k)^2-E)^{-1}-(2\pi)^{-3}\sum_{x,y\in X}[\alpha_x\delta_{xy}-g_E(x-y,k)]^{-1}\\&\quad\cdot\frac{\delta(k-k')e^{i[(\gamma+k)x-(\gamma'+k')y]}}{((\gamma+k)^2-E)((\gamma'+k')^2-E)},\end{aligned} \tag{5.9}$$

where $p=\gamma+k$ and $q=\gamma'+k'$ with $\gamma,\gamma'\in\Gamma$ and k and k' in B and $[\ ]^{-1}$ is the inverse $n\times n$ matrix. Hence we have proved

Theorem 5.1. *Let*

$$\Lambda=\{n_1a_1+n_2a_2+n_3a_3;(n_1,n_2,n_3)\in Z^3\}$$

be a discrete lattice subgroup of R^3,

$$\Gamma=\{n_1b_1+n_2b_2+n_3b_3\}, \qquad (a_i,b_j)=2\pi\delta_{ij}$$

the reciprocal lattice and

$$B=\{s_1b_1+s_2b_2+s_3b_3;\tfrac{1}{2}<s;\leqq\tfrac{1}{2}\}$$

be the corresponding Brillouin zone. Let X *be a finite set in* R^3 *and* $Y=\Lambda+X$ *and let* $\alpha_{x+\lambda}=\alpha_x$ *be a* Λ *invariant real function on* Y. *Then* H_α *of Theorem 1.1 is translation invariant under translations* $\lambda\in\Lambda$ *hence*

$$H_\alpha=\int_{\hat{\Lambda}} H_\alpha(k)dk=\frac{1}{|B|}\int_B H_\alpha(k)dk,$$

where we have identified the dual group $\hat{\Lambda}$ *with* B *via the mapping* $k\to e^{i\lambda k}$. *The reduced Hamiltonian* $H_\alpha(k)$ *is a self adjoint operator on* $l_2(\Gamma)$ *given by its resolvent kernel*

$$(H_\alpha(k)-E)^{-1}=((\gamma+k)^2-E)^{-1}\delta_{\gamma\gamma'}$$
$$-(2\pi)^{-3}\sum_{x,y\in X}[\alpha_x\delta_{xy}-g_E(x-y,k)]^{-1}\frac{e^{i(\gamma+k)x}}{(\gamma+k)^2-E}\cdot\frac{e^{-i(\gamma'+k)y}}{(\gamma'+k)^2-E},$$

where $g_E(x-y,k)$ *is given by* (5.7) *and* $[\ ]^{-1}$ *is the inverse* $n\times n$ *matrix* $n=|X|$.

It is well known that if H is a Hamiltonian which is invariant under Λ then the corresponding reduced Hamiltonian $H(k)$ has discrete spectrum with eigenvalues $E_n(k)$ [10]. The functions $E_n(k)$ over the forms $\hat{\Lambda}=R^3/\Gamma$ are called the energy bands of the Bloch Hamiltonian H. A detailed knowledge of the energy bands $E_n(k)$ is of considerable interest in the study of the solid state.

Let us therefore consider the case $|X|=1$, i.e. $X=\{0\}$. In this case $Y=\Lambda$ and $\alpha_\lambda=\alpha$ for all $\lambda\in\Lambda$. From Theorem 5.1 we have that

$$(H_\alpha(k)-E)^{-1}=((\gamma+k)^2-E)^{-1}\delta_{\gamma\gamma'}-(2\pi)^{-3}(\alpha-g_E(0,k))^{-1}\frac{1}{(\gamma+k)^2-E}\cdot\frac{1}{(\gamma'+k)^2-E}, \tag{5.10}$$

where

$$g_E(0,k)=\lim_{\omega\to\infty}(2\pi)^{-3}\left[\sum_{\substack{\gamma\in\Gamma\\|\gamma+k|\leqq\omega}}\frac{1}{(\gamma+k)^2-E}-4\pi\omega\right]. \tag{5.11}$$

The eigenvalues of $H_\alpha(k)$ are the poles of (5.10). There are two possibilities for such poles, first the zeros of $\alpha - g_E(0,k)$ and then the zeros of $(\gamma+k)^2 - E$, which are the eigenvalues of the free Hamiltonian. Let us first consider the solutions of

$$\alpha - g_E(0,k) = 0. \tag{5.12}$$

Since

$$\frac{dg_E(0,k)}{dE} = (2\pi)^{-3} \sum_{\gamma\in\Gamma} \frac{1}{((\gamma+k)^2 - E)^2} \tag{5.13}$$

we see that $E - g_E(0,k)$ is an increasing function everywhere on the real line, $g_E(0,k)$ has a positive pole of first order at the points $|\gamma+k|^2$, $\gamma\in\Gamma$ with a residue equal to the number of points in Γ which are mapped into $|\gamma+k|^2$. Hence there is exactly one solution of (5.12) in each of the bounded intervals I_n, $n=1,2,\dots$ where

$$R - |\Gamma+k|^2 = \bigcup_{n=0}^{\infty} I_n \tag{5.14}$$

and I_n are open intervals numbered in increasing order from left to right and I_0 is the unbounded interval to the left. Observing that $g_E(0,k) \to -\infty$ as $E \to -\infty$, we find that there is exactly one solution in the unbounded interval I_0. All these solutions are obviously first order poles of $(H_\alpha(k) - E)^{-1}$ and are therefore simple eigenvalues of $H_\alpha(k)$. The eigenvalue which is the solution of (5.12) in I_0 is obviously the bottom of the spectrum of $H_\alpha(k)$ and called $E_0(k)$.

The other possible poles of (5.10) are the points $E=(\gamma+k)^2$, $\gamma\in\Gamma$ which are the eigenvalues of the free Hamiltonian. It is easily seen that if $(\gamma_0+k)^2$ is a simple eigenvalue of the free Hamiltonian i.e. if there is only one $\gamma\in\Gamma$ such that $(\gamma+k)^2 = (\gamma_0+k)^2$ and that is $\gamma=\gamma_0$, then $E=(\gamma+k)^2$ is not a pole of the resolvent (5.10) because the poles in the first and in the second term in (5.10) exactly cancel each other. If however $(\gamma_0+k)^2$ has multiplicity $m+1$, i.e. there are exactly $m+1$ different elements $\gamma_0, \dots, \gamma_m$ in Γ such that $(\gamma_0+k)^2 = (\gamma_1+k)^2 = (\gamma_m+k)^2$, then (5.10) has a pole at $E=(\gamma_0+k)^2$ and the corresponding eigenspace is m dimensional and is spanned by the vectors

$$\delta_{\gamma\gamma_j} - \frac{1}{m+1} \sum_{i=0}^{m} \delta_{\gamma\gamma_i}, \qquad j=1,\dots,m, \tag{5.15}$$

where $\{\gamma_0, \dots, \gamma_m\}$ is the inverse image of $|\gamma_0+k|^2$ under the map $\gamma \to |\gamma+k|^2$.

Let now $E_0(k) \leqq E_1(k) \leqq \dots$ be the eigenvalues of $H_\alpha(k)$. If $E_n(k)$ is the unique solution of (5.12) in an interval $I_{n'}$ then E_n is simple and from (5.10) we get that the corresponding eigenfunction is $\psi_n^k(\gamma) = ((\gamma+\mathrm{k})^2 - \mathrm{E}_n(\mathrm{k}))^{-1}$. Hence we have proved

Theorem 5.2. *Let X consist of only one point, i.e. $X=\{0\}$. Then the corresponding reduced Bloch Hamiltonian $H_\alpha(k)$ is given by its resolvent kernel on $l_2(\Gamma)$*

$$(H_\alpha(k) - E)^{-1}(\gamma,\gamma') = (\gamma+k)^2 - E)^{-1}\delta_{\gamma\gamma'} - (2\pi)^{-3}(\alpha - g_E(0,k))^{-1}$$
$$\frac{1}{(\gamma+k)^2 - E} \cdot \frac{1}{(\gamma'+E)^2 - E},$$

where

$$g_E(0,k)=\lim_{\omega\to\infty}(2\pi)^{-3}\left[\sum_{\substack{\gamma\in\Gamma\\|\gamma+k|\leqq\omega}}\frac{1}{(\gamma+k)^2-E}-4\pi\omega\right].$$

$H_\alpha(k)$ has a pure point spectrum and is bounded below. Let $R-|\Gamma+k|^2=\bigcup_{n\geqq 0} I_n^k$ where I_n^k are open intervals, I_0 unbounded. Then there is exactly one simple eigenvalue $E_n(k)$ in each I_n^k with corresponding eigenfunction $\psi_n^k(\gamma)=((\gamma+k)^2-E_n(k))^{-1}$. In addition $H_\alpha(k)$ has eigenvalues at the points $|\gamma+k|^2$ for which the map $\Gamma\to R^+$ given by $\gamma\to|\gamma+k|^2$ is not simple. The multiplicity of the eigenvalue $|\gamma_0+k|^2$ is one less than the multiplicity of the map $\gamma\to|\gamma+k|^2$ at the point $|\gamma_0+k|$. The corresponding eigenspace is spanned by the vectors

$$\delta_{\gamma\gamma_j}-\frac{1}{m+1}\sum_{i=0}^{m}\delta_{\gamma\gamma_i},\qquad j=1,\ldots,m,$$

where $\{\gamma_0,\ldots,\gamma_m\}$ is the inverse image of $|\gamma_1+k|^2$ under $\gamma\to|\gamma+k|^2$.

We shall consider the eigenvalues $E_n(k)$ of $H_\alpha(k)$ of Theorem 5.2 to be periodic functions over R^3 with periods Γ, i.e. $E_n(k+\gamma)=E_n(k)$ for $\gamma\in\Gamma$. From Theorem 5.2 we see that there is a natural correspondence between the elements $\gamma\in\Gamma$ and the eigenvalues $\{E_n(k)\}$ of $H_\alpha(k)$ i.e. $\gamma\to E_\gamma(k)$ where $E_\gamma(k)$ is the largest eigenvalue smaller or equal to $|\gamma+k|^2$. Let $\gamma'\neq\gamma$ be such that $|\gamma'+k|^2$ is a largest element in $|\Gamma+k|^2$ smaller or equal to $|\gamma+k|^2$. If $|\gamma'+k|^2<|\gamma+k|^2$ then $E_\gamma(k)\in(|\gamma'+k|^2,|\gamma+k|^2)$ and if $|\gamma'+k|^2=|\gamma+k|^2$ then $E_\gamma(k)=|\gamma+k|^2$.

$\gamma\to E_\gamma(k)$ preserves multiplicity and $E_\gamma(k)=E_{\gamma'}(k)$ for $\gamma\neq\gamma'$ if and only if there is a $\gamma''\in\Gamma$ different from γ and γ' such that $|\gamma+k|^2=|\gamma'+k|^2=|\gamma''+k|^2$. Since $E_\gamma(k)$ are solutions of (5.12) they are different branches of one and the same analytic function of k. There is a unique lowest band $E_0(k)$ which is smaller than all the points $|\gamma+k|^2$, $\gamma\in\Gamma$. All the other energy bands are connected.

To prove this let γ be arbitrary in Γ such that $E_\gamma(0)$ is not the unique smallest eigenvalue $E_0(0)$, and let $E_{\gamma'}(0)$ smallest eigenvalue of $H_\alpha(0)$ larger or equal to $E_\gamma(0)$.

We want to prove that there is a $k\in R^3$ such that $E_\gamma(k)=E_{\gamma'}(k)$. If $E_\gamma(0)=E_{\gamma'}(0)$ we are finished and if not $|\gamma|^2<E_{\gamma'}(0)<|\gamma'|^2$ and $E_\gamma(0)\leqq|\gamma|^2$. Since $E_\gamma(0)>E_0(0)$ there is a $\gamma''\in\Gamma$ such that $E_{\gamma''}(0)$ is a largest eigenvalue smaller or equal to $E_\gamma(0)$, and

$$|\gamma''|^2\leqq E_\gamma(0)\leqq|\gamma|^2<E_{\gamma'}(0)<|\gamma'|^2. \tag{5.16}$$

Moreover from the definition of $E_\gamma(k)$ we have that

$$|\gamma''+k|^2\leqq E_\gamma(k)\leqq|\gamma+k|^2\leqq E_{\gamma'}(k)\leqq|\gamma'+k|^2 \tag{5.17}$$

in the neighborhood of zero where

$$|\gamma''+k|^2\leqq|\gamma+k|^2\leqq|\gamma'+k|^2. \tag{5.18}$$

By a theorem of Euclid there is a point in R^3 such that

$$|\gamma''+k|=|\gamma+k|=|\gamma'+k|, \tag{5.19}$$

in fact (5.19) defines a unique line in R^3, namely the line through the centre of the triangle $(\gamma, \gamma', \gamma'')$ and orthogonal to this triangle. This line intersects the neighborhood given by (5.18) and on this intersection we get from (5.17) that $E_\gamma(k) = E_{\gamma'}(k)$. Hence we have proved.

Theorem 5.3. *Let the assumptions be as in Theorem 5.2. The energy bands $E_n(k)$ are branches of an analytic function of k, periodic over R^3 with period Γ. There is a unique simple lowest eigenvalue $E_0(k)$ which is the only eigenvalue smaller than $|\Gamma+k|^2$. Moreover $E_0(k) < E_n(k)$ for all $n \neq 0$. There is a natural correspondence $\gamma \to E_\gamma(k)$, $\gamma \in \Gamma$ between Γ and $\mathrm{sp}\,H_\alpha(k)$, where $E_\gamma(k)$ is the largest eigenvalue smaller or equal to $|\gamma+k|^2$. $\gamma \to E_\gamma(k)$ preserves multiplicity in the sense that the multiplicity of $E_\gamma(k)$ is the number of elements in the inverse image. Moreover if $\gamma' \in \Gamma$ is so that $|\gamma'+k|^2$ is a largest element in $|\Gamma+k|^2$ smaller or equal to $|\gamma+k|^2$ then $|\gamma'+k| \leqq E_\gamma(k) \leqq |\gamma+k|^2$, and if $|\gamma'+k|^2 < |\gamma+k|^2$ then $|\gamma'+k|^2 < E_\gamma(k) < |\gamma+k|^2$. All the energy surfaces $E_\gamma(k)$ apart from the lowest $E_0(k)$ are connected, and $E_\gamma(k)$ is connected with other surfaces along lines given by $|\gamma''+k| = |\gamma+k| = |\gamma'+k|$ for γ, γ', and γ'' three different points in Γ.*

It follows from (5.11) and (5.12) that $E_0(k)$ takes its minimum at $k=0$ and maximum at $k = k_0 = (\frac{1}{2}b_1, \frac{1}{2}b_2, \frac{1}{2}b_3)$. Moreover we see that the minimum $E_0(0) < 0$ and the maximum $E_0(k_0)$ is negative if and only if $\alpha < \alpha_0$ where

$$\alpha_0 = g_0(0, k_0) = (2\pi)^{-3} \lim_{\omega\to\infty} \left[\sum_{\substack{\gamma\in\Gamma \\ |\gamma+k| \leqq \omega}} \frac{1}{(\gamma+k_0)^2} - 4\pi\omega \right]. \tag{5.20}$$

Hence we get the following theorem

Theorem 5.4. *Let the assumptions be as in Theorem 5.2. Then the spectrum of H_α is absolutely continuous and*

$$\text{if} \quad \alpha \geqq \alpha_0 \quad \text{then} \quad \mathrm{sp}\,H_\alpha = [E_0(0), \infty),$$

$$\text{if} \quad \alpha < \alpha_0 \quad \text{then} \quad \mathrm{sp}\,H_\alpha = [E_0(0), E_0(k_0)] \cup [0, \infty) \quad \text{with} \quad E_0(k_0) < 0,$$

where

$$\alpha_0 = g_0(0, k_0) = (2\pi)^{-3} \lim_{\omega\to\infty} \left[\sum_{\substack{\gamma\in\Gamma \\ |\gamma+k| \leqq \omega}} \frac{1}{(\gamma+k_0)^2} - 4\pi\omega \right]$$

and $k_0 = \frac{1}{2}(b_1, b_2, b_3)$.

6. The Grating (the Linear Interferometer)

In this section we consider a potential with support on a set of equally spaced parallel lines in the plane spanned by the second and the third axis in R^3. We take the lines to be parallel to the third axis and we want the potential to be translation invariant along the lines and equally strong on each line. This is the potential of a grating which is often used as an interferometer in spectroscopy. The corresponding Hamiltonian is now translation invariant in the direction of the third axis, and therefore the third component of the momenta is conserved. Hence the problem reduces to a problem in the plane orthogonal to the third axis, and the lines are represented by a string of equally spaced points along the second axis in the plane spanned by the first and the second axis.

Hence the problem of the grating is that of a Hamiltonian in R^2 with a potential with support on a discrete subgroup of the second axis and the potential being translation invariant under this discrete subgroup.

Let $\Lambda_1=\{na,\, n\in Z\}$, $a\in R^+$ and consider Λ_1 as a subgroup of R^2 which is a subgroup of the second component of $R\times R=R^2$. Let $Y=\Lambda_1$ and let α be a real function on Y invariant under Λ_1, i.e. $\alpha_\lambda=\alpha$. The corresponding Hamiltonian H_α is given by Theorem 1.2 as

$$(H_\alpha-E)^{-1}=(p^2-E)^{-1}-\sum_{\lambda,\lambda'\in\Lambda_1}\left[\left(\alpha-\frac{\ln\sqrt{-E}}{2\pi}\right)\delta_{\lambda\lambda'}-\tilde{G}_E(\lambda-\lambda')\right]^{-1}$$

$$\cdot(2\pi)^{-2}\frac{e^{ip\lambda}}{p^2-E}\frac{e^{-iq\lambda'}}{q^2-E}, \tag{6.1}$$

where

$$\tilde{G}_E(\lambda-\lambda')=(2\pi)^{-2}\int\frac{e^{ip(\lambda-\lambda')}}{p^2-E}dp \quad \text{for} \quad \lambda\neq\lambda' \tag{6.2}$$

and $\tilde{G}_E(0)=0$.

Now set

$$h_E(0,k)=\sum_{\lambda\in\Lambda_1}\tilde{G}(\lambda)e^{-ik\lambda}$$

$$=(2\pi)^{-2}\sum_{n\neq 0}\int_{R^2}\frac{e^{ia(p_2-k)n}}{p_1^2+p_2^2-E}dp_1dp_2\,.$$

Hence

$$h_E(0,k)=\lim_{\omega\to\infty}\left[\frac{1}{2}\sum_{\substack{|\gamma+k|\leq\omega\\ \gamma\in\Gamma_1}}((\gamma+\mathrm{k})^2-\mathrm{E})^{-1/2}-\frac{1}{4\pi}\ln(\omega^2+1)\right]-\frac{1}{4\pi}\ln(-E), \tag{6.3}$$

where $\Gamma_1=\left\{\frac{2\pi}{a}n,\, n\in Z\right\}$. Since H_α is translation invariant under Λ_1 we have that

$$H_\alpha=\int_{\hat{\Lambda}}H_\alpha(k)dk=\int_{-\pi/a}^{\pi/a}H_\alpha(k)dk, \tag{6.4}$$

where $\hat{\Lambda}_1=R/\Gamma_1$ is identified with the interval $\left[-\frac{\pi}{a},\frac{\pi}{a}\right]$. From (6.1) and (6.3) we then have

$$(H_\alpha(k)-E)^{-1}=(p_1^2+(\gamma+k)^2-E)^{-1}$$

$$-(2\pi)^{-2}\left(\alpha-\frac{\ln(-E)}{4\pi}-h_E(0,k)\right)^{-1}\frac{1}{p_1^2+(\gamma+k)^2-E}\,\frac{1}{q_1^2+(\gamma'+k)-E} \tag{6.5}$$

We have the following theorem

Theorem 6.1. *Let $\Lambda_1 = \{na, n \in Z\}$, $a \in R^+$ and consider Λ_1 to be a subgroup of the second component in $R^2 = R \times R$. Let α be a real function on Λ_1 and invariant under Λ_1, i.e. $\alpha_\lambda = \alpha$. Then the corresponding Hamiltonian $H_\alpha = \int H_\alpha(k) dk$ where $H_\alpha(k)$ is a self-adjoint operator on $L_2(R \times \Gamma_1)$, $\Gamma_1 = \left\{\frac{2\pi}{a} n, n \in Z\right\}$ with resolvent kernel*

$$(h_\alpha(k) - E)^{-1} = (p_1^2 + (\gamma + k)^2 - E)^{-1} - (2\pi)^{-2}(\alpha - g_E(0,k))^{-1} \frac{1}{p_1^2 + (\gamma + k)^2 - E} \frac{1}{q_1^2 + (\gamma' + k)^2 - E},$$

where

$$g_E(0,k) = \lim_{\omega \to \infty} \left[\frac{1}{2} \sum_{|\gamma + k| \leqq \omega} ((\gamma + \mathrm{k})^2 - \mathrm{E})^{-1/2} - \frac{1}{4\pi} \ln(\omega^2 + 1) \right].$$

Now on the interval $(-\infty, k^2)$ $g_E(0,k)$ is a monotonic function of E with range equal to R. Hence for any $\alpha \in R$ there is a unique solution $E_0(k, \alpha)$ of the equation

$$\alpha = g_E(0,k) \tag{6.6}$$

with $E_0(k,\alpha) < k^2$. It follows from the expression for the resolvent kernel in Theorem 6.1 that $E_0(k,\alpha)$ is a simple eigenvalue of $H_\alpha(k)$ with corresponding eigenfunction

$$\psi_0(p, \gamma; k) = \frac{1}{p^2 + (\gamma + k)^2 - E_0(k, \alpha)}. \tag{6.7}$$

We see that this is the only eigenvalue of $H_\alpha(k)$. Hence we have

Theorem 6.2. *The essential spectrum of $H_\alpha(k)$ is absolutely continuous and equal to $[k^2, \infty)$. $H_\alpha(k)$ has exactly one simple eigenvalue $E_0(k,\alpha)$ and this lies below the continuous spectrum with corresponding eigenfunction*

$$\psi_0(p, \gamma; k) = \frac{1}{p^2 + (\gamma + k)^2 - E_0(k, \alpha)}.$$

Remark. The scattering matrix may be computed in the same way as in Sect. 3 or 4.

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