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Edited by A. Dold and B. Eckmann

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# Schrödinger Operators, Aarhus 1985

Seminar

Edited by E. Balslev

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# C O N T E N T

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# The Schrödinger operator for a particle in a solid with deterministic and stochastic point interactions

by

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A B S T R A C T

We give a survey of recent results concerning Schrödinger operators describing the motion of a quantum mechanical particle in $\mathbb{R}^3$ or $\mathbb{R}^1$ under the influence of a potential concentrated at N centers, $N \leq \infty$.

We dedicate particular attention to the case $N = \infty$, with centers forming a periodic lattice (model of a crystal) or with centers randomly distributed with random strengths (models of disordered solids or random alloys).

## 0. Introduction

The study of the motion of quantum mechanical particles in an ordered or disordered solid presents formidable difficulties and various simplifications/idealizations have to be made. In the "one electron approximation" just one particle (electron) is considered and the centers of forces (nuclei) are fixed, belonging to a lattice (nuclear vibrations and presence of other electrons are thus neglected).
In the case where the total interaction potential between the electron and the nuclei is periodic ("Bloch/Floquet model"), structural results (band structure, estimates on number of gaps) on the spectrum are known, see e.g. [ 1 ], [ 2 ], [ 3 ], [ 4 ], [ 5 ]. In the case of randomly disturbed lattices also some general results are known, see e.g. [ 6 ], [ 7 ], [ 8 ]. However in both cases there is great interest in having "solvable models" in which all quantities can be calculated. Such models have also the important function of dealing as reference for testing approximate mathematical methods.
An important class of solvable models is provided by the so called point interaction models (also known under the name of $\delta$-interaction models or zero range models; they are also closely related to "pseudo potentials" models). These models have been introduced in solid state physics and nuclear physics since the thirties, see [ 9 ] (which surveys up to 65 work on the 1-dimensional case), [ 10 ], [ 11 ], [ 12 ]. One should also mention later applications to problems of electromagnetic theory, see e.g.[13,14]. In particular the Kronig-Penney model of a one-dimensional crystal with periodic $\delta$-interactions is well known and have played an important role as a reference model in solid state physics, see e.g. [ 15 ]. The 3-dimensional analogue of this model has only been brought under mathematical control in recent years (see e.g.[ 11 ], [16, 17, 34, 40] and references therein) and should come to play an important role also for more realistic approaches of solid state physics. The first part of each section of this paper is dedicated to a description of this model and of the corresponding results concerning the spectrum.
For the description of disordered solids, like those arising from impurities or from alloys, models with stochastic interactions have been investigated, in particular in recent years, under the stimulus of Anderson-Mott discussion of the phenomenon of localization; there is by now a quite large literature, see e.g.[ 8 ], [18], [ 11 ] and references therein. Also in this case, the study of solvable models provides new insights, as was already clear since the work around the Hutton-Saxner conjecture in one-dimension (see e.g. [9 ] and references therein). Recently the one-dimensional case of models of alloys built with $\delta$-interaction of random strength and position has been discussed in [ 6 ], [ 7 ], [19]. The case of three dimensional models with $\delta$-interactions of random strengths and positions has also been discussed recently, see [20]-[23] . We take up this subject in Sect. 2. Finally we also mention some other models involving interactions localized at certain subsets of $\mathbb{R}^3$, like those involving $\delta$-shell models, models of electrons interacting with polymers and models for self-interacting polymers, see e.g. [24] resp.25, 29] and references therein.

## 1. Schrödinger operators with non random point interactions

Let us start by explaining the meaning of the words "point interactions" in the title of this lecture. By this one understands in general, in the theory of Schrödinger operators, hence in quantum theory, the presence in the Hamiltonian of potentials, "interactions", of the form of operators multiplication by a "function" V supported on some subset of $\mathbb{R}^d$ consisting of isolated points (or, more generally, of measure zero). "Function" is to be understood in some generalized sense (even more general than distribution), and the first problem one meets is of course to define properly say $-\Delta + V$ as an operator in $L^2(\mathbb{R}^d, dx)$, with $\Delta$ the Laplacian in $\mathbb{R}^d$.

To illustrate what we have mind let us consider a couple of typical examples.

a) $d \leq 3$, $-\Delta + \lambda\delta(x)$. This model has a long history in nuclear physics, as an idealized model of a short range force (Bethe-Peierls, Thomas 1935; see e.g. [11] [12] [26]).

b) $d \leq 3$, $-\Delta + \sum_{y \in Y} \lambda_y \delta(x-y)$ for Y a discrete subset of $\mathbb{R}^d$. This model has a long history in solid state physics, at least for d = 1 and Y periodic, e.g. $\mathbb{Z}$: "Kronig-Penney" model for the motion of an electron in an idealized crystal (see e.g. [15], [11]).

c) $-\Delta + \lambda V(x)$ with $|\text{supp } V| = 0$ ($|\ |$ meaning Lebesgue measure) (e.g. supp V the surface of a sphere for d = 3: "delta shell model", see e.g. [24], [27]).

d) $-\Delta + \lambda\int_0^t \delta(x-b(s))ds$, with $\{b(s), 0 \leq s \leq t\}$ a continuous curve in $\mathbb{R}^d$, like e.g. a path of a Brownian particle (this latter case constitutes a model of a quantum mechanical particle interacting with a polymer, see e.g. [25],[28],[29]).

The questions one can ask are: can one associated with above heuristic Hamiltonians well defined self-adjoint operators H in $L^2(\mathbb{R}^d)$?
What about their spectrum, eigenfunctions etc.?

### 1.1 The case of a one center interaction in $\mathbb{R}^3$

Let us first recall some methods for defining H in the case a). The first observation is that the case $d \geq 4$ is trivial in as much as formally $H = -\Delta$ on $C^\infty_{0,0}(\mathbb{R}^d)$ (the $C^\infty$ functions of compact support vanishing in a neighborhood of zero) and $-\Delta \upharpoonright C^\infty_{0,0}(\mathbb{R}^d)$ is essentially self-adjoint for $d \geq 4$, cfr. e.g. [30], Ch. X), hence there is no self-adjoint extension of $H \upharpoonright C^\infty_{0,0}(\mathbb{R}^d)$ different from the trivial one, $-\Delta$.

We shall now examine in some details the most interesting case for physics, namely d = 3 (for the cases d = 1,2 see [11]).

a) 1. The first method for defining $H = -\Delta + \lambda\delta(x)$ in $L^2(\mathbb{R}^3)$ is to use nonstandard analysis. We shall not describe here this method (see [31], [32], [25], [11]), we just give a hint. Let $\varepsilon$ be a positive infinitesimal. By transfer $H_\varepsilon \equiv -\Delta + \lambda_\varepsilon \delta_\varepsilon$ is well defined, self-adjoint in ${}^*L^2(\mathbb{R}^3)$ with $\delta_\varepsilon(x) = (\frac{4}{3}\pi\varepsilon^3)^{-1}\ \chi_1(|x|/\varepsilon)$, a non standard realization of the $\delta$-function, $\chi_1$ being the characteristic function of a sphere of radius 1 and centre at the origin, and

$$\lambda_\varepsilon = -\frac{2}{3}\pi^3\varepsilon + \frac{(4\pi)^2}{3}\ \alpha\varepsilon^2,\ \alpha \in \mathbb{R}.$$

Then the standard part (defined by the resolvent) of $H_\varepsilon$ exists and is equal to the self-adjoint operator $-\Delta_\alpha$ describing a "point interaction of strength $\alpha$ at the origin" (we shall give below a standard description of $-\Delta_\alpha$). This non standard procedure shows also that the only possible realizations of "$-\Delta + \lambda\delta(x)$" form a one-parameter family, with parameter $\alpha \in \mathbb{R}$. In fact also $\alpha$ a positive infinite number is allowed, in which case $-\Delta_\alpha$ is simply the free Hamiltonian $-\Delta$. It also indicates that an infinitesimal negative coupling constant is needed to obtain, after taking standard parts, an Hamiltonian different from $-\Delta$.

It also turns out that the sign of the "renormalized coupling constant" $\alpha$ determines whether or not $-\Delta_\alpha$ has a bound state (eigenvalue) (at $-(4\pi\alpha)^2$), namely if $\alpha < 0$ there is an eigenvalue, if $\alpha \geqq 0$ there is no eigenvalue.

a) 2. Let us now give shortly a first standard method of constructing $-\Delta_\alpha$, for details and proofs see [ 33], [ 11]. Let V be Rollnik (i.e. $\iint |V(x)|\ |V(y)|\ |x-y|^{-2}\ dxdy < \infty$) and in $L^1(\mathbb{R}^3)$, and let $\lambda$ be $C^1(\mathbb{R})$ with $\lambda(0) = 1$. We shall study $-\Delta + \lambda(\varepsilon)\ \varepsilon^{-2}\ V(x/\varepsilon)$ as $\varepsilon \downarrow 0$. Set $v \equiv |V|^{1/2}$, $u \equiv v$ sign V, $G_k(x) \equiv \dfrac{e^{ik|x|}}{4\pi|x|}$ for $\mathrm{Im} k > 0$, $x \neq 0$, $x \in \mathbb{R}^3$ (so that $G_k(x) = (-\Delta - k^2)^{-1}(x)$ is the kernel of the resolvent of $-\Delta$).

If $\varphi \in L^2(\mathbb{R}^3)$ solves $uG_o v\varphi = -\varphi$ then define $\psi \equiv G_o v\varphi$. Then from the assumption on V we have $\psi \in L^2_{loc}(\mathbb{R}^3)$, $\nabla\psi \in L^2(\mathbb{R}^3)$, $H\psi = 0$ in the sense of distributions, where $H \equiv -\Delta + V$ (in the sense of quadratic forms). If $\psi \notin L^2(\mathbb{R}^3)$ then one says that H has a zero energy resonance (or there is such a resonance for V). If $\psi \in L^2(\mathbb{R}^3)$ then $H\psi = 0$ in sense that $\psi \in D(H)$ (the definition domain of H) and $H\psi = 0$. In this case $\psi$ is a zero energy eigenstate for H. One has, under the additional assumption $|x|\ V(x) \in L^1(\mathbb{R}^3)$: $\psi \in L^2(\mathbb{R}^3) \Leftrightarrow (v,\varphi) = -\int V\psi dx = 0$.

The following case distinction is important (we assume here $(1 + |\cdot|)\ V \in L^1(\mathbb{R}^3)$):

Case I: $-1$ is not an eigenvalue of $uG_o v \equiv K$ (this is the case when $V \geqq 0$, e.g.).

Case II: $-1$ is a simple eigenvalue of K and $\psi \notin L^2(\mathbb{R}^3)$ i.e. $\psi$ is not an eigenfunction (i.e. there is a "simple zero energy resonance").

Case III: $-1$ is an eigenvalue of K with eigenfunctions $\varphi_j$ and the corresponding $\psi_j$ are in $L^2(\mathbb{R}^3)$ for all j (in this case there is no zero energy resonance).

Case IV: $-1$ is an eigenvalue of K, with eigenfunctions $\varphi_j$ and at least one $\psi_j \notin L^2(\mathbb{R}^3)$.

Under the above assumption on the potential and on $\lambda$, and in addition assuming $\lambda'(0) \neq 0$ in cases III, IV, we have that $n - \lim_{\varepsilon \downarrow 0} (H_\varepsilon - k^2)^{-1} = (-\Delta_\alpha - k^2)^{-1}$, where n-lim means norm-limit and $\alpha = +\infty$ in cases I, III (so that in these cases $-\Delta_\alpha = -\Delta$). In case II we have $\alpha = -\lambda'(0)\,|(v,\varphi)|^{-2}$; in case IV we have $\alpha = -\lambda'(0)\{\sum_{\ell=1}^{N} |(v,\varphi_\ell)|^2\}^{-1}$ (in these formulae we have chosen suitable normalizations of the $\varphi$, $\varphi_\ell$ e.g., in case II, (sign $V\varphi,\varphi) = -1$, where (,) is the scalar product in $L^2(\mathbb{R}^3)$).

Remark: The intuitive reason for the dependence of $\alpha$ on the zero energy behaviour of $-\Delta + V$ can be found in the fact that

$$H_\varepsilon = \varepsilon^{-2} U_\varepsilon(-\Delta + \lambda(\varepsilon)V(\cdot))U_\varepsilon^{-1},$$

where $U_\varepsilon$ is the unitary scaling $(U_\varepsilon g)(x) = \varepsilon^{-3/2} g(x/\varepsilon)$, $\varepsilon > 0$ in $L^2(\mathbb{R}^3)$, hence $\sigma(H_\varepsilon) = \varepsilon^{-2}\sigma(-\Delta + \lambda(\varepsilon)V(\cdot))$, where $\sigma(\cdot)$ means spectrum. This indicates that the behaviour of $\sigma(H_\varepsilon)$ as $\varepsilon \downarrow 0$ is determined by the behaviour at 0 of $\sigma(-\Delta + \lambda(0)V(\cdot))$.

Remark: The above procedure is a construction of the point interaction Hamiltonian $-\Delta_\alpha$ as limit of Schrödinger operators with "scaled local potentials". Other regularizations of the interaction have been discussed in the literature, see e.g. [51], [11] (and references therein).

a) 3. Perhaps the most directly usable characterization of $-\Delta_\alpha$ is by its resolvent kernel:

$$(-\Delta_\alpha - k^2)^{-1} = G_k - (\overline{G_k(\cdot)}, \cdot) A G_k, \qquad (1.1)$$

with $A \equiv B^{-1}$, $B \equiv (\frac{ik}{4\pi} - \alpha)$, $\qquad$ Im $k > 0$, $k^2 \notin \sigma(-\Delta_\alpha)$,

where $\sigma(-\Delta_\alpha) = \begin{cases} [0,\infty) & \text{for } \infty \geq \alpha \geq 0 \\ \{-(4\pi\alpha)^2\} \cup [0,\infty) & \text{for } \alpha < 0. \end{cases}$

It follows easily $\sigma_{ess}(-\Delta_\alpha) = \sigma_{ac}(-\Delta_\alpha) = [0,\infty)$, $\sigma_{sc}(-\Delta_\alpha) = \emptyset$.

For $\alpha < 0$ the normalized eigenfunction $\varphi$ to the simple eigenvalue $-(4\pi\alpha)^2$ is $(-\alpha)^{1/2}\,|x|^{-1}\exp(4\pi\alpha\,|x|)$. For $\alpha > 0$, there is a resonance at $k = 4\pi i\alpha$.

a) 4. Take $\varphi_\alpha = |\alpha|^{1/2}|x|^{-1}\exp(4\pi\alpha|x|)$ for $x \neq 0$, $\alpha \in \mathbb{R}$, $\varphi \equiv 1$ for $\alpha = +\infty$. The quadratic form $f \in C_0^\infty(\mathbb{R}^3) \to \int(\nabla f)^2 \varphi_\alpha^2 dx$ in $L^2(\mathbb{R}^3, \varphi_\alpha^2 dx)$ is well defined and closable. The self-adjoint positive operator $\hat{H}_\alpha$ in $L^2(\mathbb{R}^3, \varphi_\alpha^2 dx)$ associated with its closure is unitary equivalent $-\Delta_\alpha + (4\pi\alpha)^2$ for $\alpha \in \mathbb{R}$, in fact $\hat{H}_\alpha = \varphi_\alpha^{-1}[-\Delta_\alpha + (4\pi\alpha)^2]\varphi_\alpha$. For $\alpha = +\infty$ it is $-\Delta$.

The interest of the realization $\hat{H}_\alpha$ is that $\hat{H}_\alpha = -\Delta - \beta_\alpha \cdot \nabla$ on $C_0^\infty(\mathbb{R}^3)$-functions in $L^2(\mathbb{R}^3, \varphi_\alpha^2 dx)$, hence with $\beta_\alpha \equiv \nabla \ln\varphi_\alpha$. This is a "diffusion operator", whose closure generates a Markov semigroup in $L^2(\mathbb{R}^3, \varphi_\alpha^2 dx)$, with invariant measure $\varphi_\alpha^2 dx$ (a probability measure for $\alpha < 0$). $\hat{H}_\alpha$ is the operator associated with the closed Dirichlet form $\int(\nabla f)^2 \varphi_\alpha^2 dx$ in $L^2(\mathbb{R}^3, \varphi_\alpha^2 dx)$. Thus $\hat{H}_\alpha$ has an immediate probabilistic meaning as generator of a symmetric diffusion process (whereas $-\Delta_\alpha + (4\pi\alpha)^2$ has only the interpretation of a Brownian motion disturbed by "creation of mass" at the origin). For these concepts and results see [ 35 ], [ 36 ], [ 37 ].

## 1.2 The case of point interactions at N centers

Of course there was nothing special in choosing the source in the origin, we could have treated on the same footing the operator $-\Delta + \lambda\delta_y(x)$ for any $y \in \mathbb{R}^3$.

In fact all considerations extend also to $-\Delta + \sum_{y\in Y} \lambda_y \delta_y(x)$, with Y any finite subset of $\mathbb{R}^3$. We shall limit ourselves here to give the formula for the resolvent.

Similarly as for the case $Y = \{0\}$ treated above, each coupling constant $\lambda_y$ has to be renormalized to yield a corresponding $\alpha_y \in \mathbb{R} \cup \{+\infty\}$. Denoting by $-\Delta_{\alpha,Y}$ the realization of $-\Delta + \sum_{y\in Y} \lambda_y \delta_y(x)$ as a well defined self-adjoint operator on $L^2(\mathbb{R}^3, dx)$ we get correspondingly to a 3) above:

$$(-\Delta_{\alpha,Y} - k^2)^{-1} = G_k - \sum_{y,y'\in Y} (\overline{G_k(\cdot - y)}, \cdot)\, A_{yy'}\, G_k(y' - \cdot), \tag{1.2}$$

with $k^2 \notin \sigma(-\Delta_{\alpha,Y})$, $\mathrm{Im}\, k > 0$,

$A_{yy'}$, the kernel of the operator A in $\ell^2(Y)$ defined by $A = B^{-1}$, where B is the operator in $\ell^2(Y)$ with kernel $B_{yy'} \equiv (\frac{ik}{4\pi} - \alpha_y)\, \delta(y - y') + \tilde{G}_k(y-y')$, $\tilde{G}_k(z) \equiv G_k(z)$ for $z \neq 0$, $\tilde{G}_k(z) = 0$ for $z = 0$.

For $Y = \{0\}$, $\alpha_o = \alpha$, $A_{yy'} = A$ this reduces to the formula in a) 3. i.e. in this case $-\Delta_{\alpha,Y} = -\Delta_\alpha$.

<u>Remark:</u> As discussed in [ 38 ] for $|Y| = n$ there are actually $n^2$ self-adjoint extensions of $-\Delta \restriction C^\infty_{o,o}(\mathbb{R}^3)$, where the first zero means compact support and the second vanishing at a neighborhood of Y. The above n parametric realization $-\Delta_{\alpha,Y}$ can be shown to be the one given by separated boundary conditions at each point, see [11,38,39].

<u>Remark:</u> The same results for $\sigma_{ess}$, $\sigma_{ac}$, $\sigma_{sc}$ as for $-\Delta_\alpha$ hold. The point spectrum of $-\Delta_{\alpha,Y}$ is entirely contained in $(-\infty, 0)$ and consists of at most N eigenvalues counting multiplicity and the eigenvalues are given by $k^2$ with $\mathrm{Im}\, k > 0$ s.t. $\det B(k) = 0$, the multiplicity of the zero eigenvalue of $B(k)$ being equal to the multiplicity of the eigenvalue $k^2$. See e.g. [ 11 ], where also many other results on point interactions with N centers can be found.

We shall now procede to the most interesting case for us, the case of infinitely many centers.

## 1.3 Point interactions at a discrete set of centers

We shall consider heuristic Hamiltonians of the form $-\Delta + \sum_{y\in Y} \lambda_y \delta_y(\cdot)$, with Y a discrete infinite set i.e. $Y \equiv \{y_j \in \mathbb{R}^3 \mid j \in \mathbb{N},\ \inf_{j\neq j'} |y_j - y_{j'}| > 0$ .

In analogy with our discussion in 1.1, 1.2 we shall have to define properly an

Hamiltonian $-\Delta_{\alpha,Y}$ "realizing" the above heuristic one, by "renormalizing" the coupling constants $\lambda_y$ to $\alpha_y$ with $\alpha$ a real-valued function on Y (as we know from 1.1, 1.2 the value $+\infty$ of $\alpha_y$ would simply correspond to deleating this y from Y).

We shall give a description of $-\Delta_{\alpha,Y}$ by its resolvent, using the one given in 1.2. Let thus $\tilde{Y}$ run over the finite subsets of Y and let $\tilde{\alpha} \equiv \alpha \restriction \tilde{Y}$. Then, by 1.2, $(-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1}$ is the well defined resolvent of a lower bounded self-adjoint operator $-\Delta_{\tilde{\alpha},\tilde{Y}}$. The following theorem can be proven, see e.g. [11]:

Theorem 1: For $\mathrm{Im}\, k^2 \neq 0$ the strong limit as $\tilde{Y} \uparrow Y$ of $(-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1}$ exists and is the resolvent $(-\Delta_{\alpha,Y} - k^2)^{-1}$ of a self-adjoint operator. This resolvent is given by

$$(-\Delta_{\alpha,Y} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{\infty} [\Gamma_{\alpha,Y}(k)]^{-1}_{j,j'} |G_k(\cdot - y_{j'})\rangle\langle G_k(\cdot - y_j)| \qquad (1.3)$$

$\Gamma_{\alpha,Y}(k)$ is the closed operator in $\ell^2(Y)$ given by $(\Gamma_{\alpha,Y}(k)) = -(B_{y_j,y_{j'}})^{-1}$, with $B_{y_j y_{j'}}$ defined as in 1.2 on $\ell_o(Y) \equiv \{g \in \ell^2(Y),\ \mathrm{supp}\ g \text{ finite}\}$. For $\mathrm{Im}\, k > 0$ large enough one has $(\Gamma_{\alpha,Y}(k))^{-1}$ bounded. $\Gamma_{\alpha,Y}(k)$ is analytic in k for $\mathrm{Im}\, k > 0$.

The proof exploits the monotonicity properties of the resolvent $(-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1}$ in $\tilde{Y}$, for $k^2$ sufficiently large.

Remark: It is possible to show that $-\Delta_{\alpha,Y}$ is local in the sense that if $\psi \in D(-\Delta_{\alpha,Y})$ and $\psi = 0$ in a domain U of $\mathbb{R}^3$, then $-\Delta_{\alpha,Y}\psi = 0$ in U. Moreover it is possible to approximate in norm resolvent sense $-\Delta_{\alpha,Y}$ by local scaled short range interactions, extending 1.1, a2): see [ 11 ].

## 1.4 Periodic point interactions

The case of "periodic point interactions" is of particular importance in solid state physics. In this case both $\alpha$ and Y are periodic, e.g. $Y = \mathbb{Z}^3$ and $\alpha$ constant. The corresponding Schrödinger operator $-\Delta_{\alpha,Y}$ of 1.3 is then the mathematical realization of the heuristic Hamiltonian $-\Delta + \lambda \sum_{y \in \mathbb{Z}^3} \delta_y(\cdot)$, after renormalization of the coupling constant $\lambda$ (independent of y). This Hamiltonian fits in the so called "one-electron model of a solid", in as much as the solid is exemplified by a fixed infinitely extended crystal with (infinitely massive) nuclei at the vertices, and the electron moving in the crystal interacts only with the crystal (other effects like relativistic effects, lattice vibrations, spin-orbit coupling,..., are neglected, in this picture). More generally, we can consider heuristic point interaction Hamiltonians of the following form. Let $\Lambda$ be a lattice of $\mathbb{R}^3$, i.e. $\Lambda \equiv \{\sum_{i=1}^{3} n_i a_i\}$, with $a_1, a_2, a_3$ a basis of $\mathbb{R}^3$ and $n \equiv (n_1, n_2, n_3)$ running over $\mathbb{Z}^3$.

$\Lambda$ is called a Bravais lattice.

Let $\hat{\Gamma}$ be the basic period cell or primitive cell relative to $\Lambda$ i.e. $\hat{\Gamma} = \mathbb{R}^3/\Lambda$ (so that each $x \in \mathbb{R}^3$ can be written as $x = \lambda + \hat{\gamma}$, with $\lambda \in \Lambda$ and $\hat{\gamma} \in \hat{\Gamma}$). $\hat{\Gamma}$ can be identified with the so called Wigner-Seitz cell $\{\sum_{i=1}^{3} s_i a_i\}$, $s_i \in [-\frac{1}{2}, \frac{1}{2})$.

Let $y_j$, $j = 1 \ldots N$ be N points in $\hat{\Gamma}$ i.e. $y_j \in \hat{\Gamma}$.

Then we can consider the heuristic Hamiltonian:

$$H = -\Delta + \sum_{\lambda \in \Lambda} \sum_j \lambda_j \, \delta_{y_j+\lambda}(\cdot). \tag{1.4}$$

This yields a model of a multiatomic crystal or a perfect alloy (think of $y_1 \ldots y_N$ as carrying N different atoms or nuclei, acting with coupling constants $\lambda_1,\ldots,\lambda_N$ by a $\delta$-potential on an electron entering $\hat{\Gamma}$- and translate the whole picture by any $\lambda \in \Lambda$ ).

Of course for a proper mathematical definition of a self-adjoint operator associated with the above heuristic Hamiltonian we can use the theorem in 1.3, with $Y = \{y_j + \lambda,\ \lambda_j \in \hat{\Gamma},\ \lambda \in \Lambda\}$ . Then the corresponding $-\Delta_{\alpha,Y}$ is the mathematical realization of H. For the detailed study of $-\Delta_{\alpha,Y}$, in particular its spectrum, we shall have to exploit the particular symmetry properties of $(\alpha,Y)$. It is useful to think of $-\Delta_{\alpha,Y}$ as coming from the interaction $\sum_{y \in \Lambda} \sum_j \delta_{y_j+\lambda}(\cdot)$ and reason on its invariance properties on the basis of those of the potential V, formally $\sum_{\lambda \in \Lambda} \sum_j \lambda_j \, \delta_{y_j+\lambda}(\cdot)$. More generally, it is useful to clarify the picture by studying Schrödinger operators of the form $-\Delta + V$ in $L^2(\mathbb{R}^3)$, with V the multiplication operator by a periodic, say smooth function with periods the vectors $\lambda$ in a Bravais lattice $\Lambda$. By the smoothness and periodicity of V we can expand V in Fourier series i.e. $V(x) = \sum_{\gamma \in \Gamma} V_\gamma \, e^{i\gamma x}$, with uniform convergence, where

$$V_\gamma = |\Gamma|^{-1} \int_{\hat{\Gamma}} V(\nu)\, e^{-i\gamma\nu}\, d\nu. \tag{1.5}$$

$\Gamma$ is the so called dual or reciprocal or orthogonal lattice i.e. $\Gamma = \{\sum_i n_i b_i\}$, with $b_i$, $i=1,2,3$ the dual basis of $\mathbb{R}^3$ given by $a_j b_{j'} = 2\pi\delta_{jj'}$, with $n = (n_1,n_2,n_3)$ running over $\mathbb{Z}^3$.

It is useful to consider also the Fourier transform $\hat{H}$ of H.

Let $\hat{V}(p) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} V(x) e^{-ipx} dx$ be the Fourier transform of V (which exists if we look upon V e.g. as a tempered distribution; in fact, V being bounded, $\hat{V}$ is a pseudo measure).

The Fourier inversion formula holds i.e.

$$V(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} \hat{V}(p)\, e^{ipx} dp, \tag{1.6}$$

in the sense of tempered distributions.

Let us now assume e.g. $V \in C_0^\infty(\mathbb{R}^3)$. Then the Fourier series expansion for V converges uniformly and one has

$$\hat{V}(p) = (2\pi)^{3/2} \sum_{\gamma \in \Gamma} V_\gamma \delta(p-\gamma), \tag{1.7}$$

with convergence e.g. in the weak topology on $\mathscr{S}'(\mathbb{R}^3)$.

Let $\mathfrak{F}$ be the unitary operator given by Fourier transform in $L^2(\mathbb{R}^3,dx)$. Then, as well known, $\mathfrak{F}(-\Delta)\mathfrak{F}^*$ is multiplication by $p^2$ in $L^2(\mathbb{R}^3,dp)$.
$\mathfrak{F} V \mathfrak{F}^*$ is the convolution operator in $L^2(\hat{\mathbb{R}}^3,dp)$:

$$(2\pi)^{-3/2}(\overline{\hat{V}} (p-\cdot),\cdot) = \sum_{\gamma \in \Gamma} V_\gamma \delta(p-\gamma-\cdot,\cdot). \tag{1.8}$$

Let U be the mapping from $L^2(\hat{\mathbb{R}}^3,dp)$ onto $\int_{\hat{\Lambda}}^{\oplus} \ell^2(\Gamma)d\theta \equiv L^2(\hat{\Lambda}, \ell^2(\Gamma))$ given by

$(U\hat{f})(\theta,\gamma) \equiv \hat{f}(\theta+\gamma)$, where $\hat{f} \in L^2(\hat{\mathbb{R}}^3,dp)$, with the identification $\hat{p} \leftrightarrow \theta + \gamma$, $\gamma \in \Gamma$, $\theta \in \hat{\Lambda}$,

with $\hat{\Lambda} \equiv \hat{\mathbb{R}}^3/\Gamma$ the dual group to $\Lambda$ (also called basic periodic cell or primitive cell of the dual lattice $\Gamma$). $\hat{\Lambda}$ can be identified with the Wigner-Seitz cell $\{\sum_{i=1}^{3} s_i b_i \mid s_i \in [-\frac{1}{2}, \frac{1}{2}), \ i=1,2,3\}$ of $\Gamma$, also called Brillouin zone.

Then $U\mathfrak{F}(-\Delta + V)\mathfrak{F}^* U^* = \int_{\hat{\Lambda}}^{\oplus} \hat{H}(\theta)d\theta$, with $\hat{H}(\theta)$ acting in $\ell^2(\Gamma)$ according to, as easily deduced from (1.8):

$$(\hat{H}(\theta)g)(\gamma) = |\gamma + \theta|^2 g(\gamma) + \sum_{\gamma' \in \Gamma} V_{\gamma'} g(\gamma-\gamma'). \tag{1.9}$$

The sum on the r.h.s. converges for $g \in \ell^2(\Gamma)$.
Thus $(U\mathfrak{F}(-\Delta + V)\mathfrak{F}^* U^* \hat{f})(\theta,\gamma) = (\hat{H}(\theta)\hat{f}(\theta,\cdot),\cdot)(\gamma)$, $\forall f \in L^2(\hat{\mathbb{R}}^3,dp)$. (1.10)

In particular the spectrum of $-\Delta + V$ is obtained by determining the spectrum of $\hat{H}(\theta)$. Now with $-\hat{\Delta} \equiv \mathfrak{F}(-\Delta)\mathfrak{F}^*$ we have

$$(-\hat{\Delta}(\theta)g)(\gamma) = |\gamma + \theta|^2 g(\gamma), \tag{1.11}$$

hence $\sigma(-\hat{\Delta}(\theta)) = \sigma_d(-\hat{\Delta}(\theta)) = |\Gamma + \theta|^2$, where $\sigma_d$ means discrete spectrum and $|\Gamma + \theta^2| \equiv \{|\gamma+\theta|^2 \ | \gamma \in \Gamma\}$ .

If e.g. $V_\gamma \in \ell^2$, then one shows, see e.g. [ 1 ] , [ 3 ] ,

$$\sigma(H) = \sigma(\hat{H}) = \bigcup_{\theta \in \hat{\Lambda}} \sigma(\hat{H}(\theta)), \tag{1.12}$$

with $\hat{H} \equiv \mathfrak{F} H \mathfrak{F}^*$ . $\sigma(\hat{H}(\theta))$ is purely discrete, consisting of isolated eigenvalues of finite multiplicity and $\sigma(\hat{H})$ is absolutely continuous and consists of bands separated by gaps.
How can one prove similar results in the case where V is a periodic point interaction, and hence is too singular to satisfy the above assumptions?
Two equivalent procedures can be followed. Either start with H replaced by $-\Delta_{\alpha,Y}$ and decompose according to

$$U(-\Delta_{\alpha,Y})U^* = \int_{\hat{\Lambda}}^{\oplus} (-\hat{\Delta}_{\alpha,Y})(\theta)d\theta. \tag{1.13}$$

Or use a perturbation theorem to perturb first $-\hat{\Delta}(\theta)$ to $-\hat{\Delta}(\theta)$ plus point interaction and integrate afterwards.

We shall describe here shortly the latter procedure. Formally we have to perturb $-\Delta(\theta)$ by $V(x) = -\sum_{j=1}^{N} \sum_{\lambda\in\Lambda} \mu_j\, \delta(x - y_j - \lambda)$ for some $\mu_j \in \mathbb{R}$ (which are going to be renormalized), $y_i$ being points in the basic periodic cell $\hat{\Gamma}$. In this case $V_\gamma = -|\hat{\Gamma}|^{-1} \sum_{j=1}^{N} \mu_j\, e^{-i\gamma y_j}$, $\gamma \in \Gamma$, with $|\hat{\Gamma}|$ the volume of $\Gamma$.

Introduce for any $\kappa > 0$ the operator in $\ell^2(\Gamma)$ (with cut off $\kappa$):

$$(\hat{H}^\kappa(\theta)g)(\gamma) \equiv |\gamma + \theta|^2\, g(\gamma) - |\hat{\Gamma}|^{-1} \sum_{j=1}^{N} \mu_j(\kappa)(\phi^\kappa_{y_j}(\theta),g)\, \phi^\kappa_{y_j}(\theta), \tag{1.14}$$

where $\theta \in \hat{\Lambda}$, $\gamma \in \Gamma$, $g \in \ell^2_o(\Gamma)$.

$(,)$ is the scalar product in $\ell^2(\Gamma)$.

$$\phi^\kappa_{y_j}(\theta)\,(\gamma) \equiv \chi_\kappa(\gamma + \theta)\, e^{-i(\gamma+\theta)y_j}, \tag{1.15}$$

with $\chi_\kappa$ the characteristic function of the closed ball in $\mathbb{R}^3$ with radius $\kappa$ and center at the origin. We then have the

<u>Theorem</u> **2**: Let $\hat{H}^\kappa(\theta)$ be the self-adjoint operator in $\ell^2(\Gamma)$ given by (1.14) with domain $D(\hat{H}^\kappa(\theta)) = D(-\hat{\Delta}(\theta)) = \{g \in \ell^2(\Gamma) \mid \sum_{\gamma\in\Gamma} |\gamma + \theta|^4\, |g(\gamma)|^2 < \infty\}$, $\forall\, \theta \in \hat{\Lambda}$.

Then if $\mu_j(\kappa) = (\alpha_j + \kappa/2\pi^2)^{-1}$ for some $\alpha_j \in \mathbb{R}$, then $\hat{H}^\kappa(\theta)$ converges for all $\theta \in \hat{\Lambda}$ in norm resolvent sense as $\kappa \to \infty$ to a self-adjoint operator $-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta)$, with $Y \equiv \{y_1,\dots,y_N\}$, $\alpha \equiv (\alpha_1 \dots \alpha_N)$, whose resolvent is given by

$$(-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta) - k^2)^{-1} = G'_k(\theta) + |\hat{\Gamma}|^{-1} \sum_{j,j'=1}^{N} [\Gamma_{\alpha,\Lambda,Y}(k,\theta)]^{-1}_{j,j'}\, (F_{-\bar{k},y_j}(\theta),\cdot)F_{k,y_j}(\theta), \tag{1.16}$$

for all k s.t. $k^2 \notin |\Gamma + \theta|^2$, $\mathrm{Im}\, k > 0$, $\det \Gamma_{\alpha,\Lambda,Y}(k,\theta) \neq 0, \theta \in \hat{\Lambda}$, where $\Gamma_{\alpha,\Lambda,Y}(k,\theta)$ is the $N \times N$ matrix with $jj'$-element $\alpha_j\, \delta_{jj'} - g_\kappa(y_j - y_{j'},\theta)$, with

$$g_\kappa(x,\theta) \equiv \begin{cases} |\hat{\Gamma}|^{-1} \lim\limits_{\kappa\to\infty} \sum\limits_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\le\kappa}} e^{i(\gamma+\theta)x} / (|\gamma + \theta|^2 - k^2) = \sum\limits_{\lambda\in\Lambda} G_k(x+\lambda)e^{-i\theta\lambda}, x \in \mathbb{R}^3 - \Lambda \\ (2\pi)^{-3}\, e^{-i\theta x} \lim\limits_{\kappa\to\infty} [\sum\limits_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\le\kappa}} (|\gamma + \theta|^2 - k^2)^{-1}\, |\hat{\Lambda}| - 4\pi\kappa] = \sum\limits_{\lambda\in\Lambda} \tilde{G}_k(x+\lambda)e^{-i\theta\lambda} + \frac{ik}{4\pi}, \\ \qquad x \in \Lambda, \end{cases} \tag{1.17}$$

$G'_k(\theta)$ the right hand side of(1.17), is the multiplication operator in $\ell^2(\Gamma)$ by the function $(|\gamma + \theta|^2 - k^2)^{-1}$.

The term $G_k(x + \theta)$, $x \in \mathbb{R}^3 - \Lambda$, $\theta \in \hat{\Lambda}$ appearing in the second expression for $g_k(x+\theta)$,