Point interaction Hamiltonians for crystals with random defects

by

S. Albeverio[1,2,3,7], R. Figari[2,3,4], F. Gesztesy[6], R. Høegh-Krohn†, H. Holden[5], W. Kirsch[1,3]

Abstract:

We give a short report on work done in recent years on solvable models for quantum mechanical crystals (crystals with point interactions, thus three dimensional extensions of Kronig Penney's model). We discuss the mathematical definition of the Hamiltonian and its spectral properties in the case of perfect crystals, as well as in the case of crystals with deterministic or randomly distributed point defects. We also discuss the connection of such point interactions Hamiltonians with the study of scattering by a large number of small randomly placed scatterers.

1. Introduction

In this paper we shall report on some recent mathematical work on models describing crystals with defects which are randomly distributed. In the formulation of these quantum mechanical models so called point interactions arise; these are interactions localized at points of the perturbed crystal, and are felt by the particle (electron) moving in these crystals (in the usual one-electron approximation of the motions of electrons in a crystal). The crystals we discuss here are mainly three dimensional (but similar results are obtained for two and one dimensional crystals). Despite extensive and very interesting work developed in recent years on point interactions in three dimensions, described e.g. in monographs [AGHKH], [DO], it seems that quite a few physicists, mathematical physicists and mathematicians still believe that point interactions only are possible in one dimension—an immediate association being with the Kronig–Penney model (since it has entered standard text books in solid state physics). This entire workshop has been a proof of how active is the research concerning three dimensional models with point interactions. We hope that the present contribution might also help eliminating eventually the above mentioned prejudice. In fact all is done in one dimension with point interactions can be done also in three dimensions, provided of course the point interactions are correctly defined. We shall report here mainly on work of the authors and their coworkers, in particular, as far as random perturbations are concerned, F. Martinelli. We refer to other contributions in this

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1. Fakultät für Mathematik, Ruhr-Universität Bochum, D-4630 Bochum 1 (FRG)
2. BiBoS Research Centre
3. SFB 237 Bochum–Essen–Düsseldorf
4. Dipartimento di Scienze Fisiche, Università di Napoli (Italy)
5. Matematisk Institutt, Universitetet i Trondheim, N-7034 Trondheim-NTH (Norway)
6. Department of Mathematics, University of Missouri, Columbia, Mo 65211 (USA)
7. CERFIM Research Centre, Locarno (CH)

† Matematisk Institutt, Universitetet i Oslo (Norway)
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volume for complementary topics, see also e.g. [Pa] (and references therein). Our basic reference for this paper is the monography [AGHKH], to which we also refer for more complete references. For the reader at his first contact with point interactions let us start by answering briefly the question:

1.1 What are point interactions ?

A point interaction at the origin 0 in the d-dimensional Euclidean space $\mathbb{R}^d$ should be a perturbation ("potential") localized at 0 of the free Hamiltonian, thus the Hamiltonian (Schrödinger operator) describing this interaction has the form (in suitable units)

$$H = \text{“} - \Delta + \lambda\delta(x)\text{“} \tag{1.1}$$

as an operator in $L^2(\mathbb{R}^d, dx)$ (square integrable functions over $\mathbb{R}^d$). Does H exist as a well defined self-adjoint operator, is it non trivial in the sense of being different from the free part $-\Delta$? More generally point interactions at a subset Y of R^d should be

$$H = \text{“} - \Delta + \sum_{y\in Y} \lambda_y \delta(x-y)\text{“} \tag{1.2}$$

in $L^2(\mathbb{R}^d, dx)$.
Models of this type, with different choices of Y, occur in nuclear physics, solid state physics, electromagnetism, see [AGHKH] and references therein. It is well known that there is a "no go theorem" for Y discrete (without accumulation points) if $d \geq 4$, $-\Delta$ being already essentially self-adjoint on $C_0^\infty(\mathbb{R}^d - \{0\})$ (C^∞ functions of compact support in the complement of the origin) if $d \geq 4$. [1]).

It is also well known that, as an application of Krein's theory, as first discussed by Berezin and Faddeev, when $d \leq 3$ for Y consisting of only one point there exists a 1 parameter family indexed by $\alpha \in \mathbb{R}$, of different realizations $-\Delta_\alpha \neq -\Delta$ of H. The parameter α determines for $d = 2, 3$ a renormalized coupling constant. For $d = 1$, α is simply λ. The way $-\Delta_\alpha$ arises is perhaps best seen by an heuristic argument (justifiable by nonstandard analysis [AFHKL]):

$$\left(-\Delta + \lambda V - k^2\right)^{-1} = G_k - G_k \left[\frac{1}{\lambda} + VG_k\right]^{-1} VG_k\,, \tag{1.3}$$

with $G_k \equiv \left(-\Delta - k^2\right)^{-1}$, $\quad k^2 \neq 0$, as computed rigorously for V say bounded and continuous. Setting then formally $V(x) = \delta(x)$ in this formula one sees that, for $d = 2, 3$, one has to choose $\frac{1}{\lambda} = -G_0(0) - \alpha$ to compensate the singularity of $|G_k(0)|$ ($= +\infty$ for $d = 2, 3$). By this choice of λ we get $\left[\frac{1}{\lambda} + VG_k\right] = \frac{ik}{4\pi} - \alpha$. As suggested by this (1.1) can then be defined using the final result of this formal computation, namely as the selfadjoint operator $-\Delta_\alpha$ in $L^2(\mathbb{R}^d, dx)$, $d \leq 3$ with resolvent kernel given by

$$\left(-\Delta_\alpha - k^2\right)^{-1}(x,y) = G_k(x-y) - G_k(x)\left(\frac{ik}{4\pi} - \alpha\right)^{-1} G_k(y)\,. \tag{1.4}$$

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[1]) It is a different story if instead of $L^2(\mathbb{R}^d, dx)$ one considers some other spaces, as in some uses of point interactions in electromagnetic theory, see references to work by Grossman and Wu in [AGHKH]. For recent results on point interactions situated on non discrete subsets Y see in addition to [AGHKH] and contributions to these proceedings, [Bra], [ABrR], [AMaZ1-3], [AFHKL], [AFHKKL], [Ko], [H], [Pan], [Te] and references therein.

Remark: The mentioned justification of the above formal computation by nonstandard analysis yields that, for $d = 3$, and ε infinitesimal, $-\Delta + \lambda_\alpha(\varepsilon)\delta_\varepsilon(x)$, with $\delta_\varepsilon(x)$ a nonstandard realization of the $\delta-$function (in standard terms, $\delta_{\tilde{\varepsilon}}(x)$ is a delta sequence for $\tilde{\varepsilon} \downarrow 0$), is near standard and defines $-\Delta_\alpha \neq -\Delta$ if $\lambda_\alpha(\varepsilon) = \left[-\frac{\pi^2}{4\varepsilon^2} + \frac{8\pi}{\varepsilon}\alpha\right] \frac{4}{3}\pi\varepsilon^3$, $\alpha \in \mathbb{R}$. A similar result holds also for $d = 2$. See [AFHKL] and references therein. (1.4) or the observation in the remark give a realization of $-\Delta_\alpha$ as a $\delta-$ interaction or point interaction of strength α at the origin.

Remarks 1) It is useful to remark that setting $\alpha = +\infty$ formally in (1.4) the r.h.s. reduces to G_k, so that it is natural to define $-\Delta_{+\infty} \equiv -\Delta$.
2) Besides the mentioned two ways to define $-\Delta_\alpha$, the one by the resolvent and the nonstandard analytic one, there exist other ways to define $-\Delta_\alpha$ e.g.
a)"by boundary conditions": formulated for $d = 3$, $-\Delta_\alpha$ can be characterized as the extension of $-\Delta$ on $C_0^\infty(\mathbb{R}^3 - \{0\})$ functions with domain such that if $f = D(-\Delta_\alpha)$ and $f(x) = \tilde{f}(r)$, $r \equiv |x|$, then $\frac{\partial}{\partial r}\left(r\tilde{f}(r)\right) = 4\pi\alpha\left(r\,\tilde{f}(r)\right)$ at $r = 0$.

b) "by resolvent limits": define for $\varepsilon > 0$, $H_\varepsilon = -\Delta + \lambda(\varepsilon)\varepsilon^{-2}V(x/\varepsilon)$, with V in Rollnik's class, $(1 + |\cdot|)V \in L^1(\mathbb{R}^3)$, and $\lambda \in C^1(\mathbb{R})$, $\lambda(0) = 1$, $\lambda'(0) \neq 0$ such that -1 is an eigenvalue of $v\,\mathrm{sign}V\,G_0 v$, $v \equiv |V|^{\frac{1}{2}}$ with eigenfunctions φ_j, $j = 1, \ldots, N$ in $L^2(\mathbb{R}^3, dx)$ such that the "resonance functions" $G_0 v\varphi_j$ are not in $L^2(\mathbb{R}^3, dx)$ for some j. Then H_ε converges in norm resolvent sense as $\varepsilon \downarrow 0$ to $-\Delta_\alpha$, with $\alpha = -\frac{\lambda'(0)}{\sum_{j=1}^N |(v,\varphi_j)|^2}$ This is an approximation of $-\Delta_\alpha$ by local potentials, there are also approximations by non local potentials, see again [AGHKH].

c) Another useful construction of $-\Delta_\alpha$, which provides probabilistic tools for the study of point interactions, has been first discussed in [AHKS]. Let, for $d = 3$, $\varphi_\alpha(x) \equiv |\alpha|^{\frac{1}{2}}\frac{e^{4\pi\alpha|x|}}{|x|}$, $\alpha \in \mathbb{R}$. Let $\hat{H}_\alpha$ be the self-adjoint positive operator in $L^2(\mathbb{R}^3, |\varphi_\alpha|^2\,dx)$, uniquely associated with the Dirichlet form $E(f,f) = \frac{1}{2}\int |\nabla f|^2 |\varphi_\alpha|^2 dx$ in $L^2(\mathbb{R}^3, |\varphi_\alpha|^2 dx)$
(in the sense that $\left(\hat{H}_\alpha^{\frac{1}{2}} f, \hat{H}_\alpha^{\frac{1}{2}} f\right) = E(f,f)$, $\forall f \in D(\hat{H}_\alpha^{\frac{1}{2}}) = D(E)$). Then we can define $-\Delta_\alpha$ by $-\Delta_\alpha = \varphi_\alpha \hat{H}_\alpha \varphi_\alpha^{-1} - (4\pi\alpha)^2$. $\hat{H}_\alpha$ on $C_0^\infty(\mathbb{R}^3 - \{0\})$ is given by $-\Delta - \beta_\alpha \cdot \nabla$, with $\beta_\alpha \equiv \nabla \ln \varphi_\alpha$. $\hat{H}_\alpha$ generates a diffusion Markov symmetric semigroup in $L^2(\mathbb{R}^3, |\varphi_\alpha|^2 dx)$, with invariant measure $|\varphi_\alpha|^2 dx$.

Having solved the problem of the construction of self-adjoint realizations of the one source point interaction, by one of the above methods, it is not difficult to extend the solution to other cases, of the type (1.2.) with Y consisting e.g. of N points in $\mathbb{R}^3$ or a discrete subset of $\mathbb{R}^3$ (see below). One can also discuss the case where Y is some other suitable geometrical measure zero subsets of $\mathbb{R}^3$ like e.g. S^2 (see e.g. [AGS]) or the path of Brownian motion on $\mathbb{R}^d, d \leq 5$, run in $[0,t]$ (see [AFHKL], [AFHKKL]). In this article we shall discuss some situations where the particle and the centers are in $\mathbb{R}^3$, for other cases in particular finite and infinitely many centers in $\mathbb{R}^d, d = 1, 2$, see [AGHKH] and also e.g. [DO], as well as contributions to this conference, in particular by P. Exner and P. Šeba.

1.2 N-centers point interactions

Before going over to the case of infinitely many centers, let us consider the N-centers case, given heuristically by (1.2.) with Y consisting of N points ("sources") in $\mathbb{R}^3$. We give strengths $\{\alpha_y, y \in Y\}$ corresponding to the sources $y \in Y$. The point interaction Hamiltonian for the sources y, with strengths α_y, denoted by $-\Delta_{\alpha,Y}$, is given in terms of its resolvent by

$$\left(-\Delta_{\alpha,Y} - k^2\right)^{-1} = G_k - \sum_{y,y' \in Y} \left(\overline{G_k(\cdot - y)}, \cdot\right) [\Gamma_{\alpha,Y}(k)]^{-1}_{yy'} G_k(y' - \cdot), \qquad (1.5)$$

with

$$[\Gamma_{\alpha,Y}(k)]_{y,y'} \equiv \left[\left(\frac{ik}{4\pi} - \alpha_y\right)\delta(y-y') + \tilde{G}_k(y-y')\right]_{y,y'}, y, y' \in Y \tag{1.6}$$

where $\tilde{G}_k(z) = G_k(z)$ for $z \neq 0$ and $\tilde{G}_k(z) = 0$ for $z = 0$.

Remark. Actually there exist N^2 self-adjoint extensions of $-\Delta$ restricted to C^∞ funtions of compact support outside the sources $y \in Y$, only N of which are covered by above definition. However only the ones given above do correspond to separated boundary conditions at the sources, the others are "non local" involving non separated boundary conditions, see [DaGr], [Bra]. Having the above resolvent it is possible to discuss in details spectral properties and scattering for N centers, see [AGHKH].

1.3. The case of infinitely many centers

We shall consider the case of Hamiltonians given formally by (1.2) with Y an infinite subset of $\mathbb{R}^3$, discrete in the sense that

$$Y = \{y_i, i \in \mathbb{N}\} \text{ with } \inf_{j \neq j'} |y_j - y_{j'}| > 0.$$

We give sources α_j, $j \in \mathbb{N}$ and denote for any $\tilde{Y} \subset Y$, $\tilde{Y}$ finite, by $\tilde{\alpha}$ the restriction of α to $\tilde{Y}$. One then defines the Hamiltonians for point interactions with sources Y and strengths α by the limit in the sense of strong resolvent convergence of $\left(-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2\right)^{-1}$ as $\tilde{Y} \uparrow Y$.

That this limit exists is easily seen by using monotonicity arguments, see [AGHKH]. Since by (1.2) we have good control on the approximants it is possible to get information on the limit, especially in the case where (α, Y) have suitable symmetry properties, see [AGHKH]. Such a case is the one of crystals, which we shall handle in the next chapter.

2. Periodic point interactions and crystals.

We shall consider in the one electron model of a solid the case of a multiatomic crystal or a perfect alloy, with point sources located at the points of a subset Y of $\mathbb{R}^3$ of the form

$$Y = \Lambda + Y_0, \text{ with } \Lambda \equiv \left\{\sum_{i=1}^{3} n_i a_i, (n_1, n_2, n_3) \in \mathbb{Z}^3\right\}$$

a Bravais lattice and Y_0 a finite number of points of $\mathbb{R}^3$. Let $\hat{\Gamma} \equiv \mathbb{R}^3/\Lambda$ be the basic periodic or primitive cell or Wigner-Seitz cell, i.e.

$$\hat{\Gamma} \equiv \left\{\sum_{i=1}^{3} s_i a_i, s_i \in \left[-\frac{1}{2}, \frac{1}{2}\right)\right\}.$$

Let b_j be dual basis vectors in the sense that

$$a_i b_j = 2\pi\delta_{ij}, \quad i, j = 1, 2, 3.$$

Let

$$\Gamma \equiv \left\{\sum_{i=1}^{3} n_i b_i, (n_1, n_2, n_3) \in \mathbb{Z}^3\right\}.$$

Γ is called the dual lattice.

$$\hat{\Lambda} \equiv \mathbb{R}^3/\Gamma \equiv \left\{ \sum_{i=1}^{3} s_i b_i, s_i \in \left[-\frac{1}{2}, \frac{1}{2} \right) \right\}$$

is the so called Wigner-Seitz cell of the dual lattice Γ or Brillouin zone. $\hat{\Gamma}$ is the dual group of Λ and is the basic periodic cell or primitive cell of the dual lattice. One has the direct decomposition $L^2\left(\hat{\Lambda}, l^2(\Gamma)\right) = \int_{\hat{\Lambda}}^{\oplus} l^2(\Gamma) d\theta$. We can look upon $\theta + \gamma, \gamma \in \Gamma$ as coordinates corresponding to $\hat{p} \in \mathbb{R}^3$. Our periodic Hamiltonian $\hat{H}$, describing crystals (in Fourier space), is unitarily equivalent to a direct integral:

$$\hat{H} \cong \int_{\hat{\Lambda}}^{\oplus} \hat{H}(\theta) d\theta,$$

for some $\hat{H}(\theta)$ acting in $l^2(\Gamma)$.

The study of the spectrum of $\hat{H}$ is then reduced to the study of the spectrum of $\hat{H}(\theta)$.

If $\hat{H}$ is the momentum space realization of a Hamiltonian, then $\hat{H}(\theta)$ is called the reduced Hamiltonian. E.g. if H is $-\Delta$, then $-\hat{\Delta}(\theta)$ is the operator of multiplication by $|\gamma + \theta|^2$ in $l^2(\Gamma)$ and the spectrum of $-\hat{\Delta}(\theta)$ is the discrete set $|\Gamma + \theta|^2$, so that $\sigma(-\Delta) = \bigcup_{\theta \in \hat{\Lambda}} \sigma(-\hat{\Delta}(\theta)) d\theta$ consists of bands, the spectrum in each band being purely absolutely continuous. We shall now discuss the Hamiltonians corresponding to point interactions located at the points $Y_0 + \Lambda$. Formally it is given by $-\Delta + V(x)$, with

$$V(x) = - \sum_{\substack{y_j \in Y_0 \\ j=1,\ldots,N}} \sum_{\lambda \in \Lambda} \mu_j \delta(x - y_j - \lambda), \tag{2.1}$$

with (unrenormalized) strengths $\mu_j \in \mathbb{R}$, $j = 1, \ldots, N$ (with N number of points in Y_0).

The following Theorem, proved in [AGHKH], shows how to construct the point interaction Hamiltonian corresponding to the interaction given by the above formal expression (2.1):

Theorem 2.1 Let

$$\left(\hat{H}^K(\theta) g\right)(\gamma) \equiv |\gamma + \theta|^2 g(\gamma) - \frac{1}{|\hat{\Gamma}|} \sum_{j=1}^{N} \mu_j^k \left(\phi_{y_j}^K(\theta), g\right) \phi_{y_j}^K(\theta),$$

with $K > 0$ a cut-off, $(,)$ the scalar product on $l^2(\Gamma)$, and

$$\phi_{y_j}^K(\theta, \gamma) \equiv \chi_K(\gamma + \theta) e^{-i(\gamma+\theta)y_j},$$

χ_K being the characteristic functions of the closed ball of radius K centered at the origin. We have that

$$D\left(\hat{H}^K(\theta)\right) = D\left(-\hat{\Delta}(\theta)\right) = \left\{ g \in l^2(\Gamma) |, \sum_{\gamma \in \Gamma} |\gamma + \theta|^4 |g(\gamma)|^2 < \infty \right\}.$$

Choose $\mu_j^K \equiv \left(\alpha_j + \frac{K}{2\pi^2}\right)^{-1}$, with $\alpha_j \in \mathbb{R}$. Then $\hat{H}^K(\theta)$ converges in norm resolvent sense as $K \longrightarrow \infty$ to a self-adjoint operator $-\hat{\Delta}_{\alpha,\Lambda,Y_0}(\theta)$, the reduced Hamiltonian for point interactions on $\Lambda + Y_0$. This operator is given by its resolvent through the formula

$$\left(-\hat{\Delta}_{\alpha,\Lambda,Y_0}(\theta) - k^2\right)^{-1} = G_k(\theta) + |\hat{\Gamma}|^{-1} \sum_{j,j'=1}^{N} \left[-\Gamma_{\alpha,\Lambda,Y_0}(h,\theta)\right]_{jj'}^{-1} \left(F_{-\bar{k},y_{j'}}(\theta,\cdot),\cdot\right) F_{k,y_j}(\theta,\cdot),$$

$$[\Gamma_{\alpha,\Lambda,Y_0}(k,\theta)]_{j,j'} \equiv \alpha_j \delta_{jj'} - g_k(y_j - y_{j'},\theta),$$

with

$$g_k(x,\theta) \equiv \begin{cases} \frac{1}{|\Gamma|} \lim_{K\to\infty} \sum_{\gamma\in\Gamma, |\gamma+\theta|\le K} \frac{e^{i(\gamma+\theta)x}}{|\gamma+\theta|^2 - k^2} & \text{for } x \in \mathbb{R}^3 - \Lambda \\ (2\pi)^{-3} e^{-i\theta x} \lim_{K\to\infty} \left[-4\pi K + \sum_{\gamma\in\Gamma |\gamma+\theta|\le K} \left(|\gamma+\theta|^2 - k^2\right)^{-1} |\hat{\Lambda}| \right] & \text{for } x \in \Lambda. \end{cases}$$

$$F_{k,y}(\theta,\gamma) \equiv \frac{e^{-i(\gamma+\theta)y}}{|\gamma+\theta|^2 - k^2}, G_k(\theta) \equiv \left(|\gamma+\theta|^2 - k^2\right)^{-1}.$$

The periodic point interaction Hamiltonian with sources on $\Lambda + Y_0$ and strengths $\alpha_{y_j} = \alpha_{y_j+\lambda}$ (independent of $\lambda \in \Lambda$) is given by $-\Delta_{\alpha,\Lambda+Y_0} \cong \int_{\hat{\Lambda}}^{\oplus} (-\Delta_{\alpha,\Lambda,Y_0}(\theta))\, d\theta$, hence determined by the above resolvent. ∎

In the simplest case $Y_0 = \{0\}$, writing $-\hat{\Delta}_{\alpha,\Lambda}$ for $-\hat{\Delta}_{\alpha,\Lambda+\{0\}}$, we have the following spectral results:

Theorem 2.2 $\sigma\left(-\hat{\Delta}_{\alpha,\Lambda}(\theta)\right)$ is purely discrete consisting of isolated eigenvalues of finite multiplicity. We have $\mathbb{R} - |\Gamma+\theta|^2 = \bigcup_{n=0}^{\infty} I_n(\theta)$, with $I_0(\theta) = (-\infty, \theta^2)$, $I_n(\theta)$ being bounded disjoint open intervals for $n \ge 1$, each containing exactly one eigenvalue $E_n^{\alpha,\Lambda}(\theta)$ for $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$. These eigenvalues are increasing in α. In addition a point $E^{\Lambda}(\theta) \in |\Gamma+\theta|^2$ is an eigenvalue of $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ of multiplicity $m \ge 1$ if and only if there exist $\gamma, ..., \gamma_m \in \Gamma$ such that $E^{\Lambda}(\theta) = |\gamma_0+\theta|^2 = ... = |\gamma_m+\theta|^2$.

For the proof see [AGHKH]. Having this result one then gets information on the spectrum of the point interaction Hamiltonian for a crystal Λ:

Theorem 2.3 The spectrum $\sigma(-\Delta_{\alpha,\Lambda})$, of a crystal with point interactions on a lattice Λ, with strengths α equal at each point of the lattice, is purely absolutely continuous and has the form of the union of two intervals

$$\sigma\left(-\Delta_{\alpha,\Lambda}\right) = \left[E_0^{\alpha,\Lambda}(0), E_0^{\alpha,\Lambda}(\theta_0)\right] \cup \left[E_1^{\alpha,\Lambda}, \infty\right),$$

with

$$\theta_0 \equiv -\frac{1}{2}(b_1 + b_2 + b_3),$$

$$E_1^{\alpha,\Lambda} \equiv \min\left\{E_{b_-}^{\alpha,\Lambda}(0), \frac{1}{4}|b_-|^2\right\} = \min_{\theta\in\hat{\Lambda}}\left[E_{b_-}^{\alpha,\Lambda}(\theta)\right],$$

with

$$|b_-| \le b_j, j = 1,2,3, \quad b_- \in \{b_1, b_2, b_3\}.$$

We have $E_1^{\alpha,\Lambda} > 0$ for all $\alpha \in \mathbb{R}$. Moreover $E_0^{\alpha,\Lambda}(\theta_0) < 0$ if $\alpha < \alpha_{0,\Lambda} \equiv g_0(0,\theta_0)$ (in this case we have thus effectively a gap!). The spectrum of $\sigma\left(-\Delta_{\alpha,\Lambda}\right)$ is monotone increasing in α. One has

$$E_0^{\alpha,\Lambda}(0) \longrightarrow \begin{cases} 0 & \text{as } \alpha \longrightarrow +\infty \\ -\infty & \text{as } \alpha \longrightarrow -\infty \end{cases}$$

and

$$E_0^{\alpha,\Lambda}(\theta_0) \longrightarrow \begin{cases} |\theta_0|^2 & \text{as } \alpha \longrightarrow +\infty \\ -\infty & \text{as } \alpha \longrightarrow -\infty \end{cases}$$

There exists an $\alpha_{1,\Lambda} \in \mathbb{R}$ such that

$$\sigma\left(-\Delta_{\alpha,\Lambda}\right) = \left[E_0^{\alpha,\Lambda}(0), \infty\right) \qquad \forall \alpha \ge \alpha_{1,\Lambda}$$

(i.e. for large enough strengths the gap closes).

Remark. a) There exist some extensions of this result to the case where the basic cell consists of more than one point i.e. $|Y_0| > 1$. E.g. in such a case $\sigma(-\Delta_{\alpha,Y_0+\Lambda}) \cap (-\infty, 0)$ consists of at most $|Y_0|$ disjoint closed bands, see [AGHKH] and references therein.
b) One can approximate $-\Delta_{\alpha,Y_0+\Lambda}$ in the norm resolvent sense by scaled short range Hamiltonians, which can be exploited for obtaining information on crystals with interactions not of the point interaction type.

3. Random point interactions, defect crystals.

We consider the models of Sect. 2 with the sources on $Y_0 + \Lambda$ replaced by random sources located at the random subset $Y(\omega)$ of $\mathbb{R}^3$, with ω a point in a probability space Ω, $Y(\omega)$ being for each ω a countable subset $\{y_j(\omega), j \in \mathbb{N}\}$ of $\mathbb{R}^3$ such that $\inf_{j,j' \in \mathbb{N}} |y_j(\omega) - y_{j'}(\omega)| > 0$.
Let $\alpha(\omega) = \{\alpha_{y_j}(\omega), j \in \mathbb{N}\}$ be a Y-indexed family of random strengths (real valued variables). For each ω, by the methods indicated in Sect. 1.3, we can define a point interaction Hamiltonian

$$H_\omega = -\Delta_{\alpha(\omega),Y(\omega)}, \qquad \omega \in \Omega.$$

A particularly interesting case is the following. Let $X_\lambda, \lambda \in \Lambda$ be i.i.d. $\{0,1\}$-valued random variables associated with the points of a Bravais lattice Λ_0. Set $p = P(X_\lambda = 1)$. Choose $Y(\omega)$ to be the set of occupied sites in Λ i.e. $Y(\omega) = \{\lambda \in \Lambda, X_\lambda(\omega) = 1\}$. Assume $\{\alpha_\lambda, \lambda \in Y\}$ are i.i.d. random variables with supp P_{α_0} compact. Then H_ω has the interpretation of a point interaction Hamiltonian describing a crystal with randomly distributed defects. If $\Lambda(\omega) = \Lambda$ then it is natural to talk of a random alloy, with types of alloys described by the state space of α. Using the fact that both α and Y are i.i.d. we have the following theorem:

Theorem 3.1 $(H_\omega, \omega \in \Omega)$ is an ergodic family of self adjoint operators in $L^2(\mathbb{R}^3)$ (relative to the natural shift operator in path space). The spectrum $\sigma(H_\omega)$ and its different parts like $\sigma_{ess}(H_\omega)$, and the closure $\overline{\sigma_p(H_\omega)}$ of the point spectrum of H_ω, are non random subsets of $\mathbb{R}$, almost surely. Moreover, the discrete spectrum $\sigma_d(H_\omega)$ is void, almost surely. Finally, for any $\tau \in \mathbb{R}$ there exists a subset Ω_τ of Ω of probability 1 such that τ is not an eigenvalue of finite multiplicity of H_ω for $\omega \in \Omega_\tau$.

Remark. This result belongs to a type of results established in various contexts by Pastur, Kirsch-Martinelli, Englisch-Kürsten, see e.g. [AGHKH], [Ki], [KiMa] and references therein.

It is useful to refer to the family $\Phi(\omega) \equiv \{\alpha_\lambda(\omega), X_\lambda(\omega), \lambda \in \Lambda\}$ as to a "stochastic potential". Let $H(\Phi(\omega)) \equiv H_\omega \equiv -\Delta_{\alpha(\omega),Y(\omega)}$ be the corresponding Hamiltonian. We call any $\phi \equiv \{(\xi_\lambda, \eta_\lambda) \in \text{supp} P_{\alpha_0} \times \{0,1\}, \lambda \in \Lambda\}$ an admissible potential. The set of all admissible potentials is denoted by $\mathcal{A}$. Let us set $\Lambda(\phi) \equiv \{\lambda \in \Lambda, \eta_\lambda = 1\}$ and $H(\phi) \equiv -\Delta_{\alpha(\phi),\Lambda(\phi)}$. We call $\phi \in \mathcal{A}$ periodic with periods $L_i, i = 1,2,3$ if there exist linearly independent $L_i \in \Lambda - \{0\}$ such that $\xi_{\lambda+L_i} = \xi_\lambda$ and $\eta_{\lambda+L_i} = \eta_\lambda$ for all $\lambda \in \Lambda$ and all $i = 1,2,3$. This means that the charges as well as the occupied sites are L_i-invariant. We call $\mathcal{P}$ the family of all periodic admissible potentials. We then have

Theorem 3.2 The spectrum $\sigma(H(\phi))$ of the Hamiltonian $H(\phi)$ for any admissible potential ϕ is contained in Σ with $\Sigma = \sigma(H(\Phi(\omega)))$ for almost every $\omega \in \Omega$. Moreover $\Sigma = \bigcup_{\phi \in \mathcal{A}} \sigma(H(\phi)) = \overline{\bigcup_{\phi \in \mathcal{P}} \sigma(H(\phi))}$.

Proof: This also follows from the references mentioned in the previous theorem, see e.g. [AGHKH].

Remark: One can show in addition that:

a) Given $p \leq 1$ the set Σ depends only on $\mathrm{supp}P_{\alpha_0}$

b) Σ has a band structure, see [AGHKH].

It is possible to give a rather detailed study of the variation of the negative part of the spectrum of $H(\phi(\omega))$ as one removes some of the point interactions. In fact we have

Theorem 3.3

$$\begin{aligned} \text{Let } \mu &\equiv \inf[\mathrm{supp}P_{\alpha_0}], \\ \nu &\equiv \sup[\mathrm{supp}P_{\alpha_0}]. \end{aligned}$$

Assume that either $E_0^{\nu,\Lambda}(0) \leq E_0^{\mu,\Lambda}(\theta_0)$ or $\mathrm{supp}P_{\alpha_0} = [\mu, \nu]$. Then the assumption $p = 0$ implies

$$\begin{aligned} \Sigma &= \left[E_0^{\mu,\Lambda}(0), E_0^{\nu,\Lambda}(\theta_0)\right] \cup \left[E_1^{\mu,\Lambda}, \infty\right] \\ &= \sigma(-\Delta_{\mu,\Lambda}) \cup \sigma(-\Delta_{\nu,\Lambda}). \end{aligned} \tag{3.1}$$

If $\nu < \alpha_{0,\Lambda}$ we have

$$\Sigma \cap (-\infty, 0) = \left[E_0^{\mu,\Lambda}(0), E_0^{\nu,\Lambda}(\theta_0)\right]$$

and if $\mu \geq \alpha_{1,\Lambda}$ we have $\Sigma = \sigma(-\Delta_{\mu,\Lambda})$.

Remark. a) If $0 < p < 1$ the same results hold, but (3.1) should be replaced by

$$\Sigma = \left[E_0^{\mu,\Lambda}(0), E_0^{\nu,\Lambda}(\theta_0)\right] \cup [0, \infty) = \sigma(-\Delta_{\mu,\Lambda}) \cup \sigma(-\Delta_{\nu,\Lambda}) \cup [0, \infty).$$

b)For $\mu > \alpha_{1,\Lambda}$ we have the result that $\sigma(H_\omega) = \sigma(-\Delta_{\mu,\Lambda})$ almost surely, i.e. the spectrum does not change if starting from the random Hamiltonian we create or switch off points with arbitrary strength.

c) For results on random Hamiltonians formally given by

$$H(\omega) = -\Delta + \lambda \int_0^t \delta(x - b(s,\omega))ds$$

with $b : [0,t] \longrightarrow \mathbb{R}^d$ a Brownian motion in $\mathbb{R}^d, d \leq 5$ see [AFHKL] [AFHKKL] and references therein. Such Hamiltonians arise in the description of the scattering of a quantum mechanical particle by a polymer. Moreover, via the Feynman-Kac formula, they also enter the construction of polymer measures of the heuristic form

$$\exp\left[-\lambda \int_0^t \int_0^t \delta(b(s_1) - \tilde{b}(s_2))ds_1 ds_2\right] dP(b)d\tilde{P}(\tilde{b}),$$

with (b, P), $(\tilde{b}, \tilde{P})$ two independent Brownian motions in $\mathbb{R}^d, d \leq 4$. The densities of such measures also occur in Symanzik's representations of self-interacting scalar quantum fields described by interaction densities $v(s)$ which are functions of s^2, like e.g. in the $(\varphi^4)_d$-model, see [AFHKL].

4. Point interactions and scattering by a large number of small randomly placed scatterers

In the definition of the N center point interaction (1.5.) all the physical constants characterizing the strength of the interaction, the energy of the quantum particle and the mutual distances of the scatterers are contained in the matrix $\Gamma_{\alpha,Y}(k)$.

In particular they appear in Γ as the inverses of three lengths: the $\alpha_y, y \in Y = \{Y_1, ..., Y_N\}$ represent the inverses of an "effective linear size " of the scatterers, (see [AGHKH]), k is proportional to the inverse of the wave length associated with the quantum particle and the $G_k(y-y')$ are proportional to the inverses of the distances between the scatterers. In this section we shall study some limits $N \longrightarrow \infty$, different from those studied in Sect. 2,3, but also of physical relevance cfr e.g. [Lo]. We report here on work in [FHT] - [FOT].

In the following the orders of magnitude of the above lengths will be expressed as powers of the number N of the scatterers and the volume of the system will be considered fixed and finite (of course only the dimensionless ratios of the lengths are to be considered as meaningful parameters). We shall consider separately three situations, which we shall denote by cases 1), 2), 3).

Case 1:

$$\inf_{y,y' \in Y} |y - y'| = 0(N^{-\frac{1}{3}}), k^{-1} = 0(1), \alpha_y^{-1} = 0(N^{-1})$$

. In this case there is a large number N of scatterers in a finite volume, each one of strength being of order N^{-1}. The wavelength of the quantum particle is large with respect to the scatterers effective length and to the interparticle distance.

Physically, in this case one expects a finite effective potential depending only on the local strength per unit volume of the scatterers.

Case 2:

$$\inf_{y,y' \in Y} |y - y'| = 0\left(N^{-\frac{1}{3}}\right), k^{-1} = 0\left(N^{-\frac{1}{3}}\right), N^{\frac{1}{2}}\alpha_y^{-1} = 0(N^{-\frac{1}{3}}).$$

In this case the wavelength is of the same order as the interparticle distance. Each scatterer has infinitesimal strength but the "surface per unit volume" is kept constant.

The limit problem is expected to contain information about the local statistics of the interparticle distances. It is the relevant limit, for example, in modelling scattering of neutrons by liquids (scattering due only to the nuclei of the atoms in the liquid). In fact this kind of scattering experiments are often performed to investigate the range of solid-like order in the interparticle distances in fluids.

Case 3: All the lengths are of order $N^{-\frac{1}{3}}$. This case is in fact a genuine infinite volume limit case. There are no negligible terms in the Γ matrix.

This case is the relevant one for modelling amorphous or perfect crystalline solids, as discussed in Sect. 2,3. In what follows we give results for cases 1) and 2), for dimension $d = 3$ (the case $d = 2$ can be worked out as the $d = 3$ case, whereas the case $d = 1$ is much simpler).

Case 1 Let $Y^{(N)} = \left\{y_1^{(N)}, ..., y_N^{(N)}\right\}$ be a sequence of N-tuples of points in $\mathbb{R}^3$ such that

$$\frac{1}{N}\sum_{i=1}^{N} \delta_{y_i^{(N)}} \underset{N\uparrow\infty}{\overset{w}{\longrightarrow}} \rho(x)dx$$

with $\rho(x) \geq 0$, $\rho(\cdot) \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, $\int_{\mathbb{R}^3} \rho(x)dx = 1$, the convergence being weak convergence of probability measures on $\mathbb{R}^3$.

Some technical assumptions on the distribution of the $y_i^{(N)}$ will be needed; e.g.

$$\inf_{i,j} \left| y_i^{(N)} - y_j^{(N)} \right| \geq cN^{-\alpha} \text{ for some } \alpha \in \left(\frac{1}{3}, 1\right)$$

$$\frac{1}{N^2} \sum_{\substack{i,j \\ i \neq j}} \frac{1}{\left| y_i^{(N)} - y_j^{(N)} \right|^2} \leq c \qquad \forall N$$

If, for example, the $y_i^{(N)}$ are chosen to be N independent, identically distributed (i.i.d.) random points of $\mathbb{R}^3$ with common distribution density ρ, the above stated assumptions are satisfied by any configuration of a set of measure increasing to 1 when N goes to infinity.
Let $\alpha^{(N)} = \{\alpha_y, y \in Y^{(N)}\}$. We are looking for the existence of a limit operator for the sequence $-\Delta_{N\alpha^{(N)},Y^{(N)}}$ and for an explicit characterization of the limit. If all the $\alpha_j^{(N)}$ are bounded away from 0 and $\inf_{j \neq j'} \alpha_j^N \left| y_j^{(N)} - y_{j'}^{(N)} \right| \gg 1$, as a first order in a perturbation expansion, we get, as $N \longrightarrow \infty$:

$$\left[\Gamma_{N\alpha^{(N)},Y^{(N)}}\right]_{j,j'} \sim N\alpha_j^{(N)} \delta_{j,j'}$$

and

$$\left(-\Delta_{N\alpha^{(N)},Y^{(N)}} - k^2\right)^{-1}(x,y) \sim G_k(x,y) +$$

$$+\frac{1}{N} \sum_{j=1}^{N} G_k\left(x, y_j^{(N)}\right) G_k\left(y_j^{(N)}, y\right) \left(\alpha_j^{(N)}\right)^{-1} \tag{4.1}$$

If the $\alpha_j^{(N)}$ are chosen to be the values $\alpha\left(y_j^{(N)}\right)$ in $y_j^{(N)}$ of a function which is continuous (outside a set of $\rho(x)dx$ measure 0) and $0 < a \leq |\alpha| \leq b < \infty$, the right hand side of (4.1) converges to

$$G_k(x,y) + \int_{\mathbb{R}^3} G_k(x,z) \frac{\rho(z)}{\alpha(z)} G_k(z,y) dz =$$

$$= (-\Delta - k^2)(x,y) + \left[(-\Delta - k^2)^{-1} \frac{\rho}{\alpha} (-\Delta - k^2)^{-1}\right](x,y) \quad . \tag{4.2}$$

(4.2) is the first term of a perturbation expansion of $(-\Delta + \frac{\rho}{\alpha} - k^2)$; up to the first order $-\Delta_{N\alpha^{(N)},Y^{(N)}}$ behaves for large N like $(-\Delta - \frac{\rho}{\alpha})$.
In fact the result is true up to any order in the expansion. One has in particular the following

Theorem 4.1.: Under the assumptions made before

$$s - \lim_{N \uparrow \infty} \left(-\Delta_{N\alpha^{(N)},Y^{(N)}} + \lambda\right)^{-1} = \left(-\Delta - \frac{\rho}{\alpha} + \lambda\right)^{-1} \equiv A_\rho^\lambda$$

for $\lambda > 0$ sufficiently large.
For a detailed proof and further comments see [FHT]. If the $y_i^{(N)}$ are i.i.d. random points with common distribution density ρ the above stated theorem can be looked upon as an operational law of large number. The corresponding central limit theorem can also be proved:

Theorem 4.2.: For any $f, g \in L^2(\mathbb{R}^3)$ the random variable

$$N^{\frac{1}{2}} \left(f, \left[\left(-\Delta_{N\alpha^{(N)},Y^{(N)}} + \lambda\right)^{-1} - A_\rho^\lambda\right] g\right) \equiv \xi^{(N)}(Y^{(N)})$$

converges in distribution when N goes to $+\infty$ to the gaussian random variable ξ^λ with mean 0 and variance.

$$E(\xi^\lambda) = \left(A_\rho^\lambda f A_\rho^\lambda g, \alpha^{-2} A_\rho^\lambda f A_\rho^\lambda g\right)_{L_\rho^2} - \left(A_\rho^\lambda f, \alpha^{-1} A_\rho^\lambda g\right)_{L_\rho^2}^2$$

(here $L_\rho^2 = L^2(\mathbb{R}^3, \rho dx)$).
For the proof and further comments see [FHT] and [FOT].

Remark: If V is any function in $L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ and we take ρ, α as

$$\rho(x) = |V(x)| / \int_{\mathbb{R}^3} |V(x)| dx$$

$$\alpha(x) = (\text{sign } V)(x) / \int_{\mathbb{R}^3} |V(x)| dx$$

so that $\frac{\rho}{\alpha} = V$, then Theorems 4.1, 4.2 express the fact that any one particle Hamiltonian with a potential V of class $L^1 \cap L^2$ can be arbitrarily well approximated by a Hamiltonian with zero range potential on an increasing number of points.

Case 2: In experiments of neutron scattering, neutrons with a wavelength of a few Ångstrøms are used to investigate samples of condensed matter. The average interparticle distances are of the same order of the wavelength, while the range of the interaction of the neutrons with the nuclei of the atoms is of the order
10^{-13} cm.

A first order expansion for the differential cross section $d\sigma/d\Omega$ for a formal potential $2\pi b \sum_{i=1}^{N} \delta(x - y_i^{(N)})$ (in the usual units such that $\hbar = m = 1$) gives

$$\left(\frac{d\sigma}{d\Omega}\right)(x) = b^2 \sum_{i,j}^{N} e^{ix(y_i^{(N)} - y_j^{(N)})}$$

where x is the transferred momentum and $y_i^{(N)}$ are the positions of the scatterers.

Notice that the formal expansion cannot be continued beyond the first order term since infinities due to the singularity of the G_k at coinciding points would appear in each higher order term. For the N-centers point interaction the above mentioned result is exact for N large in the scaling described above as pertaining to case 2 (which in a box of volume proportional to N can be redefined as $|y_i - y_j| = 0(1), k^{-1} = 0(1), N^{\frac{1}{2}} \alpha_j^{-1} = 0(1)$). In fact let $\left(\frac{d\sigma}{d\Omega}\right)^{\frac{1}{2}}_{N^{\frac{1}{2}}\alpha, Y^{(N)}}$ be the differential cross section corresponding to N-center zero range interactions, all of the same strength $N^{-\frac{1}{2}}\alpha^{-1}$, placed at the points $\{y_1^{(N)}, ..., y_N^{(N)}\}$. Under some technical assumptions on the distribution of the $y_i^{(N)}$, it is possible to prove that

$$\lim_{N \nearrow \infty} \left| \left(\frac{d\sigma}{d\Omega}\right)_{N^{\frac{1}{2}}\alpha, Y^{(N)}} - \frac{1}{N\alpha^2} \sum_{i,j} e^{ik\left(y_i^{(N)} - y_j^{(N)}\right)} \right| = 0 \tag{4.3}$$

For this see [DFZ].

Notice that if the $y_i^{(N)}$ are distributed according to an homogeneous point process in $\mathbb{R}^3$ of density ρ and if the static pair correlation function given by

$$\frac{g(r)}{4\pi r^2} dr = Pr\left\{ \left| y_i^{(N)} - y_j^{(N)} \right| \in (r, r + dr) \middle| y_i^{(N)} \right\}$$

is decaying fast enough to ρ for large r, the common limit of the two quantities appearing in (4.3) is $\frac{1}{\alpha^2} + \frac{\rho}{\alpha^2}\hat{g}(x)$ ($\hat{g}$ denotes the Fourier transform of g).

It should be stressed that for the N-centers point interaction the terms of the perturbation expansion, disappearing in the limit $N \longrightarrow \infty$, are explicitly known.

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