# Band edge localization in randomly perturbed crystals

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## 1 The results

Random Schrödinger operators, i.e. families of Schrödinger operators $H_\omega$ depending on a random parameter $\omega \in \Omega$, a suitable probability space, are used in mathematical physics as a quantum mechanical model of disordered solids. Working in the one-electron approximation, i.e. studying the motion of a single electron in the force field of fixed disordered nuclei, the spectral characteristics of $H_\omega$ can be interpreted in terms of the dynamics of the electron (see the discussion of the RAGE theorem in [15, Ch.XI.17] and the references given therein): If $H_\omega$ has pure point spectrum almost surely (for almost every $\omega \in \Omega$), then the electron wave function essentially remains restricted to a bounded region for all times. In this case the solid is interpreted as being an electrical *insulator*. If, on the other hand, the spectrum is continuous, then the motion of the electron is unbounded in the time mean, where no time mean has to be taken in the case of absolutely continuous spectrum. In solid state physics this is seen as corresponding to a *conductor*.

Here we study a model for a crystal with randomly distributed impurities. The model is given by the random Schrödinger operator

$$H_\omega = -\Delta + V_{per} + V_\omega \tag{1.1}$$

in $L^2(\mathbb{R}^d)$. The potential of the crystal is given by a real valued $\mathbb{Z}^d$-periodic function $V_{per}$ on $\mathbb{R}^d$, which in addition satisfies the technical requirement $V_{per} \in L^p_{loc}(\mathbb{R}^d)$, where $p = 2$ if $d \leq 3$, and $p > d/2$ if $d \geq 4$. The impurities are thought to be alloy like, i.e. fixed to the period lattice, and described by an Anderson type random potential

$$V_\omega(x) = \sum_{k \in \mathbb{Z}^d} q_k(\omega) f(x-k). \tag{1.2}$$

Our assumptions on the *single site potential* $f$ and the random coupling constants $q_k$ are as follows:

Let $f \in L^p(\mathbb{R}^d)$ with $p$ as above have compact support, and let $f \geq \chi_{\Lambda_s(0)}$ for some $s > 0$. Here $\chi_A$ denotes the characteristic function of some subset $A$ of $\mathbb{R}^d$, and $\Lambda_s(0)$ is the cube of sidelength $s$ with center 0.

The $q_k$ are independent, identically distributed real random variables on a probability space $(\Omega, \mathbb{P})$. They are assumed to have absolutely continuous distribution with density $g \in L^\infty(\mathbb{R})$, where $\operatorname{supp} g = [q_-, q_+]$, a compact interval. Thus, for example, one can choose

$$(\Omega, \mathbb{P}) = \left( [q_-, q_+]^{\mathbb{Z}^d}, \bigotimes_k g(q_k) dq_k \right)$$

and

$$q_k(\omega) = \omega_k \quad \text{for } \omega \in \Omega.$$

The random Schrödinger operator $H_\omega$ as defined by (1.1) and (1.2) has first been studied for the special case $V_{per} = 0$. In this case the almost sure spectrum of $H_\omega$ is a half line $[E_0, \infty)$, and for the choice $f = \chi_{\Lambda_1(0)}$ Kotani and Simon [14] have shown localization at low energies, i.e. that there is a $\delta > 0$ such that $H_\omega$ almost surely has dense pure point spectrum in $[E_0, E_0 + \delta)$ with exponentially decaying eigenfunctions. Combes and Hislop [3] have extended this result to more general $f$ using an additional disorder assumption on $V_\omega$.

If $V_{per} \neq 0$, then, in general, the spectrum of the periodic Schrödinger operator $H_{per} = -\Delta + V_{per}$ has band structure and, under some weak additional assumptions, is purely absolutely continuous, cf. [15, Ch.XVI]. It is not difficult to show that under the above assumptions one gets band structure also for the spectrum of $H_\omega$. In fact, the following formula holds $\mathbb{P}$-almost surely:

$$\sigma(H_\omega) = \bigcup_{q \in [q_-, q_+]} \sigma \left( H_{per} + q \sum_{k \in \mathbb{Z}^d} f(\cdot - k) \right) =: \Sigma, \tag{1.3}$$

for a proof see [12]. This implies band structure, where points in the boundary $\partial\Sigma$ of $\Sigma$ are given by band edges of either $H_{per} + q_+ \sum_k f(\cdot - k)$ or $H_{per} + q_- \sum_k f(\cdot - k)$. Energies at these boundary points correspond to the rare events that all coupling constants $q_k(\omega)$ are near $q_+$ or $q_-$. Thus $\partial\Sigma$ is a *fluctuation boundary* and physically one expects localization for energies lying close to it. This is confirmed by our main result:

**Theorem 1.1.** *Assume that there exists $\tau > d$ such that $g$ satisfies*

$$\int_{q_-}^{q_-+h} g(s)\,ds \le h^\tau \quad \textit{and} \quad \int_{q_+-h}^{q_+} g(s)\,ds \le h^\tau \quad \textit{for small } h > 0. \tag{1.4}$$

*Then in a neighborhood of $\partial\Sigma$ the spectrum of $H_\omega$ is pure point $\mathbb{P}$-almost surely with exponentially decaying eigenfunctions.*

Near the bottom of the spectrum we have the following result on localization:

**Theorem 1.2.** *Assume that $V_{per}$ is reflection symmetric with respect to all coordinate axes. Then in a neighborhood of* $\inf\Sigma$ *the spectrum of $H_\omega$ is pure point $\mathbb{P}$-almost surely with exponentially decaying eigenfunctions.*

At the bottom of the spectrum we are able to apply a known result of Kirsch and Simon [11] on the Lifshitz tail behavior of the density of states. This allows us to drop the decay assumption (1.4) on $g$ in Theorem 1.2, but the results from [11] need $V_{per}$ to be reflection symmetric. The idea that Lifshitz tails should imply localization was to our knowledge first rigorously established by Klopp in [13].

There is recent work of Barbaroux, Combes and Hislop [2] which is closely related to our Theorem 1.1. They provide a general framework for band edge localization, which includes periodic Schrödinger operators as a special case, but also applies to certain models involving magnetic fields. Results on band edge localization for several other models have been given by Figotin and Klein, who studied random lattice operators [6], acoustic models [7] (see also [17]), and models from electrodynamics [8].

Full proofs of Theorems 1.1 and 1.2 and some generalizations are given in [12], where the various methods involved in the argument are described in detail. Even after a number of improvements in the presentation of the proofs have been found compared to former discussions of localization, this still involves considerable technical effort. Therefore we use the following section to outline the strategy used in the proofs by stating several intermediate results and sketching their proofs.

## 2 The proofs

### 21 The Simon-Wolff criterion and localization

The phenomenon of dense point spectrum has been found to be highly unstable under perturbations, see e.g. [4]. While this has proven to be an obstacle in establishing a general mathematical theory of localization, there is at least one criterion for localization which has turned out to be widely applicable. It was originally formulated in a paper by Simon and Wolff [16] for the case of lattice Schrödinger operators with random potential of Anderson type. The continuum version which we use below was essentially provided by Combes and Hislop in [3]. A drawback of this method is that it needs absolute continuity of the distribution of the random coupling constants $q_k$ in (1.2), while other methods (e.g. [5]) principally can treat more singular distributions.

In order to apply the Simon-Wolff (Combes-Hislop) criterion, we use the following result, where $R(z, \omega) := (H_\omega - z)^{-1}$.

**Theorem 2.1.** *Let $Q : \mathbb{R}^d \to \mathbb{R}$ be bounded, measurable and of compact support. Under the assumptions of Theorem 1.1 (resp. Theorem 1.2) there exists a neighborhood $U$ of $\partial\Sigma$ (resp. $\inf \Sigma$) such that the following holds with probability one:*

*(a) For almost every $E \in U$*

$$\sup_{\varepsilon \neq 0} \| R(E + i\varepsilon) Q \| < \infty. \tag{2.1}$$

*(b) For almost every $E \in U$ there exist $C$ and $\gamma > 0$ such that*

$$\sup_{\varepsilon \neq 0} \| \chi_{\Lambda_1(x)} R(E + i\varepsilon) Q \| \leq C e^{-\gamma |x|} \tag{2.2}$$

*for every $x \in \mathbb{Z}^d$.*

Ideas on how to prove this result are discussed in the next subsection. Once Theorem 2.1 is established, then the Simon-Wolff criterion says that (a) implies pure point spectrum of $H_\omega$ in $U$ for almost every $\omega$, while the stronger result (b) is needed to show that eigenfunctions decay exponentially for $E \in U$ and almost every $\omega$. Thus Theorems 1.1 and 1.2 are both consequences of Theorem 2.1. A detailed proof is provided in [12], offering a variant of the treatment in

[16] respectively [3]. The first step is to show that Theorem 2.1 implies that polynomially bounded eigensolutions are automatically exponentially decaying:

**Lemma 2.2.** *To every $\omega \in \Omega$ there exists a subset $S_\omega \subset U$ (the neighborhood found in Theorem 2.1) such that $|U \setminus S_\omega| = 0$ and the following holds:*

*If $E \in S_\omega$ and $\varphi$ is a weak solution of $(H_\omega + \lambda f)\varphi = E\varphi$ with $(1+|\cdot|^2)^{-s/2}\varphi \in H^1$ (the first order Sobolev space) for some $s \in \mathbb{R}$, then there exist $C$ and $\gamma > 0$ such that*

$$|\varphi(x)| \leq Ce^{-\gamma|x|} \quad \textit{for every } x \in \mathbb{R}^d.$$

The existence of polynomially bounded solutions required in Lemma 2.2 is a standard result from the theory of generalized eigenfunction expansions:

**Lemma 2.3.** *Let $H = -\Delta + V$ in $L^2(\mathbb{R}^d)$, where $V$ is uniformly locally in $L^p$ with $p = 2$ if $d \leq 3$ and $p > \frac{d}{2}$ if $d \geq 4$. Let $\mu$ be a spectral measure and $s > d/2$.*

*Then for $\mu$-almost every $E \in \mathbb{R}$ there exists a non-trivial weak solution $\varphi$ of $H\varphi = E\varphi$ with $\varphi \in H^1_{-s}$.*

Lemmas 2.2 and 2.3 are now used as follows to prove Theorems 1.1 and 1.2: By an application of Fubini's theorem and the absolutely continuous distribution of the $q_k$, it is sufficient to fix $\omega$ and prove localization of $H_\lambda = H_\omega + \lambda f$ in $U$ for almost every $\lambda$. This follows readily from Lemmas 2.2 and 2.3 after it is checked that the exceptional set $U \setminus S_\omega$ from Lemma 2.2 effects the spectrum of $H_\lambda$ only for $\lambda$'s in a nullset. This is established by using a result on *spectral averaging* (taken from [3]) as final input.

## 22 Multiscale analysis

With one exception, Aizenman and Molchanov's work [1] on lattice operators, all proofs of multidimensional localization which can be found in the literature have used the method of multiscale analysis. This method was first used in the context of random Schrödinger operators by Fröhlich and Spencer [9] and has meanwhile undergone a number of extensions and simplifications. We use it to prove Theorem 2.1. To set up this iterative procedure for proving (2.1) and (2.2) we use the following results as input. Detailed proofs for all of them are given in [12].

(a) The band edges of periodic Schrödinger operators change linearly under periodic perturbations of fixed sign:

**Theorem 2.4.** *Let $V, W \in L^p_{loc}$ be $\mathbb{Z}^d$–periodic and $p$ as above. Assume that $W \geq 0$ is such that the interior of $\{x; W(x) \geq \alpha\}$ is non-empty for some $\alpha > 0$. Let $H = -\Delta + V$, $H(\lambda) = H + \lambda W$ and denote by $a(\lambda) \in \partial\sigma(H(\lambda))$ a band edge varying continuously with $\lambda \in (-\lambda_0, \lambda_0)$. Then there exists $\lambda_1 > 0$ and $C > 0$ such that*

$$|a(\lambda) - a(0)| \geq C|\lambda| \text{ for } |\lambda| \leq \lambda_1.$$

This result, whose proof depends mainly on unique continuation methods and analytic perturbation theory, is basic for turning the physical idea of a fluctuation boundary into a rigorous treatment of localization.

(b) We need a *Wegner estimate* for box hamiltonians, i.e. operators of the form

$$H_\Lambda(\omega) = H_{per} + V_\omega \quad \text{in } L^2(\Lambda),$$

where $\Lambda = \Lambda_\ell(i)$, $\ell \in \mathbb{N}$, $i \in \mathbb{Z}^d$, and periodic boundary conditions are imposed.

**Theorem 2.5.** *Let $a \in \partial\Sigma$. Then there is an open interval $I$ containing $a$ and a $C_W$ such that for all intervals $J \subset I$ and all $\Lambda = \Lambda_\ell(i)$ with $\ell \in \mathbb{N}, i \in \mathbb{Z}^d$ we have:*

$$\mathbb{P}\{\sigma(H_\Lambda(\omega)) \cap J \neq \emptyset\} \leq C_W |J||\Lambda|^2.$$

This estimate expresses that it is quite unlikely to "hit" an eigenvalue of $H_\Lambda(\omega)$ for fixed $\Lambda$ and varying $\omega$. Recently, Kirsch [10] has introduced a method which allows to conclude a Wegner estimate from estimates on the spatial distribution of eigenfunctions of box hamiltonians. Based on this method we get Theorem 2.5 as a consequence of

**Proposition 2.6.** *Let $a \in \partial\Sigma$. Then there is an open interval $I$ containing $a$ and $C > 0$ such that for all $\Lambda = \Lambda_\ell(i)$ with $\ell \in \mathbb{N}, i \in \mathbb{Z}^d$, all $\omega \in \Omega$ and all normalized eigenfunctions $\psi$ of $H_\Lambda(\omega)$ corresponding to an eigenvalue $\mu \in I$ we have:*

$$\sum_{k \in \Lambda} \int_{\Lambda_s(k)} |\psi(x)|^2 dx \geq C.$$

The idea of the proof of Proposition 2.6 is that the spectral boundary can be shifted away from $a$ by adding a suitable periodic perturbation with support in $\bigcup_k \Lambda_r(k)$ $(r < s)$ to $V_\omega$, cf. Theorem 2.4. $\psi$ remains to be an eigensolution in the complement $F$ of $\bigcup_k \Lambda_s(k)$. But the new operator has a spectral gap near $a$. A simple tunneling estimate shows that not all of $\psi$'s support can be concentrated in $F$.

(c) Finally, Theorem 2.4 and assumption (1.4) on the distribution of the $q_k$ can be turned into a high probability estimate for a lower bound on the distance of the spectrum of a box hamiltonian to a band edge $a \in \partial\Sigma$:

**Theorem 2.7.** *Assume (1.4) and let $a \in \partial\Sigma$. Then for any $\xi \in (0, \tau - d)$ there is a $\beta > 0$ and $\ell^* = \ell^*(\tau, \xi)$ such that*

$$\mathbb{P}\{dist(\sigma(H_\Lambda(\omega)), a) > \ell^{\beta-1}\} > 1 - \ell^{-\xi} \tag{2.3}$$

*for $\Lambda = \Lambda_\ell(0)$ and $\ell \geq \ell^*$.*

It is here where the argument can be improved for $a = \inf \Sigma$ if $V_{per}$ is reflection symmetric. In this case results from [11] can be used to show that (2.3) holds for any $\xi > 0$, $\beta \in (-1, 1)$ and sufficiently large $\ell$, thus not requiring (1.4).

Theorem 2.7 is the starting point of the multiscale procedure, since by using a Combes-Thomas argument it can be turned into a decay estimate for resolvents of box hamiltonians similar to (2.2). Unfortunately, the decay rate found from this depends on $\ell$ and actually tends to 0 as $\ell$ becomes large, thus not leading to a global decay estimate as required for (2.2).

The idea now is to partition a larger box of sidelength $\ell'$ into smaller boxes of sidelength $\ell$ and varying centers $x$ and to "expand" the resolvent of $H_{\Lambda_{\ell'}(0)}(\omega)$ into resolvents of $H_{\Lambda_\ell(x)}(\omega)$. To apply this expansion successfully one needs two inputs:

(i) One needs to find a sequence of boxes $\Lambda_\ell(x)$ joining opposite sides of $\Lambda_{\ell'}(0)$ and such that the resolvents of $H_{\Lambda_\ell(x)}(\omega)$ all have "good" initial decay properties. Combinatorics show that this is the case with an even higher probability than probability (2.3) for an individual box $\Lambda_\ell(x)$ to be "good".

(ii) A basic estimate for $\|(H_{\Lambda_{\ell'}(0)}(\omega) - E)^{-1}\|$ is needed for every $E$ in a neighborhood of $a$ and with sufficiently large probability. This is a consequence of the Wegner estimate (Theorem 2.5).

One ends up with a resolvent decay estimate for the scale $\ell'$ with only slightly decreased decay rate than for $\ell$, but with higher probability. An iteration of this step and a limiting argument including a summation over "shells" finally leads to the almost sure estimates claimed in Theorem 2.1. For details we again refer to [12].


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