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Infinite Representability of Schrödinger Operators with Ergodic Potential

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Analog zum Begriff der endlichen Darstellbarkeit in der Banachraumtheorie wird der Begriff der Darstellbarkeit und der unendlichfachen Darstellbarkeit für selbstadjungierte Operatoren eingeführt. Es wird gezeigt, daß die unendlichfache Darstellbarkeit des Operators A in B zur Folge hat, daß das wesentliche Spektrum von B das Spektrum des Operators A enthält. Durch Anwendung auf ergodische Schrödingeroperatoren ergibt sich u. a. ein neuer Beweis für den Zusammenhang zwischen Spektrum und Zustandsdichte sowie dafür, daß das Spektrum nicht zufällig ist. Für das Spektrum des Hamiltonoperators im Falle eines substitutionellen Mischkristalls wird eine Formel angegeben, welche eine Klärung des Bowingeffektes gestattet. Ähnliche Resultate wurden unabhängig von KIRSCH und MARTINELLI gefunden.

По аналогии с понятием конечной представимости в теории банаховых пространств вводится понятие представимости и бесконечнократной представимости для самосопряженных операторов. Доказывается, что из бесконечнократной представимости оператора A в B следует, что существенный спектр оператора B содержит спектр оператора A. Приложение к эргодическим операторам Шредингера даёт, между прочим, новое доказательство неслучайности спектра таких операторов и связи между спектром и плотностью состояний. Для спектра оператора Гамильтона в случае подстановочного кристалла смеси получается формула, которая допускает выяснить суть прогибательного эффекта. Подобные результаты независимо получили также Кирш и МАРТИНЕЛЛИ.

Analogous to the notion of finite representability in the theory of Banach spaces, the notions of the representability and the infinite representability of self-adjoint operators are introduced. It is proved that the infinite representability of the operator A in B yields that the essential spectrum of B contains the spectrum of A. This result applied to ergodic Schrödinger operators yields a new proof for the nonrandomness of the spectrum and for the connection between the spectrum and the density of states. A formula for the spectrum of the Hamiltonian of a substitutional alloy is presented, which clarifies the bowing effect. Similar results were found independently by KIRSCH and MARTINELLI.

1. Representability of Self-adjoint Operators

In order to compare the spectra of self-adjoint operators, we use the concept of the infinite representability of an operator in another one. This notion is similar to the concept of finite representability of normed spaces developed in [17, 28, 29]. It means that the (not necessary finite dimensional) restrictions of an operator do not much differ from appropriately chosen restrictions of the other operator.

Definition 1.1.: Let A, B be self-adjoint operators in a Hilbert space H. We call A *infinitely representable* in B, if there is an increasing sequence $\{D_k\}$, $k \in \mathbf{N}$, of linear subspaces of dom A and a sequence $\{U_k\}$ of unitary operators, such that

i) $\bigcup_{k \in \mathbf{N}} D_k$ is dense in dom A with respect to the topology defined by the scalar product $\langle z, z\rangle + \langle Az, Az\rangle$,

ii) $U_k(D_k) \subset \operatorname{dom} B$ and for every $\varepsilon > 0$ there is a $k_0 \in \mathbf{N}$, such that for all $k > k_0$ and all $z \in D_k$

$$\langle (A - U_k^* B U_k) z, z\rangle \leqq \varepsilon(\|Az\| + \|z\|)^2,$$

iii) for $k \neq l$ $U_k(D_k)$ is orthogonal to $U_l(D_l)$.

If only i) and ii) are satisfied, then A is called *representable* in B.

Remark 1.2: Of course, every operator is representable in itself (take $U_k := I$, the identity), but not every operator is infinitely representable in itself.

For the proof of the following theorem we need a finite dimensional criterion that a point belongs to the essential spectrum. It is well known (e.g. [1]) that a number λ lies in the essential spectrum $\sigma_{\text{ess}}(A)$ of an operator A, iff there is an orthonormal sequence $\{e_n\}$ in dom A, such that $\lim\limits_{n\to\infty} \|Ae_n - \lambda e_n\| = 0$. We use the following finite dimensional variant of this criterion.

Lemma 1.3: *$\lambda \in \mathbf{R}$ belongs to the essential spectrum of a self-adjoint operator A, iff for every $\varepsilon > 0$ and $k \in \mathbf{N}$ there is an orthonormal sequence $\{e_1, \ldots, e_k\} \subset H$ and a sequence $\{z_1, \ldots, z_k\} \subset \operatorname{dom} A$, such that $\|e_i - z_i\| < \varepsilon$ and $\|Az_i - \lambda z_i\| < \varepsilon$ for $i \in \{1, \ldots, k\}$.*

Proof: The above mentioned criterion shows the necessity of the conditions. Now we prove indirectly that the conditions are sufficient. Let us assume $\lambda \notin \sigma_{\text{ess}}(A)$. Then A has a spectral representation

$$A = \int_{-\infty}^{\lambda-\delta} \mu\, dE_\mu + \lambda P + \int_{\lambda+\delta}^{\infty} \mu\, dE_\mu$$

with $\delta > 0$ and a finite dimensional orthoprojector P ($P = 0$ is also possible). For $z \in \operatorname{dom} A$ this means $\|(A - \lambda I + \delta P) z\| \geqq \delta \|z\|$. Let $\{f_1, \ldots, f_l\}$ be an orthonormal basis for the range of P. We choose $k > 4l$ and $\varepsilon > 0$ in such a way that $1 - 2\varepsilon - \varepsilon/\delta > 1/2$. If $\{z_1, \ldots, z_k\}$ and $\{e_1, \ldots, e_k\}$ fulfil the conditions of the lemma then

$$\delta(1 - \varepsilon) \leqq \delta \|z_i\| \leqq \|(A - \lambda I + \delta P) z_i\| \leqq \|Az_i - \lambda z_i\| + \delta \|P(e_i - z_i)\|$$
$$+ \delta \|Pe_i\| \leqq \varepsilon + \delta\varepsilon + \delta \|Pe_i\|,$$

i.e. $1/2 \leqq \|Pe_i\|$. By summation of the squares we get

$$k/4 \leqq \sum_{i=1}^{k} \|Pe_i\|^2 = \sum_{i=1}^{k} \sum_{j=1}^{l} |\langle e_i, f_j\rangle|^2 \leqq \sum_{j=1}^{l} \|f_j\|^2 = l.$$

This contradiction shows that the assumption $\lambda \notin \sigma_{\text{ess}}(A)$ is false ∎

Theorem 1.4: i) *If A is representable in B, then $\sigma(A) \subset \sigma(B)$* and $\sigma_{\text{ess}}(A) \subset \sigma_{\text{ess}}(B)$.

ii) *If A is infinitely representable in B, then $\sigma(A) \subset \sigma_{\text{ess}}(B)$.*

Remark 1.5: KÜRSTEN [26] proved the following version of this theorem for form-bounded perturbations. Let $q(f, g) := \int (fg + \operatorname{grad} f \cdot \operatorname{grad} g)\, d^n x$, the scalar product in $W_1^2(\mathbf{R}^n)$, and $\langle f, g\rangle := \int fg\, d^n x$. For $0 < a$ and $0 < b < 1$ we regard the set $\Gamma_{a,b}$ of those linear functionals V on the linear hull of $\{f^2 \mid f \in W_2^1(\mathbf{R}^n)\}$ which fulfil for arbitrary $f \in W_2^1(\mathbf{R}^n)$ the inequality $-a\langle f, f\rangle - bq(f, f) \leqq V(f^2) \leqq aq(f, f)$. Due to the formula $fg = \big((f + g)^2 - (f - g)^2\big)/4$ $V(fg)$ can be defined for $V \in \Gamma_{a,b}$. For every $V \in \Gamma_{a,b}$ there is an uniquely defined self-adjoint operator whose quadratic form is $q(f, g) + V(fg) - \langle f, g\rangle$ (with the form domain $W_2^1(\mathbf{R}^n)$) [19]. This operator is called $-\Delta + V$. Let $B_r \subset \mathbf{R}^n$ be the ball with center 0 and radius r. Further, we define the shift operator on $L^1(\mathbf{R}^n)$ $(T_x h)(y) := h(y - x)$ and the shift operator on $\Gamma_{a,b}$ $(T_x' V)(h) := V(T_x h)$. For $M \subset \Gamma_{a,b}$ and $V \in \Gamma_{a,b}$ we call V f-representable in M, if for every $\varepsilon > 0$ and every $r > 0$ there is $x \in \mathbf{R}^n$ and a functional $U \in M$, such that for all $f \in W_2^1(\mathbf{R}^n)$ with supp $f \subset B_r$

$$(V - T_x'U)(f^2) \leqq \varepsilon q(f, f). \tag{1}$$

Let $V, U \in \Gamma_{a,b}$. Then V is infinitely f-representable in U, iff for every $\varepsilon > 0$ and every $r > 0$ there is a $x \in \mathbf{R}^n \setminus B_r$, such that for all $f \in W_2^1(\mathbf{R}^n)$ with supp $f \subset B_r$ inequality (1) holds.

Now we are able to formulate Theorem 1.4 for form-bounded perturbations.

Theorem 1.4': i) *If V is f-representable in M, then*

$$\sigma(-\Delta + V) \subset \overline{\bigcup_{U \in M} \sigma(-\Delta + U)}.$$

ii) *If V is infinitely f-representable in $\{U\}$ then*

$$\sigma(-\Delta + V) \subset \sigma_{\text{ess}}(-\Delta + U).$$

This extension is necessary when one considers one-dimensional potentials consisting of randomly distributed δ-distributions (cf. [11]).

Proof of Theorem 1.4: i) We assume the representability of A in B and $\lambda \in \sigma_{\text{ess}}(A)$. In accordance with Lemma 1.3 we find for every $\bar{\varepsilon} > 0$ ($\bar{\varepsilon}$ is chosen in dependence on λ and ε) and $k \in \mathbf{N}$ an orthonormal sequence $\{e_1, \ldots, e_k\}$ and a sequence $\{z_1, \ldots, z_k\} \subset$ dom A, such that $\|e_i - z_i\| < \bar{\varepsilon}$, $\|Az_i - \lambda z_i\| < \bar{\varepsilon}$. Since $\bigcup_{l \in \mathbf{N}} D_l$ is dense in dom A with respect to the graph norm (cf. Def. 1.1) there are vectors $y_1, \ldots, y_k$ in $\bigcup_{l \in \mathbf{N}} D_l$, such that $\|e_i - y_i\| < 2\bar{\varepsilon}$ and $\|Ay_i - \lambda y_i\| < 2\bar{\varepsilon}$. We conclude that $\{y_1, \ldots, y_k\}$ already lies in a subspace D_m, $m \in \mathbf{N}$. For a sufficiently large $p \geqq m$ we take the unitary operator U_p from Definition 1.1. The vectors $\{U_p e_i\}$, $\{U_p y_i\}$ and B fulfil the conditions of Lemma 1.3, because for given $\varepsilon > 0$ we can choose $\bar{\varepsilon} > 0$, such that $\|U_p(e_i - y_i)\| < 2\bar{\varepsilon} < \varepsilon$ and

$$\begin{aligned}
\|(B - \lambda) U_p y_i\| &= \|(U_p^* B U_p - \lambda) y_i\| \leqq \|(A - U_p^* B U_p) y_i\| + \|(A - \lambda) y_i\| \\
&\leqq \bar{\varepsilon}(\|Ay_i\| + \|y_i\|) + \|(A - \lambda) y_i\| \\
&\leqq (1 + \bar{\varepsilon}) \|(A - \lambda) y_i\| + \bar{\varepsilon}(1 + |\lambda|) \|y_i\| \\
&\leqq (1 - \bar{\varepsilon}) 2\bar{\varepsilon} + \bar{\varepsilon}(1 + |\lambda|)(1 + 2\bar{\varepsilon}) \leqslant \varepsilon.
\end{aligned}$$

But Lemma 1.3 states that λ belongs to $\sigma_{\text{ess}}(B)$.

We prove $\sigma(A) \subset \sigma(B)$ in the same manner, but use the following criterion: $\lambda \in \sigma(A)$ (for $A = A^*$) iff for every $\varepsilon > 0$ there is a normed vector $z \in$ dom A, such that $\|Az - \lambda z\| < \varepsilon$.

ii) From $\|Ay - \lambda y\| < 2\bar{\varepsilon}$, $y \in D_m$, $\|y\| < 1 + 2\bar{\varepsilon}$ we conclude $\|(B - \lambda) U_k y\| < \varepsilon$ for all $k \geqq p$. The statement follows from $U_k y \perp U_l y$ and the above lemma ∎

2. Schrödinger Operators with Ergodic Potential

In this chapter we derive the conclusions from Theorem 1.4 for Schrödinger operators with an arbitrary stationary and ergodic potential.

Let $(\Omega, \mathfrak{B}, \nu)$ be a measure space with $\Omega \subset L^p_{\mathrm{loc,unif}}(\mathbf{R}^n)$ (for definition cf. [34: Th. 13.96]) or $\Omega \subset l^\infty(\mathbf{Z}^n)$ with $p = 2$ for $n \leqq 3$, $p > 2$ for $n = 4$ and $p = n/2$ for $n \geqq 5$. Δ denotes the (discrete) Laplacian on $L^2(\mathbf{R}^n)$ $\left(l^2(\mathbf{Z}^n)\right)$, ν is a probability measure (σ-additive!), $\mathfrak{B}$ is the σ-algebra generated by cylindrical sets [36].

Theorem 2.1: i) *If ν is stationary with respect to the translations in $\mathbf{R}^n$ $(\mathbf{Z}^n)$ (i.e. the translations are measure preserving), then the operator $H^\omega := -\Delta + V^\omega$, $V^\omega \in \Omega$, on $L^2(\mathbf{R}^n)$ $\left(l^2(\mathbf{Z}^n)\right)$ has no discrete spectrum for a.e. ω.*

ii) *If ν is ergodic (for definition cf. [16]), then almost all operators H^ω have the same spectrum as a set.*

Proof: i) From [34: Th. 13.96] we conclude that every H^ω is a self-adjoint operator on dom $(-\Delta)$. We want to show that a.e. H^ω is infinitely representable in itself. The statement then follows from Theorem 1.4 ii). Take $D_k := \{z \in \mathrm{dom}\,(-\Delta) \mid \mathrm{supp}\, z \subset N_k\}$ with $N_k := \{x = (x_1, \ldots, x_n) \in \mathbf{R}^n \mid |x_i| \leqq k \ \forall\, i\}$. We construct U_k by induction beginning with $U_1 := I$. Because of the separability of $L^p(N_k)$ we can choose a countable set $\{V_k{}^i\}$, such that for every $V \in L^p(N_k)$ there is at least one $V_k{}^i$ in the $(1/2k)$-environment of V. Fix $i \in \mathbf{N}$. For a.e. V^ω such that $V^\omega|_{N_k}$ lies in the $(1/2k)$-environment of $V_k{}^i$, recurrence [16: Satz 4.1.2] yields that for arbitrary large R_k there is a vector $x_k \in \mathbf{R}^n$, such that

$$|x_k{}^\omega| > R_k{}^\omega \quad \text{and} \quad \|V^\omega(x - x_k{}^\omega)|_{N_K} - V_k{}^i\|_p < 1/2k.$$

Take for $U_k{}^\omega$ the translation $z(x) \to z(x + x_k{}^\omega)$. Then for $z \in L^2(N_k) \cap \mathrm{dom}\,(-\Delta)$

$$\begin{aligned} \left\|\left(V^\omega(x) - V^\omega(x - x_k{}^\omega)\right) z\right\|_2 &\leqq \|(V^\omega(x) - V^\omega(x - x_k)|_{N_k}\|_p \,\|z\|_{(2-1/p)^{-1}} \\ &\leqq 1/k \cdot (c\,\|-\Delta z\|_2 + \|z\|_2) \end{aligned}$$

(cf. the proof of Theorem 10.20 in [33]). Take $R_k{}^\omega := |x_{k-1}^\omega| + nk$ to ensure that $U_k(D_k) \perp U_l(D_l)$ for all $k > l$.

ii) In analogy to i) one can prove that for a.e. V^ω, $V^{\omega'}$ H^ω is infinitely representable in $H^{\omega'}$: Let us denote by $E_k{}^i$ the set

$$\{V^\omega \mid \exists\, x_k{}^\omega \in \mathbf{R}^n \text{ with } \|V^\omega(x - x_k{}^\omega)|_{N_k} - V_k{}^i\|_p < 1/2k\}.$$

$E_k{}^i$ is invariant with respect to all translations in $\mathbf{R}^n$, $E_k{}^i$ can have only measure 0 or 1 ∎

Remark 2.2: As the proof shows we did not need the stationarity of the measure; recurrence is sufficient.

PASTUR [31: Th. 3] proved our Theorem 2.1 for random Jacobi matrices, and also that every point in the essential spectrum is with probability 1 not an eigenvalue of finite multiplicity. KIRSCH and MARTINELLI [21: Prop. 2 and Cor.] carried over this result to random Schrödinger operators.

KUNZ and SOUILLARD [24: Lemma 4.3] proved for random Jacobi matrices, that the discrete, the pure point, the absolutely continuous and the singular continuous parts of the spectrum (σ_d, σ_{pp}, σ_{ac} and σ_{sc}) are a nonrandom set for a.e. $V^\omega \in \Omega$. This result was also carried over by KIRSCH and MARTINELLI [24: Th. 1 and Th. 2] to random Schrödinger operators. The proofs are based on abstract manipulations with random spectral projectors. Our method cannot reproduce the mentioned results, but has the advantage that it works sometimes for random and recurrent, but not stationary potentials (cf. § 3).

For some random potentials it is known whether σ_{pp}, σ_{sc} or σ_{ac} is a nonvoid set. For example, almost periodic potentials V can be regarded as a special case of ergodic potentials, as pointed out by PASTUR [31]: Take for Ω the hull of V [2], the Haar measure on Ω is an ergodic σ-additive measure. Thus Theorem 2.1 can be applied, where the word "almost" can be omitted: For every V^ω, $V^{\omega'} \in \Omega$ H^ω is infinitely representable in $H^{\omega'}$.

Periodic potentials as a special case of almost periodic potentials can be regarded as a special case of ergodic potentials, too. Under mild regularity conditions the Hamiltonian $H := -\Delta + V$ has for periodic potential V only an absolutely continuous spectrum [34: Th. 13.100].

In the last few years many results concerning the detailed structure of the spectra of Hamiltonians with almost periodic potential have been proved. Examples with nonvoid σ_{pp}, σ_{sc} and σ_{ac} have been found (cf. the reviews of BELLISSARD [5] and SIMON [37]). In one dimension physisists expect that a.e. H^ω has for a "truly random" potential no continuous spectrum; for some classes of measures this has been rigorously proved [15, 7, 10]. GOLDSHADE [14] announced a proof for the same fact in the quasi-one-dimensional model of a wire with a finite number of files.

Remark 2.3: $(-\Delta + V^\omega)$ on $L^2(\mathbf{R}^3)$ is the quantum mechanical operator for the energy of a particle, $-\Delta$ is its kinetic part and V^ω is the random potential. For the operator on $L^2(\mathbf{R}^1)$ one can give another interpretation after the transformation $x \to t$ (time): $y'' = V^\omega(t)\, y$ is the equation for a vibrating system with randomly varying parameter.

In analogy to Thomas' result for local perturbations of periodic potentials [34: Th. 13. 102] we prove the following theorem in which $L^p + L_0^\infty := \{f = f_p + f_\infty \mid f_p \in L^p, f_\infty \in L^\infty, \lim\limits_{|x|\to\infty} f_\infty(x) = 0\}$.

Theorem 2.4: *Let $V^\omega \in \Omega$, $V_0 \in L^p(\mathbf{R}^n) + L_0^\infty(\mathbf{R}^n)$ with p and Ω as in Theorem 2.1. Then for a.e. V^ω $\sigma_{ess}(H^\omega + V_0) = \sigma(H^\omega)$.*

Proof: Because a.e. H^ω is infinitely representable in $H^\omega + V_0$, the inclusion $\sigma(H^\omega) \subset \sigma_{ess}(H^\omega + V_0)$ is trivial. For the inverse inclusion we want to show that $V_0 \in L^p(\mathbf{R}^n) \cap L^2(\mathbf{R}^n)$ is a relatively compact perturbation of $(-\Delta + V^\omega)^{[n/4]+1}$ ($[a]$ denotes the entire part of a) in order to apply Cor. 3 of [34: Th. 13.14]:

$$\begin{aligned} &V_0(-\Delta + V^\omega)^{-[n/4]-1} \\ &= V_0(-\Delta + 1)^{-[n/4]-1} \{(-\Delta + 1)^{[n/4]+1} (-\Delta + V^\omega)^{-[n/4]-1}\}. \end{aligned}$$

The expression in the curly brackets is a bounded operator because V^ω is a $(-\Delta)$-bounded operator with relative bound zero [34: Th. 13.96]. But $V_0(-\Delta + 1)^{-[n/4]-1}$ is a Hilbert-Schmidt operator with kernel $V_0(x) \left((p^2 + 1)^{-[n/4]-1}\right)^\vee (x - y)$ ($(\cdot)^\vee$ denotes the inverse Fourier transform of $(\cdot)$), because $V_0 \in L^2$ and $(-\Delta + 1)^{-[n/4]-1}$ has the Fourier transform $(p^2 + 1)^{-[n/4]-1} \in L^2(\mathbf{R}^n)$. The self-adjointness of $-\Delta + V_0 + V^\omega$ on dom $(-\Delta + V^\omega)$ can be easily seen: V_0 and V^ω are $(-\Delta)$-bounded with relative bound zero, i.e. $-\Delta + V_0 + V^\omega$ is self-adjoint on dom $(-\Delta)$, but dom $(-\Delta)$ = dom $(-\Delta + V^\omega)$. The extension for $V_0 \in L^p + L_0^\infty$ can be done as in [34: Example 6 to Th. 13.14], where the gap between the spaces L_0^∞ and L_ϵ^∞ can be filled as in [13] . ∎

Finally we want to show that the spectrum of an ergodic Hamiltonian coincides with the support of the *density of states measure* $d\mathcal{N}$. This measure is defined by $\mathcal{N}(E) := \lim_{\Lambda\to\mathbf{R}^n} N_E(H_\Lambda{}^\omega)/|\Lambda|$, where $\Lambda \subset \mathbf{R}^n$ are, for example, cubes. $H_\Lambda{}^\omega$ is the Hamiltonian restricted to Λ with periodic boundary conditions and N_E is the number of eigenvalues smaller than E. The a.s. existence of the limit and the independence of V^ω was proven by BENDERSKII and PASTUR [6] for a large class of ergodic potentials; for a more general class cf. [23].

Theorem 2.5: i) *If V^ω is ergodic and $E \in \sigma(H^\omega)$ for a.e. V^ω, then $\mathcal{N}(E+\varepsilon) - \mathcal{N}(E-\varepsilon) > 0$ for every $\varepsilon > 0$.*

ii) *If the space dimension is 1 and $\mathcal{N}(E+\varepsilon) - \mathcal{N}(E-\varepsilon) > 0$ for every $\varepsilon > 0$, then $E \in \sigma(H^\omega)$ for a.e. V^ω.*

Proof: i) Choose $\{V_k{}^i\}$ as in Theorem 2.1 and take for given $\delta > 0$ a sufficiently large $k \in \mathbf{N}$, such that there is a function $z(x) \in D_k$ and an index $i \in \mathbf{N}$ with $\|(-\Delta + V_k{}^i - E)\, z\| < \delta\, \|z\|$, $\nu(B_k{}^i) =: \nu_0 > 0$, where $B_k{}^i := \{V^\omega \mid \|V^\omega(x)|_{N_k} - V_k{}^i\|_p < \delta\}$. $\chi_k{}^i(V^\omega)$ denotes the characteristic function of $B_k{}^i$. The individual ergodic theorem [16: § 3.3] yields for a.e. $V^\omega \in \Omega$

$$\lim_{\Lambda\in\mathbf{R}^n} \int_\Lambda \chi_k{}^i\big(V^\omega(x-\bar{x})\big)\, d^n\bar{x}/|\Lambda| = \int_\Omega \chi_k{}^i\big(V^\omega(x)\big)\, d\nu(V^\omega) = \nu_0.$$

If $\|V^\omega(x-\bar{x})|_{N_k} - V_k{}^i(x)\| < \delta$, then $\bar{z} := z(x+\bar{x})$ fulfils

$$\|(H^\omega - E)\, \bar{z}\| \leqq \big\|\big(-\Delta + V_k{}^i(x)\big)\, z\big\| + \big\|\big(V^\omega(x-\bar{x}) - V_k{}^i(x)\big)\, z\big\| < \varepsilon\, \|z\|$$

for sufficiently small δ. For $|\bar{x} - \bar{\bar{x}}| \geqq 2kn^{1/2}$, $\bar{z}$ and $\bar{\bar{z}}$ have disjoint support. Thus $\mathcal{N}(E+\varepsilon) - \mathcal{N}(E-\varepsilon) \geqq (2kn^{1/2})^{-n}\, \nu_0$, since the number of eigenvalues of $H_\Lambda{}^\omega$ in $[E-\varepsilon; E+\varepsilon)$ is at least the number of $\bar{x} \in \Lambda$ with $V^\omega(x-\bar{x})|_{N_k} \in B_k{}^i$ and mutual distance at least $2kn^{1/2}$.

ii) For given $\varepsilon > 0$ choose Λ sufficiently large that $|N_{E+\varepsilon}(H_\Lambda{}^\omega) - N_{E-\varepsilon}(H_\Lambda{}^\omega)| \geqq 3$. $z_1, z_2, z_3 \in L^2[-l/2; l/2]$ are the corresponding eigenfunctions on $\Lambda = [-l/2; l/2]$. Define $z := \sum_{i=1}^{3} c_i z_i$, where $\{c_i\}$ is a nontrivial triple such that $z(-l/2) = z'(-l/2) = 0$. Since z fulfils periodic boundary conditions, it can be extended to the whole of $\mathbf{R}^1$ by $z(x) := 0$ for $|x| \geqq l/2$, and then $\|(H^\omega - E)\, z\| \leqq \varepsilon\, \|z\|$. Since ε was arbitrary, $E \in \sigma(H^\omega)$ ∎

Remark 2.6: It is easy to prove Theorem 2.5 ii) also for dimension $n > 1$ and almost periodic potential, random potential with occupation property (cf. § 3) or discrete models. In the first case one can use a theorem by MARCHENKO [30: Th. 2]. The condition $\mathcal{N}(E+\varepsilon) - \mathcal{N}(E-\varepsilon) > 0$ yields $E \in \sigma_\infty$ (in his notation) for an arbitrary set of parallelepipeda $\{\Omega_k\}$, if $|\Omega_k|/|\partial\Omega_k| \to \infty$ (under this condition $\mathcal{N}(E) = \lim_{\Omega_k\to\mathbf{R}^n} N_E(H_{\Omega_k})/|\Omega_k|$). But MARCHENKO showed how to choose Ω_k in order to ensure $\sigma_\infty = \sigma(H)$. In the second case the condition $\mathcal{N}(E+\varepsilon) - \mathcal{N}(E-\varepsilon) > 0$ also yields $E \in \overline{\bigcup_{\lambda'} \sigma(H_\Lambda{}^\omega)}$, and the occupation property states that for a.e. V^ω $\sigma(H^\omega) = \overline{\bigcup \sigma(H_\Lambda{}^\omega)}$. For discrete models the proof can be done as in one dimension: Choose Λ sufficiently large that $N_{E+\varepsilon}(H_\Lambda{}^\omega) - N_{E-\varepsilon}(H_\Lambda{}^\omega) \geqq |\partial\Lambda|$; $z_i \in L^2(\Lambda)$ are the eigenfunctions of $H_\Lambda{}^\omega$ with eigenvalues in $[E-\varepsilon; E+\varepsilon)$. Define $z := \sum_{i=1}^{|\partial\Lambda|} c_i z_i$, where $\{c_i\}$ is a nontrivial set of coefficients, such that $z(x) = 0$ for $x \in \Lambda$ with $\operatorname{dist}(x, \partial\Lambda) \leqq 1$ and continue as in the proof of Theorem 2.5 ii).

Pastur [31] proved the identity $\sigma(H^\omega) = \operatorname{supp} d\mathcal{N}$ for ergodic potentials, Avron and Simon [3] repreated Pastur's proof for almost periodic potentials in arbitrary dimension and Johnson and Moser [18] proved the same in one dimension by a completely other method.

3. Models with the Occupation Property

Let $a_1, \ldots, a_n$ be n independent vectors in $\mathbf{R}^n$ and V_i, $i \in \mathbf{N}$, real potentials in $\mathbf{R}^n$, such that there is a sequence $\{s_t\} \in l^1(\mathbf{Z}^n)$, such that for every $i \in \mathbf{N}$ and $t = (t_1, \ldots, t_n) \in \mathbf{Z}^n$

$$\left(\int_{C_t} |V_i(x)|^p \, d^n x\right)^{1/p} \leqq s_t,$$

where $C_t := \{x \in \mathbf{R}^n \mid x = \sum x_j a_j,\ t_j \leqq x_j < t_j + 1\}$ are the shifted basis cells and p as in § 2. Further let $[\mathbf{N}^{\mathbf{Z}^n}, B^{\mathbf{Z}^n}, \mu]$ be the measure space describing the random occupation of the lattice points by different types of atoms. Then $V^\omega(x) := \sum_{t \in \mathbf{Z}^n} V_{\omega_t}(x - \sum t_j a_j)$ is the potential of an alloy with countable many components.

Definition 3.1: The measure space $[\mathbf{N}^{\mathbf{Z}^n}, \mu]$ possesses the *occupation property*, if for every finite subset $T \subset \mathbf{Z}^n$ and every $\tilde{\omega} \in \mathbf{N}^T$ and μ-a.e. $\omega \in \mathbf{N}^{\mathbf{Z}^n}$ there is a vector $t_0 \in \mathbf{Z}^n$, such that $\tilde{\omega}_{t-t_0} = \omega_t$ for every $t \in T$.

The occupation property was defined in [11]. It describes a natural property of substitutional alloys, generalizing the independent occupation of lattice points by different kinds of atoms. For example, all random models where the absence of the continuous part in the spectrum has been proved [15, 7, 10] can be regarded as substitutional alloys with the occupation property. We want to emphasize that also non-ergodic measures can possess the occupation property, for such an example (crystal growth process starting with a given configuration) cf. [11].

We denote with S the closure of the union of the spectra of all operators H^ω with periodic potential $V^\omega \in \Omega$. In [11, 12] the following theorem has already been announced.

Theorem 3.2: *For every $V^\omega \in \Omega$ $\sigma(H^\omega) \subset S$. If the occupation property is fulfilled then for a.e. $V^\omega \in \Omega$ $\sigma(H^\omega) = S$.*

Proof: The definition of the occupation property yields that every operator with periodic potential in Ω is infinitly representable in a.e. H^ω, i.e. $S \subset \sigma(H^\omega)$. We define H as the direct sum of all Hamiltonians H^ω with periodic potential in Ω. Then $\sigma(H) = S$. Secondly, every operator H^ω is infinitely representable in H, i.e. $\sigma(H^\omega) \subset S$ ∎

Remark 3.3: This proof is related to Kürsten's proof in [25]. Kirsch and Martinelli [22] found independently the same result for a much more restricted class of substitutional alloys; their proof is related to ours. After preparing a first version of our paper we realized that the idea of the proof is already contained in a paper by Lifshic [27]. He made the inclusion $\sigma(H^1) \cup \sigma(H^2) \subsetneq \sigma(H^\omega)$ plausible, where H^ω is the Hamiltonian of a binary alloy and H^1, H^2 are the Hamiltonians of the pure crystals with potential V_1 and V_2, resp. Not all physicists saw that his idea was correct independently of the dimension of the space [20]. The problem of determining the spectrum of a substitutional alloy is intimately connected with the Saxon-Hutner conjecture, which is correct only in some special cases; for an extensive discussion cf. [11].

Remark 3.4: Theorem 3.2 contradicts the general wisdom on energy gaps in alloys [4, 8, 9, 35, 38, 39]. "Bowing" is the notation for the effect that the width of the gaps is expected to be a nonlinear function of the concentration of the atomic types. Theorem 3.2 states that the width of the gaps is constant if the concentration of all components is nonzero and that it is not greater than the gap in every pure component. The seeming difference between Theorem 3.2 and the experiments may be explained by the existence of tail functions in the density of states: The density of states decreases exponentially at the band edges, i.e. in those parts of the spectrum where Theorem 3.2 predicts a positive density and the experiments do not show it [27].

PURKERT and VOM SCHEIDT [32] proved that the differences of eigenvalues of the "averaged" Schrödinger equation on a compact set can differ from the mean value of the differences of the eigenvalues of the random Schrödinger operator. But the interpretation of their result as a proof for the bowing effect is very questionable:

i) The width of the gaps in the spectrum of an averaged Schrödinger operator (the so-called "virtual crystal approximation") depends nonlinearly on the concentration and the width of the gaps in an alloy spectrum is different from it. Thus it is not proven that the width of the gaps in the alloy spectrum depends nonlinearly on the concentration.

ii) PURKERT and VOM SCHEIDT investigated a Schrödinger operator on a finite interval with random potential and random boundary conditions. This model has no bands, but separated eigenvalues. In contrast to the models of Theorem 2.1, the spectrum depends on the individual potentials $V^\omega \in \Omega$.

Remark 3.5: In order to apply Theorem 3.2 to the models in [7; 10, 15] one has to explain how to treat an uncountable set of potentials $\{V_\alpha\}$. Because $L^p(C)$ (C is a basic cell) is separable one can choose a dense countable set $\{V_{\alpha_i}\} \subset \{V_\alpha\}$. Then the occupation property has the following form:

For every finite subset $T \subset \mathbf{Z}^n$, every $\varepsilon > 0$, every $\overline{\omega} \in \mathbf{N}^T$ and a.e. $V^\omega \in \Omega$ there is a vector $l \in \mathbf{Z}^n$, such that

$$\left\| \left(V^\omega(x - \sum l_j a_j) - \sum_{t \in T} V_{\alpha_{\overline{\omega}_t}}(x - \sum t_j a_j) \right)_{\big| \bigcup_{t \in T} C_t} \right\|_p < \varepsilon,$$

where C_t are the shifted basic cells. But we can more easily reproduce the statements in [10, 15] about the spectrum from Theorem 1.4 directly: E.g. for the model of [15] $\sigma(H^\omega) = \left[\inf_{t \in K} F(t); \infty\right)$ for a.e. V^ω, since $H := -d^2/dx^2 + \inf_{t \in K} F(t)$ is infinitely representable in a.e. $H^\omega \geqq H$. In addition, MOLCHANOV [40] used the occupation property in order to prove in a very tricky way the positivity of the Ljapunov exponent.

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REFERENCES

[1] AKHIESER, N. J., and J. M. GLAZMAN: Theory of linear operators in Hilbert space (russ.), vol. 2. Khark. Gos. Univ.: Kharkov 1978.

[2] AVRON, J., and B. SIMON: Almost Periodic Schrödinger Operators I. Commun. Math. Phys. 82 (1981), 101–120.

[3] AVRON, J., and B. SIMON: Almost Periodic Schrödinger Operators II. Duke Math. J. 50 (1983), 369–391.

[4] Baldereschi, A., and K. Maschke: Band structure of semiconductor alloys beyond the virtual crystal approximation. Solid State Commun. **16** (1975), 99–102.
[5] Bellissard, J.: Schrödinger operators with almost periodic potentials: an overview. In: Lecture Notes in Physics: Vol. 153. Springer-Verlag: Berlin—Heidelberg—New York 1982, p. 356.
[6] Benderskii, M., and L. A. Pastur: On the spectrum of the one-dimensional Schrödinger equation with a random potential (russ.). Mat. Sbornik 82 (1970), 245–256.
[7] Bentosela, F., Carmona, R., Duclos, P., Simon, B., Souillard, B., and R. Weder: Schrödinger operators with electric field and random or deterministic potential. Commun. Math. Phys. 88 (1983), 367–397.
[8] Berolo, O., Woolley, J. C., and J. A. van Vechten: Effect of Disorder on the Conduction Band Effective Mass, Valence-Band Spin-Orbit Splitting and the Direct Band Gap in III–V Alloys. Phys. Rev. **B 8** (1973), 3794–3798.
[9] Cardona, M.: Optical Properties of the Silver and Cuprous Halides. Phys. Rev. **129** (1963), 69–78.
[10] Delyon, F., Kunz, H., and B. Souillard: One-dimensional wave equations in disordered media. J. Phys. **A 16** (1983), 25–42.
[11] Englisch, H.: One-dimensional Schrödinger Operators with Ergodic Potential. Z. Anal. Anw. 2 (1983), 411–426.
[12] Englisch, H.: The spectrum of Schrödinger operators with ergodic potential. In: Ergodic Theory and Related Topics. Proc. Conf. Vitte/Hiddensee (GDR), October 19–23, 1981 (Ed.: H. Michel). Akademie-Verlag: Berlin 1982, pp. 49–52.
[13] Englisch, H., and R. Englisch: Hohenberg-Kohn-theorem and non-V-representable densities. Physica 121 A (1983) 253–268.
[14] Goldshade, I. Ya.: The structure of the spectrum of a random difference Schrödinger operator (russ.). Dokl. akad. nauk SSSR **31** (1976), 273–277.
[15] Goldshade, I. Ya., Molchanov, S. A., and L. A. Pastur: A random one-dimensional Schrödinger operator has a pure point spectrum (russ.). Funkt. anal. i pril. **11** (1977), 1–10.
[16] Jacobs, K.: Neuere Methoden und Ergebnisse der Ergodentheorie. Springer-Verlag: Berlin—Göttingen—Heidelberg 1960.
[17] James, R. C.: Some self-dual properties of normed linear spaces. Ann. Math. Studies **69** (1972), 159–175.
[18] Johnson, R., and J. Moser: The Rotation Number for Almost Periodic Potentials. Commun. Math. Phys. **84** (1982), 403–438.
[19] Kato, T.: Perturbation theory for linear operators. Springer-Verlag: Berlin—Heidelberg—New York 1966.
[20] Kirkpatrick, S., Velicky, B., and H. Ehrenreich: Electronic Densities of States in the Coherent Potential Approximation, Appendix B. Phys. Rev. **B 1** (1970), 3250–3263.
[21] Kirsch, W., and F. Martinelli: On the ergodic properties of the spectrum of general random operators. J. reine angew. Math. **334** (1982), 141–156.
[22] Kirsch, W., and F. Martinelli: On the spectrum of Schrödinger operators with a random potential. Commun. Math. Phys. 85 (1982), 329–350.
[23] Kirsch, W., and F. Martinelli: On the density of states of Schrödinger operators with a random potential. J. Phys. **A 15** (1982), 2139–2156.
[24] Kunz, H., and B. Souillard: Sur le spectre des opérateurs aux différences finies aléatoires. Commun. Math. Phys. 78 (1980), 201–246.
[25] Kürsten, K.-D.: Über zufällige Störungen der Basis der Exponentialfunktionen im Raum $L^2[-\pi,\pi]$. Z. Anal. Anw. **1**, (1982) 4, 31–36.
[26] Kürsten, K.-D.: Über das Spektrum von Schrödingeroperatoren mit formbeschränktem Potential. Wiss. Z. Karl-Marx-Univ. Leipzig, Math.-Naturwiss. R. **33** (1984) 56 bis 62.
[27] Lifshic, I. M.: On the structure of the energy spectrum and the quantum states of disordered condensed systems (russ.). Usp. fiz. nauk 83 (1964), 617–663.
[28] Lindenstrauss, J., and A. Pełczynski: Absolutely summing operators in L_p-spaces and their applications. Studia math. **29** (1968), 275–326.
[29] Lindenstrauss, J., and H. P. Rosenthal: The L_p-spaces. Israel J. Math. **7** (1969), 325–349.

[30] MARCHENKO, A. V.: On the approximation of the spectrum of an elliptic operator with almost periodic coefficients (russ.). Mat. zametki **25** (1979), 713–724.

[31] PASTUR, L. A.: Spectral Properties of Disordered Systems in the One-Body Approximation. Commun. Math. Phys. **75** (1980), 179–196.

[32] PURKERT, W., and J. VOM SCHEIDT: Stochastic eigenvalue problems for differential equations. Rept. math. Phys. **15** (1979), 205–227.

[33] REED, M., and B. SIMON: Methods of modern mathematical physics, vol. II. Academic Press: New York–San Francisco–London 1975.

[34] REED, M., and B. SIMON: Methods of modern mathematical physics, vol. IV. Academic Press: New York–San Francisco–London 1978.

[35a] SAKAI, S., and T. SUGANO: Theoretical Study on the Energy Band Structure of Ternary Alloy Semiconductors. J. fac. engineer. univ. Tokyo (B) **35** (1979), 259–311.

[35b] SCHULZE, K.-R., NEUMANN, H., and K. UNGER: Band Structure of $Ga_{1-x}In_xAs$. Phys. stat. sol. (b) **75** (1976), 493–500.

[36] SCHWARTZ, L.: Radon measures on arbitrary topological spaces and cylindrical measures. Oxford Univ. Press: London 1973.

[37] SIMON, B.: Almost periodic Schrödinger operators, a review. Adv. Appl. Math. **3** (1982), 463.

[38] STROUD, D.: Band Gaps of Semiconductor Alloys. Phys. Rev. **B 5**, (1972), 3366–3369.

[39] VAN VECHTEN, J. A., and T. K. BERGSTRESSER: Electronic Structure of Semiconductor Alloys. Phys. Rev. **B 1** (1970), 3351–3358.

[40] MOLCHANOV, S. A.: The structure of eigenfunctions of one-dimensional unordered structures (russ.). Izv. akad. nauk SSSR, ser. mat. **42** (1978), 70–103.

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