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One-dimensional Schrödinger Operators with Ergodic Potential

H. Englisch

Im ersten Teil der Arbeit werden die Ergebnisse von Luttinger und Dworin zu folgender Problemstellung von Saxon/Hutner verallgemeinert: Unter welchen Bedingungen gehört eine Energie E zur Resolventenmenge eines Mischkristallhamiltonians, vorausgesetzt, sie gehört zur Resolventenmenge der Hamiltonian aller reinen Komponenten. Symmetrische Potentiale spielen dabei eine besondere Rolle. Im dritten Teil wird die Grundzustandsenergie in Abhängigkeit vom ergodischen Potential V untersucht. Zum Vergleich werden Beispiele mit fastperiodischem Potential V angegeben. So wird Gordons Resultat zu Eigenwerten bei fastperodischem Potential im zweiten Teil verallgemeinert.

В первой части статьи обобщаются результаты Луттингера и Дворина к следующей проблеме Саксона и Хутнера: При каких условиях энергия E принадлежит резольвентному множеству гамильтониана кристалла смеси, если предполагается, что она принадлежит резольвентному множеству всех чистых компонент? При этом симметрические потенциалы играют особую роль. В третьей части исследуется основное состояние в зависимости от эргодического потенциала V. Для сравнения рассматриваются примеры с почти-периодическими потенциалами. При этом во второй части обобщается результат Гордона о собственных значениях при почти-периодическом потенциале.

In the first part of the paper the results of Luttinger and Dworin concerning the following problem of Saxon/Hutner are generalized: Which conditions guarantee that an energy value E lies in the resolvent set of the Hamiltonian for an alloy, presupposing that E lies in the resolvent set of the Hamiltonians of all pure components. Symmetric potentials play an particular role in this. In the third part the ground state energy is investigated for different types of the ergodic potential V. For comparison, examples with almost periodic potentials are given. E.g. Gordon's result concerning eigenvalues for almost periodic potentials is generalized in the second part.

1. Gaps in the spectrum of substitutional alloys

1.1. Reed/Simon [34: p. 360] present the following one-electron model for a binary alloy in one dimension: Let V_1, V_2 be two potentials on $[0; 1)$. Let ω denote a two sided sequence $\{\omega_n\}$, $n \in \mathbf{Z}$, of 1 and 2. Given ω, let V^ω be the function on $\mathbf{R}$ such that $V^\omega := V_1(x - n)$ on $[n; n + 1)$ if $\omega_n = 1$ and $V^\omega := V_2(x - n)$ on $[n; n + 1)$ if $\omega_n = 2$. Define $H^\omega := -d^2/dx^2 + V^\omega(x)$ as an operator on $L^2(\mathbf{R})$. Let p be the density of the second component in the alloy (with the potential V_2). On $\{1; 2\}^{\mathbf{Z}}$ put the product measure with $\mu(\{1\}) = 1 - p$, $\mu(\{2\}) = p$ on each factor.

Englisch/Kürsten [8] investigated the generalized model of an alloy with countably many components in $\mathbf{R}^n$, where the occupation of the lattice points by atoms need not be independent and the potential caused by one atom ranges over more than one basic cell:

Def. 1.2. Let $a_1, \ldots, a_n$ be n independent vectors in $\mathbf{R}^n$ (the physical case is $n = 3$) and V_i, $i \in N$, real potentials in $\mathbf{R}^n$ such that

$$\exists \{s_t\} \in l^1(\mathbf{Z}^n) \;\forall\, i \in \mathbf{N} \;\forall\, t = (t_1, \ldots, t_n) \in \mathbf{Z}^n : \left(\int\limits_{C_t} |V_i(x)|^p \, d^n x \right)^{1/p} \leqq s_t ,$$

where $C_t := \{x \in \mathbf{R}^n : x = \sum x_j a_j, \, t_j \leqq x_j < t_j + 1\}$ are the shifted basic cells and $p = 2$ for $n \leqq 3$, $p > 2$ for $n = 4$ and $p = n/2$ for $n \geqq 5$.

Further, $[\mathbf{N}^{\mathbf{Z}^n}, B^{\mathbf{Z}^n}, \mu)$ should be a measure space describing the random occupation of lattice points by different kinds of atoms. Let $V^\omega(x) := \sum\limits_{t \in \mathbf{Z}^n} V_{\omega_t}(x - \sum t_j a_j)$, then $H^\omega := -\triangle + V^\omega$ is the Hamiltonian of the alloy with countably many components.

In one dimension every type of atom, i, can possess a different lattice constant a_i, i.e. $V^\omega(x) := \sum\limits_{t \in \mathbf{Z}} V_{\omega_t}\left(x - \sum\limits_{s=1}^{t} a_{\omega_s}\right)$. The condition concerning the local L^p-norms now reads

$$\left(\int\limits_{[t;t+1)} |V_i(x)|^2 \, dx \right)^{1/2} \leqq s_t \cdot \min\{1; 1/a_i\} .$$

Def. 1.3. 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 $\omega_{t-t_0} = \tilde{\omega}_t$ for every $t \in T$.

Remark 1.4: This condition is fulfilled for example in the following cases:

a) The atoms occupy the lattice points independently (cf. 1.1).

b) For space dimension $n = 1$ the occupation is described by a Markov chain in which for sufficiently small $\varepsilon_i > 0$ and for all but finite transition matrices $P(t)$, $t \in \mathbf{Z}$, all matrix elements fulfil $p_{ij} \geqq \varepsilon_i$.

c) There is a finite set $T_0 \subset \mathbf{Z}^n$ and $\varepsilon_i > 0$ such that for every $t_0 \in \mathbf{Z}^n \setminus T_0$ and every finite set $T \subset \mathbf{Z}^n$ with $t_0 \notin T$ and every $\tilde{\omega} \in \mathbf{Z}^T$, the conditional probabilities fulfil $\mu\{\omega_{t_0} = i \mid \forall\, t \in T : \omega_t = \tilde{\omega}_t\} \geqq \varepsilon_i$; i.e. one can describe crystal growth processes starting from a given configuration on T_0.

d) 1.3 is equivalent to the condition that for μ-a.e. $\omega \in \mathbf{N}^{\mathbf{Z}^n}$, the hull

$$h(\omega) := w\text{—cl}\,\{\tilde{\omega} \mid \exists\, t_0 \in \mathbf{Z}^n \;\forall\, t \in \mathbf{Z}^n : \omega_t = \tilde{\omega}_{t-t_0}\}$$

is $\mathbf{N}^{\mathbf{Z}^n}$; i.e. μ-a.e. orbit (with respect to all shifts in $\mathbf{Z}^n$) is dense in $\mathbf{N}^{\mathbf{Z}^n}$. ($w$-cl denotes the weak closure; the weak topology in $\mathbf{N}^{\mathbf{Z}^n}$ is given by the generating system of open sets

$$\left\{ U_{(T,\tilde{\omega})} := \{\omega \in \mathbf{N}^{\mathbf{Z}} \mid \forall\, t \in T : \omega_t = \tilde{\omega}_t\} \mid T \subset \mathbf{Z}^n \text{ finite}, \; \tilde{\omega} \in \mathbf{N}^T \right\}.)$$

e) For measures μ, ergodic with respect to the translations in $\mathbf{Z}^n$, 1.3 is equivalent to the condition that every w-open set has a positive μ-measure.

1.5. Let us denote by S the union of all spectra $\sigma(H^\omega)$ of all operators H^ω with periodic potentials V^ω (i.e. there are n independent vectors $r_1, \ldots, r_n \in \mathbf{Z}^n$ with: $\forall\, i \in \{1, \ldots, n\} \;\forall\, t \in \mathbf{Z}^n \; \omega_t = \omega_{t+r_i}$), by $\bar{S}$ we denote the closure of S in the ordinary topology of $\mathbf{R}$. Then in [8] it was proved:

Theorem 1.6: a) *If an alloy satisfies the conditions of 1.2, then for each* $\omega \in \mathbf{N}^{\mathbf{Z}^n}$, $\sigma(H^\omega) \subseteqq \bar{S}$.

b) *If the occupation property also holds, then for* μ-a.e. $\omega \in \mathbf{N}^{\mathbf{Z}^n}$, $\sigma(H^\omega) = \bar{S}$.

Remark 1.7: The SAXON-HUTNER conjecture [37] states that for every ω $\sigma(H^\omega) \subseteqq \overline{\bigcup\limits_i \sigma(H^i)}$, where $H^i := -\triangle + \sum\limits_{t \in \mathbf{Z}^n} V_i(x - \sum t_j a_j)$ is the Hamiltonian of the periodic crystal formed only by V_i-potentials. Th. 1.6 shows that this conjecture cannot be true in general. The first counterexamples were given by JAMES/GINZBARG [20] and KERNER [22].

KIRSCH/MARTINELLI [24] found independently of us a result where the statement and the proof is closely related to Th. 1.6. The statement $\sigma(H^\omega) \supseteqq \overline{\bigcup_i \sigma(H^i)}$ is contained without rigorous proof in a paper of LIFSHITZ [28] and HORI [15], who announced it as a result of YOUNG/DWORIN.

In order to give a further characterization of $\bar{S}$, we recall the following results for Schrödinger operators with periodic potential from [34; Th. 13.89, 13.97, 13.100]:

Lemma 1.8: *Let V be a periodic potential whose Fourier series is in l^p with $p < (n-1)/(n-2)$ for $n > 3$ and $p = 2$ for $n \leqq 3$. Then $H := -\triangle + V$ has a pure absolutely continuous spectrum (we abbreviate it by $\sigma(H) = \sigma_{ac}(H)$). $\sigma(H) = \bigcup_{i\in\mathbb{N}} \bigcup_{\theta\in[0;2\pi)^n} E_i(H(\theta))$, where $H(\theta)$ is the operator $-\triangle + V$ restricted to the first basic cell with boundary conditions*

$$\varphi(x + a_j) = \exp(i\theta_j)\, \varphi(x), \qquad \partial\varphi(x + a_j)/\partial x_j = \exp(i\theta_j)\, \partial\varphi(x)/\partial x_j,$$
$$\theta_j \in [0; 2\pi), \qquad j \in \{1, \ldots, n\}$$

and E_i denotes the i^{th} eigenvalues. In one dimension we have

$$\sigma(-d^2/dx^2 + V) = \bigcup_{i\in\mathbb{N}} \left(\left[E_{2i-1}(H(0));\ E_{2i-1}(H(\pi))\right] \cup \left[E_{2i}(H(\pi));\ E_{2i}(H(0))\right]\right)$$

If V has the period a and y_0, y_1 are the solutions of the differential equation $(-d^2/dx^2 + V - E)\, y = 0$ with the initial conditions $y_0(0) = y_1'(0) = 1$, $y_0'(0) = y_1(0) = 0$, then the transition matrix $C(E)$ is defined by

$$C(E) := \begin{pmatrix} c_{11}(E) & c_{12}(E) \\ c_{21}(E) & c_{22}(E) \end{pmatrix} := \begin{pmatrix} y_0(a) & y_1(a) \\ y_0'(a) & y_1'(a) \end{pmatrix}.$$

Then $E \in \sigma(H)$ is equivalent to $|\mathrm{Tr}\, C(E)| \leqq 2$, where Tr denotes the trace, and then $\mathrm{Tr}\, C(E) = 2 \cdot \cos\theta(E)$.

Let us define

$$V_{\inf} := \inf_i V_i(x) \quad \text{and} \quad V_{\sup}(x) := \sup_i V_i(x)$$

and

$$H^{\inf/\sup} := -\triangle + \sum_{t\in\mathbb{Z}} V_{\inf/\sup}(x - \sum t_j a_j).$$

From Th. 1.6, Lemma 1.8 and the min–max principle we get immediately

Lemma 1.9: $\forall\, \omega \in \mathbb{N}^{\mathbb{Z}^n}$:

$$\sigma(H^\omega) \subseteqq \bigcup_i \left[\inf_\theta E_i(H^{\inf}(\theta));\ \sup_\theta E_i(H^{\sup}(\theta))\right].$$

The applicability of the min–max principle to the gap problem in alloys has already been seen by TAYLOR [42]; KIRSCH/MARTINELLI [24] have also used it.

Remark 1.10: If $V_{\inf}$ and $V_{\sup}$ are contained in $\{V_i\}$ (without loss of generality we assume $V_1 = V_{\inf}$ and $V_2 = V_{\sup}$) then one may conjecture that for μ-a.e. ω

$$\sigma(H^\omega) = \bigcup_i \left[\inf_\theta E_i(H^1(\theta));\ \sup_\theta E_i(H^2(\theta))\right].$$

The conjecture is based on the following interpolation argument (we take for simplicity the dimension of the space $n = 1$): By $V^{n,m}$ we denote the periodic potential with period $n+m$ consisting of n potentials V_1 and m potentials V_2; let $H^{n,m} := -d^2/dx^2 + V^{n,m}$. The min—max principle yields

$$E_{2i}\big(H^1(0)\big) = E_{2i(n+m)}\big(H^{n+m,0}(0)\big) \leqq E_{2i(n+m)}\big(H^{n,m}(0)\big) \leqq E_{2i(n+m)}\big(H^{n-1,m+1}(0)\big) \leqq E_{2i}\big(H^2(0)\big)$$

(for odd eigenvalues an analogous statement holds, beginning with $E_{2i+1}\big(H^1(0)\big) = E_{2i(n+m)+1}\big(H^{n+m,0}(0)\big)$.) For $(n+m) \to \infty$ the eigenvalues seem to fill the interval $\big[E_{2i}\big(H^1(0)\big); E_{2i}\big(H^2(0)\big)\big]$. But from $\big[E_i\big(H^1(0)\big); E_i\big(H^2(0)\big)\big] \subseteqq \sigma(H^\omega)$ would follow

$$\Big[\inf_\theta E_i\big(H^1(\theta)\big);\ \sup E_i\big(H^2(\theta)\big)\Big] \subseteqq \sigma(H^\omega),$$

since

$$\Big[\inf_\theta E_i\big(H^1(\theta)\big);\ E_i\big(H^1(0)\big)\Big] \quad \text{and} \quad \Big[E_i\big(H^2(0)\big);\ \sup_\theta E_i\big(H^2(\theta)\big)\Big]$$

lie in $\sigma(H^\omega)$ for μ-a.e. ω, if the occupation property holds. But in general the eigenvalues $E_{2i(n+m)}\big(H^{n,m}(0)\big)$ do not lie dense in the interval $\big[E_{2i}\big(H^1(0)\big); E_{2i}\big(H^2(0)\big)\big]$, as the following generalization of a result by Luttinger (cf. Remark 1.13) shows:

Theorem 1.11: *Let H^ω be Hamiltonians built up by potentials $V_i \in L^2[0; 1]$.*
a) *If the occupation property holds and*
aa) *there is an $i \in \mathbf{N}$, such that $|\mathrm{Tr}\, C_i(E)| \leqq 2$ or*
ab) *there is a $c \in \mathbf{R}$, such that for all $\varepsilon > 0$ there is an $i \in \mathbf{N}$, such that $V_i(x) \geqq c$ and $|\mathrm{Tr}\, C_i(E)| \leqq 2 + \varepsilon$,*

then $E \in \sigma(H^\omega)$ for μ-a.e. ω.

b) *If there is an $\varepsilon > 0$, such that for all $E' \in [E - \varepsilon; E + \varepsilon]$ there is a regular (2×2)-matrix X, such that for all $i \in \mathbf{N}$ $\bar{c}_{11}^i(E')\, \bar{c}_{22}^i(E') > 1$ and for all $i, j \in \mathbf{N}$ $\bar{c}_{11}^i(E')\, \bar{c}_{12}^i(E') \times \bar{c}_{11}^j(E')\, \bar{c}_{12}^j(E') > 0$, where $\bar{c}_{kl}^i$ are the matrix elements of $\bar{C}_i := X^{-1} C_i X$, then for every ω $E \notin \sigma(H)$.*

Proof: aa) is a direct conclusion of Th. 1.6 and Lemma 1.8.
ab) Now assume $|\mathrm{Tr}\, C_i| = 2 + \varepsilon$ with $\varepsilon < 1$. Then the absolute values of both eigenvalues $v_i^\pm$ of C_i, given by $|v_i^\pm| = (2+\varepsilon)/2 \pm \sqrt{(2+\varepsilon)^2/4 - 1}$, are smaller than $1 + 2\varepsilon^{1/2}$. But this means $|y_E(x)| \leqq K \cdot (1 + 2\varepsilon^{1/2})^{|x|}$ for an arbitrary solution of the differential equation $(H^i - E)\, y_E = 0$, where K depends on the initial conditions. Due to Šnol [11: § 54] this yields $\sigma(H^i) \cap [E - c_0\varepsilon^{1/2}; E + c_0\varepsilon^{1/2}) \neq \emptyset$ (c_0 depends only on c) and by Th. 1.6 $E \in \sigma(H^\omega)$ for μ-a.e. ω.
b) Define $\tilde{C}_i(E') := \mathrm{sign}\, \bar{c}_{11}^i(E') \cdot Y^{-1} \bar{C}_i(E')\, Y$ with $Y(E') := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ if $\bar{c}_{11}^i(E') \times \bar{c}_{12}^i(E') < 0$ and $Y(E') := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ elsewhere. Then $\tilde{C}_i(E')$ has only positive matrix elements. Thus also $\prod_{j=1}^k \tilde{C}_{i_j}(E')$ has for arbitrary $k \in \mathbf{N}$, $i_j \in \mathbf{N}$ only positive matrix elements. Since $\det \prod_{j=1}^k \tilde{C}_{i_j}(E') = \det \prod C_{i_j}(E') = 1$ this implies $2 < \mathrm{Tr} \prod_{j=1}^k \tilde{C}_{i_j}(E') = \mathrm{Tr}\, |\prod C_{i_j}(E')|$. Lemma 1.8 ensures that every $E' \in (E - \varepsilon; E + \varepsilon)$ lies in the resolvent set of every periodic Hamiltonian built up by V_i-potentials. Now we can apply Th. 1.6 ∎

Corollary 1.12: *Let H^ω be Hamiltonians built up by symmetric potentials V_i, $i \in \{1, \ldots, k\}$ with supports $[0; a_i]$ and symmetry axes $a_i/2$. If for every i $E \notin \sigma(H^i)$ and for every $i, j \in \{1, \ldots, k\}$ $c_{11}^i c_{12}^i c_{11}^j c_{12}^j > 0$, than $E \notin \sigma(H^\omega)$.*

Proof: The symmetry of V_i yields $c_{11}^i = c_{22}^i$ [19], i.e. $|\mathrm{Tr}\, C_i| > 2$ induces $c_{11}^i c_{12}^i > 1$ ∎

Remark 1.13: For $k = 2$ this corollary is implicitly contained in a paper by LUTTINGER [29]. His requirement

$$\operatorname{sign}(\lambda_1\lambda_2) := \operatorname{sign}\left(c_{12}^1 c_{12}^2/((1 + c_{11}^1)(1 + c_{11}^2))\right) = 1$$

is equivalent to $c_{11}^1 c_{12}^1 c_{11}^2 c_{12}^2 > 0$ because of $|c_{11}^i| > 1$. The condition $V_i(x) \geqq c$ in Th. 1.11ab) can be weakened, since SIMON [41] sharpened Šnol's result. The statement and proof of Th. 1.11b) is related to a paper by FURSTENBERG/KESTEN [10], who also regarded random products of matrices with positive elements.

Now we give a counterexample for the conjecture in 1.10: Take V symmetric with respect to the axis 1/2, supp $V \subseteqq [0; 1]$, such that $-d^2/dx^2 + \sum_{t \in Z} V(x - t)$ has a least 2 open gaps, e.g. the 1st and the 2nd gap. Then there are at least 2 indices $i, j \in \{1, 2, 3\}$ with $i < j$ and $c_{11}(E_i)\, c_{12}(E_i)\, c_{11}(E_j)\, c_{12}(E_j) > 0$, where $E_1 < E_1(0) < E_2 < E_2(0) < E_3 < E_3(0)$ is choosen in such a way that E_2, E_3 lie in a gap. Take $V_1 := V$ and $V_2 := V + E_j - E_i$. Then E_j does not lie in $\sigma(H^\omega)$ for any Hamiltonian describing an alloy with components V_1 and V_2, though $E_j \in \left[E_{j-1}^1(0); E_{j-1}^2(0)\right]$. For simplicity let us assume $i = 1, j = 2$. The last statement can be somewhat sharpened: $\left(E_1^1(\pi); \min\left(E_2^1(\pi), E_1^2(0)\right)\right) \cap \sigma(H^\omega) = \emptyset$. This is proved in the next lemma.

Lemma *1.14*: *If E, E' lie in the same gap of the operator $-d^2/dx^2 + V$ with V periodic and symmetric, then* $\operatorname{sign}\left(c_{11}(E)\, c_{12}(E)\right) = \operatorname{sign}\left(c_{11}(E')\, c_{12}(E')\right)$.

Proof: If E, E' lie in the same gap, then for every $E'' \in [E; E']$ $|c_{11}(E'')| > 1$ and $c_{12}(E'') \neq 0$. The continuity of $c_{11}(E'')$ and $c_{12}(E'')$ yields sign $c_{11}(E) =$ sign $c_{11}(E')$ and sign $c_{12}(E) =$ sign $c_{12}(E')$ ∎

Remark 1.15: Though it is not obvious, Th. 1.11b) is equivalent to the criteria of LEHMANN [26] and HORI/MATSUDA [16].

Cor. 1.12 is further equivalent to the criterium of TONG/TONG [44]. In order to demonstrate the equivalence, we begin with an explaination of the idea of Hori/Matsuda: They considered the action of the transition matrix C on the projective real line $\mathbf{R}$ (i.e. $-\infty$ is identified with ∞) $x/y \in \mathbf{R} \xrightarrow{C} (c_{11}x + c_{12}y)/(c_{21}x + c_{22}y) \in \mathbf{R}$. An interval of $\mathbf{R}$ (which is $\neq \mathbf{R}$, but which can contain the point ∞) is called a trapping region if all transition matrices map the interval into itself. The Hori-Matsuda-criterion states that the existence of trapping regions for all $E' \in [E - \varepsilon; E + \varepsilon]$, $\varepsilon > 0$ implies that E lies in a gap of the spectrum. (The original formulation [16] contained an unimportant oversight: The authors did not notice that the spectrum is a closed set: thus they allowed, for example, parabolic transformations.) With the help of Th. 1.6 and Lemma 1.8 it is easy to see that the criterion is correct: The transition matrix for an arbitrary periodic potential, formed by the given potentials, maps the trapping region — a compact set — into itself, i.e. this transformation possesses at least one fixed point. This implies that the absolute value of the trace of the unimodular transition matrix is not less than two.

As the next step we reformulate the Hori-Matsuda-criterion: A trapping region can only exist for $E' \in [E - \varepsilon; E + \varepsilon]$, if each transition matrix has two real eigenvalues. The eigenvalue with modulus greater (less) than 1 corresponds to a stable (unstable) fixed point ("sink" ("source") in the notation of [16]). A trapping region obviously exists if one can divide the projective line $\mathbf{R}$ into two intervals; one containing all stable fixed points, the other all unstable [16: Th. 2]. This last statement is the starting point for Lehmann and Tong/Tong: Both reformulated this condition in terms of some parameters of the transition matrix. For the case of symmetric potentials their conditions coincide with the Hori-Matsuda-criterion, for asymmetric only LEHMANN

[26: (7)] found an equivalent condition. Since Tong/Tong assume a particular division of $\mathbf{R}$, they got a weaker result than Hori/Matsuda or Lehmann. Though the articles [16, 26] are closely connected, LEHMANN [26; § 5] did not realize it.

The equivalence of the Hori-Matsuda-condition and ours can be seen in the following way. If all stable, but not unstable fixed points of the transition matrices C_i lie in an open interval J, then take that X which transforms $\mathbf{R}^+$ into J. The stable fixed points of $\bar{C}_i$ lie in $\mathbf{R}^+$, the unstable in $\mathbf{R}^-$. An explicit calculation shows that for all i the matrix elements of $\bar{C}_i$ have the same sign; i.e. 1.11b) is fulfilled.

Conservely, if all matrix elements of $\bar{C}_i$ are positive then the Frobenius-Perron theorem [34: p. 350] (or an inversion of the above mentioned explicit calculation) yields that all stable fixed points lie in $\mathbf{R}^+$, all unstable fixed points in $\mathbf{R}^-$. Thus the fixed points of C_i lie in $J := X\mathbf{R}^+$, the unstable in $\mathbf{R} \setminus J$. For practical use Th. 1.11b) is only convenient for the case where X is the unit matrix I. If the potentials are symmetric this choice yields a criterion (cf. 1.12) equivalent to the Hori-Matsuda criterion; but for asymmetric potentials Th. 1.11b) with $X = I$ is equivalent to the criterion by TONG/TONG [44], i.e. it is more restrictive than the Hori-Matsuda criterion.

Now we want to extend the Hori-Matsuda concept of a trapping region. But for practical calculations this concept is not so elegant as the original one: If for some $\varepsilon > 0$ and all $E' \in [E - \varepsilon; E + \varepsilon]$ there are k proper (i.e. $\neq \mathbf{R}$) intervals J_i of the projective line $\mathbf{R}$ such that every C_i maps $\bigcup_{i=1}^{k} J_i$ into one of these intervals, then E lies in a gap of the spectrum. The proof can be carried out in the same way as we sketched the proof for the original Hori-Matsuda criterion.

Corollary 1.16: *Let $V_a := a \cdot \delta(x - 1/2)$, where δ denotes the δ-distribution, $a \in [k^+; c] \cup [-c; k^-]$ with $k^- < 0$, $k^+ > 0$. If $E \notin \left(\sigma(H^{k^+}) \cup \sigma(H^{k^-})\right)$ and*
a) $E \geqq 0$ or
b) $E < 0$, $E \notin \sigma(H^{-c})$ *and* $c_{11}^{k} c_{11}^{-c} > 0$,
then $E \notin \sigma(H^\omega)$ for any H^ω built up by V_a-potentials.

Proof: These potentials do not satisfy the condition $V \in L^2(\mathbf{R})$, but they are form-bounded with respect to $-d^2/dx^2$ (cf. [8]). The condition $|a| \leqq c$ ensures the form-boundedness of V^ω; thus H^ω is self-adjoint. We explicitly calculate (cf. [6: (31)]) $c_{11}^a = \cos E^{1/2} + a(4E)^{-1/2} \sin E^{1/2}$ for $E \geqq 0$ and $c_{11}^a = \mathrm{ch}(-E)^{1/2} + a(-4E)^{-1/2} \times \mathrm{sh}\,(-E)^{1/2}$ for $E < 0$. Obviously the condition $|c_{11}^{k^+}| > 1$, $|c_{11}^{k^-}| > 1$ and $E \geqq 0$ or $|c_{11}^{-c}| > 1$ and $c_{11}^{k} c_{11}^{-c} > 0$ yields $|c_{11}^a| > 1$ for every $a \in [k^+; \infty) \cup (-c; k^-]$. LUTTINGER [29] proved that $c_{11}^a c_{12}^a$ has a sign independent of a if $|c_{11}^a| > 1$. Thus we can apply 1.11b), though the set of allowed a is uncountable: Approximate V^ω by random potentials formed by a countable set of V_a-potentials.

Remark 1.17: If all a are positive or negative then a shorter proof is possible with the help of 1.9 (cf. [24: Prop. 4.4]).

Corollary 1.18: *Let $V_a := k \cdot \delta(x)$ be potentials on the interval* $[0; a]$ (cf. 1.2) *with $a \in [a'; a' + b]$. If*
a) $E \geqq 0, l < 0, \exists n \in \mathbf{N}: n\pi - 2 \cdot \arctan\left(k(4E)^{-1/2}\right) < a'E^{1/2} < n\pi - bE^{1/2}$ *or*
b) $E \geqq 0, k \geqq 0, \exists n \in \mathbf{N}: n\pi < a'E^{1/2} < n\pi + 2 \cdot \arctan\left(k(4E)^{-1/2}\right) - bE^{1/2}$ *or*
c) $E < 0, k \geqq 0$ *or*
d) $E < 0,\ k < 0,\ a'(-E)^{1/2} > 2\mathrm{Arth}\left(-k(-4E)^{-1/2}\right)$ *for* $k(-4E)^{-1/2} > -1$ *or* $a'(-E)^{1/2} > 2\,\mathrm{Arcth}\left(-k(-4E)^{-1/2}\right)$ *for* $k(-4E)^{-1/2} < -1$
then $E \notin \sigma(H^\omega)$ for any H^ω built up by V_a-potentials.

Proof: The inequalities express that for $a \in [a'; a' + b]$ $|c_{11}^a| > 1$. BORLAND [3] has already proved that the conditions a) and b) are sufficient, and so we will only show it for d) in the case $-k(-4E)^{-1/2} > 1$ (the other calculations are similar). $\operatorname{ch}\left(a'(-E)^{1/2}\right) + k(-4E)^{-1/2} \operatorname{sh}\left(a'(-E)^{1/2}\right) < -1$ is equivalent to $(c^2 - 1)^{-1/2} \times \operatorname{ch}\left(a'(-E)^{1/2}\right) + c(c^2 - 1)^{-1/2} \operatorname{sh}\left(a'(-E)^{1/2}\right) < -(c^2 - 1)^{-1/2}$, where we have abbreviated $c := k(-4E)^{-1/2}$. $\operatorname{Arsh}\left((c^2 - 1)^{-1/2} - a'(-E)^{1/2}\right) < -\operatorname{Arsh}(c^2 - 1)^{-1/2}$; i.e. $a'(-E)^{1/2} > 2 \cdot \operatorname{Arsh}(c^2 - 1)^{-1/2} = 2 \cdot \operatorname{Arcth} - c$. Choose $X = I$. The transition matrix $C_{a'}$ for a $k \cdot \delta$-potential, surrounded symmetrically by two regions of length $a'/2$ of zero potential consists only of negative elements. Since an arbitrary random chain can be cut into pieces of $k \cdot \delta$-potential surrounded by zero potential of length $a'/2$ and of pure zero potential of arbitrary length, the condition of 1.11 b) is fulfilled: For negative energy the transiton matrix for a zero potential of arbitrary length consists only of positive matrix elements ∎

Remark 1.19: Since the method of HORI/MATSUDA [16] is nothing other than Borland's method [3] applied to general potentials, it is obvious that LEHMANN [26] must reproduce Borland's conditions for the potential of cor. 1.18. It seems that the explicit condition 1.18d) for $E < 0$ is new, but the qualitative behaviour (no condition for an upper limit of a) has been already given in LEHMANN [26]).

Remark 1.20: FRISCH/LLOYD [9] investigated the same model, where $a \in \mathbb{R}^+$ is Poisson-distributed. Since for μ — a.e. ω there are arbitrarily long intervals $J \subset \mathbb{R}$ with $V^\omega|_J = 0$, H^ω has no gaps for $E \geqq 0$. For $E < 0$ there are also no gaps: A set of random potentials generated by a poisson distribution possesses the occupation property. The ground state energies $E_1{}^a(0)$ depend continuously on a; i.e. for $k < 0$ $\operatorname{supp} E_1{}^a(0) = (-\infty; 0]$. Thus 1.6 yields $(-\infty; 0] \subsetneqq \sigma(H^\omega)$ for μ-a.e. ω and $k < 0$. For $k \geqq 0$ V^ω is positive; i.e. $E \notin \sigma(H^\omega)$ for $E < 0$.

Now we want to derive a conclusion from 1.12 for the ground state energy.

Corollary 1.21: *Let V_i by symmetric semibounded potentials with support* $[0; 1]$. *Then for every ω $\inf \sigma(H^\omega) \geqq \inf_i \inf \sigma(H^i)$. The equality holds for μ-a.e. ω if the occupation property holds.*

Proof: 1.6 yields that for a.e. ω $\inf \sigma(H^\omega) \leqq \inf_i \inf \sigma(H^i)$, if the occupation property holds. Now assume $E < \inf_i \inf \sigma(H^i)$. Choose $E_i < \inf_x V_i(x)$. If y_1 is the solution of $(H^i - E_i)\, y_1 = 0$, $y_1(0) = 0$, $y_1'(0) = 1$, then $y_1(x) > 0$ for all sufficiently small $x > 0$. But then $y_1''(x) = (V_i - E_i)\, y_1(x) > 0$; i.e. y_1' is increasing and this ensures $c_{12}(E_i) = y_1(1) > 0$. 1.14 ensures $c_{12}(E) > 0$. From $c_{11}\left(\inf \sigma(H^i)\right) = 1$ follows $c_{11}(E) > 0$. With the help of 1.12 we get $\inf \sigma(H^\omega) \geqq \inf_i \inf \sigma(H^i)$ for every ω ∎

Remark 1.22: For asymmetric potentials 1.21 does not hold: Take for example a positive function $y \in C^2[0; 1]$ with $y'(0) = y'(1) = 0$ and $y(0) \neq y(1)$. Define $v_1(x) := y''(x)/y(x)$ and $V_2(x) := V_1(1 - x)$; thus $\sigma(H^1) = \sigma(H^2)$. $w_1(x) := \sum_{i \in \mathbb{Z}} \left(y(1)/y(0)\right)^i y(x - i)$ is an everywhere positive, exponentially increasing or decreasing solution of $H^1 w_1 = 0$; i.e. $0 < \inf \sigma(H^1)$ by Sturm's oscillation theorem [4] and 1.8. Take $H^{12} := -d^2/dx^2 + \sum_{i \in \mathbb{Z}} \left(V_1(x - 2i) + V_2(x - 2i - 1)\right)$. Then $w(x) := \sum_{i \in \mathbb{Z}} \left(y(x - 2i) + y(-x - 2i)\right)$ is periodic, everywhere positive solution of $H^{12} w = 0$, i.e. $0 = \inf \sigma(H^{12}) \geqq \inf \sigma(H^\omega)$ for μ-a.e. ω (cf. 1.8). This example with $\inf \sigma(H^{12}) < \inf \sigma(H^i)$ seems to be connected with Luttinger's theorem on symmetric rearrangement (cf. [39: Th. 13.12]): Take $y := 1 + 3x^2/2 - x^3$. Then $y'(0) = y'(1) = 0$; $V_1 = y''/y$

is decreasing on $[0; 1]$ and $y > 0$ on the same interval. $V_{12}(x) := V_1(x) + V_2(x-1)$ with $V_2(x) := V_1(1-x)$ is the symmetrically rearranged potential of $V_{11}(x) := V_1(x) + V_1(x-1)$ on $L^2[0; 2]$ with $\inf \sigma(-d^2/dx^2 + V_{12}) < \inf \sigma(-d^2/dx^2 + V_{11})$, where the operators are taken with respect to periodic boundary conditions.

DWORIN [6] and MATSUDA [30] (cf. also MATSUDA/OKADA [31]) gave a condition for $E \notin \sigma(H^\omega)$, which cannot be derived from 1.11. Dworin's condition is not exact. We present it in a more general form which is compatible with the closedness of the spectrum.

Theorem **1.23:** *V_i should satisfy the conditions of 1.2 If there is an $\varepsilon > 0$, such that for all $E' \in [E-\varepsilon; E+\varepsilon]$ there is a regular (2×2)-matrix X, such that for all $i, j \in \mathbb{N}$*

$$|\bar{c}^i_{11}(E') + \bar{c}^j_{22}(E')\, \bar{c}^i_{12}(E')/\bar{c}^j_{12}(E')| \geqq 2$$

and

$$|\bar{c}^i_{22}(E') + \bar{c}^j_{11}(E')\, \bar{c}^i_{12}(E')/\bar{c}^j_{12}(E')| \geqq 2,$$

where $\bar{c}^i_{kl}$ are the matrix elements of $\bar{C}_i := X^{-1}C_iX$, then for every ω $E \notin \sigma(H^\omega)$.

Proof: Dworin showed that for large x these conditions imply the independence of the ratio $y'(x)/y(x)$ from the initial conditions in $x = 0$, where $y(x)$ is a solution of $H^\omega y = E'y$. (Dworin's remark that $y(m)/y(m-1)$ converges is wrong.) If a periodic potential has a transition matrix $C(E')$ with $|\mathrm{Tr}\, C(E')| < 2$, then $(H^\omega - E')\, y = 0$ has two independent solutions, y_+ and y_-, fulfilling some ± 0-boundary condition (cf. 1.8) and $y'(x)/y(x) = (c_+y_+' + c_-y_-')/(c_+y_+ + c_-y_-)$ also depends asymptotically on the initial conditions, i.e. on c_+/c_-. But if for all $E' \in [E-\varepsilon; E+\varepsilon]$ all periodic Hamiltonians H^ω have $|\mathrm{Tr}\, C(E')| \geqq 2$, then the analyticity and nonconstancy of $\mathrm{Tr}\, C(E')$ yields $|\mathrm{Tr}\, C(E')| > 2$ for $E' \in (E-\varepsilon; E+\varepsilon)$ and one can apply 1.6 and 1.8 ∎

If we put $X := I$ the resulting conditions of 1.23 are not symmetric. Thus one can formulate another simple set of sufficient conditions which are not equivalent to the above set for $X = I$. In contrast, the conditions of 1.11b) are symmetric for $X = I$, even when they do not seem to be symmetric: If $c^i_{11}c^i_{22} > 1$, then the independence of $c^i_{11}c^i_{12}$ from i with respect to the sign is equivalent to the independence of sign $(c^i_{11}c^i_{21})$, because $c^i_{12}c^i_{21} > 0$.

Corollary **1.24:** *If for every $i, j \in \mathbb{N}$ and every $E' \in [E-\varepsilon; E+\varepsilon]$ for some $\varepsilon > 0$,*

$$|c^i_{11}(E') + c^j_{22}(E')\, c^i_{21}(E')/c^j_{21}(E')| \geqq 2$$

and

$$|c^i_{22}(E') + c^j_{11}(E')\, c^i_{21}(E')/c^j_{21}(E')| \geqq 2,$$

then $E \notin \sigma(H^\omega)$ for very ω.

Proof: Put $X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ ∎

Remark **1.25:** With the help of [30: 3.27] it is easy to verify that Matsuda's condition [30: 6.9] is equivalent to Dworin's condition [6: 28]. In MATSUDA/OKADA [31] this condition was derived once more; now they used a convergence theorem for continued fractions as Dworin did.

The original formulation [6, 30] corresponds to the choice $X = I$. Our formulation is indeed less restrictive, as the following example demonstrates: $C_1 := \begin{pmatrix} 2 & 3 \\ 1 & 2 \end{pmatrix}$ and

$C_2 := \begin{pmatrix} +5 & -24 \\ -1 & +5 \end{pmatrix}$ fulfil the conditions of cor 1.24, but not those of 1.23 with $X = I$. Dworin obtained Luttinger's result [29: cf. 1.16], but a weaker result than Borland [3: cf. 1.18]. Also our generalized version 1.23 of the Dworin-Matsuda criterion leads sometimes to more restricted results than Theorem 1.11b): Choose $C_a := \begin{pmatrix} \operatorname{ch} a & \operatorname{sh} a \\ \operatorname{sh} a & \operatorname{ch} a \end{pmatrix}$, $\varepsilon^{-1} > a > \varepsilon$. These matrices fulfil the conditions of 1.11b). But $\bar{c}_{12}^a = (x_{11}^2 - x_{12}^2)(\operatorname{sh} a)/\det X$ and the invariance of the trace yields $\bar{c}_{11}^a = \operatorname{ch} a + t \operatorname{sh} a$, $\bar{c}_{22}^a = \operatorname{ch} a - t \cdot \operatorname{sh} a$ with t depending on X. We find $|\bar{c}_{11}^a + \bar{c}_{22}^b \bar{c}_{12}^a / \bar{c}_{12}^b| = |\operatorname{ch} a + \operatorname{ch} b \cdot \operatorname{sh} a / \operatorname{sh} b| =: A_{a,b}$. Since $\lim_{a \to 0, b \to \infty} A_{a,b} = 1$ there is certainly a pair (a, b) such that (C_a, C_b) does not fulfil 1.23, if $\varepsilon > 0$ is sufficiently small.

Neither can 1.23 be derived from 1.11b): The above matrices, C_1, C_2 fulfil the conditions of 1.23, but not those of 1.11b): The stable fixed point $3^{1/2}$ of the transformation associated with C_1 lies between the unstable fixed point $24^{1/2}$ of C_2 and the unstable fixed point $-3^{1/2}$ of C_2.

From Lehmann's paper [26: explanation to fig. 2] one gets the impression that his criteria are necessary for the occurence of gaps. The above example shows that this is wrong. Further he wrote: "In jeder bezüglich der Zusammensetzung und der Anordnung der Potentiale beliebigen Legierung sind die Energiebereiche verboten, die auch in jeder aus den Komponenten dieser Legierung aufbaubaren binären Legierung verboten sind." ("In every arbitrary — with respect to the order of the potentials — alloy those energy regions are forbidden which are also forbidden in every binary alloy consisting of any two components of this alloy.") This statement is also incorrect, but one can modify it in order to get a correct statement:

An energy region is forbidden for an m-ary alloy, if for every two transition matrices the condition 1.11b) is satisfied. The proof is simple if we take the equivalent formulation of Hori/Matsuda [16]: If for every two matrices the two stable fixed points can be separated from the unstable, then this is also possible for the set of all fixed points. That Lehmann's statement quoted above is wrong we can see from the following counterexample: $A := \begin{pmatrix} 1/3 & 1 \\ 1 & 6 \end{pmatrix}$, $B_\varepsilon := \begin{pmatrix} 6 + 2\varepsilon & 1 \\ 1 + 2\varepsilon/2 & 1/3 \end{pmatrix}$, $C_\varepsilon := \begin{pmatrix} 2 & 1 \\ -9 - 2\varepsilon & -4 - \varepsilon \end{pmatrix}$. Then for sufficiently small $\varepsilon > 0$ any two arbitrary transition matrices belong to an energy gap of the coresponding binary alloy since (A, B_ε) fulfils the conditions of 1.11b) and both (A, C_ε) and $(B_\varepsilon, C_\varepsilon)$ fulfil those of 1.23 (with $X = I$) But for $\varepsilon = 0$ $\operatorname{Tr}(AB_0C_0) = 0$, the continuity yields that for sufficiently small ε $|\operatorname{Tr}(AB_\varepsilon C_\varepsilon)| < 2$; i.e. the alloy consisting of components with transition matrices A, B_ε and C_ε has for the same energy no gap.

Khomskii [23] showed that using Hadamard's theorem for the determinant of matrices one can sometimes get statements on gaps. He was able to reproduce the results of Luttinger and Borland (cf. 1.16 and 1.18). His method seems to be not as general as those used in 1.11b) or 1.23, since a difference equation must be derived from the differential equation, and it is not obvious how to do this for other cases than the one mentioned; the calculations in [23: § 7 + 8] use the special nature of the potential. On the other hand his method works for some discretisized models (e.g. tight-binding model) in 3 dimensions, where the methods based on the transition matrix break down, there being no useful analogy to the transition matrix for more than one dimension.

The papers of Tong/Tong [44] and Lehmann [26] contain conjectures concerning those energies which occur in a gap of at least one ordered alloy. A solution of this problem will be presented in a forthcoming paper [7].

2. Eigenvalues in the spectrum

2.1 While for potentials generated by diffusion processes a.e. solution of $(H^\omega - E)\,y = 0$ increases or decreases exponentially [32], one can give explicit counterexamples for an exponential behaviour in the model of an alloy: If for a fixed energy $E \in \left(\bigcap_i \sigma(H^i)\right)$ and an unimodular (2×2)-matrix C and every $i \in \mathbf{N}$ there is an exponent $p(i) \in \mathbf{R}$ with $|\mathrm{Tr}\, C| < 2$, $C_i(E) = C^{p(i)}$ (C_i is the transition matrix for the i^{th} component, cf. 1.8), then for every ω $(H^\omega - E)\,y = 0$ has only bounded solutions with $\limsup_{|x|\to\infty} |y(x)| \neq 0$. TONG [43] proved for a model with constant potential and random interspace between them that for a countable number of energies all transition matrices commute and thus not all solutions of the differential equation increase or decrease exponentially. A weaker result was rediscovered by DENBIGH/RIVIER [5], though they mention the review paper by ISHII [17], where Tong's result occurs. For an occupation of the lattice points given by an ergodic Markov process, a result of ROYER [35], VIRTSER [45] and GUIVARCH [14] yields that the spectrum has no absolutely continuous part.

2.2. The type of spectrum of H^ω does not only depend on the type of process giving the potentials, it also depends on the dimension of the space. For example, GOLDSHADE e.a. [12] proved for the one-dimensional Schrödinger equation with a particular random potential that $\sigma(H^\omega) = \sigma_p$ — the point spectrum — for a.e. ω, whereas one expects in higher dimensions that the absolutely continuous spectrum σ_{ac} is non-void. All known examples (cf. [8]) do not contradict the following conjecture: If the potential is given by a weakly mixing process (for definitions cf. [18]) then in 1 dimension $\sigma(H^\omega) = \sigma_{\mathrm{p}}$ for a.e. ω. Let us consider the mixing properties of the model for an alloy: The occupation given by an ergodic (with respect to $\mathbf{Z}^n$) Markov process is isomorphic to a Bernoulli shift (for definition cf. [33]), but the ergodic (with respect to $\mathbf{R}^n$) potentials of the alloy given by $\{\omega, \overline{\omega}\} \in \mathbf{N}^{\mathbf{Z}^n} \times [0;1)^n \to V^{\omega;\overline{\omega}}(x) := V^\omega(x - \sum \overline{\omega}_j a_j)$ are not weakly mixing with respect to all translations in $\mathbf{R}^n$.

The reverse of the above conjecture is certainly not true: SARNAK [36] has given examples of non-selfadjoint operators with almost periodic potential such that $\sigma(H) = \sigma_{\mathrm{p}}$. SCHARF [38: p. 595] has given a special class of examples of limit periodic potentials such that the Schrödinger operator has at least one eigenvalue. JOHNSON/MOSER [21] have constructed a special class of quasiperiodic potentials with the same property. GORDON [13] showed in an existency proof that for given frequencies there is a quasiperiodic potential possessing these frequencies and $\sigma_{\mathrm{p}}(-d^2/dx^2 + V) \neq \emptyset$. We will prove Gordon's statement for arbitrary dimensions in a constructive way. We found the examples independently of [13, 21, 38], but the example is very similar to that of [21].

Theorem 2.3: *Let G_i be arbitrary dense subgroups of* $\mathbf{R}$. *Then there is an almost periodic function V in $C(\mathbf{R}^n)$, having $G_1 \times \cdots \times G_n$ as frequency module, such that $-\triangle + V$ has at least one eigenvalue.* (For definitions cf. [40].)

Proof: Because of the density of G_i we can pick out a generating set $\{y_{k,i} \in G_i;\ k \in \mathbf{N}\}$ with $|y_{k,i} - k| < 1/2$. Let us inverstigate $f_i(x_i) := \sum_{k=2}^{\infty} \ln^{-2} k\left(-1 + \cos(x_i/y_{k,i})\right) \leqq 0$. For $|x| > 8$ we estimate

$$f_i(x) < \sum_{k=[|x|/2]}^{[|x|]} \ln^{-2} k\left(-1 + \cos(x/y_{k,i})\right)$$

$$< \left(-1 + \cos(10/(4 - 1/2))\right) \sum_{[|x|/2]}^{[|x|]} \ln^{-2} k < -c\,|x| \cdot \ln^{-2} |x|,$$

where $[x]$ denotes the entire part of x. Thus $\exp\left(\sum_{i=1}^{n} f_i(x_i)\right)$ is an eigenfunction for the operator $-\triangle + \sum_i \left(f_i'(x_i)^2 + f_i''(x_i)\right)$. But $V := f_i'(x_i)^2 + f_i''(x_i)$ is an almost periodic potential, because $f_i' = \sum_n - \sin(x_i/y_{n,i})/(y_{n,i} \ln^2 n)$ has an absolutely convergent Fourier decomposition, since $\sum_m^{\infty} n^{-1} \ln^{-2} n < c \cdot \ln^{-1} m$. f_i'' also has an absolutely convergent Fourier decomposition ∎

Remark 2.4: There is a conjecture, much stronger than 2.3: For some Hamiltonian H^ω with almost periodic potential $\sigma(H^\omega) = \sigma_p$ for a.e. ω [40]! Perhaps, in our example for V, the set of ω with $\sigma_p(-\triangle + V^\omega) \neq \emptyset$ (V^ω is from the hull of V; for definition cf. 1.4d) with $t, t_0 \in \mathbf{R}$) has measure 0.

On the other hand Molčanov and Pastur (private communication) emphasize that for the model of an alloy the singular continuous spectrum $\sigma_{sc}(H)$ (for definition cf. [40]) may be nonvoid for a.e. ω. If this happens this would be interesting in connection with the intuitive idea: "The greater the disorder, the greater the tendency to localization". Some random alloys seem to be less disordered than some almost periodic structures!

3. The dependence of the ground state energy on the coupling constant

3.1. In 2.2 we discussed the possibility to determine the type of the spectrum from the mixing properties of the process defining the potential. Kotani [25] poses another problem: to find a connection between mixing properties and the behaviour of the density of states $N(E)$ (for definition cf. [25]). He conjectures that strong mixing properties imply a strong increase of $N(E)$ near ess inf $V(x)$. He illustrates his conjecture with two examples: the periodic potential and potentials generated by a Poisson process. Further, he investigates 3 different types of potentials generated by a Poisson process, each with a different behaviour of $N(E)$ near ess inf $V(x)$, but it is not clear in which sense these 3 types have different mixing properties.

We wish to investigate the ground state energy in dependence on the mixing properties of the ergodic potential. The ground state energy is related to the density of states by $\inf_E \sigma(-\triangle + \lambda V) = \inf_E \operatorname{supp} N(E; -\triangle + \lambda V)$. More precisely, we investigate the limits $\lim_{\lambda\to 0} \inf \sigma(-\triangle + \lambda V)$ and $\lim_{\lambda\to\infty} \inf \sigma(-\triangle + \lambda V)$. The last expression gives no differentiation of the processes with different mixing properties; such a general result also holds for $\lim_{E\to\infty} N(E)$ [25, Th. 5].

Theorem 3.2: *Let* $V \in L^p_{\mathrm{loc}}(\mathbf{R}^n)$ *(uniformly!) with* $p = 2$ *for* $n \leqq 3$, $p > 2$ *for* $n = 4$ *and* $p = n/2$ *for* $n \geqq 5$. *Then* $\lim_{\lambda\to\infty} \lambda^{-1} \inf_E \sigma(-\triangle + \lambda V) = \operatorname{ess\,inf}_x V(x)$.

Proof: We denote $M_\varepsilon := \left\{\bar{x} \mid V(\bar{x}) \leqq \operatorname{ess\,inf}_x V(x) + \varepsilon\right\}$, i.e. $\mu(M_\varepsilon) > 0$, where μ is the Lebesgue measure in $\mathbf{R}^n$. Let us choose a set $B_{\delta,\varepsilon}$ depending on some δ with

a) $\mu(M_\varepsilon \triangle B_{\delta,\varepsilon}) < \delta$. (The symbol $\triangle$ denotes the symmetric difference of sets.)
b) $B_{\delta,\varepsilon}$ is an element of the algebra (not σ-algebra!) generated by the sets $\prod_i [a_i; b_i]$ with arbitrary $a_i, b_i \in \mathbf{R}$.

Because V lies uniformly locally in some L^p, V lies uniformly in L^1_{loc}, i.e. $\|V_{|B_{\delta,\varepsilon}\setminus M_\varepsilon}\|_1 < \varepsilon'$, where ε' depends on δ. Now take a bounded function $\psi_\varepsilon \in \operatorname{dom}(-\triangle)$ with

$\operatorname{supp}\psi_\varepsilon \subset B_{\delta,\varepsilon}$, $\|\psi_\varepsilon\|_2 = 1$ and $\|\psi_\varepsilon\|_\infty < \big(\mu(B_{\delta,\varepsilon}) - \delta\big)^{-1/2}$. Then

$$\begin{aligned}\operatorname{ess\,inf} V &\leqq \inf \sigma(-\triangle/\lambda + V) \leqq \langle\psi_\varepsilon, (-\triangle + \lambda V)\,\psi_\varepsilon\rangle/\lambda \\ &= \langle\psi_\varepsilon, -\triangle\psi_\varepsilon\rangle/\lambda + \langle\psi_\varepsilon, V\psi_\varepsilon\rangle \\ &\leqq c_\varepsilon/\lambda + (1-\varepsilon)\,(\operatorname{ess\,inf} V + \varepsilon) + \|\psi_\varepsilon\|_\infty\,\|V_{|B_{\delta,\varepsilon}\setminus M_\varepsilon}\|_1 \\ &\leqq c_\varepsilon/\lambda + (1-\varepsilon)\,(\operatorname{ess\,inf} V + \varepsilon) + \big(\mu(B_{\delta,\varepsilon}) - \delta\big)^{-1}\,\varepsilon'\end{aligned}$$

with an ε-dependent constant c_ε. Choose δ and thus ε' so small that $\big(\mu(B_{\delta,\varepsilon}) - \delta\big)^{-1}$ $H \times \varepsilon < \varepsilon$ ∎

Remark **3.3.**: Let us give the following generalization for the notion of the i^{th} eigenvalue E_i of an operator H [34: § 13]: $E_i := \inf\limits_{\mathscr{H}_i} \max\limits_{\psi\in\mathscr{H}_i} \langle\psi, H\psi\rangle$, where $\mathscr{H}_i \subset \mathscr{H}$ denotes an arbitrary i-dimensional subspace of the Hilbert space $\mathscr{H}$. Then the conditions of 3.2 imply a stronger conclusion: $\lim\limits_{\lambda\to\infty} \lambda^{-1}E_i(-\triangle + \lambda V) = \operatorname{ess\,inf}\limits_x V(x)$.

The proof of 3.2 has to be changed only slightly: Divide $B_{\delta,\varepsilon}$ into i sets $B^j_{\delta,\varepsilon}$, $j \in \{1, \ldots, i\}$, lying in the algebra generated by $\prod\,[a_i; b_i)$ and having equal measure. Take $\psi_\varepsilon{}^j \in \operatorname{dom}(-\triangle)$ with $\operatorname{supp}\psi_\varepsilon{}^j \in B^j_{\delta,\varepsilon}$, $\|\psi_\varepsilon{}^j\|_2 = 1$, $\|\psi_\varepsilon{}^j\|_\infty < \big(\mu(B^j_{\delta,\varepsilon}) - \delta\big)^{-1/2}$ and define $\mathscr{H}_i$ as the linear span of $\{\psi_\varepsilon{}^j\}$.

The proof of 3.2 is the joint work of the author and K.-D. Kürsten, the next theorem is the work of the author and M. Endrullis:

Theorem **3.4:** *Let V be a periodic potential in $L^p_{\text{loc}}(\mathbf{R}^n)$ with p as in 3.2 Let us assume that V is normalized, i.e. $\int\limits_{C_0} V(x)\,d^nx = 0$ (C_0 is the basic cell, cf. 1.2), and $V \not\equiv 0$. Then* $0 > \lim\limits_{\lambda\to 0} \inf\limits_E \sigma(-\triangle + \lambda V)/\lambda^2 > -\infty$.

Proof: The key of the proof is to show that perturbation theory is applicable. Ordinary perturbation theory works with isolated eigenvalues, but $-\triangle$ on $L^2(\mathbf{R}^n)$ does not have any eigenvalues. The infimum of the spectrum of $(-\triangle + \lambda V)$ regarded as an operator on $L^2(\mathbf{R}^n)$ is equal to the infimum of the spectrum of $(-\triangle + \lambda V)$ regarded as an operator on $L^2(C_0)$ with periodic boundary conditions. For $n = 1$ this result is contained in 1.8, for $n > 1$ it was mentioned in [2]. One can prove the case $n > 1$ analogously to that of $n = 1$, because the ground state of $-\Delta$ on $L^2(C_0)$ with periodic boundary conditions is a single eigenvalue (0) with strictly positive eigenvector (the constant), as an explicit calculation shows. Thus this operator generates a positivity improving semi-group [34: Th. 13.44]. Now $-\Delta$ has on $L^2(\mathbf{R}^n)$ a discrete spectrum and V is $(-\Delta)$-bounded, i.e. perturbation theory is directly applicable. The infimum of $\sigma(-\triangle + \lambda V)$ is thus an analytic function $E_1(\lambda)$ of λ: $E_1(\lambda) = E_1(0) + a_1\lambda + a_2\lambda^2 + \cdots$ with $E_1(0) = \inf\sigma(-\Delta) = 0$. The normalization of V yields $a_1 = 0$. Further $a_2 = -\sum\limits_{t\in\mathbf{Z}^n\setminus\{0\}} |\langle\psi_0, V\psi_t\rangle|^2/(E_t - E_0)$, where $\{\psi_t\}$ is an orthonormal basis of eigenvectors of $-\triangle$ regarded as an operator on $L^2(C_0)$ and E_t denotes the eigenvalue associated with ψ_t. Since ψ_0 is a constant, $\langle\psi_0, V\psi_t\rangle$ is proportional to $\tilde{V}_t$, the Fourier coefficients of V with respect to $\{\psi_t\}$. $V \not\equiv 0$ yields that at least one coefficient is not zero. Since V is normalized, this coefficient is not the coefficient V_0. Thus $a_2 = -c \sum\limits_{t\in\mathbf{Z}^n\setminus\{0\}} |\tilde{V}_t|^2/(E_t - E_0) < 0$ ∎

For almost periodic potentials the situation is more complicated. First we state the simple part, which holds for all ergodic potentials.

Lemma 3.5: *Let V^ω be and ergodic potential* (for def. cf. [18]) *uniformly in $L^p_{\mathrm{loc}}(\mathbf{R}^n)$ with p as in 3.2 Let us assume that a.e. V^ω is normalized, i.e.* $M(V^\omega) := \lim_{T\to\infty} (2T)^{-n} \int_{-T}^{T} \cdots \int_{-T}^{T} V^\omega(x)\, d^n x = 0$. *Then for every λ and a.e. ω* $\inf \sigma(-\triangle + \lambda V^\omega) \leqq 0$.

Remark 3.6. If V is not normalized, then put $\left(\inf \sigma(-\triangle + \lambda V) - \lambda M(V)\right)$ instead of $\left(\inf \sigma(-\triangle + \lambda V)\right)$ in 3.4 and 3.5.

Proof of 3.5: For arbitrary large R we choose a function $\psi_R \in \operatorname{dom}(-\triangle)$ by $\psi_R(x) := \begin{cases} 1 & |x| \leqq R \\ \varphi(|x| - R) \text{ for } & R < |x| < R+1, \\ 0 & |x| \geqq R+1 \end{cases}$ where $\varphi(x) \in C^2(\mathbf{R})$ is a function with $\varphi(x) = 1$ for $x \leqq 0$, $\varphi(x) = 0$ for $x \geqq 1$ and $\varphi(x) > 0$ elsewhere. Then $\inf \sigma(-\triangle + \lambda V^\omega) \leqq \lim_{R\to\infty} \langle \psi_R, (-\triangle + \lambda V^\omega)\psi_R\rangle / \langle \psi_R, \psi_R\rangle = 0$ because of the normalization of V^ω, $\langle \psi_R, -\triangle\psi_R\rangle$ increasing as R^{n-1}, and $\langle \psi_R, \psi_R\rangle$ increasing as R^n ∎

Theorem 3.7: a) *Let V_i be periodic potentials uniformly in $L^p_{\mathrm{loc}}(\mathbf{R}^n)$ with p as in 3.2, normalized* (cf. 3.4) *and not necesserily with the same periods. Then the almost periodic potential* $V_{\mathrm{ap}} := \sum^m V_i$ *satisfies* $\liminf_{\lambda\to 0} \sigma(-\triangle + \lambda V_{\mathrm{ap}})/\lambda^2 > -\infty$.

b) *There is for arbitrary $\varepsilon > 0$ a normalized almost periodic potential V_ε with*

$$\liminf_{\lambda\to 0} \sigma(-d^2/dx^2 + V_\varepsilon)/(\lambda\, |\log \lambda|^\varepsilon) < 0.$$

Proof: a) The inequality $\inf \sigma(A + B) \geqq \inf \sigma(A) + \inf \sigma(B)$ yields $\inf \sigma(-\triangle + \sum \lambda V_i) \geqq \sum \inf \sigma(-\triangle/m + \lambda V_i)$. Now we can apply 3.4.

b) Take $V := \sum_n - n^{-1-\varepsilon} \cos(x/2^n)$. Then we have for ψ_R of 3.5 and $\lambda > 0$ $\inf \sigma(H_\lambda) \leqq \langle \psi_R, H_\lambda \psi_R\rangle / \langle \psi_R, \psi_R\rangle \leqq \left(c_1 - \lambda \int_{-R}^{R} \sum n^{-1-\varepsilon} \cos(x/2^n)\right)(2R + c)^{-1} \leqq \left(c_1 - 2\lambda \sum 2^n n^{-1-\varepsilon} \times \sin(R/2^n)\right)/(2R + c)$. We put: $R = 2^m \pi$, where $m \in \mathbf{N}$ and $\lambda^{-2} < R \leqq 2\lambda^{-2}$. We find $\sum_{n=1}^{m} 2^n n^{-1-\varepsilon} \sin(2^m \pi/2^n) = 0$ and

$$\sum_{n=m+1}^{\infty} 2^n n^{-1-\varepsilon} \sin(R/2^n) > 2/\pi \sum_{n=m+1}^{\infty} R n^{-1-\varepsilon} > c_2 R m^{-\varepsilon} > c_3\, |\log \lambda|^\varepsilon/\lambda^2 .$$

The c_i denote some ε-dependent constants and H_λ denotes $-d^2/dx^2 + \lambda V_\varepsilon$. Finally $\inf \sigma(H_\lambda) < (c_1 - 2\lambda c_3\, |\log \lambda|^\varepsilon)/(4/\lambda^2 + c) \leqq c_4(-\lambda)\, |\log \lambda|^\varepsilon)$ ∎

Remark 3.8: Because of 3.5 $\inf \sigma(H_\lambda)$ is nonanalytic in $\lambda = 0$, i.e. we have a new behaviour in comparison with the periodic potential. It is easy to construct examples in more-dimensional spaces in the same manner.

Now we want to compare 3.7 b) with the potential generated by Markov processes (cf. [12]): For these latter potentials it holds that $\inf_E \sigma(H_\lambda{}^\omega) = \inf_x \left(\lambda V^\omega(x)\right)$ for a.e. V^ω. Obviously, in this case also $\inf \sigma(H_\lambda{}^\omega)$ is nonanalytic in $\lambda = 0$, but it is analytic elsewhere. Finally we get the behaviour of $\inf \sigma(H_\lambda{}^\omega)$ for the alloy (for def. cf. 1.2 and 1.3) from 1.21 and 3.4.

Lemma 3.9: a) *Let V_i be finitely many symmetric normalized potentials in $L^2[0; 1]$, which are bounded below, or*

b) *Let V_i be countably many potentials in $L^p(\mathbf{R}^n)$, satisfying* 1.2. *V_1 should be normalized* (cf. 3.5) *and for every $x \in \mathbf{R}^n$ and every $i \in \mathbf{N}$ $V_1(x) \leqq V_i(x)$.*

Then for a.e. ω and processes possessing the occupation property it holds that

$$0 > \liminf_{\lambda\to 0} \sigma(-\triangle + \lambda V^{\omega})/\lambda^2 > -\infty .$$

Proof: b) It is a conclusion of 1.6b), 1.9 and 3.4.

Remark **3.10:** For processes without the occupation property the inequality $\liminf_{\lambda\to 0} \sigma(-\triangle + \lambda V^{\omega})/\lambda^2 > -\infty$ remains true. The function $\inf \sigma(H_\lambda{}^{\omega})$ is analytic for real λ with the possible exception of the following set of points $\{\lambda \mid \exists\{i, j\} : i \neq j, \inf \sigma(H_\lambda{}^i) = \inf \sigma(H_\lambda{}^j)\}$ (for definition of H^i cf. 1.7), which has not points of accumulation. In case b) the ground state energy is analytic for every $\lambda > 0$. The statement of 3.9a) may be surprising because, it says that for some special alloys where the potential of each constituent is normalized have a behaviour of the ground state energy which seems to be typical for ordered (periodic) systems; whereas some almost periodic potentials show a behaviour which is typical for random systems (cf. 3.8). In the general case, where only the hole potential of the alloy is normalized, but not each single potential of the constituents, one has the behaviour of $\inf \sigma(H_\lambda{}^{\omega})$ near $\lambda = 0$ like in a random system. Because it is difficult to say in which sense an alloy where all single potentials are normalized is less random than an almost periodic potential, the following conjecture which is similar to Kotani's (3.1) or that of 2.3, does not make much sense: Strong mixing properties imply a strong decrease of $\inf \sigma(H_\lambda{}^{\omega})$ for λ near 0.

Remark to 2.4: Bellissard e.a. [46] proved the conjecture quoted at the beginning of 2.4.

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VERFASSER:

Dr. HARALD ENGLISCH
Sektion Mathematik der Karl-Marx-Universität Leipzig
DDR-7010 Leipzig, Karl-Marx-Platz 10