Commun. Math. Phys. 103, 167–176 (1986)

Communications in
Mathematical
Physics

Internal Lifschitz Singularities of Disordered Finite-Difference Schrödinger Operators

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Abstract. The integrated density of states has $\mathbf{C}^{\infty}$-like singularities, $\ln|k(E)-k(E_c)| = -|E-E_c|^{-\nu/2}\varphi_c(E)$, with $\varphi_c > 0$, a milder function at the edges of the spectral gaps which appear when the distribution function of the potential $d\mu$ has a sufficiently large gap. The behaviour of φ_c near E_c is determined by the local continuity properties of $d\mu$ near the relevant edge: $\varphi_c(E) = \mathcal{O}(1)$ if $d\mu$ has an atom and $\varphi_c = \mathcal{O}(\ln|E-E_c|)$ if μ is (absolutely) continuous and power bounded.

Introduction

Let $H_\omega = T + V_\omega$ be a tight-binding Schrödinger operator with disordered potential on $\mathbb{Z}^\nu$ (or an infinite sublattice of it):

$$(H_\omega f)(n) = \sum_m I(n-m)f(m) + V_\omega(n)f(n). \tag{1.1}$$

Here I has compact support and $V_\omega(n)$ are independent, identically distributed (iid) random variables. The (compact) support of their common distribution function $d\mu$ contains at least two points.

Such operators appear in many models for electrons in disordered systems either as finite difference approximations of Schrödinger operators or as restrictions of such operators to subspaces spanned by localized (atomic or Wannier) basis sets.

Let $\mathcal{N}(E, A)$ be the number of eigenvalues of the operator A which are less than E. The integrated density of states (IDS) for H may be defined by

$$k(E) = \lim_{\Lambda \uparrow \mathbb{Z}^\nu} |\Lambda|^{-1} \mathcal{N}(E, H_\omega^\Lambda), \tag{1.2}$$

where H_ω^Λ is a restriction of H to the compact $\Lambda \subset \mathbb{Z}^\nu$ and $|\Lambda|$ is the number of points in Λ.[1]

1 For Schrödinger operators on $\mathbb{R}^\nu$, $|\Lambda|$ is the Lebesgue measure of Λ

Under rather reasonable physical assumptions (ergodicity and exponential mixing for the process V_ω, see e.g. [7, 9, 13]) – which in our case are evidently true – the limit in Eq. (1.2) exists for a.e. ω and does not depend on ω, the sequence $\{\Lambda\}$ or the boundary conditions used to define H_ω^Λ.

For periodic operators $k(E)$ is piecewise $\mathbf{C}^\infty$ having algebraic singularities at the spectral (band) edges and at some internal points (van Hove singularities).

Much less is known in the disordered case. Intuitively one would expect the disorder to smoothen the singularities in $k(E)$. For absolutely continuous $d\mu$ Wegner [17] has shown that $k(E)$ is Lipschitz continuous. Craig and Simon [2] proved that $k(E)$ is log Hölder continuous for general μ. Recently Simon and Taylor [15] proved that $k \in \mathbf{C}^\infty$ for the one-dimensional Anderson model.

A nice physical argument by Lifschitz [8] predicts that near fluctuative spectral (band) edges, where only large-scale fluctuations of the potential, resembling ordered domains, contribute to $k(E)$, it has an essential singularity of C^∞ type:

$$\varrho(E) = \frac{dk}{dE}(E) \sim \exp[-|E-E_c|^{-\nu/2}\varphi_c(E)], \tag{1.3}$$

for $\operatorname{Sp} H_\omega \ni E \to E_c$, with $\varphi_c(E)$ a milder function.

Near the lowest edge of $\operatorname{Sp} H_\omega$, the IDS has been proven to have this Lifschitz behaviour for a large class of discrete [4, 11, 14] and continuum models [1, 3, 6] (see also references in [9] and [14]). For the Lorentz model of dilute, short-range scatterers several terms in the asymptotic expansion of $\varphi_c(E)$ were obtained [10].

In [11] φ_c was shown to be $\mathcal{O}(1)$ if $\mu[a] > 0$, where $a = \min \operatorname{supp} \mu$ and $\mathcal{O}(\ln|E-E_c|)$ if $\mu[a, a+\varepsilon] = \mathcal{O}(\varepsilon^\lambda)$, $\lambda > 0$, for $E \downarrow \min \operatorname{Sp} H_\omega$.[2]

For many physically interesting models $\operatorname{Sp} H_\omega$ has gaps. Lifschitz's arguments predict singularities of type Eq. (1.3) at the corresponding spectral edges.

The purpose of this paper is to prove that $k(E)$ has essential singularities of the Lifschitz type at the edges of the gaps which appear in $\operatorname{Sp} H_\omega$ if $\operatorname{supp} \mu$ has sufficiently large gaps.

Theorem 1.1 (Kunz and Souillard [7]). *Let $H_\omega = T + V_\omega$. Then, for a.e. ω,*

a) $$\operatorname{Sp} H_\omega \supset \operatorname{Sp} T + \operatorname{supp} \mu,$$

b) $$\operatorname{Sp} H_\omega \subset [\inf \operatorname{Sp} T, \sup \operatorname{Sp} T] + \operatorname{supp} \mu.$$

In this paper we shall consider only $T = T_0$, with T_0 the finite difference laplacian defined by Eq. (1.1), where

$$I(m) = \begin{cases} 2\nu J, & m = 0; \\ -J, & |m| = 1; \\ 0, & \text{otherwise}. \end{cases} \tag{1.4}$$

2 $f(x) = \mathcal{O}(g(x))$ as $x \to x_0$ is used in this paper as shorthand for $\exists C_1, C_2 \neq 0$, with $C_1 C_2 > 0$ such that $C_1 \leqq \liminf \frac{f(x)}{g(x)} \leqq \limsup \frac{f(x)}{g(x)} \leqq C_2$

Then, $\mathrm{Sp}\,T_0=[0,4\nu J]$ has no gaps and by Theorem 1.1

$$\mathrm{Sp}\,H_\omega=[\inf\mathrm{Sp}\,T_0,\ \sup\mathrm{Sp}\,T_0]+\mathrm{supp}\,\mu, \tag{1.5}$$

with probability one.

Let $\mathrm{supp}\,\mu=\cup[a_i,b_{i+1}]$, with $b_i<a_i\leqq b_{i+1}$. Let $\mathscr{C}=\{c;\,b_c+4\nu J<a_c\}$. Then $\bigcup\limits_{c\in\mathscr{C}}(b_c,a_c)$ belongs to the resolvent set of H_ω and these are the only gaps in its spectrum.

Definitions. 1. The pair E_c, x_c where $E_c=a_c$, $x_c=a_c$ or $E_c=b_c+4\nu J$, $x_c=b_c$; $c\in\mathscr{C}$ are a *spectral edge* of H_ω and the *associated edge of the measure* $d\mu$.

2. The edge is of *type A* if $\mu(x_c-\varepsilon,x_c+\varepsilon)=\mathcal{O}(\varepsilon^\lambda)$, $\lambda>0$ and of *type B* if $\mu[x_c]>0$.[3]

The main result of this paper is

Theorem 1.2. *Let $H_\omega=T_0+V_\omega$ be given by Eqs. (1.1) and (1.5); E_c and x_c a spectral edge and the associated edge of $d\mu$;*

Then, $k(E)$ has an essential singularity of Lifschitz type at E_c:

$$\ln|k(E)-k(E_c)|=-|E-E_c|^{-\nu/2}\varphi_c(E), \tag{1.6}$$

for $\mathrm{Sp}\,H_\omega\ni E\to E_c$. *Here φ_c is a milder function:*

$$\varphi_c(E)=\begin{cases}\mathcal{O}(\ln|E-E_c|), & x_c\in A;\\ \mathcal{O}(1), & x_c\in B;\end{cases}\qquad \mathrm{Sp}\,H_\omega\ni E\to E_c. \tag{1.7}$$

As a corollary to Theorem 1.2, a theorem proved by Kirsch and Martinelli [6] for a class of disordered Schrödinger operators and by Simon [14] for the Anderson model is generalized to the internal singularities:

Corollary 1.3. *In the assumptions of Theorem 1.2*

$$\lim_{\mathrm{Sp}\,H_\omega\ni E\to E_c}\frac{\ln|\ln|k(E)-k(E_c)||}{\ln|E-E_c|}=-\frac{\nu}{2}, \tag{1.8}$$

for all the spectral edges of H_ω.

Our basic tool is the following

Proposition 1.4. *Let $\mathbb{Z}^\nu(\mathbb{R}^\nu)$ be tiled with nonoverlapping congruent domains: $\mathbb{Z}^\nu(\mathbb{R}^\nu)=\bigcup\limits_\alpha \Lambda_\alpha$, $\Lambda_\alpha\cap\Lambda_\beta=\emptyset$, $\Lambda_\alpha=\Lambda+n_\alpha$, $n_\alpha\in\mathbb{Z}^\nu$.*

Let H_ω be bounded from above and below by direct sums of statistically independent domain Hamiltonians:

$$\bigoplus_\alpha H_\omega^{\Lambda_\alpha,L}\leqq H_\omega\leqq\bigoplus_\alpha H_\omega^{\Lambda_\alpha,U}. \tag{1.9}$$

Then,

$$|\Lambda|^{-1}\{\mathcal{N}(E,H_\omega^{\Lambda,U})\}_{\mathrm{av}}\leqq k(E)\leqq|\Lambda|^{-1}\{\mathcal{N}(E,H_\omega^{\Lambda,L})\}_{\mathrm{av}}, \tag{1.10}$$

where $\{\circ\}_{\mathrm{av}}$ is the expectation value with respect to the ensemble of potentials $V_\omega(n)$.

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3 The edges of the *Anderson* model are of type *A*, while those of the *binary alloy* model are of type *B*

Proposition 1.4, together with a reasonable choice of approximating Hamiltonians allows the bounding of $k(E)$ to be reduced to estimating several eigenvalues of the approximating Hamiltonians which lie close to E.

This approach, which has been widely used for estimating $k(E)$ near the bottom of the spectrum [5, 6, 11, 14], is simpler and more general than the functional integration methods [1, 3, 4, 10], whose application requires quite specific (and irrelevant to leading order) assumptions on the analytic properties of the logarithm of the Laplace transform of $d\mu$.

2. Approximating Hamiltonians and Reduction to Lowest Edge

Let $\Lambda \subset \mathbb{Z}^\nu$ be a domain and $\partial\Lambda = \{n \in \Lambda, \exists m \in \mathbb{Z}^\nu \backslash \Lambda, |m-n|=1\}$ its frontier. We shall consider three types of boundary conditions defining restrictions of the operator T_0 to functions with $\operatorname{supp} f \subset \Lambda$.

a) $T_0^{\Lambda,P} = P_\Lambda T_0 P_\Lambda$, where the projection P_Λ is the characteristic function of Λ:

$$(T_0^{\Lambda,P} f)(n) = 2\nu J f(n) - J \sum_{\substack{|i|=1 \\ n+i \in \Lambda}} f(n+i)\,; \tag{2.1}$$

b) Dirichlet boundary conditions:

$$T_0^{\Lambda,D} = T_0^{\Lambda,P} + K_{\partial\Lambda}\,, \tag{2.2}$$

with

$$(K_{\partial\Lambda} f)(n) = \zeta(n) J f(n)\,, \tag{2.3}$$

where $\zeta(n)$ is the number of bonds between n and sites in $\mathbb{Z}^\nu \backslash \Lambda$. Evidently $\zeta(n)=0$, $n \notin \partial\Lambda$;

c) Neumann boundary conditions:

$$T_0^{\Lambda,N} = T_0^{\Lambda,P} - K_{\partial\Lambda}\,. \tag{2.4}$$

These operators satisfy the evident inequalities

$$0 \leqq T_0^{\Lambda,N} \leqq T_0^{\Lambda,P} \leqq T_0^{\Lambda,D} \leqq 4\nu J\,. \tag{2.5}$$

One may readily see [11, 14] that for any tiling of $\mathbb{Z}^\nu$,

$$\bigoplus_\alpha T_0^{\Lambda_\alpha,N} \leqq T_0 \leqq \bigoplus_\alpha T_0^{\Lambda_\alpha,D}\,. \tag{2.6}$$

Hence, adding the diagonal operator V_ω to Eq. (2.6) will yield approximating Hamiltonians for Proposition 1.4.

Remark. For general T, Eq. (1.1), the approximating Hamiltonians may be obtained by adding/subtracting to $\bigoplus_\alpha P_{\Lambda_\alpha} H_\omega P_{\Lambda_\alpha}$ the direct sum of $K_{\partial\Lambda_\alpha}$ with

$$(K_{\partial\Lambda} f)(n) = f(n) \sum_{m \in \mathbb{Z}^\nu \backslash \Lambda} |I(n-m)|\,.$$

An useful property of the restrictions of T_0 defined above is that subtracting one from $4\nu J$ yields another:

Lemma 2.1. *Let $H_\omega^{\Lambda,\circ}$, with $\circ = P, D, N$, be given by Eqs.* (2.1)–(2.4). *Then* $\forall x \in \mathbb{R}$,

$$H_\omega^{\Lambda,P} = x + 4\nu J - U^* H_{\omega x}^{\Lambda,P} U, \tag{2.7}$$

$$H_\omega^{\Lambda,D} = x + 4\nu J - U^* H_{\omega x}^{\Lambda,N} U, \tag{2.8}$$

where the unitary operator $(Uf)(n) = (-1)^{n_1 + \dots + n_\nu} f(n)$ *and*

$$V_{\omega x}(n) = x - V_\omega(n). \tag{2.9}$$

Proof. It is sufficient to note that the diagonal matrix elements of $H_\omega^{\Lambda,P}$ are equal to $2\nu J + V_\omega(n)$ and that U changes the signs of the off-diagonal ones. □

By the preceding lemma one needs to investigate only the edges of the lower component of $\mathrm{Sp}\, H_\omega$.

If $\mathrm{supp}\,\mu$ has a gap it is useful to partition Λ into a lower and an upper subdomain with respect to the values of $V_\omega(n)$.

Let $V_\omega(n) \in [a, b] \cup [c, d]$, $n \in \Lambda$, with $a \leqq b < c \leqq d$. Then

$$\Lambda = \mathscr{A}_{\Lambda\omega} \cup \mathscr{B}_{\Lambda\omega}, \tag{2.10}$$

$$\mathscr{A}_{\Lambda\omega} = \{n \in \Lambda,\ V_\omega(n) \in [a, b]\}, \qquad \mathscr{B}_{\Lambda\omega} = \Lambda \backslash \mathscr{A}_{\Lambda\omega}. \tag{2.11}$$

The indices of $\mathscr{A}$, $\mathscr{B}$ will be omitted whenever it does not lead to confusion.

Lemma 2.2. *Let* $\mathrm{supp}\,\mu \subset [a, b] \cup [c, d]$ *with* $\beta = b + 4\nu J < c$. *Let* $E \leqq \beta$ *and the domain* Λ *is partitioned into lower and upper domains, Eqs.* (2.10), (2.11). *Then a.e.*

$$\mathcal{N}(E, H_\omega^{\Lambda,D}) \geqq |\mathscr{A}| - \lim_{x \uparrow \infty} \mathcal{N}(\beta - E, H_{\tilde\omega}^{\Lambda,N}), \tag{2.12}$$

where

$$V_{\tilde\omega}(n) = \begin{cases} b - V_\omega(n), & n \in \mathscr{A}; \\ x, & n \in \mathscr{B}. \end{cases} \tag{2.13}$$

Proof. By the min-max principle the first $|\mathscr{A}|$ eigenvalues of $H_\omega^{\Lambda,D}$ are bounded from above by the eigenvalues of $P_{\mathscr{A}} H_\omega^{\Lambda,D} P_{\mathscr{A}}$.

Neglecting the other eigenvalues which are $\geqq c > \beta$,

$$\mathcal{N}(E, H_\omega^{\Lambda,D}) \geqq \mathcal{N}(E, P_{\mathscr{A}} H_\omega^{\Lambda,D} P_{\mathscr{A}}). \tag{2.14}$$

By Lemma 2.1 $P_{\mathscr{A}} H_\omega^{\Lambda,D} P_{\mathscr{A}}$ is unitarily equivalent to $\beta - P_{\mathscr{A}} H_{\omega b}^{\Lambda,N} P_{\mathscr{A}}$, defined by setting $x = b$ into Eq. (2.9), since $P_{\mathscr{A}}$ commutes with U.

The relation

$$\mathcal{N}(E, C) = \dim \mathscr{H} - \mathcal{N}(-E, -C), \tag{2.15}$$

is valid a.e.[4] for any Hermitian matrix C on a finite dimensional space $\mathscr{H}$.

Thus, from Eqs. (2.14), (2.15), and (2.7) follows a.e.

$$\mathcal{N}(E, H_\omega^{\Lambda,D}) \geqq |\mathscr{A}| - \mathcal{N}(\beta - E, P_{\mathscr{A}} H_{\omega b}^{\Lambda,N} P_{\mathscr{A}}). \tag{2.16}$$

4 Because $\mathcal{N}(E, \circ)$ is continuous from the left; redefining $\mathcal{N}$ at discontinuities to be half the sum of its left and right limits would eliminate this restriction, but we shall use the standard definition

To complete the proof we need the following lemma which is readily established by direct calculations:

Lemma 2.3. *Let* $\mathscr{A}\subset\Lambda\subset\mathbb{Z}^\nu$, $\mathscr{B}=\Lambda\backslash\mathscr{A}$, $H=T+V=H^*$, $(Vf)(n)=V(n)f(n)$, $V_x=P_\mathscr{A}VP_\mathscr{A}+xP_\mathscr{B}$. *Then* $\forall z\in\mathbb{C}$ *with* $\operatorname{Im}z\neq 0$,

$$\lim_{x\to\infty}(z-T-V_x)^{-1}=P_\mathscr{A}{}^\mathscr{H}[z\mathbb{1}_\mathscr{A}-P_\mathscr{A}HP_\mathscr{A}]^{-1}, \tag{2.17}$$

uniformly in the resolvent norm for z in compact sets with $\operatorname{Im}z\neq 0$.

The eigenvalues of $P_\mathscr{A}H_{\omega b}^{\Lambda,N}P_\mathscr{A}$ are given by the poles of its resolvent in $\mathscr{A}$. Since the restriction does not depend on $P_\mathscr{B}V_{\omega b}P_\mathscr{B}$, one may replace $V_{\omega b}$ by Eq. (2.13).
Analytic continuation of Eq. (2.17), together with the fact that the other eigenvalues of $H_{\tilde\omega}^{\Lambda,N}$ go to $+\infty$ as $x\uparrow\infty$ completes the proof. □

Lemma 2.4. *In the assumptions of Lemma 2.2*

$$\mathscr{N}(E,H_\omega^{\Lambda,N})\leqq|\mathscr{A}|-\max\left[0,\lim_{x\uparrow\infty}\mathscr{N}(\beta-E,H_{\tilde\omega}^{\Lambda,D})-|\partial\mathscr{A}_1|\right], \tag{2.18}$$

where $\partial\mathscr{A}_1=\{n\in\partial\mathscr{A};\ \exists m\in\mathscr{B}=\Lambda\backslash\mathscr{A},\ |m-n|=1\}$ *and* $V_{\tilde\omega}$ *is given by Eq.* (2.13).

Proof. Let us uncouple $\mathscr{A}$ and $\mathscr{B}$ by inserting Neumann conditions at the broken bonds

$$H_\omega^{\Lambda,N}\geqq H_\omega^{\mathscr{A},N}\oplus H_\omega^{\mathscr{B},N}. \tag{2.19}$$

Since $\operatorname{Sp}H_\omega^{\mathscr{B},N}\geqq c>\beta$, for $E\leqq\beta$ only the eigenvalues of $H_\omega^{\mathscr{A},N}$ contribute. By the same arguments as in the proof of Lemma 2.2,

$$\mathscr{N}(E,H_\omega^{\Lambda,N})\leqq\mathscr{N}(E,H_\omega^{\mathscr{A},N})=|\mathscr{A}|-\mathscr{N}(\beta-E,H_{\omega b}^{\mathscr{A},D}). \tag{2.20}$$

Substituting $V_{\tilde\omega}$ in $H_{\omega b}^{\Lambda,D}$ and taking $x\uparrow\infty$ would yield $P_\mathscr{A}H_{\omega b}^{\Lambda,D}P_\mathscr{A}=H_{\omega b}^{\mathscr{A},P}+P_\mathscr{A}K_{\partial\Lambda}P_\mathscr{A}$ instead of the required $H_{\omega b}^{\mathscr{A},D}=H_{\omega b}^{\mathscr{A},P}+K_{\partial\Lambda}$.
The (diagonal) matrix element of their difference

$$K_1=K_{\partial\mathscr{A}}-P_\mathscr{A}K_{\partial\Lambda}P_\mathscr{A}\geqq 0, \tag{2.21}$$

are nonzero only on $\partial\mathscr{A}_1$ – the part of $\partial\mathscr{A}$ that has nearest neighbours in $\mathscr{B}\subset\Lambda$.
A rough estimate of the effect of this semipositive perturbation is

$$\mathscr{N}(E,P_\mathscr{A}H_{\tilde\omega}^{\Lambda,D}P_\mathscr{A})-\mathscr{N}(E,H_{\tilde\omega}^{\mathscr{A},D})\leqq\operatorname{rank}K_1=|\partial\mathscr{A}_1|. \tag{2.22}$$

Together with the obvious inequality $\mathscr{N}(E,\circ)\geqq 0$ this yields Eq. (2.18). □

Lemmas 2.1, 2.2, and 2.4 allow us to replace the estimates of $\mathscr{N}(E,\circ)$ in Proposition 1.4 for E near an arbitrary spectral edge E_c of H_ω by estimates of $\mathscr{N}(E,\circ)$ for some effective Hamiltonians near the bottom of their spectrum.

Using the estimates of [14] one could proceed to prove directly Corollary 1.3.

Since we want to prove the sharper estimates, Eq. (1.7), which show how the function φ_c depends on the local properties of $d\mu$ near the relevant edge, in the next section, which has some overlap with [11], some bounds on the lowest eigenvalues and $\mathscr{N}(E,\circ)$ near the bottom of the spectrum are given.

3. Estimates for $\mathcal{N}(E, \circ)$ and the Lowest Eigenvalue

Lemma 3.1. *Let $H = T + V$, with $V(n) \geqq 0$ and the compact $\Lambda \subset \mathbb{Z}^\nu$. Let $\mathcal{A} = \{n \in \Lambda;\ V(n) = 0\}$, $\mathcal{B} = \Lambda \backslash \mathcal{A}$. Then*

a) $$\mathcal{N}(E, H^{\Lambda,D}) \geqq \max[0, \mathcal{N}(E, T^{\Lambda,D}) - |\mathcal{B}|]\,; \tag{3.1}$$

b) $$\mathcal{N}(E, H^{\Lambda,N}) \leqq \mathcal{N}(E, T^{\Lambda,N}) - \Theta[\lambda_1(H^{\Lambda,N}) - E]\Theta[E - \lambda_1(T^{\Lambda,N})]\,, \tag{3.2}$$

where $\lambda_1(\circ)$ is the lowest eigenvalue of $\circ$.

Proof. a) follows from the equivalent of Eq. (2.22) – a semipositive V may not push the n^{th} eigenvalue of $H^{\Lambda,D}$ beyond the $(n + \operatorname{rank} V)^{\text{th}}$ one of $T^{\Lambda,D}$. b) follows by taking $\lambda_i(H^{\Lambda,N}) \geqq \lambda_i(T^{\Lambda,N})$, $i \geqq 2$. □

To apply Eq. (3.2) we need a lower bound on $\lambda_1(H^{\Lambda,N})$. In the case of positive V it may be obtained from Thirring's inequality [16]. The following lemma will allow us to avoid taking the inverse of V.

Lemma 3.2. *Let $H = H_0 + V$; $H_0 \geqq 0$, $H_0\varphi = 0$, $\lambda_2(H_0) \geqq \lambda_2 > 0$; $V \geqq 0$. Then*

$$\lambda_1(H) \geqq W - \sqrt{W^2 - \lambda_2 \langle V \rangle}\,, \tag{3.3}$$

where $\langle \circ \rangle = (\circ \varphi, \varphi)$,

$$W = \frac{1}{2}\left(\lambda_2 + \frac{\langle V^2 \rangle}{\langle V \rangle}\right). \tag{3.4}$$

Proof. Let $\omega > 0$. Then $V + \omega > 0$ is invertible and applying Thirring's inequality to $(H_0 - \omega) + (V + \omega)$ yields

$$\lambda_1(H) \geqq -\omega + \min[\lambda_2, \langle (V + \omega)^{-1} \rangle^{-1}]\,. \tag{3.5}$$

The right-hand side of Eq. (3.5) is concave in ω. Therefore, it has an unique maximum for $\omega \geqq 0$. If $\lambda_2 > \langle V^{-1} \rangle^{-1}$ it is attained for ω_0 – the solution of

$$\lambda_2 \langle (V + \omega_0)^{-1} \rangle = 1\,.$$

Instead of solving this equation, let us substitute the inequality

$$\left\langle \frac{1}{V + \omega} \right\rangle = \frac{1}{\omega}\left[1 - \left\langle V^{1/2} \frac{1}{V + \omega} V^{1/2} \right\rangle\right] \leqq \frac{1}{\omega}\left[1 - \frac{\langle V \rangle^2}{\langle V^2 \rangle + \omega \langle V \rangle}\right] \tag{3.6}$$

into Eq. (3.5). Solving the quadratic equation for best ω yields Eq. (3.4). □

Remark. The bound (3.5) is expressed in terms of the same quantities as Temple's inequality, which does not require the (semi) positivity of V. If $\lambda_2 > \langle V^2 \rangle / \langle V \rangle > \langle V \rangle$, Temple's inequality gives

$$\lambda_1(H) \geqq \lambda_L \geqq \langle V \rangle - \frac{\langle V^2 \rangle - \langle V \rangle^2}{\lambda_2 - \langle V \rangle}\,. \tag{3.7}$$

For $\langle V \rangle < \lambda_2 < \langle V^2 \rangle / \langle V \rangle$ the right-hand side is negative although we know $\lambda_1(H) > 0$. One may improve this by considering $H \geqq H_0 + gV$, $0 \leqq g \leqq 1$, using Eq. (3.7) and choosing the best $g \leqq 1$. The resulting bound is still smaller than Eq. (3.4).

A similar approach may be used to worsen the Thirring bounds for several eigenvalues to obtain manageable equations for lower bounds from variational upper bounds when calculating $[PV^{-1}P]^{-1}$ is a difficult task but PVP and PV^2P are available [12].

4. Proof of Theorem 1.2

Using the lemmas in Sect. 2 near any spectral edge $k(E)$ is bracketed by expressions of type $\{|\mathscr{A}|+F\}_{\mathrm{av}}$, where $\{|\mathscr{A}|\}_{\mathrm{av}}$ is equal to the average number of sites having the values of the potential in the lower component of $\operatorname{supp}\mu$ – which is equal to $k(E_c)$ – and F involves bounds on $\mathscr{N}(E, H_{\mathrm{eff}})$ near the lowest spectral edge for an approximating Hamiltonian H_{eff}.

Thus we need to prove the estimates Eq. (1.7) only near the bottom of the spectrum.

A positive measure $d\mu$ may be arbitrarily well approximated by ladder measures – weighted sums of Dirac measures – which appear as the natural approximants. For our purposes two-step ladders (binary alloy model measures) will be sufficient.

Let $\mu(x)=\mu(-\infty, x)$, $\operatorname{supp}\mu\subset[a,b]$.

Definition. Let $\xi\in(a,b)$, $p=\mu[a,\xi)$, $q=1-p$. The measures β and γ defined by

$$\beta(x)=p\Theta(x-\xi)+q\Theta(x-b)\leqq\mu(x)\leqq p\Theta(x-a)+q\Theta(x-\xi)=\gamma(x)\,, \tag{4.1}$$

are a pair of *binary alloy measures bracketing* μ.

Remark. Proposition 1.4 remains valid if one replaces the averages over the ensemble generated by $\otimes d\mu$ by the average over the relevant binary alloy approximant: $\otimes d\beta$ for the upper bound and $\otimes d\gamma$ for the lower one.

Let $\Lambda=\{1,2,\dots,N\}^\nu$, a hypercube of side N. Then the eigenvalues of $T_0^{\Lambda,\circ}$ are given by

$$\lambda_{\mathbf{Q}}=4J\sum_{s=1}^{\nu}\sin^2\left(\frac{\pi Q_s}{2N}\right), \tag{4.2}$$

where $\mathbf{Q}=(Q_1,Q_2,\dots,Q_\nu)\in\{0,1,\dots,N-1\}^\nu$ for $\circ=N$ and $\mathbf{Q}\in\{1,2,\dots,N\}^\nu$ for $\circ=D$.

Substituting the inequality (3.1) into the lower bound in Proposition 1.4 and using the Remark above to replace $d\mu$ by $d\gamma$ one obtains by considering only the contributions of $\mathscr{A}$,

$$k(E)\geqq N^{-\nu}\{\max[0, N(E-\xi, T_0^{\Lambda,D})-|\mathscr{B}_\omega|]\}_{\mathrm{av}}\geqq N^{-\nu}p^{N^\nu}\Theta\left(E-\frac{\nu J\pi^2}{N^2}\right). \tag{4.3}$$

Choosing $N=1+\operatorname{Int}\sqrt{\nu J\pi^2/(E-\xi)}$, one may find a constant $C_1>0$, independent of p and E, such that for small enough $E-a>0$,

$$\ln k(E)\geqq C_1\max_{a<\xi<E}\frac{\ln p}{(E-\xi)^{\nu/2}}. \tag{4.4}$$

If the estimate followed from Lemma (2.4) the $|\partial\mathscr{A}_1|$ term which was to be subtracted from $\mathcal{N}(E, T_0^{A,D})$ is zero for the configuration $\Lambda=\mathscr{A}$, considered in the second inequality (4.3).

For measures of type (4.1) $V(n)$ may take only two values. In this case the bound (3.3) coincides with the best Thirring bound from Eq. (3.5):

$$\lambda_1(H_\omega^{A,N}) \geqq F(|\mathscr{B}|) = a + W - \sqrt{W^2 - \pi^2 J|\mathscr{B}|(\xi-a)/N^{2+\nu}}\,, \tag{4.5}$$

where

$$W = \frac{1}{2}\left(\xi - a + \frac{\pi^2 J}{N^2}\right), \tag{4.6}$$

and $|\mathscr{B}|$ is the number of sites with $V(n)=\xi>a$.

Then, for $N<\sqrt{\pi^2 J/(E-a)}$, Proposition 4.1 with Lemma 3.1b and Eq. (4.5) give, using again the Remark,

$$k(E) \leqq N^{-\nu} \sum_{m=0}^{M} C_{N^\nu}^m p^{N^\nu - m} q^m\,, \tag{4.7}$$

where $M=M(E,N)$ is the integer part of the solution of the equation

$$F(m)=E\,, \tag{4.8}$$

with F defined in Eq. (4.5).

If $M<qN^\nu$ the inequality (4.7) remains valid if the summation is replaced by M times the summand for $m=M$.

Let $x=MN^{-\nu}$. Taking the logarithm of Eq. (4.7) and using Stirling's formula for the factorials, one may find a constant $C_2>0$ independent of E, ξ, $p\xi$ such that for small enough ξ, $E-a<\xi-a$

$$\ln k(E) \leqq \frac{C_2}{(E-a)^{\nu/2}} \min_{\frac{E-a}{\xi-a}<x<q} S(x,\xi)\,. \tag{4.9}$$

Here

$$S(x,\xi) = \left[\frac{x(\xi-a)+a-E}{\xi-E}\right]^{\nu/2} \left[x\ln\frac{q}{x} + (1-x)\ln\frac{p}{1-x}\right]. \tag{4.10}$$

The optimization with respect to N was replaced by optimization with respect to x, using the solution of Eq. (4.8).

If the edge is of type B one may take $\xi\downarrow a$ in Eq. (4.4). Then $p=\mu[a]>0$ and the estimate (1.7 B) is true in the lim inf sense. For the upper bound let $E<a+\dfrac{1-\mu[a]}{2}(\xi_0-a)$, where $\xi_0=\max\mu^{-1}\left(\dfrac{1+\mu[a]}{2}\right)$. Then, $\limsup_{E\downarrow a} S[\tfrac{1}{2}(1-\mu[a]), \xi_0]$ is finite and negative and Eq. (1.7 B) is true also in the lim sup sense.

For an edge of type A, choose $\xi=(1-\chi)a+\chi E$, with $\chi\sim|\ln(E-a)|^{-1}$ for small enough E. Then, since for edges of type A $\ln p=\mathcal{O}(\ln(\xi-a))$, taking the lim inf as $E\downarrow a$ of Eq. (4.4) yields the lim inf half of Eq. (1.7 A).

Taking $x=\nu/(\nu+2)$ and $\xi=E+(E-a)|\ln(E-a)|$ in the bound (4.10) yields the remaining lim sup half of Eq. (1.7 A). □

The Corollary (1.3) follows now from Eq. (1.7) since

$$\lim_{\mathrm{Sp}\,H \ni E \to E_c} \ln|\varphi_c(E)/\ln|E-E_c|| = 0 .$$

Acknowledgement. I thank Prof. Barry Simon for his interest in this paper and for sending me some of his results prior to publication.

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Communicated by B. Simon

Received June 26, 1985; in revised form September 3, 1985