The band edges of a frustrated random Schrödinger operator

H Englisch† and A MacKinnon‡

† Naturwissenschaftlich-Theoretisches Zentrum der Karl-Marx-Universität, Leipzig, DDR-7010, German Democratic Republic
‡ Blackett Laboratory, Imperial College, London SW7 2BZ, UK

Abstract. A discrete Schrödinger operator with off-diagonal disorder is subject to the effects of frustration more usually associated with spin-glass theory. It is shown that the bands coincide with those of the corresponding ordered system, but Lifshitz tails occur at the band edges. On the contrary, the Saxon–Hutner conjecture and diagrammatic analysis would lead to misleading suggestions about the spectrum.

1. Introduction

A standard model in the theory of disordered solids is the Anderson model (Anderson 1958, Simon 1985) with diagonal disorder $V^\omega(n)$ as a tight-binding Hamiltonian

$$\mathbf{H}^\omega y(n) = -\sum_{j=1}^{d}[y(n+a_j) + y(n-a_j)] + V^\omega(n)y(n) \qquad n \in \mathbb{Z}^d \quad (1)$$

where n is a d-dimensional vector with integer components denoting a position on a lattice and $a_j \in \mathbb{Z}^d$ is the vector with 1 in the jth coordinate and 0 otherwise. V^ω denotes the random realisation of the potential.

Important questions concerning $\mathbf{H}^\omega$ are:

(i) Where is the spectrum (band and edges)?

(iii) How much spectrum is there (density of states)?

(iii) What kind of spectrum is there (localised or extended states)?

We consider the first two questions for the Hamiltonian with off-diagonal disorder

$$\mathbf{H}^\omega y(n) = -\sum_{j=1}^{d}\exp(i\theta_{n,j}^\omega)y(n+a_j) + \exp(i\theta_{n,-j}^\omega)y(n-a_j) \qquad (2)$$

with

$$\theta_{n,-j}^\omega = -\theta_{n-\delta_j,j}^\omega \qquad (2')$$

where condition (2′) guarantees the self-adjointness of the Hamiltonian. The ordered crystal with period 1 in every direction a_j fulfils the condition

$$\theta^\omega_{n,j} = \theta_j \qquad \theta_j = -\theta_{-j} \tag{3}$$

and has a spectrum which coincides with that of the standard case $\theta_1 = \ldots = \theta_d = 0$, namely the interval $[-2d, 2d]$. This follows from the gauge transformation for the generalised eigenfunctions $y(n) = x(n)\exp[-i(n_1\theta_1 + \ldots + n_d\theta_d)]$. For every random one-dimensional Hamiltonian (2) there also exists a gauge transformation which maps (2) onto the standard Hamiltonian with $\theta_1 = 0$. In that case the transformation becomes $y(n) = x(n)\exp[-i(\theta^\omega_{0,1} + \cdots + \theta^\omega_{n-1,1})]$. But for $d \geq 2$ and general random $\theta^\omega_{n,j}$ such a gauge transformation cannot be found due to frustration, a gauge-invariant notion from spin-glass theory (Toulouse 1977). Frustration in our problem means that for an elementary plaquette $(n, n + a_i, n + a_i + a_j, n + a_j)$ the sum

$$(\theta^\omega_{n,i} + \theta^\omega_{n+a_i,j} + \theta^\omega_{n+a_i+a_j,-i} + \theta^\omega_{n+a_j,-j})\bmod 2\pi \tag{4}$$

does not vanish. The consequences of this fact for the spectrum of (2) are discussed in section 4, whereas sections 2 and 3 are respectively devoted to the questions of where such a Hamiltonian arises and how one can get wrong suggestions about its spectrum.

At the end of the introduction the notion of off-diagonal disorder should be made more precise. The easiest assumption is that the random variable $\theta^\omega_{n,j}$ is independently and identically distributed for $j \in (1, \ldots, d)$. If, for example, $\theta^\omega_{n,j}$ can only take the values 0 and π then the resulting Hamiltonian looks very similar to the $\pm J$-spin-glass model (Toulouse 1977). But the assumption of an independent distribution is unnecessarily strong. The most natural physical condition is the ergodicity of the disorder, i.e. the indecomposability of the underlying spatial homogeneous probability measure (Endrullis and Englisch 1984, section 1). The ergodicity guarantees the self-averaging of such spectral quantities as the bands and the density of states. But, for example, periodic off-diagonal terms can be considered as given by a very special ergodic measure (Endrullis and Englisch, section 2.1). Since one expects that statements concerning the size of the bands and the behaviour of the density of states at the band edges only hold for typical disorder, ergodicity is too weak an assumption for our purposes. For simplicity we will consider in this paper only independent identically distributed disorder. With the notion of the occupation property (Englisch 1983) an extension of the results concerning the bands is easy. A more specialised model has already been treated, e.g., by Wegner (1980).

2. The origin of the model

The problem of frustration occurs in a remarkably large number of tight-binding Hamiltonians. Perhaps the simplest is the ordered two-dimensional (2D) triangular lattice. With all off-diagonal matrix elements between nearest neighbours equal to unity, the spectrum is the interval $[-3, 6]$, rather than $[-6, 6]$ as one might naïvely expect. In order to construct an eigenvector corresponding to -6 it would be necessary for it to change sign between each pair of neighbours; clearly impossible on a triangular lattice.

In fact the problem will occur on any lattice containing odd numbered rings of atoms, including all close-packed lattices. Another important class of solids subject to this form of frustration is formed by glasses and amorphous semiconductors.

Another source of frustration is due to magnetic fields, which are usually introduced into a tight-binding model through the Peierls (Luttinger 1951, Harper 1955) factor in which

$$V_{(m,n)(m',n')} \mapsto \begin{cases} V_0 & m = m', \; n = n' \pm 1 \\ V_0 \exp(\pm in e \Phi/\hbar) & m = m' \pm 1, \; n = n' \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

where (m, n) represent sites on a 2D square lattice and Φ is the magnetic flux in an elementary plaquette.

In an obvious generalisation (2) above, with random $\theta_{n,j}^{\omega}$, represents a system containing random magnetic fields, e.g. due to magnetic impurities.

A related system is one involving spin–orbit coupling (Jüngling and Oppermann 1980). In this case the off-diagonal matrix element in (2) maps onto a 2 × 2 matrix $V_{\sigma,\sigma'}$ which is subject to the constraint

$$V_{-\sigma,-\sigma'} = \sigma\sigma' V_{\sigma,\sigma'}^* \quad (6)$$

where (σ, σ') can take the values ± 1 only, and V^* represents the complex conjugate of V. The four spin states belonging to two neighbouring sites now form a frustrated plaquette for which the the sum of phases, defined in (4), is an odd multiple of π.

3. Misleading approaches

In an ordered but frustrated system, the impossibility of constructing an *antiferro-magnetic* state or anything approaching such a state implies that the spectrum is significantly narrower than the interval $\{-Z, Z\}$, where Z is the connectivity of the lattice. Is this also true for a glass or for a system frustrated due to off-diagonal disorder? In this paper we are concentrating on the latter case represented by (2). We believe, however, that the results are more general.

3.1. Diagrammatic analysis

The density of states can be investigated by studying the trace of the resolvent or Green function defined in terms of matrices $\mathbf{G}$ and $\mathbf{H}$ by

$$\mathbf{G}(z) = [z - \mathbf{H}^{\omega}]^{-1} \quad (7)$$

where $z = E + i\eta$. This can be expanded in the form

$$\mathbf{G}(z) = z^{-1} + z^{-1}\mathbf{H}^{\omega}\mathbf{G}(z) \quad (8a)$$

$$= z^{-1} + z^{-1}\mathbf{H}^{\omega}z^{-1} + z^{-1}\mathbf{H}^{\omega}z^{-1}\mathbf{H}^{\omega}z^{-1}$$

$$+ z^{-1}\mathbf{H}^{\omega}z^{-1}\mathbf{H}^{\omega}z^{-1}\mathbf{H}^{\omega}z^{-1} + \cdots \quad (8b)$$

$$\text{Tr}\,\mathbf{G}(z) = z^{-1}\sum_{n=0}^{\infty} z^{-n}\text{Tr}\,\{(\mathbf{H}^{\omega})^n\} \quad (8c)$$

which can be visualised as a sum over all possible walks around the lattice which return to their starting point.

Our Hamiltonian contains only off-diagonal matrix elements between nearest neighbours and these have the form $\exp(i\theta)$ uniformly distributed around the unit circle. In this case the only terms which survive averaging of (8c) are those which contain the product of each matrix element with its complex conjugate. This implies that each bond must be traversed in both directions or not at all. The simplest class of terms in (8c) which fulfil this condition are those which take N steps from the origin and then return along the same path. Note in particular that terms involving simple loops always average to zero.

Compare now the Bethe lattice (Bethe 1935) or Cayley tree (Cayley 1889) of the same coordination, $2d$, as the system we are considering. Since the Bethe lattice contains no rings of atoms, all the terms in (8b) must consist of contributions from bonds which are traversed in both directions. In fact for each term in the expansion for the Bethe lattice there is a corresponding term in the expansion of H^ω. We are thus in a position to carry out a partial summation of (8c) for this group of terms.

Using the renormalised perturbation expansion technique (Economou, 1983) the diagonal element of the Green function on a particular site of the Bethe lattice $G(z)$ can be written in terms of the truncated Green function $G'(z)$ on the neighbouring site. This is defined in terms of the series (8) above except that original site is excluded from all terms in the summation. Hence

$$G(z) = [z - 2dG'(z)]^{-1}. \tag{9}$$

Note however that if any single site is excluded from the sum then all sites beyond that site are also automatically excluded. Thus $G'(z)$ represents the Green function at the end of a tree from which a complete branch has been removed, so that the end site is $(2d - 1)$-fold coordinated whereas all other sites remain $2d$-fold coordinated. Equation (9) could be interpreted as describing the process of joining $2d$ truncated trees together to form a completely $2d$-fold coordinated tree.

In a similar way it is possible to join $(2d - 1)$ truncated trees together to form another truncated tree. In this case however the old and new trees will be identical since they are both infinite but truncated trees. Hence we can write

$$G'(z) = [z - (2d - 1)G'(z)]^{-1} \tag{10a}$$

$$= \frac{1}{2} \frac{z \pm \sqrt{z^2 - 4(2d - 1)}}{(2d - 1)} \tag{10b}$$

$$G(z) = -\frac{1}{2} \frac{(2d - 2)z - 2d[z^2 - 4(2d - 1)]^{1/2}}{z^2 - (2d)^2}. \tag{10c}$$

This approximation yields a spectrum in the interval $[-\sqrt{4(2d - 1)}, \sqrt{4(2d - 1)}]$ rather than $[-2d, 2d]$.

It remains to identify those terms in (8c) which are not included in the Bethe approximation. Such terms must depend on the ring structure of the lattice but still contain each step in both directions. On a square lattice the simplest such term has the form

$$0 \to 1 \to 2 \to 3 \to 0 \to 4 \to 5 \to 6 \to 0 \to 3 \to 2 \to 1 \to 0 \to 6 \to 5 \to 4 \to 0$$

which consists of a walk round the ring $0 \to 1 \to 2 \to 3 \to 0$ followed by the ring $0 \to 4 \to 5 \to 6 \to 0$. The first ring is then traversed in reverse followed by the

second ring again in reverse. This term arises in 16th order of the expansion (8c). At this order there are 48 such terms compared with 20 275 660 for the Bethe lattice. This latter figure was calculated by expanding (9) using the computer algebra system muMATH (Rich and Stoutmeyer 1982, Wooff and Hodgkinson 1987).

We may conclude therefore that the Bethe lattice represents a very good approximation for the behaviour of the density of states of H^ω. However, the terms we have identified which are not correctly taken into account may be associated with multiple scattering from small clusters. We should expect therefore that localised states will not be correctly reproduced.

3.2. The Saxon–Hutner conjecture

While the foregoing analysis suggests a band which is too small, the ideas presented now actually lead to the correct band, but to too large a density of states at the band edges.

The density of states $N(E)$ of periodic Hamiltonians at a band edge E_b has the form

$$N(E) \sim c_d m^{d/2} |E - E_b|^{-1+d/2} \tag{11}$$

where c_d is a dimension-dependent constant and m the effective mass, whereas typically disordered Hamiltonians have the Lifshitz asymptotics (Lifshitz 1965)

$$N(E) \sim \exp(-c|E - E_b|^{-d/2}). \tag{12}$$

Originally the Saxon–Hutner conjecture (Saxon and Hutner 1949) states that an energy lies in the gap of an alloy if it lies in a gap for all pure crystals built from the constituents of the alloy. It has been known for a long time that this conjecture is not generally true (cf Englisch 1983), the correct statement was given independently by Kirsch and Martinelli (1982) and by Englisch and Kürsten (1984) (we neglect the closure of the union of all $\sigma(H^{\omega\mathrm{per}})$):

$$E \notin \sigma(H^\omega) \qquad \text{iff for all } H^{\omega\mathrm{per}} \ E \notin \sigma(H^{\omega\mathrm{per}}) \tag{13}$$

where σ denotes the spectrum and $H^{\omega\mathrm{per}}$ is an arbitrary periodic realisation with periods which are multiples equivalent to that of the elementary cell. At first reading there may appear to be no difference between these two statements. The difference lies in the size of the periods: Saxon and Hutner consider only periodic realisations with a period coinciding with the elementary cell. It is possible for energy intervals to exist at which there are states in the alloy and only in some of the periodic realisations with larger period, but not in any of the periodic realisations with period being the elementary cell.

The Saxon–Hutner conjecture is connected with the density of states through the classification of the Soviet school (Lifshitz *et al* 1982) into fluctuating band edges with asymptotics (12) and stable band edges with asymptotics (11). The second case can also occur in random systems if the energy considered is a band edge for all periodic realisations of the disorder with arbitrary lengths of the periods.

We saw in the introduction that $-2d$ and $2d$ are the band edges for (2)+(3), i.e. crystals with period 1 in every direction a_j. Following the intuition of Lifshitz (1965) one could believe that (2) with random $\theta^\omega_{n,j}$ has a stable band edge with the asymptotics (11). But the counter-example in the next section shows that one cannot neglect periodic realisations with larger periods when differentiating between (11) and (12).

4. The bands and Lifshitz tails for frustrated Schrödinger operators

From relation (13) and the knowledge of the spectrum for (2)+(3), we can immediately conclude $[-2d, 2d] \in \sigma(\mathsf{H}^\omega)$ for random $\theta^\omega_{n,j}$. In order to prove

$$\sigma(\mathsf{H}^\omega) = [-2d, 2d] \tag{14}$$

we have to show the inverse conclusion:

Lemma.

$$-2d(\boldsymbol{y}^\dagger \boldsymbol{y}) \leq (\boldsymbol{y}^\dagger \mathsf{H}^\omega \boldsymbol{y}) \leq 2d(\boldsymbol{y}^\dagger \boldsymbol{y})$$

where $\boldsymbol{y}$ denotes a vector whose elements are $y(n)$ and $\boldsymbol{y}^\dagger$ is its Hermitian conjugate.

Proof. We only show the first inequality, the second follows from the first with the help of the transformation $y(n) = x(n)(-1)^{n_1 + \cdots + n_d}$:

$$
\begin{aligned}
-\boldsymbol{y}^\dagger \mathsf{H}^\omega \boldsymbol{y} &= \sum_n \sum_j \exp(\mathrm{i}\theta^\omega_{n,j}) y(n)^* y(n + a_j) + \exp(-\mathrm{i}\theta^\omega_{n,j}) y(n) y(n + a_j)^* \\
&\leq \sum_n 2d\, y(n)^* y(n) \\
&= 2d\boldsymbol{y}^\dagger \boldsymbol{y}
\end{aligned}
\tag{15}
$$

according to the inequality

$$ab + a^* b^* \leq |a|^2 + |b|^2. \tag{16}$$

In (16) we have an equality iff $a = b^*$. Therefore, in (15) the equality holds iff for all n and j

$$y(n + a_j) = y(n) \exp(-\mathrm{i}\theta^\omega_{n,j}). \tag{17}$$

Considering an elementary plaquette it is obvious that (17) cannot be satisfied simultaneously for all n and j if (4) differs from 0 for at least one triple (n, i, j).

Here we see that the analogy with the frustration in spin-glass theory is very tight. Frustration, in our framework, not only means the absence of a global gauge transformation, but also the impossibility of a simultaneous minimisation of all summands in an energy expression.

In order to prove in our model the lower bound for $N(E)$ in (12), one can follow the ideas of Simon (1985) by choosing boxes with nearly no frustration. We expect that the upper bound in (12) is also correct, though we cannot directly adopt the proof by Simon (1985). There a decrease of the potential leads to a decrease of $\boldsymbol{y}^\dagger \mathsf{H}^\omega \boldsymbol{y}$, whereas an increase of frustration tends to shrink the spectrum from both sides.

Let us consider for $d = 2$ the Hamiltonian (2) with

$$\theta^\omega_{n,1} = 0 \qquad \theta^\omega_{n,2} = \begin{cases} 0 & \text{for } n_1 \text{ even} \\ k & \text{for } n_1 \text{ odd} \end{cases} \qquad k \in [0, \pi]. \tag{18}$$

The direct integral decomposition given by Reed and Simon (1978, theorem 13.97) also applies to the case of operators with off-diagonal periodicity. The eigenvalue equation for (2) in the elementary cell $\{0, 1\} \times \{0\}$ with generalised periodic boundary conditions

$$y(n + 2a_1) = \exp(i\vartheta_1)y(n) \qquad y(n + a_2) = \exp(i\vartheta_2)y(n) \tag{19}$$

has the form

$$0 = \det \begin{pmatrix} -2\cos\vartheta_2 - E & -1 - \exp(i\vartheta_1) \\ -1 - \exp(-i\vartheta_1) & -2\cos(\vartheta_2 + k) - E \end{pmatrix}$$

$$= E^2 + 4\cos(\tfrac{1}{2}k)\cos(\vartheta_2 + \tfrac{1}{2}k)E + 4\cos^2(\tfrac{1}{2}k)\cos^2(\vartheta_2 + \tfrac{1}{2}k) \tag{20}$$

$$\quad - 4\sin^2(\tfrac{1}{2}k)\sin^2(\vartheta_2 + \tfrac{1}{2}k) - 2 - 2\cos\vartheta_1$$

$$E = -2\cos(\tfrac{1}{2}k)\cos(\vartheta_2 + \tfrac{1}{2}k) \pm \{4\sin^2(\tfrac{1}{2}k)[1 - \cos^2(\vartheta_2 + \tfrac{1}{2}k)] + 2 + 2\cos\vartheta_1\}^{1/2}.$$

The lower band edge is found for $\vartheta_1 = 0$ and a minus sign before the square root. The corresponding value for ϑ_2 is either given by $z = \cos(\vartheta_2 + \tfrac{1}{2}k) = 1$, i.e. by $\vartheta_2 = -\tfrac{1}{2}k$, or for an optimal $z \in (-1, 1)$ as the solution of the equation for the first derivative

$$dE/dz = -2\cos(\tfrac{1}{2}k) + 4\sin^2(\tfrac{1}{2}k)z[4 + 4\sin^2(\tfrac{1}{2}k)(1 - z^2)]^{-1/2} = 0 \tag{21}$$

i.e. for

$$k > 2\sin^{-1}\left(\frac{\sqrt{5}}{2} - \frac{1}{2}\right)^{1/2} \tag{22}$$

by

$$\vartheta_2 = -\tfrac{1}{2}k + \cos^{-1}[\sin^{-2}(\tfrac{1}{2}k) - \sin^2(\tfrac{1}{2}k)]^{1/2}. \tag{23}$$

The lower band edge E_1 for k contradicting (22) is

$$E_1 = -2\cos(\tfrac{1}{2}k) - 2 \tag{24}$$

and for k fulfilling (22)

$$E_1 = -2\frac{[1 + \sin^2(\tfrac{1}{2}k)]^{1/2}}{\sin\tfrac{1}{2}k}. \tag{25}$$

E_1 is an increasing function of k, the frustration according to formula (4). The upper band edge E_u equals $-E_1$, which follows either from a gauge transformation or directly from (15) with the plus sign before the root and with π added to the former ϑ_2. We restricted k to $[0, \pi]$ since for $k \in [\pi, 2\pi]$ the Hamiltonian is equivalent to that with $\tilde{k} = 2\pi - k$. For the maximal frustration $k = \pi$ the band is the minimal interval $[-2\sqrt{2}, 2\sqrt{2}]$, where we have at $E = 0$ a zero in the density of states. Remembering that for periodic Hamiltonians the density of states is proportional to the measure of the set $\{(\vartheta_1, \vartheta_2)\}$ with fixed E (Reed and Simon 1978, theorem 13.101) we get $E = 0$ only for $\vartheta_1 = \pi$ and $\vartheta_2 = \tfrac{1}{2}\pi$ in formula (14).

Let us finally mention that the band edge E_1 does not generally appear for periodic boundary conditions as in the familiar case of Schrödinger operators with periodic potential (cf Simon 1985, theorem 13.89e) for an argument which also applies to $d = 2$. Similar examples as (17) can also be treated for $d > 2$.

5. Conclusions

In analysing the properties of the frustrated Schrödinger operator represented by (2) we have derived two apparently contradictory conclusions.

(i) The density of states is very well represented by that of the Bethe Lattice which has band edges at $E = \pm 2\sqrt{2d-1}$.

(ii) The Saxon–Hutner conjecture and related arguments show that the rigorous bounds on the spectrum are at $E = \pm 2d$.

Except for the trivial case $d = 1$ the former argument gives a band which is too narrow.

The true form of the density of states is probably such that there is an apparent band edge, represented by a very rapid fall in the density of states, at $E \approx \pm 2\sqrt{2d-1}$ with a weak Lifshitz tail out to $E = \pm 2d$. Although we have studied a particular model we believe that this behaviour is a general property of frustrated random Hamiltonians.

Acknowledgments

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