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On thermodynamic observables and the Anderson model

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Abstract. A thermodynamic observable is approximately additive under the decomposition of the volume. This property is of particular relevance to disordered systems. If scaled by the size of the system (N) a thermodynamic observable converges with probability one to a non-random limit as $N \to \infty$ inasmuch as one may apply the ergodic theorem. We present a simple argument to prove that the density of states in the Anderson model is a thermodynamic observable. Both diagonal and off-diagonal disorder are discussed, and the relation to the replica method is indicated.

1. Thermodynamic observables

Randomness has added a new feature to the study of physical systems. Whereas a regular system gives rise to processes with reproducible answers, a random system has observables which vary when we go from one sample to another. More precisely, when we determine the outcomes α_i of a sequence of experiments on the observable A, we have in general $\alpha_i \neq \langle \alpha \rangle$. That is, the α_i differ from their mean value and we may get another answer if we go from α_i to α_{i+1}.

On the other hand some observables may become non-random as the size of the system goes to infinity ($N \to \infty$). These we call *self-averaging* observables. So A is a self-averaging observable if the difference between α_i and $\langle \alpha \rangle$ becomes arbitrarily small as $N \to \infty$. An example is provided by the free energy per site, $N^{-1} \ln Z_N$. See a previous paper (van Hemmen and Palmer 1982).

One may wonder, however, what is the mechanism behind self-averaging. In this paper we shall isolate a property which is common to most self-averaging observables: at 'minimal' cost we can break them up into many *independent* parts which have the same distribution as the original observable as $N \to \infty$. Such an observable we call *thermodynamic*. We express this more clearly below.

A thermodynamic observable, say W_N, is to be associated with the size N of the system. N may be the number of spins or, in the Anderson model, the number of lattice points contained in a certain volume. We imagine the system to be split up into many disjoint subsystems labelled by an index j and, for the moment, we fix the size M of each of the subsystems. Then W_N is approximately additive under the decomposition of the volume,

$$W_N = \sum_j W_M^{(j)} + R_N$$

where the $W_M^{(j)}$ are independent, identically distributed random variables and R_N is typically an error term which stems from neglecting the interaction *between* the

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subsystems; R_N is such that $N^{-1}R_N$ is small as M is large. We now send first N, then M to infinity. By the law of large numbers $N^{-1}W_N$ converges to a limit which does *not* depend on the specific random configuration one has taken and, hence, $N^{-1}W_N$ is self-averaging. In fact, the convergence is thermodynamic. The reader may consult van Hemmen and Palmer (1982) for a definition of this notion, which implies that the large-volume limit $N \to \infty$ and the replica limit $n \to 0$ may be interchanged. For the moment we need not be more precise since keeping in mind $N^{-1} \ln Z_N$ as a typical example suffices throughout what follows.

Recently (Pruisken and Schäfer 1981) the replica method was used to elucidate the localisation problem associated with the Anderson (1958) model. However, the validity of the replica method remains an open problem. It is therefore worthwhile to study the density of states in the Anderson model (prior to the localisation) and to show that it is a thermodynamic observable. This will be done in the present paper. In contrast to Pastur (1973) and Fukushima *et al* (1975) we can dispense with the restriction to diagonal disorder and are able to handle off-diagonal disorder as well. Moreover, the relation to the replica method becomes particularly transparent.

The key to our method is a peculiarity in a theorem of Ledermann (1944, see also van Hemmen and Vertogen 1975) which apparently has been overlooked up to now:

If in a Hermitian matrix the elements of p rows and their corresponding columns are modified *in any way whatever*, provided that the matrix remains Hermitian, the number of eigenvalues, which lie in any interval, cannot increase or decrease by more than $2p$.

In § 2 we define the Anderson model, formulate the main theorem, and prove it. As a simple corollary we obtain an explicit formula for the integrated density of states in § 3. A discussion is to be found in § 4.

2. The Anderson model

The Anderson model describes one electron hopping on a d-dimensional cubic lattice and experiencing the influence of a random potential V. Its Hamiltonian is given by

$$\mathcal{H} = -\Delta + V \tag{1}$$

where Δ is the discretised Laplacian

$$(-\Delta \boldsymbol{x})_i = (2d)x_i - \sum_{\langle i,j \rangle} x_j \tag{2}$$

describing the hopping from a site i to its nearest neighbours j. The operator $-\Delta$ is the lattice analogue of the kinetic energy. The randomness is contained in the potential V

$$(V\boldsymbol{x})_i = \xi_i x_i \tag{3}$$

i.e. there is only diagonal disorder. The ξ_i are independent, identically distributed random variables whose distribution need not be specified here. Note that the Hamiltonian $\mathcal{H}$ describes one particle only.

Theorem. Let Λ_N be a sequence of cubes of increasing volume which finally fill the whole space, let $\mathcal{H}_N$ be the restriction of $\mathcal{H}$ to Λ_N (supplied with some boundary condition), and let $\sigma(\mathcal{H}_N)$ denote the set of eigenvalues of $\mathcal{H}_N$. Then the integrated

density of states of $\mathcal{H}$

$$F(\lambda) = \lim_{N\to\infty} \frac{1}{N} \#\{\lambda_j \in \sigma(\mathcal{H}_N): \lambda_j \leq \lambda\} \equiv \lim_{N\to\infty} F_N(\lambda; \boldsymbol{\xi}) \tag{4}$$

exists and does not depend on $\boldsymbol{\xi}$ *with probability one.* Hence

$$F(\lambda) = \lim_{N\to\infty} \langle F_N(\lambda; \boldsymbol{\xi}) \rangle \tag{5}$$

where the angular brackets denote an average over the ξ_i. Furthermore, the convergence in (4) is *thermodynamic*, so that the replica limit $n \to 0$ and the large-volume limit $N \to \infty$ may be interchanged freely (van Hemmen and Palmer 1979, 1982).

For the proof of (4) and (5) we choose a sequence of cubes Λ_N of increasing size N. The side of a cube is taken to be km, so that $N = (km)^d$. We pick a specific configuration $\boldsymbol{\xi}$, fix λ, and associate $F_N(\lambda; \boldsymbol{\xi}) = N^{-1} \#\{\lambda_i \in \sigma(\mathcal{H}_N): \lambda_i \leq \lambda\}$ with $N^{-1} \ln Z_N$.

Suppose first that $d = 1$. Then $N = km$, and $\mathcal{H}_N$ is a matrix

$$\mathcal{H}_N = \begin{pmatrix}
\ddots & \ddots & \ddots & & & & & & \\
\ddots & -1 & 2+\xi_m & (-1) & & & & & \\
 & & (-1) & 2+\xi_{m+1} & -1 & & & & \\
 & & & -1 & \ddots & \ddots & & & \\
 & & & & \ddots & & -1 & & \\
 & & & & & -1 & 2+\xi_{2m} & (-1) & \\
 & & & & & & (-1) & 2+\xi_{2m+1} & -1 \\
 & & & & & & & -1 & \ddots
\end{pmatrix}$$

which we imagine to be split up into k blocks of size m. If the -1 outside the blocks (encircled in the diagram) were not there, then $\mathcal{H}_N$ would decompose into a direct sum of non-interacting Hamiltonians $\mathcal{H}_j$, which belong to *disjoint* regions, say Λ^j, $1 \leq j \leq k$, and the spectrum of $\mathcal{H}_N$ would be the union of the spectra of the $\mathcal{H}_j$, i.e.

$$\mathcal{H}_N = \bigoplus_{j=1}^{k} \mathcal{H}_j \Rightarrow \sigma(\mathcal{H}_N) = \bigcup_{j=1}^{k} \sigma(\mathcal{H}_j).$$

This decomposition may be obtained if we modify $\mathcal{H}_N$ by deleting the -1 outside the blocks. (In the case of periodic boundary conditions we also have to delete two matrix elements in the top right-hand and bottom left-hand corner.) Since we modify at most $(k+1)$ rows of the matrix $\mathcal{H}_N$ together with their corresponding columns, the number of eigenvalues less than or equal to λ cannot increase or decrease by more than $2(k+1)$ (Ledermann 1944; see also van Hemmen and Vertogen 1975, § 4). Moreover, the densities of states in the disjoint regions Λ^j correspond to *independent*, identically distributed random variables. With this idea in mind we turn to the general case and consider a subdivision of Λ_N into $K = k^d$ disjoint subcubes Λ^j of side m and $M = m^d$ sites each; $j = 1, \ldots, k^d$. We modify $\mathcal{H}_N$ at the borders of the subcubes so as to decompose it into k^d non-interacting Hamiltonians $\mathcal{H}(\Lambda^j)$. Using Ledermann's theorem we then find

$$F_N(\lambda; \boldsymbol{\xi}) = \frac{1}{k^d} \sum_{j=1}^{k^d} F_M(\lambda; \boldsymbol{\xi}_j) + \frac{1}{N} R_N \tag{6}$$

where ξ_j is ξ restricted to the subcube $\Lambda^j \subseteq \Lambda_N$ and R_N is a surface term; $N^{-1}R_N = O(m^{-1})$. Equation (6) may be compared with equation (9) of van Hemmen and Palmer (1982). The $F_M(\lambda; \xi_j)$, $1 \leq j \leq k^d$, are independent, identically distributed random variables. The theorem, including thermodynamic convergence, now follows by sending first K, thus N, and then M to infinity.

Two extensions deserve mention. First, *off*-diagonal disorder does not change the above argument. Second, for (4) and (5) to hold the stochastic variables ξ_i need not be independent. Instead of independence it would suffice to require that the process be homogeneous and ergodic (Walters 1975).

Except for the thermodynamic convergence, the theorem above was first proved by Pastur (1973) for the special case of the Schrödinger equation in $\mathbb{R}^3$; see also Fukushima *et al* (1975). Pastur's proof needs the Feynman–Kac formula and, therefore, cannot accommodate the case with off-diagonal disorder—in contrast to the present approach. We now want to obtain an explicit formula for $F(\lambda)$.

3. The density of states reconsidered

We need some definitions. Let $\mathbb{1}_{(-\infty,\lambda]}(x)$ be one for $-\infty < x \leq \lambda$, and zero for $x > \lambda$. Define the spectral family of $\mathcal{H}$ and $\mathcal{H}_N$ by

$$E_\lambda = \mathbb{1}_{(-\infty,\lambda]}(\mathcal{H}) \tag{7}$$

and

$$E_\lambda^N = \mathbb{1}_{(-\infty,\lambda]}(\mathcal{H}_N). \tag{8}$$

Both depend on the randomness, i.e. ξ. We have

$$\frac{1}{N} \operatorname{Tr} E_\lambda^N = \frac{1}{N} \sum_{\lambda_j \leq \lambda} 1 = F_N(\lambda; \xi). \tag{9}$$

The proposition below is also valid for off-diagonal disorder, but for the sake of definiteness we consider the Anderson model (1) and assume $|\xi_i| \leq B$.

Let the inner product $\Sigma_n \bar{f}_n g_n$ between two elements f and g of $l^2(\mathbb{Z}^d)$ be denoted by (f, g). Finally, let us write δ_j for the sequence on $\mathbb{Z}^d$ which is one at the site j and zero elsewhere. The δ_j form a complete orthonormal set.

Proposition. Let

$$F(\lambda) = \lim_{N \to \infty} \langle F_N(\lambda; \xi) \rangle. \tag{10}$$

Then

$$F(\lambda) = \langle (\delta_0, E_\lambda \delta_0) \rangle \tag{11}$$

at each λ at which F is continuous. As in (5), angular brackets denote an average over the randomness.

Before turning to the proof, I would like to give equations (10) and (11) some intuitive appeal. For a finite system ($N < \infty$) the density of states is given by

$$F_N(\lambda; \xi) = \frac{1}{N} \sum_{j \in \Lambda_N} (\delta_j, E_\lambda^N \delta_j)$$

which is equation (9) with N as the number of sites in Λ_N. As $N \to \infty$ we expect that $(\delta_j, E_\lambda^N \delta_j)$ approaches $(\delta_j, E_\lambda \delta_j)$, at least at all continuity points λ of E_λ, and thus

$$F(\lambda) = \lim_{N\to\infty} F_N(\lambda; \boldsymbol{\xi}) = \lim_{N\to\infty} \frac{1}{N} \sum_{j\in\Lambda_N} (\delta_j, E_\lambda \delta_j) = \langle (\delta_0, E_\lambda \delta_0) \rangle$$

by the ergodic theorem (Walters 1975). In this way we would have understood directly that the integrated density of states $F(\lambda)$ exists with probability one and does not depend on the specific random configuration $\boldsymbol{\xi}$. As a convenient by-product we should have obtained an explicit formula for F which relates it to the average of a quantity containing $\mathcal{H}$, the Hamiltonian of the *infinite* system. Such a representation may be of advantage in estimating $F(\lambda)$. However, though equation (11) is correct, the simplicity of the argument above is a bit specious. There is *no* uniform estimate of $|(\delta_j, E_\lambda^N \delta_j) - (\delta_j, E_\lambda \delta_j)|$ and thus we have to proceed more indirectly.

Since the integrated density of states is a thermodynamic observable (§ 2), the limit of $F_N(\lambda) \equiv \langle F_N(\lambda; \boldsymbol{\xi}) \rangle$ as $N \to \infty$, i.e. the function F, is well defined for any λ. Moreover $F(-\infty) = 0$, $F(+\infty) = 1$, and $\lambda_1 \leq \lambda_2$ implies

$$F(\lambda_1) = \lim_{N\to\infty} F_N(\lambda_1) \leq \lim_{N\to\infty} F_N(\lambda_2) = F(\lambda_2). \tag{12}$$

So F is the point-wise limit of a sequence of distribution functions (Ash 1972) and it would be a distribution function itself if it were right continuous. But it is continuous, except for at most countably many points where it may jump. There we modify F so as to be right continuous, and call the modification F_+. Then F_+ is a distribution function which is the limit of F_N at each λ at which F_+ is continuous (that is, equals F). Hence (Ash 1972, § 4.5.4)

$$\lim_{N\to\infty} \int_{-\infty}^{+\infty} f(\lambda)\, \mathrm{d}F_N(\lambda) = \int_{-\infty}^{+\infty} f(\lambda)\, \mathrm{d}F_+(\lambda) \tag{13}$$

for all bounded continuous f. To prove our proposition it suffices to prove equality of F_+ and $\langle (\delta_0, E_\lambda \delta_0) \rangle$, the latter also being a distribution function.

Let $l^2(\Lambda_N)$ be the set of all sequences with coordinates in Λ_N only; plainly $(g, g) < \infty$ for any g in $l^2(\Lambda_N)$. The trace on $l^2(\Lambda_N)$ may be written either as a sum over sites or as a sum over eigenstates of $\mathcal{H}_N$. Thus

$$\frac{1}{N} \sum_{j\in\Lambda_N} (\delta_j, \mathrm{e}^{\mathrm{i}t\mathcal{H}_N} \delta_j) = \frac{1}{N} \operatorname{Tr} \mathrm{e}^{\mathrm{i}t\mathcal{H}_N} = \int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}t\lambda}\, \mathrm{d}F_N(\lambda; \boldsymbol{\xi}). \tag{14}$$

As $N \to \infty$ the Ledermann theorem implies that we may assume periodic boundary conditions for $\mathcal{H}_N$. Averaging (14) and using the translation invariance of $\langle (\delta_j, \exp(\mathrm{i}t\mathcal{H}_N)\delta_j) \rangle$ as a function of j we then obtain

$$\langle (\delta_0, \mathrm{e}^{\mathrm{i}t\mathcal{H}_N} \delta_0) \rangle = \int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}t\lambda}\, \mathrm{d}F_N(\lambda). \tag{15}$$

And sending N to infinity we find, using (13),

$$\lim_{N\to\infty} \langle (\delta_0, \mathrm{e}^{\mathrm{i}t\mathcal{H}_N} \delta_0) \rangle = \int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}t\lambda}\, \mathrm{d}F_+(\lambda). \tag{16}$$

Whatever $\boldsymbol{\xi}$, $(\delta_0, \exp(\mathrm{i}t\mathcal{H}_N)\delta_0)$ converges to $(\delta_0, \exp(\mathrm{i}t\mathcal{H})\delta_0)$ (Reed and Simon 1972).

Since the latter may be written $\int \exp\{it\lambda\}\, d(\delta_0, E_\lambda \delta_0)$, we end up with†

$$\int_{-\infty}^{+\infty} e^{it\lambda}\, d\langle(\delta_0, E_\lambda \delta_0)\rangle = \int_{-\infty}^{+\infty} e^{it\lambda}\, dF_+(\lambda). \tag{17}$$

By the uniqueness of the Fourier transform the proposition follows. It was announced, without proof, by Fukushima *et al* (1975). Part of the present argument has been patterned after a suggestion by Fukushima (1978).

4. Discussion

The spatial structure of the Hamiltonian $\mathscr{H}$ is of prime importance in showing that a certain observable related to $\mathscr{H}$, such as the free energy or the density of states, is self-averaging or thermodynamic. If the observable is (approximately) additive under the decomposition of the volume and the randomness of the system is determined by a homogeneous and ergodic stochastic process, all we can say is that the observable is self-averaging. That is, the behaviour of the observable becomes non-random as $N \to \infty$. The limit $N \to \infty$ idealises the macroscopic size of the system we are interested in. To obtain the slightly stronger notion of thermodynamic convergence we need to assume a bit more; for example, disjoint regions are stochastically independent. The proof of the additivity itself depends on the observable whose behaviour we want to predict or verify. In the case of the free energy the main tool was the Bogoliubov–Peierls inequality, in the present situation we could take advantage of the Ledermann theorem.

The importance of an observable becoming non-random as $N \to \infty$, in spite of the disorder in the system, can hardly be overestimated. It means that a theory can predict *reproducible* answers. If the stronger notion of thermodynamic convergence applies, the thermodynamic limit $N \to \infty$ and the replica limit $n \to 0$ may be interchanged, and the replica method becomes available as an analytic tool.

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† Here the tightness of the measures pays.

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