Journal of Statistical Physics, Vol. 80, Nos. 5/6, 1995

Rigorous Mean-Field Model for Coherent-Potential Approximation: Anderson Model with Free Random Variables

Peter Neu[1] **and Roland Speicher**[2]

Received October 25, 1994; final March 15, 1995

A model of a randomly disordered system with site-diagonal random energy fluctuations is introduced. It is an extension of Wegner's n-orbital model to arbitrary eigenvalue distribution in the electronic level space. The new feature is that the random energy values are not assumed to be independent at different sites, but free. Freeness of random variables is an analog of the concept of independence for noncommuting random operators. A possible realization is the ensemble of randomly rotated matrices at different lattice sites. The one- and two-particle Green functions of the proposed Hamiltonian are calculated exactly. The eigenstates are extended and the conductivity is nonvanishing everywhere inside the band. The long-range behavior and the zero-frequency limit of the two-particle Green function are universal with respect to the eigenvalue distribution in the electronic level space. The solutions solve the CPA equation for the one- and two-particle Green function of the corresponding Anderson model. Thus our (multisite) model is a rigorous mean-field model for the (single-site) CPA. We show how the Lloyd model is included in our model and treat various kinds of noises.

KEY WORDS: Disordered systems; random matrices; coherent-potential approximation.

1. INTRODUCTION

During the last decades randomly disordered systems have gained much interest in statistical physics. Especially since Anderson's paper[1] in 1958 these systems have attracted many physicists due to the localization phenomenon. However, realistic multisite models like the Anderson model

[1] Institut für Theoretische Physik, Universität Heidelberg, 69120 Heidelberg, Germany.
[2] Institut für Angewandte Mathematik, Universität Heidelberg, 69120 Heidelberg, Germany.

0022-4715/95/0900-1279$07.50/0

are in general unsolvable beyond the one-dimensional case. Exact calculations are only possible in one pathological case—namely for the Lloyd model[2] with Cauchy-distributed disorder.

The Anderson model describes the hopping of an electron in a d-dimensional disordered lattice $\mathbf{Z}^d$. The Hamiltonian is

$$H = H_0 + H_1 \tag{1.1}$$

where H_0 is the deterministic, translational-invariant Hamiltonian

$$H_0 = \sum_{r, r' \in Z^d} v_{|r-r'|} |r\rangle\langle r'| \tag{1.2}$$

and where the random disorder is assumed to be diagonal in the sites and independent between different sites, i.e.,

$$H_1 = \sum_{r \in Z^d} f_r |r\rangle\langle r| \tag{1.3}$$

with f_r being identically distributed, independent random variables. Although H_1 is a quite simple operator, its relation to H_0 is complicated and in the present form the Anderson model is not exactly solvable.

To circumvent this dilemma, two strategies have been developed: One is to approximate the multisite model by single-site models which can be solved exactly[3–7]; the other is to develop models which become exactly solvable in the mean-field limit of infinite dimension d, infinite interaction range R, or infinite number of angular momentum states n at each lattice site.[8,9] Among the former the most realistic ones are those single-site models which apply the *coherent-potential approximation* (CPA)[5–7]; among the latter Wegner's *n-orbital model*[8] is most frequently studied. Wegner's generalization of the Anderson model consists in putting n electronic states at each site and describing the disorder by Gaussian random matrices in the electronic states. Whereas for $n = 1$ this reduces to the Anderson model with Gaussian disorder, the opposite limit $n \to \infty$ becomes exactly solvable. Interestingly, this solution coincides with a CPA solution of the Anderson model where the single-site disorder is distributed according to Wigner's semicircle law.[10,11]

This fact has gained much interest in the debate about the range of validity of the CPA and its connection with the mean-field models. As mentioned by Khorunzhy and Pastur,[9] the infinite-d, -R, and -n limits do not coincide with the CPA in general; however, they have similar properties.

The starting point of our investigation is the following observation: The main reason for the difficulty in solving the Anderson model is that the

assumption of independence of the f_r at different sites cannot be translated into a tractable relation between H_0 and H_1. Hence, in our approximation of the Anderson model, we replace the assumption of independence by a "noncommutative" independence: we assume the f_r to be *free*. Freeness has been introduced in mathematics in the context of von Neumann algebras by Voiculescu[12] and has been extended to noncommutative probability theory by Voiculescu[12–16] and Speicher.[17–19] The assumption of freeness will allow us to calculate all physical quantities in our model exactly.

Freeness and random matrices are intimately connected with each other: Arbitrary Hermitian $n \times n$ matrices randomly rotated against each other—via unitary random matrices—are in the limit $n \to \infty$ a possible representation of free random variables.[14, 20] This relation will provide the following concrete realization of our model[21]: At each lattice site r we have n electronic levels $|r\alpha\rangle$ numbered by $\alpha = 1,..., n$. Let $f = (\langle\alpha| f |\beta\rangle)_{\alpha,\beta=1}^{n}$ be a fixed operator in the electronic level space and put

$$f_r := u_r f u_r^{\dagger} \tag{1.4}$$

where the u_r are unitary random matrices in the electronic level space chosen independently for different sites r. This means that we act at each site r with a copy f_r of the given operator f, but that the basis for f_r and the basis for $f_{r'}$ are rotated randomly against each other for all pairs of different sites $r \neq r'$.

From this point of view our model has a mean-field character and can be considered as a generalization of Wegner's *n-orbital model*[8] to arbitrary eigenvalue distributions in the electronic level space. In his original formulation, Wegner chose the $f_r = ((1/\sqrt{n}) f_r^{\alpha\beta})_{\alpha,\beta=1}^{n}$ as Gaussian random matrices at each r, such that the entries $f_r^{\alpha\beta}$ and $f_{r'}^{\gamma\delta}$ are independent for different sites $r \neq r'$. Thus in the limit $n \to \infty$, he was restricted to Wigner's semicircular eigenvalue distribution.[10, 11] It is this last restriction which we will show to be the reason that the CPA and the hitherto considered mean-field models coincide only for the semicircle distribution. On the contrary, we can show that the solution of our model and the solution of the corresponding Anderson model in the CPA approximation coincide always if the disorder is distributed according to the same distribution in both cases. Thus our (multisite) model is a rigorous mean-field model for the (single-site) CPA.

The long-range behavior and the zero-frequency limit of the two-particle Green function are universal with respect to the eigenvalue distribution in the electronic level space. Independently of the distribution of the disorder we find Wegner's result for the Gaussian ensemble[8] that (i)

eigenstates separated by an energy ω are correlated over a length L which diverges like $|\omega|^{-1/2}$ for $\omega \to 0$, and (ii) the two-particle Green function for energies in opposite halves of the complex place differing by ω approaches a constant for $d > 2$, diverges logarithmically for $d = 2$, and like $|\omega|^{d/2-1}$ for $0 \leqslant d < 2$.

The paper is organized as follows: In Section 2 we introduce the concept of free random variables and outline their connection with random matrices and their description by noncrossing cumulants. In Section 3 we introduce our model and calculate the one- and two-particle Green function and the conductivity exactly. Section 4 is devoted to the connection of our model with the CPA. In Section 5 we discuss our model for various kinds of disorder, and show how the Lloyd model is included in our model; finally, in Section 6 we summarize our main results.

2. FREENESS, RANDOM MATRICES, AND NONCROSSING CUMULANTS

2.1. The Concept of Freeness and Random Matrices

The concept of *freeness* was introduced by Voiculescu[12] in order to treat noncommutative random variables in an analogous way as commutative (classical) random variables are treated by the concept of *independence*. From an operational point of view independence and freeness are nothing but rules for the calculation of mixed moments of random variables $X_1, X_2, \ldots$, if the moments of all X_r are given separately. Thus, independence of the X_r means

$$\langle X_{r(1)} X_{r(2)} X_{r(3)} \cdots \rangle = \left\langle \prod_{i:\, r(i)=1} X_{r(i)} \right\rangle \left\langle \prod_{i:\, r(i)=2} X_{r(i)} \right\rangle \cdots \tag{2.1}$$

Freeness replaces this now by the following rule:

Definition. $X_1, X_2, \ldots$ are *free* if we have for all $m \in \mathbf{N}$ and for all polynomials $p_1(X)$, $p_2(X), \ldots, p_m(X)$ of one variable X that

$$\langle p_1(X_{r(1)})\, p_2(X_{r(2)}) \cdots p_m(X_{r(m)}) \rangle = 0 \tag{2.2}$$

whenever

$$\langle p_k(X_{r(k)}) \rangle = 0 \tag{2.3}$$

for all $k = 1, \ldots, m$ and $r(k) \neq r(k+1)$ for all $k = 1, \ldots, m-1$ (i.e., consecutive indices are different).

First, one should convince oneself that this is really a rule for calculating all mixed moments of the X_r's. Let us consider the case of two variables $X = X_1$ and $Y = X_2$. For $\langle XY \rangle$ the definition yields that $\langle XY \rangle = 0$ if $\langle X \rangle = \langle Y \rangle = 0$. If X and Y have nonvanishing mean, then by using (2.2) for the polynomials $p_1(X) = X - \langle X \rangle \mathbb{1}$ and $p_2(Y) = Y - \langle Y \rangle \mathbb{1}$ one easily finds $\langle XY \rangle = \langle X \rangle \langle Y \rangle$. Whereas this is the same result as for independent X and Y, the calculation of $\langle XYXY \rangle$ via

$$0 = \langle (X - \langle X \rangle \mathbb{1})(Y - \langle Y \rangle \mathbb{1})(X - \langle X \rangle \mathbb{1})(Y - \langle Y \rangle \mathbb{1}) \rangle$$

yields

$$\langle XYXY \rangle = \langle X^2 \rangle \langle Y \rangle^2 + \langle X \rangle^2 \langle Y^2 \rangle - \langle X \rangle^2 \langle Y \rangle^2 \tag{2.4}$$

and shows thereby that independence ($\langle XYXY \rangle = \langle X^2 \rangle \langle Y^2 \rangle$) and freeness are quite different concepts. Furthermore, freeness is really a noncommutative concept: If X, Y are free, we have $\langle XXYY \rangle = \langle X^2 \rangle \langle Y^2 \rangle$, which shows [cf. (2.4)] that X and Y do not commute. Hence X and Y cannot be represented by classical c-number random variables.

There exists a canonical representation of free random variables by special kinds of random matrices: Let $U(n)$ be the ensemble of unitary $n \times n$ matrices equipped with the canonical invariant Haar measure. Take two deterministic $n \times n$ matrices A and B (e.g., diagonal matrices) and rotate them against each other randomly, i.e., $X := A$ and $Y := uBu^\dagger$ with $u \in U(n)$. Then, in the limit $n \to \infty$, X and Y are free with respect to $\langle n^{-1} \operatorname{tr}[\ldots] \rangle_{\text{av}}$, where $\langle \ldots \rangle_{\text{av}}$ denotes the average over the ensemble of unitary matrices. Note that $n^{-1} \operatorname{tr}[\ldots]$ gives the eigenvalue distribution of our $n \times n$ matrices. This connection between freeness and unitary random matrices was first discovered by Voiculescu[14] and further developed by Speicher.[20] Another representation for free random variables with a special kind of distribution by deformed creation and annihilation operators will be discussed in Section 5.

Let us now check that the assumption of freeness of the f_r in the Hamiltonian H_1 results in a definite relation between H_0 and H_1, namely they are also free.

Theorem 1. Let the Hamiltonian H be given by (1.1)–(1.3). If the $f_1, f_2, \ldots$ are free with respect to $\langle \ldots \rangle_{\text{ens}}$, then H_0 and H_1 are also free with respect to $\langle \ldots \rangle$. Here $\langle \ldots \rangle = \langle\langle r_0 | \ldots | r_0 \rangle\rangle_{\text{ens}}$, independent of r_0, and $\langle \ldots \rangle_{\text{ens}}$ denotes the average over the disorder.

Proof. Consider polynomials $p_1, p_2, \ldots$ and $q_1, q_2, \ldots$ with $\langle p_i(H_0) \rangle = 0 = \langle q_j(H_1) \rangle$ for all i, j. Then we have to show that

$$\langle p_1(H_0)\, q_1(H_1)\, p_2(H_0)\, q_2(H_1) \ldots \rangle = 0 \tag{2.5}$$

and

$$\langle q_1(H_1)\, p_1(H_0)\, q_2(H_1) p_2(H_0) \ldots \rangle = 0 \tag{2.6}$$

We only treat the first case; the second is analogous. Note that $\langle r|\, q_j(H_1)\, |r'\rangle = \delta_{r,r'}\, q_j(f_r)$. Then

$$\begin{aligned}
&\langle p_1(H_0)\, q_1(H_1)\, p_2(H_0)\, q_2(H_1) \ldots \rangle \\
&\quad = \langle\langle r_0|\, p_1(H_0)\, q_1(H_1)\, p_2(H_0) q_2(H_1) \ldots\, |r_0\rangle\rangle_{\text{ens}} \\
&\quad = \sum_{r(1),\, r(2), \ldots} \langle\langle r_0|\, p_1(H_0)\, |r(1)\rangle\, q_1(f_{r(1)}) \\
&\qquad \times \langle r(1)|\, p_2(H_0)\, |r(2)\rangle\, q_2(f_{r(2)}) \ldots\, |r_0\rangle\rangle_{\text{ens}} \\
&\quad = \sum_{r(1),\, r(2), \ldots} \langle r_0|\, p_1(H_0)\, |r(1)\rangle \langle r(1)|\, p_2(H_0)\, |r(2)\rangle \ldots \\
&\qquad \times \langle q_1(f_{r(1)})\, q_2(f_{r(2)}) \ldots \rangle_{\text{ens}}
\end{aligned} \tag{2.7}$$

Since with H_0 also $p_i(H_0)$ is translationally invariant, $\langle r_0|\, p_i(H_0)\, |r_0\rangle \equiv \langle p_i(H_0)\rangle = 0$ implies $\langle r(i)|\, p_{i+1}(H_0)\, |r(i)\rangle = 0$ for all i, and we can restrict the sum to $r(i)$'s with $r(i) \neq r(i+1)$ for all i. However, for these terms we know that $\langle q_1(f_{r(1)})\, q_2(f_{r(2)}) \ldots \rangle_{\text{ens}} = 0$ due to the freeness of the f_j's and $\langle q_j(f_{r(j)})\rangle_{\text{ens}} = \langle q_j(H_1)\rangle = 0$. ∎

2.2. Description of Free Random Variables by Noncrossing Cumulants

In the physics of disordered systems, usually Green functions are calculated. This leads to the evaluation of mixed moments of—in our case—free random variables. The abstract definition of freeness ensures that all mixed moments are determined, but we do not have a concrete formula for them so far. An efficient machinery for concrete calculations is provided by the noncrossing cumulants.

Let $X_1, X_2, \ldots$ be free random variables. Then we consider quantities $k_m(Y_1, \ldots, Y_m)$ for all $m \geq 1$, where the arguments Y_i are noncommutative polynomials in $X_1, X_2, \ldots$. These k_m are called *noncrossing cumulants* and one way to define them is the following recurrence formula between the moments and the cumulants:

$$\begin{aligned}
\langle Y_1 \ldots Y_m \rangle = \sum_{p=0}^{m-1} \sum_{\substack{i(1), \ldots, i(p) \\ \subset \{2, \ldots, m\}}} & k_{p+1}(Y_1, Y_{i(1)}, Y_{i(2)}, \ldots, Y_{i(p)}) \\
& \times \langle Y_2 \ldots Y_{i(1)-1} \rangle \langle Y_{i(1)+1} \ldots Y_{i(2)-1} \rangle \ldots \langle Y_{i(p)+1} \ldots Y_m \rangle
\end{aligned} \tag{2.8}$$

Starting with $k_1(Y_1) = \langle Y_1 \rangle$, (2.8) may be used to determine $k_m(Y_1, ..., Y_m)$ successively. The noncrossing cumulants were introduced in ref. 19 and further elaborated with regard to stochastic dynamics in ref. 22. Examples are (in an obvious notation) $k_2(1, 2) = \langle 12 \rangle - \langle 1 \rangle \langle 2 \rangle$; for the special case of centered Y_i ($\langle Y_i \rangle = 0$ for $i = 1, ..., 4$), we have $k_4(1, 2, 3, 4) = \langle 1234 \rangle - \langle 12 \rangle \langle 34 \rangle - \langle 14 \rangle \langle 23 \rangle$.

It follows from the results of ref. 19 that also the following generalization of (2.8) holds:

$$\begin{aligned}
&\langle Y_1 \dots Y_m Y_{m+1} \dots Y_{m+l} \rangle \\
&\quad = \langle Y_1 \dots Y_m \rangle \langle Y_{m+1} \dots Y_{m+l} \rangle \\
&\qquad + \sum_{p=1}^{m} \sum_{q=1}^{l} \sum_{\substack{i(1),\dots,i(p) \\ \subset \{1,\dots,m\}}} \sum_{\substack{j(1),\dots,j(q) \\ \subset \{m+1,\dots,m+l\}}} k_{p+q}(Y_{i(1)}, \dots, Y_{i(p)}, Y_{j(1)}, \dots, Y_{j(q)}) \\
&\qquad \times \langle Y_1 \dots Y_{i(1)-1} \rangle \langle Y_{i(1)+1} \dots Y_{i(2)-1} \rangle \dots \langle Y_{j(q)+1} \dots Y_{m+l} \rangle
\end{aligned} \tag{2.9}$$

Thus, the noncrossing cumulants give the corrections to the frequently assumed factorization of $\langle Y_1 \dots Y_m Y_{m+1} \dots Y_{m+l} \rangle$ into $\langle Y_1 \dots Y_m \rangle \langle Y_{m+1} \dots Y_{m+l} \rangle$.

To derive the connection between freeness and noncrossing cumulants we will use another characterization of the noncrossing cumulants [which is equivalent to (2.8), (2.9)], namely, they are uniquely determined by

$$k_1(Y) = \langle Y \rangle \tag{2.10}$$

$$\begin{aligned}
&k_m(Y_1, ..., Y_i, Y_{i+1}, ..., Y_m) \\
&\quad = k_{m-1}(Y_1, ..., Y_i Y_{i+1}, ..., Y_m) \\
&\qquad - \sum_{k=0}^{i-1} k_{m+k-i}(Y_1, ..., Y_k, Y_{i+1}, ..., Y_m)\, k_{i-k}(Y_{k+1}, ..., Y_i) \\
&\qquad - \sum_{l=i+1}^{m-1} k_{m+i-l}(Y_1, ..., Y_i, Y_{l+1}, ..., Y_m)\, k_{l-i}(Y_{i+1}, ..., Y_l)
\end{aligned} \tag{2.11}$$

Note that in the first term of the rhs of (2.11) Y_i and Y_{i+1} are multiplied with each other, and that in the second and third terms $Y_{k+1}, ..., Y_i$ and $Y_{i+1}, ..., Y_l$ are skipped in k_{m+k-i} and k_{m+i-l}, respectively. Equation (2.11) allows to reduce all higher cumulants to k_1. It is quite easy to derive from (2.10), (2.11) the following properties:

Remarks. 1. $k_m(Y_1, ..., Y_m)$ is a multilinear function in $Y_1, ..., Y_m$.

2. $k_m(Y_1, ..., Y_m) = 0$ for $m \geqslant 2$ if at least for one i we have $Y_i = \mathbb{1}$ [of course $k_1(\mathbb{1}) = 1$].

Up to now we have not used any freeness; we have just defined noncrossing cumulants as special polynomials in the moments. That this definition gives us indeed the right tool for handling freeness is shown by the next proposition (for a more detailed proof see ref. 19):

Proposition 1. For each $i=1,...,m$ let Y_i be a polynomial in one variable $X_{r(i)}$ for some $r(i)$, $Y_i=p_i(X_{r(i)})$, and assume $X_1, X_2,...$ to be free. Then $k_m(p_1(X_{r(1)}),..., p_m(X_{r(m)}))=0$ whenever there exists at least one pair i, j with $i\neq j$ and $r(i)\neq r(j)$ (i.e., such that Y_i and Y_j are free).

Proof. By (2.11) we can glue together neighboring Y_i, Y_{i+1} with $r(i)=r(i+1)$ and hence we can assume that $r(i)\neq r(i+1)$ for all $i=1,...,m-1$. Next, we write again $Y_i=(Y_i-\langle Y_i\rangle 1)+\langle Y_i\rangle 1$ and, by Remarks 1 and 2, we can restrict ourselves to the case where all Y_i are centered, i.e., $\langle Y_i\rangle=0$ for all $i=1,...,m$. But then we can reduce—by using (2.11) [or equivalently (2.8)] and induction—$k_m(Y_1,..., Y_m)$ to $k_1(Y_1 \dots Y_m)\equiv\langle Y_1 \dots Y_m\rangle$, which vanishes by the definition of the freeness. ∎

Thus, the quite implicit definition of freeness, namely that very special mixed moments in free variables vanish, has now been replaced by the statement that all noncrossing cumulants with at least two different free variables vanish without any restriction on $\langle p_i(X_{r(i)})\rangle$ (cf. the definition of freeness). So we have, e.g., $k_3(X_1, X_1^2, X_2)=0$ if X_1 and X_2 are free—independent of the values of $\langle X_1\rangle$, $\langle X_1^2\rangle$, and $\langle X_2\rangle$—whereas $k_3(X_1, X_1^2, X_1)\neq 0$ in general. It is this very property of free random variables which will allow us to calculate the one-particle and the two-particle Green functions of our model in the next section exactly. Note that the noncrossing cumulants play exactly the same role for free random variables as the usual cumulants do for independent random variables.

3. SITE-DIAGONAL ANDERSON MODEL AND FREENESS

3.1. The Model

We consider now the following model of a randomly disordered system: The Hamiltonian H is given by $H=H_0+H_1$, where H_0 and H_1 are defined in (1.2) and (1.3), respectively, and where we assume the f_r to be identically distributed and free with respect to the average $\langle\dots\rangle_{\text{ens}}$. Due to our discussion on the relation between freeness and random matrices, we also have the concrete realization of our model as a generalized *n-orbital model* [cf. Eq. (1.4)]. According to our remarks around Eq. (2.4), the

$f_r \equiv (u_r f u_r^\dagger)_{\alpha\beta=1}^n$ become free in the limit $n \to \infty$. Thus, freeness is the correct mathematical notion for the $n \to \infty$-limit.

It is interesting to note that freeness is already to some extent contained in the original Anderson model (f_r being independent, random c-numbers). For instance we find in this case for $\langle H_0 H_1 H_0 H_1 \rangle$ the same result as in (2.4):

$$\begin{aligned}
\langle H_0 H_1 H_0 H_1 \rangle &= \langle\langle r_0 |\, H_0 H_1 H_0 H_1 \,| r_0 \rangle\rangle_{\text{ens}} \\
&= \left\langle \sum_r v_{|r-r_0|} f_r v_{|r_0-r|} f_{r_0} \right\rangle_{\text{ens}} \\
&= \sum_{r \neq r_0} v_{|r-r_0|} v_{|r_0-r|} \langle f_r \rangle_{\text{ens}} \langle f_{r_0} \rangle_{\text{ens}} + v_0^2 \langle f_{r_0}^2 \rangle_{\text{ens}} \\
&= \langle H_1 \rangle^2 \left(\sum_r v_{|r-r_0|} v_{|r_0-r|} - v_0^2 \right) + \langle H_1^2 \rangle\, v_0^2 \\
&= \langle H_1 \rangle^2 \langle H_0^2 \rangle + \langle H_1^2 \rangle \langle H_0 \rangle^2 - \langle H_1 \rangle^2 \langle H_0 \rangle^2 \quad (3.1)
\end{aligned}$$

Thus, the usual Anderson model yields freeness between H_0 and H_1 for small moments, but something uncontrollable for higher moments, which precludes the model being exactly solvable.

3.2. One-Particle Green Function

We want to calculate the averaged one-particle Green function (1PG) defined by

$$G(r, r'; z) := \left\langle\!\!\left\langle r \left| \frac{1}{z-H} \right| r' \right\rangle\!\!\right\rangle_{\text{ens}} \tag{3.2}$$

In matrix notation this reads

$$G(r, r'; z) = n^{-1} \sum_\alpha \langle\langle r, \alpha |\, [z-H]^{-1} \,| r', \alpha \rangle\rangle_{\text{ens}}$$

Let us first concentrate on its diagonal part $G(r_0, r_0; z)$, which is independent of r_0 due to translation invariance. Let us introduce the short-hand notation $G(z) := G(r_0, r_0; z)$ and $\langle \ldots \rangle := \langle\langle r_0 | \ldots | r_0 \rangle\rangle_{\text{ens}}$, thus

$$G(z) = \left\langle \frac{1}{z-(H_0+H_1)} \right\rangle = \sum_{n=0}^{\infty} \frac{\langle (H_0+H_1)^n \rangle}{z^{n+1}} \tag{3.3}$$

On calculating this quantity we assume that we know the 1PG of H_0 and H_1 separately,

$$G_0(z) = \left\langle \frac{1}{z - H_0} \right\rangle = \sum_{n=0}^{\infty} \frac{\langle H_0^n \rangle}{z^{n+1}} \equiv \sum_{n=0}^{\infty} \frac{\langle r_0 | H_0^n | r_0 \rangle}{z^{n+1}} \tag{3.4}$$

$$G_1(z) = \left\langle \frac{1}{z - H_1} \right\rangle = \sum_{n=0}^{\infty} \frac{\langle H_1^n \rangle}{z^{n+1}} \equiv \sum_{n=0}^{\infty} \frac{\langle f_{r_0}^n \rangle_{\text{ens}}}{z^{n+1}} \tag{3.5}$$

Thus, our problem consists in calculating moments of $H_0 + H_1$ given the moments of H_0 and H_1 separately, where due to our assumption of the f_r being free and by Theorem 1, H_0 and H_1 are free. In analogy to the usual convolution, which describes the sum of independent random variables, we have to calculate the so-called *free convolution*[13, 15] of the free random variables H_0 and H_1. At this point the difficulties with the usual Anderson model become evident: Independence of $f_1, f_2, \ldots$ does not imply a definite relation between H_0 and H_1 so that no well-defined notion of convolution between the distributions of H_0 and H_1 exists.

Theorem 2. Let the Hamiltonian H be given by (1.1)–(1.3), where $f_1, f_2, \ldots$ are free and identically distributed. Then the diagonal part of the 1PG is given by

$$G(z) = G_0[z - R_1[G(z)]] \tag{3.6}$$

where R_1 is determined by

$$G_1(z) = \frac{1}{z - R_1[G_1(z)]} \tag{3.7}$$

The off-diagonal part of the 1PG is given via the Fourier transform

$$G(r, r'; z) = \int_q \tilde{G}(q; z)\, e^{iq(r - r')} \tag{3.8}$$

by

$$\tilde{G}(q; z) = \frac{1}{z - \tilde{v}(q) - R_1[G(z)]} \tag{3.9}$$

where

$$v_{r-r'} = \int_q \tilde{v}(q)\, e^{iq(r - r')}$$

Here,

$$\int_q := \frac{\mathscr{V}}{(2\pi)^d} \int_{1\mathrm{BZ}} d^d q$$

$\mathscr{V}$ is the volume of the first Brillouin zone (1BZ).

Remark. Note that the diagonal part $G(z)$ entirely determines the off-diagonal part since with $\tilde{G}_0(q; z) = [z - \tilde{v}(q)]^{-1}$, Eqs. (3.8) and (3.9) are equivalent to

$$G(r, r'; z) = G_0(r, r'; z - R_1[G(z)]) \tag{3.10}$$

Proof. We first prove Theorem 2 for the diagonal part of the 1PG. Proposition 1 implies that the noncrossing cumulants of $H = H_0 + H_1$ are additive, i.e.,

$$k_m(H) = k_m(H_0) + k_m(H_1) \tag{3.11}$$

with the short-hand notation $k_m(H) := k_m(H, ..., H)$. Hence the free convolution is linearized by the noncrossing cumulants as the usual convolution is linearized by the usual cumulants. It remains to derive a relation between the noncrossing cumulants and the 1PG. If we specialize (2.8) to $Y_1 = ... = Y_m = H$ we obtain

$$\langle H^m \rangle = \sum_{p=1}^{m} \sum_{\substack{j(1),...,j(p)=0 \\ j(1)+\cdots+j(p)=m-p}}^{m-p} k_p(H) \langle H^{j(1)} \rangle \ldots \langle H^{j(p)} \rangle \tag{3.12}$$

If we now define

$$R(w) := \sum_{m=0}^{\infty} w^m k_{m+1}(H) \tag{3.13}$$

then we find with (3.3), (3.12) the relation

$$G(z) = \frac{1}{z - R[G(z)]} \tag{3.14}$$

Thus, R can be considered as the self-energy of $G(z)$, which depends self-consistently on $G(z)$ itself. Relation (3.14) and its equivalent form

$$G[R(w) + w^{-1}] = w \tag{3.15}$$

are due to Voiculescu,[15] who calls R the R-transform of H. The derivation given here using noncrossing cumulants was first given in ref. 19; for a dynamical generalization see ref. 22. In the same way we can write

$$G_0(z) = \frac{1}{z - R_0[G_0(z)]} \tag{3.16}$$

$$G_1(z) = \frac{1}{z - R_1[G_1(z)]} \tag{3.17}$$

where

$$R_0(w) := \sum_{m=0}^{\infty} w^m k_{m+1}(H_0) \tag{3.18}$$

$$R_1(w) := \sum_{m=0}^{\infty} w^m k_{m+1}(H_1) \tag{3.19}$$

Because of (3.11) R is also additive

$$R(w) = R_0(w) + R_1(w) \tag{3.20}$$

Defining y by $G(z) = G_0(y)$, we get

$$z - R_0[G(z)] - R_1[G(z)] = y - R_0[G_0(y)] = y - R_0[G(z)]$$

and thus $z - R_1[G(z)] = y$, from which we finally derive (3.6), which proves together with (3.17) the first assertion of our theorem. Note that (3.6) reduces to (3.7) if we put $H_0 = 0$: then $G_0(z) = z^{-1}$ and $G = G_1$. Note also that there is only an apparent asymmetry between H_0 and H_1, since we may write in the same way

$$G(z) = G_1[z - R_0[G(z)]] \tag{3.21}$$

Let us now treat the off-diagonal part of the 1PG. Again, our assumption of freeness of the f_r will guarantee that we can derive an exact expression for $G(r, r', z)$. Using Dyson's equation gives

$$\begin{aligned} G(r, r'; z) &= G_0(r, r'; z) \\ &\quad + \sum_{m=1}^{\infty} \sum_{r_1, \ldots, r_m} \langle G_0(r, r_1; z) f_{r_1} G_0(r_1, r_2; z) f_{r_2} \cdots f_{r_m} G_0(r_m, r'; z) \rangle_{\text{ens}} \\ &= G_0(r, r'; z) + \sum_{m=1}^{\infty} \sum_{r_1, \ldots, r_m} G_0(r, r_1; z) \cdots G_0(r_m, r'; z) \langle f_{r_1} \cdots f_{r_m} \rangle_{\text{ens}} \end{aligned}$$

$$= G_0(r, r'; z) + \sum_{m=1}^{\infty} \sum_{r_1, \ldots, r_m} G_0(r, r_1; z) \ldots G_0(r_m, r'; z)$$
$$\times \sum_{p=0}^{m-1} \sum_{\substack{i(1), \ldots, i(p) \\ \subset \{2, \ldots, m\}}} k_{p+1}(f_{r_1}, f_{r_{i(1)}}, \ldots, f_{r_{i(p)}})$$
$$\times \langle f_{r_2} \cdots f_{r_{i(1)-1}} \rangle \langle f_{r_{i(1)+1}} \cdots f_{r_{i(2)-1}} \rangle \cdots \langle f_{r_{i(p)+1}} \cdots f_{r_m} \rangle \tag{3.22}$$

where we have used the recurrence formula (2.8) for the noncrossing cumulants. Due to the freeness of the f_r and Proposition 1, only such terms contribute where $r_1 = r_{i(1)} = \ldots = r_{i(p)}$, which yields after some resummations

$$G(r, r'; z) = G_0(r, r'; z)$$
$$+ \sum_{p=1}^{\infty} \sum_{r_1} G_0(r, r_1; z)\, k_{p+1}(f_{r_1})\, G(r_1, r_1; z)^p\, G(r_1, r'; z)$$
$$= G_0(r, r'; z) + R_1[G(z)] \sum_{r_1} G_0(r, r_1; z)\, G(r_1, r'; z) \tag{3.23}$$

where we have used $k_p(f_{r_1}) = k_p(H_1)$ and $G(z) = G(r_1, r_1; z)$. Note that, once $G(z)$ is known, (3.23) is a linear system of equations for $G(r, r'; z)$ which can be solved by Fourier transformation. Then, Eq. (3.23) reads

$$\tilde{G}(q; z) = \tilde{G}_0(q; z) + R_1[G(z)]\, \tilde{G}_0(q; z)\, \tilde{G}(q; z) \tag{3.24}$$

which yields with

$$\tilde{G}_0(q; z) = \frac{1}{z - \tilde{v}(q)} \tag{3.25}$$

the second assertion, Eq. (3.9), of our theorem. ∎

We finally comment on the analytic structure of the solution (3.6). By definition $G(z)$, $G_0(z)$, and $G_1(z)$ are holomorphic functions in the upper complex half-plane $\mathbf{C}^+$. However, it is *a priori* not clear whether $G(z)$ initially defined by Eq. (3.6) only in a neighborhood of ∞ has an analytic continuation to $\mathbf{C}^+$.

Clearly, the implicit definition of $G(z)$ by (3.6) is unique except for the critical points $z \in \mathbf{C}^+$ where $G'(z) = 0$. Let us denote this set by $D = \{z \in \mathbf{C}^+ \mid G'(z) = 0\}$ and by $\Delta = G(D)$ their critical values; analogously, we define D_j and Δ_j for $j = 0, 1$. Then Voiculescu has shown[16] for compactly supported measures of H_0 and H_1 and $G(z)$ implicitly given by (3.6) that:

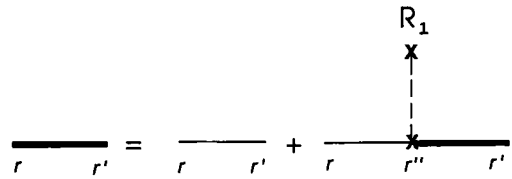

Fig. 1. Diagrammatic representation of Eq. (3.23). $R_1[G(z)]$ can be interpreted as an effective local potential which scatters the propagating electron incoherently at each lattice site.

1. $G(\mathbf{C}^+) \subset G_0(\mathbf{C}^+) \cap G_1(\mathbf{C}^+)$.
2. $R_j[G_j(z)]$ $(j=0, 1, 2)$ has an analytic continuation from ∞ to $\mathbf{C}^+$ (here $G_2 \equiv G$, $R_2 \equiv R$).
3. If $\Delta_0 \cap \Delta_1 = \varnothing$, the function $y(z) := z - R_1[G(z)]$ has an analytic continuation from ∞ to $\mathbf{C}^+$.

The assumption $\Delta_0 \cap \Delta_1 = \varnothing$ implies that if $w^{-1} + R_0(w)$—which is the inverse of G_0 [cf. Eq. (3.15)]—has a branching point of order $p > 1$ at ζ_0, then ζ_0 is not a branching point of $w^{-1} + R_1(w)$ and hence ζ_0 is a branching point of order exactly p for $w^{-1} + R(w)$.[16] This guarantees the uniqueness of the analytic continuation of Eq. (3.6). This assumption is not restrictive for practical purposes in physics as long as the measures of H_0 and H_1 do not coincide. However, in this case we know due to the freeness of H_0 and H_1 (cf. Theorem 1) that $R(w) = 2R_0(w) = 2R_1(w)$.

Before we develop further our formalism for the 2PG, let us give $R_1[G(z)]$ a clear physical interpretation. The diagrammatic representation of Eq. (3.23) is shown in Fig. 1, in obvious notation. Thus, $R_1[G(z)]$ behaves like an effective local potential which scatters the propagating electron incoherently at each lattice site. The total scattered wave is the sum of the contributions from each lattice site without interference terms. From this viewpoint our model has CPA character. We will come back to this in Section 4.

3.3. Two-Particle Green Function

In this section the averaged two-particle Green function (2PG)

$$\mathcal{G}(r, s, s', r'; z_1, z_2) := \left\langle\!\!\left\langle r \left| \frac{1}{z_1 - H} \right| s \right\rangle \left\langle s' \left| \frac{1}{z_2 - H} \right| r' \right\rangle\!\!\right\rangle_{\text{ens}} \tag{3.26}$$

will be calculated. In matrix notation this reads

$$\mathscr{G}(r, s, s', r'; z_1, z_2) = n^{-1} \sum_{\alpha, \beta} \langle\langle r, \alpha | [z_1 - H]^{-1} | s, \beta \rangle \langle s', \beta | [z_2 - H]^{-1} | r', \alpha \rangle\rangle_{\text{ens}}$$

We define the 2PG of H_1 by

$$\mathscr{G}_1(z_1, z_2) := \left\langle \frac{1}{z_1 - H_1} \frac{1}{z_2 - H} \right\rangle = \left\langle \frac{1}{z_1 - f_{r_0}} \frac{1}{z_2 - f_{r_0}} \right\rangle_{\text{ens}} \tag{3.27}$$

From the identity

$$\begin{aligned}(z_1 - z_2) \sum_s \left\langle\!\!\left\langle r \left| \frac{1}{z_1 - H} \right| s \right\rangle \left\langle s \left| \frac{1}{z_2 - H} \right| r' \right\rangle\!\!\right\rangle_{\text{ens}} &= \left\langle\!\!\left\langle r \left| \frac{z_1 - z_2}{(z_1 - H)(z_2 - H)} \right| r' \right\rangle\!\!\right\rangle_{\text{ens}} \\ &= G(r, r'; z_2) - G(r, r'; z_1)\end{aligned} \tag{3.28}$$

one obtains the *sum rule*

$$(z_1 - z_2) \sum_s \mathscr{G}(r, s, s, r'; z_1, z_2) = G(r, r'; z_2) - G(r, r'; z_1) \tag{3.29}$$

which reduces for $\mathscr{G}_1$ to

$$(z_1 - z_2)\, \mathscr{G}_1(z_1, z_2) = G_1(z_2) - G_1(z_1) \tag{3.30}$$

The 2PG of our model is now given by the following theorem.

Theorem 3. Let the Hamiltonian H be given by (1.1)–(1.3) where $f_1, f_2, \ldots$ are free and identically distributed. Let further $G(z)$ and $G(r, r'; z)$ be given by (3.6)–(3.9). Then, for $\operatorname{Im} z_{1/2} \neq 0$

$$\begin{aligned}\mathscr{G}(r, s, s', r'; z_1, z_2) = {} & G(r, s; z_1)\, G(s', r'; z_2) \\ & + \mathscr{R}_1[G(z_1), G(z_2)] \\ & \times \sum_{r''} G(r, r''; z_1)\, \mathscr{G}(r'', s, s', r''; z_1, z_2)\, G(r'', r'; z_2)\end{aligned} \tag{3.31}$$

where $\mathscr{R}_1(w_1, w_2)$ is determined by

$$\mathscr{R}_1(w_1, w_2) = \frac{R_1(w_1) - R_1(w_2)}{w_1 - w_2} \tag{3.32}$$

Remark. Note that, once the 1PG is known, (3.31) is a linear system of equations for the 2PG.

Proof. Again we use Dyson's equation to obtain

$$\begin{aligned}\mathcal{G}(r, s, s', r'; z_1, z_2) &= \left\langle \left\{ G_0(r, s; z_1) + \sum_{m=1}^{\infty} \sum_{r_1, \ldots, r_m} G_0(r, r_1; z_1) f_{r_1} \ldots f_{r_m} G_0(r_m, s; z_1) \right\} \right. \\ &\quad \left. \times \left\{ G_0(s', r'; z_2) + \sum_{l=1}^{\infty} \sum_{s_1, \ldots, s_l} G_0(s', s_1; z_2) f_{s_1} \ldots f_{s_l} G_0(s_l, r'; z_2) \right\} \right\rangle_{\text{ens}} \end{aligned} \tag{3.33}$$

As before, we can express this in terms of the noncrossing cumulants by using relation (2.9) for $\langle f_{r_1} \ldots f_{r_m} f_{s_1} \ldots f_{s_l} \rangle$. Due to the freeness of $f_1, f_2, \ldots$ we can again use Proposition 1 and therefore we can restrict the summation in (2.9) to terms with

$$r_{i(1)} = \cdots = r_{i(p)} = s_{j(1)} = \cdots = s_{j(q)}$$

After some resummation we finally obtain

$$\begin{aligned}\mathcal{G}(r, s, s', r'; z_1, z_2) &= G(r, s; z_1)\, G(s', r'; z_2) \\ &\quad + \sum_{p, q=1}^{\infty} \sum_{r''} k_{p+q}(H_1)\, G(r, r''; z_1)\, G(r'', r''; z_1)^{p-1} \\ &\quad \times \mathcal{G}(r'', s, s', r''; z_1, z_2)\, G(r'', r''; z_2)^{q-1}\, G(r'', r'; z_2)\end{aligned} \tag{3.34}$$

Defining

$$\begin{aligned}\mathcal{R}_1(w_1, w_2) &:= \sum_{p, q=1}^{\infty} k_{p+q}(H_1)\, w_1^{p-1} w_2^{q-1} \\ &= \sum_{n=1}^{\infty} k_n(H_1) \sum_{\substack{p, q \geq 1 \\ p+q=n}} w_1^{p-1} w_2^{q-1} \\ &= \sum_{n=1}^{\infty} k_n(H_1) \frac{w_1^n - w_2^n}{w_1 - w_2}\end{aligned} \tag{3.35}$$

yields, with (3.19), Eqs. (3.32) and (3.31). ∎

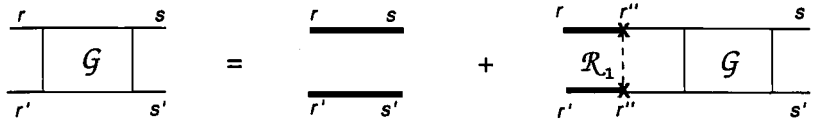

Fig. 2. Diagrammatic representation of Eq. (3.31). $\mathcal{R}_1[G(z_1), G(z_2)]$ can be interpreted as an effective local electron–electron interaction. Equation (3.31) has a ladder structure.

Following Wegner[8] [his Eqs. (4.18)–(4.21)], one easily shows that Eq. (3.31) is consistent with the sum rule (3.29). Using this sum rule together with (3.32) yields the relation

$$\mathcal{R}_1[G(z_1), G(z_2)] \sum_s \mathcal{G}(r, s, s, r; z_1, z_2) = -\frac{R_1[G(z_1)] - R_1[G(z_2)]}{z_1 - z_2} \tag{3.36}$$

which closely resembles a Ward identity. Since $R_1[G(z_1)]$ is the self-energy of the 1PG the lhs may be interpreted as a vertex function. The structure of Eq. (3.31) permits still another characterization of $\mathcal{R}_1[G(z_1), G(z_2)]$ as a local effective electron–electron interaction. This becomes particularly pronounced if one represents (3.31) diagrammatically as in Fig. 2. Thus Eq. (3.31) has a ladder structure with an effective electron–electron interaction $\mathcal{R}_1[G(z_1), G(z_2)]$. This interaction is a contact interaction, i.e., after averaging, the two electrons propagate independently through the lattice unless they meet at same site. As for the 1PG, our model resembles the CPA in character. We come back to this in Section 4.

3.4. Long-Range Behavior and Conductivity

3.4.1. Long-Range Behavior. To discuss the long-range behavior of the 2PG, let us consider its connected part for $r = r'$ and $s = s'$

$$C(r, s; z_1, z_2) := \mathcal{G}(r, s, s, r; z_1, z_2) - G(r, s; z_1) G(s, r; z_2) \tag{3.37}$$

and its Fourier transform

$$\tilde{C}(q; z_1, z_2) = \sum_r C(0, r; z_1, z_2)\, e^{iqr} \tag{3.38}$$

The disconnected part of the 2PG yields only a short-range contribution and will not be discussed in the following.

Defining $\mathscr{G}_{12}(r, s; z_1, z_2) := G(r, s; z_1)\, G(s, r; z_2)$ and its Fourier transform

$$\tilde{\mathscr{G}}_{12}(q; z_1, z_2) := \sum_r G(r, 0; z_1)\, G(0, r; z_2)\, e^{iqr}$$

$$= \int_{q'} \tilde{G}(q'; z_1)\, \tilde{G}(q' - q; z_2) \tag{3.39}$$

with $\tilde{G}(q; z)$ given by (3.9) and using (3.31), one obtains with the abbreviation $\mathscr{R}_1 \equiv \mathscr{R}_1[G(z_1), G(z_2)]$

$$\tilde{C}(q; z_1, z_2) = \mathscr{R}_1(\tilde{\mathscr{G}}_{12}(q; z_1, z_2))^2 + \mathscr{R}_1 \tilde{\mathscr{G}}_{12}(q; z_1, z_2)\, \tilde{C}(q; z_1, z_2) \tag{3.40}$$

which has the solution

$$\tilde{C}(q; z_1, z_2) = \frac{\mathscr{R}_1(\tilde{\mathscr{G}}_{12}(q; z_1, z_2))^2}{1 - \mathscr{R}_1 \tilde{\mathscr{G}}_{12}(q; z_1, z_2)} \tag{3.41}$$

Now we want to show that $\tilde{C}(0; z_1, z_2)$ diverges if z_1 and z_2 approach the same energy E from different halves of the complex plane along the branch cut of G, that is, for

$$\varrho(E) \equiv \frac{1}{2\pi i}[G(E - i0^+) - G(E + i0^+)] \neq 0 \tag{3.42}$$

This follows from the decomposition

$$\tilde{G}(q; z_1)\, \tilde{G}(q; z_2) = \frac{\tilde{G}(q; z_2) - \tilde{G}(q; z_1)}{z_1 - R_1[G(z_1)] - z_2 + R_1[G(z_2)]} \tag{3.43}$$

where we have used (3.9), which yields

$$\tilde{\mathscr{G}}_{12}(0; z_1, z_2) = \frac{1}{\mathscr{R}_1} + \frac{z_2 - z_1}{\mathscr{R}_1(z_1 - z_2) - \mathscr{R}_1^2(G(z_2) - G(z_1))} \tag{3.44}$$

Thus the denominator of (3.41) vanishes for $q = 0$ and $\lim z_{1/2} = E$, since the second term of (3.44) vanishes because of (3.42). From this one concludes that $\tilde{C}(q; z_1, z_2)$ has a diffusive pole.

To make this explicit we take

$$z_1 = E + \frac{1}{2}\omega, \qquad z_2 = E - \frac{1}{2}\omega \tag{3.45}$$

where E is real and ω has an imaginary part of sign s. Inserting this in (3.44) and assuming following Wegner[8] cubic symmetry with coordination number n, one finds by expanding around $q=0$ in leading order for small ω and q^2

$$n\tilde{C}(q; z_1, z_2) = \left(-\frac{i\omega s}{2\pi\varrho(E)} + Aq^2 \right)^{-1} \tag{3.46}$$

with

$$\begin{aligned} A &= -\left(\frac{\mu(E)}{\varrho(E)}\right)^2 \left.\frac{\partial \tilde{\mathscr{G}}_{12}(q; z_1, z_2)}{\partial q^2}\right|_{q=0} \\ &= \frac{1}{2d}\left(\frac{\mu(E)}{\varrho(E)}\right)^2 \sum_r r^2 G(0, r; z_1)\, G(r, 0; z_2) \end{aligned} \tag{3.47}$$

Here we have used (3.32) to write

$$\begin{aligned} &\mathscr{R}_1[G(E+i0^+), G(E-i0^+)] \\ &\quad = \frac{R_1[G(E-i0^+)] - R_1[G(E+i0^+)]}{G(E-i0^+) - G(E+i0^+)} = \frac{\mu(E)}{\varrho(E)} \end{aligned} \tag{3.48}$$

with the measure of $R_1[G(z)]$

$$\mu(E) := \frac{1}{2\pi i}\{R_1[G(E-i0^+)] - R_1[G(E+i0^+)]\} \tag{3.49}$$

In the case of the Gaussian ensemble with covariance M we will show in Section 5 that $\mu(E) = M\varrho(E)$, i.e., $\mathscr{R}_1 \equiv M$, so that we find Wegner's result[8] [his Eqs. (4.40)–(4.41)]. Thus Eq. (3.46) merely differs from the corresponding solution for the Gaussian ensemble by a redefinition of the constant A. The function $\tilde{C}(q; z_1, z_2)$ essentially determines the long-range and the $\omega \to 0$ limit of the 2PG. Without further calculations one concludes from this that the qualitative behavior of the long-range and the $\omega \to 0$ limit of the 2PG does not depend on the distribution of the disorder in the electronic level space.

In more detail, following Wegner[8] (his Section V), one sees from (3.46) with the definition of the wave vector

$$\kappa = \left(\frac{-i\omega s}{2\pi A\varrho(E)}\right)^{1/2}, \qquad \operatorname{Re}\kappa > 0 \tag{3.50}$$

that eigenstates separated by an energy difference ω are correlated in phase over a length

$$L = |\kappa|^{-1} = [2\pi A \varrho(E)/|\omega|]^{1/2} \tag{3.51}$$

which diverges as $|\omega|^{-1/2}$ as $\omega \to 0$. Furthermore, by Fourier backtransformation and dimensional analysis one finds for fixed $r \ll L$ and energies in opposite halves of the complex plane differing by ω that $C(0, r; z_1, z_2)$ approaches a finite value provided $d > 2$, diverges logarithmically as a function of ω for $d = 2$, and like $|\omega|^{d/2-1}$ for $0 \leqslant d < 2$, respectively, for $\omega \to 0$. This implies that for $d > 0$ the eigenstates are extended since C does not diverge as fast as $|\omega|^{-1}$. Up to a redefinition of the constant A this is the same result as for the Gaussian ensemble[8].

3.4.2. Conductivity. The 2PG determines the conductivity $\sigma_T(\omega)$ via the Kubo–Greenwood relation[9]

$$\sigma_T(\omega) = \frac{2e^2}{\pi \mathscr{V}} \int_{-\infty}^{\infty} \omega^{-1} \left[n_F\left(E - \frac{\omega}{2}\right) - n_F\left(E + \frac{\omega}{2}\right) \right] \sigma(\omega, E)\, dE \tag{3.52}$$

Here, $n_F(E) = \{\exp[(E - E_F)/T] + 1\}^{-1}$ is the Fermi distribution, E_F is the Fermi energy, and $\sigma(\omega, E)$ is the current–current or the density–density spectral function[8].

At $T = 0$ and in the dc limit $\omega \to 0$ the conductivity is given by the spectral function itself

$$\sigma_{T=0}(\omega) = \frac{2e^2}{\pi \mathscr{V}} \sigma(\omega, E_F), \qquad \omega \to 0 \tag{3.53}$$

where the spectral function $\sigma(\omega, E_F)$ is given by the connected part of the 2PG,[8] yielding

$$\begin{aligned} \sigma_{T=0}(\omega \to 0) &= \frac{e^2 n}{4\pi^2 \mathscr{V}} \omega^2 \sum_s \frac{\partial}{\partial q^2} \tilde{C}\left(q; E_F + \frac{\omega}{2} + is0^+, E_F - \frac{\omega}{2} + is0^+\right)\Big|_{q=0} \\ &= \frac{2\pi e^2 n A}{\mathscr{V}} \varrho^2(E_F) \end{aligned} \tag{3.54}$$

Using the definition of A in (3.47) and the Fourier transform (3.9), we can also give this result as follows:

$$\sigma_{T=0}(\omega \to 0) = \frac{2\pi e^2 n B}{\mathscr{V}} \mu^2(E_F) \tag{3.55}$$

where $\mu(E_F)$ is the spectral function of $R_1[G(z)]$ [cf. (3.49)] and

$$B := A\left(\frac{\varrho(E_F)}{\mu(E_F)}\right)^2 = -\frac{\partial \tilde{\mathscr{G}}_{12}(q; z_1, z_2)}{\partial q^2}\bigg|_{q=0} \tag{3.56}$$

The last two equations show that the dc conductivity at zero temperature is essentially given by the square of the spectral function of the Fourier transform of the 1PG. Again this result differs from that for the Gaussian ensemble by a mere redefinition of the constant A. From this one concludes that the conductivity is nonvanishing everywhere inside the band, and that localization cannot occur in our model.

4. COHERENT-POTENTIAL APPROXIMATION

One of the most effective approximation methods for the Anderson model is the (single-site) *coherent-potential approximation* (CPA) initially proposed by Soven[5] and Taylor.[6] Its main idea can be summarized as follows[3,4]: One introduces an effective homogeneous medium with the propagator $G_0(r, s; z-\Sigma)$ with an effective potential Σ in which the electron moves and demands

$$G(r, s; z) = G_0(r, s; z - \Sigma(z)) \tag{4.1}$$

In other words, the CPA calculates G from an effective Hamiltonian $H_{\text{eff}} = H_0 + \sum_r \Sigma\, |r\rangle\langle r|$. The coherent potential Σ is determined in such a way that the difference between the actual and the effective Hamiltonian, $H - H_{\text{eff}}$, produces on the average zero scattering at one site, i.e., the averaged single-site t matrix vanishes

$$\langle t(z)\rangle := \left\langle \frac{f_r - \Sigma}{1 - (f_r - \Sigma)\, G(z)} \right\rangle = 0 \tag{4.2}$$

where $G(z) \equiv G(r, r; z)$ is given by

$$G(z) = G_0(z - \Sigma(z)) \tag{4.3}$$

Due to the translation invariance, $t(z)$ is site independent. Velický[7] has worked out this concept for the 2PG and has found the following CPA equation for the 2PG:

$$\begin{aligned}\mathscr{G}(r, s, s', r'; z_1, z_2) &= G(r, s; z_1)\, G(s', r'; z_2) \\ &\quad + \mathscr{L}(z_1, z_2) \sum_{r''} G(r, r''; z_1)\, \mathscr{G}(r'', s, s', r''; z_1, z_2)\, G(r'', r'; z_2)\end{aligned} \tag{4.4}$$

where G is given by (4.1) with Σ satisfying (4.2) and

$$\mathcal{L}(z, z') = \frac{\langle t(z)\, t(z')\rangle}{1 + G(z)\langle t(z)\, t(z')\rangle\, G(z')} \tag{4.5}$$

Here $\langle t(z)\, t(z')\rangle$ contains all contributions from repeated scattering at the same site. Thus the 2PG is given as the sum of single-site contributions in agreement with the general CPA philosophy.

In view of (4.1) and (4.4) the solutions of our model (3.6) and (3.31) have CPA character. This was already realized by Wegner[8] and Khorunzhy and Pastur[9] for the n-orbital model. Wegner showed that the $n \to \infty$ limit of his model yields the CPA solution of the Anderson model provided that the f_r are distributed according to the semicircle law.[8] In general the connection between the CPA and models like Wegner's n-orbital model is not clear (see the discussion in ref. 9).

Here, we will show that the concept of freeness allows us to put the CPA on a firm mathematical basis, namely, we can prove the following theorem:

Theorem 4. Let the Hamiltonian H be given by (1.1)–(1.3) where $f_1, f_2, \ldots$ are *free* and identically distributed according to a distribution P. Then, the solution for the 1PG given by Theorem 2 and the solution for the 2PG given by Theorem 3 are identical to the CPA solution of the Anderson model where the $f_1, f_2, \ldots$ are *independent* and identically distributed with the same P.

Proof. We first prove the assertion of the theorem for the 1PG. We show that (3.6) and (3.7) solve the CPA equations (4.1) and (4.2) if we identify $\Sigma(z) = R_1[G(z)]$. Using this to rewrite the CPA condition (4.2) as

$$\langle t(z)\rangle = \sum_{n=1}^{\infty} \langle [f_r - R_1(w)]^n\rangle\, w^{n-1} \tag{4.6}$$

where $w := G(z)$, one finds

$$\begin{aligned}
\langle t(z)\rangle + \frac{1}{w} &= \sum_{n=0}^{\infty} \langle [f_r - R_1(w)]^n\rangle\, w^{n-1} \\
&= \sum_{n=0}^{\infty} \sum_{k=0}^{n} \binom{n}{k} \langle f_r^k\rangle [-R_1(w)]^{n-k}\, w^{n-1} \\
&= \sum_{k=0}^{\infty} \langle f_r^k\rangle \left\{ \sum_{n=k}^{\infty} \binom{n}{k} [-wR_1(w)]^{n-k} \right\} w^{k-1}
\end{aligned}$$

$$= \frac{1}{w^2} \sum_{k=0}^{\infty} \frac{\langle f_r^k \rangle}{[R_1(w) + 1/w]^{k+1}}$$

$$= \frac{1}{w^2} G_1 \left[R_1(w) + \frac{1}{w} \right]$$

$$= \frac{1}{w} \tag{4.7}$$

i.e., $\langle t(z) \rangle = 0$. Here, we have used the equivalent form of (3.7), $G_1[R_1(w) + 1/w] = w$, and the identity

$$\sum_{n=k}^{\infty} \binom{n}{k} a^{n-k} = \frac{1}{(1-a)^{k+1}} \tag{4.8}$$

To prove the assertion of the theorem for the 2PG we show that $\mathscr{L}(z, z') = \mathscr{R}_1[G(z), G(z')]$. We first calculate the average of the product of the single-site t matrices

$$\Lambda(z, z') := \langle t(z)\, t(z') \rangle = \left\langle \frac{f_r - \Sigma}{1 - (f_r - \Sigma) G} \frac{f_r - \Sigma'}{1 - (f_r - \Sigma')\, G'} \right\rangle \tag{4.9}$$

where we have used the abbreviations $G = G(z)$, $G' = G(z')$, $\Sigma = \Sigma(z)$, $\Sigma' = \Sigma(z')$. The average can be evaluated using (4.2). Identifying $\Sigma(z) = R_1[G(z)]$, one finds

$$\Lambda(z, z') = \frac{R_1[G] - R_1[G']}{G - G' + GG'(R_1[G'] - R_1[G])} \tag{4.10}$$

which reduces with Eq. (3.32) to

$$\Lambda(z, z') = \mathscr{R}_1[G, G']/(1 - \mathscr{R}_1[G, G']\, GG') \tag{4.11}$$

Solving this equation for $\mathscr{R}_1$ yields the rhs of (4.5) and therefore proves the second assertion of our theorem. ∎

In the CPA both the 1PG and the 2PG are entirely determined by the coherent potential $\Sigma(z)$ which follows self-consistently from (4.2) and (4.3). In our model $\Sigma(z)$ is given by Voiculescu's R-transform R_1 of the disorder. Thus the prescription (3.7) for calculating R_1 can be considered as the formal solution of the CPA equations for arbitrary disorder.

5. DISCUSSION OF SPECIFIC DISTRIBUTIONS

5.1. Deterministic Noise

Let us start with the trivial case where all f_r are deterministic, attaining the constant γ, i.e., they have a $\delta(f_r - \gamma)$ distribution for all r. Then, $G_1(z) = [z-\gamma]^{-1}$, hence $R_1(w) = \gamma$ [cf. Eq. (3.7)], hence $\mathscr{R}_1(w_1, w_2) = 0$ [cf. Eq. (3.32)]. This yields the following solution for the Green functions:

$$G(z) = G_0(z-\gamma)$$

$$\tilde{G}(q; z) = \frac{1}{z - \tilde{v}(q) - \gamma} \tag{5.1}$$

$$\mathscr{G}(r, s, s', r'; z_1, z_2) = G(r, s; z_1)\, G(s', r'; z_2)$$

i.e., the connected part C of the 2PG vanishes. Since for deterministic f_r there is no difference between independence and freeness, this is also the exact solution of the original Anderson model. Of course, it is just given by a trivial energy shift γ of the unperturbed solution.

5.2. Cauchy (Lorentz) Noise: The Lloyd Model

Consider now the Lloyd model where the f_r are distributed according to a Cauchy distribution with parameter γ, i.e.,

$$dP(f_r = \varepsilon) = \frac{1}{\pi} \frac{\gamma}{\gamma^2 + \varepsilon^2}\, d\varepsilon \tag{5.2}$$

Note that moments and thus also cumulants of H_1 do not exist in this case, but nevertheless our main formulas for the connection between $G_1(z)$ and $R_1(w)$ can be justified in this case, too.[23, 24] We have

$$G_1(z) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\gamma}{\gamma^2 + \varepsilon^2} \frac{1}{z - \varepsilon}\, d\varepsilon = \frac{1}{z + i\gamma} \tag{5.3}$$

hence $R_1(w) = is\gamma$, with s being the sign of the imaginary part of w. Using (3.32), one sees that $\mathscr{R}_1(w_1, w_2) = 0$ if w_1 and w_2 are on the same halves of the complex plane, and

$$\mathscr{R}_1(w_1, w_2) = \frac{2is_1\gamma}{w_1 - w_2} \tag{5.4}$$

if w_1 and w_2 are on opposite halves. Thus in the former case, we find the same result as in (5.1) with γ replaced by $i\gamma$. In the latter case the connected part C of the 2PG does not vanish, so that one finds a finite conductivity

$$\sigma_{T=0}(\omega \to 0) = \frac{2e^2 nB}{\pi \mathscr{V}} \gamma^2 \tag{5.5}$$

with $B = -[\partial \tilde{\mathscr{G}}_{12}(q)/\partial q^2]|_{q=0}$.

5.3 Gaussian Random Matrix Noise: The Wegner Model

Wegner's model consists in choosing the f_r to be—in the limit $n \to \infty$—symmetric $n \times n$ Gaussian random matrices with the entries of f_r and of $f_{r'}$ being independent for $r \neq r'$. As explained in Sections 2.1 and 3.1, this means nothing but that the f_r are free. Thus Wegner's model is the special case of ours where the distribution of the f_r is given by the eigenvalue distribution of symmetric Gaussian random matrices, i.e., by Wigner's semicircle law,

$$P(f_r = \varepsilon) = \frac{1}{2\pi M} (4M - \varepsilon^2)^{1/2} \, d\varepsilon \tag{5.6}$$

for $\varepsilon^2 \leqslant 4M$ and zero elsewhere. The fact that Gaussian random matrices are free explains quite naturally Wegner's observation that his model gives the same result as the CPA with a semicircle distribution applied to the Anderson model.

For the semicircle law one has

$$G_1(z) = \frac{z - (z^2 - 4M)^{1/2}}{2M} = \frac{1}{z - MG_1(z)} \tag{5.7}$$

which yields $R_1(w) = Mw$. This means that only the second noncrossing cumulant is different from zero and thus we have $\mathscr{R}_1(w_1, w_2) = M$. This gives the following solution:

$$G(z) = G_0[z - MG(z)] \tag{5.8}$$

$$\tilde{G}(q; z) = \frac{1}{z - \tilde{v}(q) - MG(z)} \tag{5.9}$$

$$\tilde{C}(q; z_1, z_2) = \frac{M(\tilde{\mathscr{G}}_{12}(q; z_1, z_2))^2}{1 - M\tilde{\mathscr{G}}_{12}(q; z_1, z_2)} \tag{5.10}$$

$$\sigma_{T=0}(\omega \to 0) = \frac{2\pi e^2 nA}{\mathscr{V}} \varrho^2(E) \tag{5.11}$$

with $A = -M^2[\partial \tilde{\mathcal{G}}_{12}(q)/\partial q^2]|_{q=0}$. These formulas were found by Wegner[8] and later rederived by Khorunzhy and Pastur.[9] The deformed semicircle law (5.8) has also appeared earlier in the work of Pastur[25] as the solution for the problem of determining the eigenvalue distribution of a sum $W+D$ of a symmetric Gaussian random matrix W and a nonrandom diagonal matrix D. By our remarks in Section 2, this latter problem is nothing but calculating the free convolution of the distribution of W and of D, and hence, in the light of Theorem 1, the coincidence of Wegner's and Pastur's result appears as no surprise.

One should also note that in the context of the free convolution the semicircle distribution plays the same role as the Gaussian distribution for the classical convolution. This can be seen, for instance, from the fact that only the second noncrossing cumulant is different from zero for the semicircle distribution, similarly as only the second usual cumulant is nonvanishing for the Gaussian distribution. For more details on the "free Gaussian" and related topics, such as free central limit theorem or free Poisson law, we refer to refs. 15, 17, and 23.

5.4. q-Noise: An Interpolation

In ref. 26 we introduced a new class of stochastic processes which interpolate continuously between classical, Gaussian, random matrix, dichotomic, and Poisson processes. This construction can be adapted for quenched multisite disorder as follows: Let the disorder at each site r be given by

$$\hat{f}_r := \sigma(a_r + a_r^\dagger) + \xi a_r^\dagger a_r \tag{5.12}$$

in terms of deformed annihilation and creation operators a_r, $a_r^\dagger$ on some Hilbert space $\mathcal{H}$. These operators satisfy at each site r the deformed canonical commutation relations

$$a_r a_r^\dagger - q a_r^\dagger a_r = \mathbf{1} \tag{5.13}$$

$$a_r |0\rangle = 0 \tag{5.14}$$

where $\mathbf{1}$ and $|0\rangle$ denote the identity operator and the vacuum in $\mathcal{H}$, respectively. At different sites $r \neq r'$ the operators are assumed to be free, implying that $\hat{f}_1, \hat{f}_2, \ldots$ are free, i.e.,

$$a_r a_{r'}^\dagger \equiv 0, \qquad r \neq r' \tag{5.15}$$

The deformation parameter q is real and varies continuously in the interval $-1 \leqslant q \leqslant 1$. For $\xi = 0$, the limiting cases $q = 1$ and $q = -1$ describe

Gaussian and dichotomic disorder, respectively, whereas the case $q=0$ corresponds to Wegner's n-orbital model. The $\xi a_r^\dagger a_r$ term allows us to include Poisson-like disorder.[26, 27]

Equation (5.15) is an alternative representation of those free random variables which can be represented by deformed creation and annihilation operators. To make the construction clear, let us formulate the original Anderson model for Gaussian site-diagonal disorder ($q=1$, $\xi=0$) in this language: $\hat{f}_r := \sigma(a_r + a_r^\dagger)$ with $a_r a_{r'}^\dagger - a_{r'}^\dagger a_r = \delta_{r,r'}\mathbf{1}$ for all r, r', in particular, $a_r a_{r'}^\dagger = a_{r'}^\dagger a_r$ for $r \neq r'$, which is clearly different from (5.15).

We can now identify moments of the random variables f_r in (1.3) with the Hilbert space vacuum expectation values of products of $\hat{f}_r$ by means of a generalized Wick theorem.[26, 28] By using the partial cumulants we have calculated the 1PG of H_1 [cf. Eq. (36) in ref. 26]

$$
\begin{aligned}
G_1(z) &= \frac{1}{z - R_1[G_1(z)]} \\
&= \cfrac{1}{z - \cfrac{\sigma^2 q^{(0)}}{z - \xi q^{(0)} - \cfrac{\sigma^2 q^{(1)}}{z - \xi q^{(1)} - \cfrac{\sigma^2 q^{(2)}}{z - \xi q^{(2)} - \cfrac{\sigma^2 q^{(3)}}{\ddots}}}}} \\
&=: 1/(z - (\sigma^2 q^{(0)}/(z - \xi q^{(0)} - (\sigma^2 q^{(1)}/(z - \xi q^{(1)} \\
&\quad - (\sigma^2 q^{(2)}/(z - \xi q^{(2)} - (\sigma^2 q^{(3)}/\ldots)\ldots)
\end{aligned}
\tag{5.16}
$$

where

$$
q^{(k)} := 1 + q + q^2 + \cdots + q^k = \frac{1 - q^{k+1}}{1 - q} \tag{5.17}
$$

Thus,

$$
\begin{aligned}
R_1[G(z)] = {} & G(z)\,\sigma^2 q^{(0)}/(1 + G(z)(R_1[G(z)] - \xi q^{(0)}) \\
& + (G(z)^2\ \sigma^2 q^{(1)}/(1 + G(z)(R_1[G(z)] - \xi q^{(1)}) \\
& + (G(z)^3\,\sigma^2 q^{(2)}/(1 + G(z)(R_1[G(z)] - \xi q^{(2)}) \\
& + (G(z)^4\,\sigma^2 q^{(3)}/\ldots)\ldots)
\end{aligned}
\tag{5.18}
$$

which together with

$$G(z) = G_0[z - R_1[G(z)]] \tag{5.19}$$

is a closed set of nonlinear self-consistent equations for the 1PG and $R_1(w)$. The continued fraction (5.18) can be summed in closed form for $q = -1$, where one finds, for $\xi = 0$, $R_1[G(z)] = \{[1 + 4\sigma^2 G^2(z)]^{1/2} - 1\}/2G(z)$, and for $q = 0$, where one finds, for $\xi = 0$, $R_1[G(z)] = \sigma^2 G(z)$ and thereby Wegner's model with $\sigma^2 = M$.

6. SUMMARY

In this paper we have applied the concept of free random variables, invented by Voiculescu in a mathematical context, to the tight-binding Hamiltonian with site-diagonal disorder of an electron in a periodic solid. The difference of our model from the usual Anderson model lies in the fact that instead of assuming the disorder to be independent at different lattice sites, we have assumed it to be free.

Both freeness and independence can be considered as a rule for calculating mixed moments of random variables. In contrast to the case of independent disorder, free noise does imply a treatable relation between H_0 and H_1: they are also free. This finally allows us to close the infinite hierarchy of equations of motion and to calculate all physically relevant quantities.

In Section 3 we have argued that in the limit $n \to \infty$ free noise can be represented by $n \times n$ random matrices which are randomly rotated against each other at different lattice sites, starting from a matrix with fixed but arbitrary eigenvalue distribution in the limit $n \to \infty$. In this sense, our model is an extension of Wegner's n-orbital model for the Gaussian ensemble to arbitrary eigenvalue distribution in the energy level space. A striking property of our model is that both the long-range behavior and the zero-frequency limit of the 2PG are universal with respect to the eigenvalue distribution in the energy level space.

One surprising feature of the Wegner model is that its solution coincides with a special CPA solution. This generalizes also to our model. In Section 4 we have shown that our solution for the 1PG and the 2PG also solves the CPA equations for the Anderson model with the same distribution of disorder. Note that we specify our model rigorously in the beginning and that we are able to calculate all quantities without any further approximation. Thus our multisite model is a rigorous mean-field model for the usual single-site CPA. The R-transform of Voiculescu, R_1, may be considered as the formal solution of the CPA equations for arbitrary disorder. It possesses the physical interpretation as an effective local potential; the corresponding quantity for the 2PG, $\mathscr{R}_1$, can be considered as an effective local electron–electron interaction. Cleary, as seen in Section 5, aside

from some specific distributions, both functions cannot be calculated analytically. However, due to the mentioned universality, the Wegner model is exemplary in many respects and it might be sufficient to restrict oneself to this case in the general frame of a mean-field approximation.

Furthermore, our description using the theory of free random variables and the notion of noncrossing cumulants allows a straightforward generalization to the case of dynamical disorder and thus promises to give a rigorous model for dynamical CPA. These subjects will be pursued further in forthcoming investigations.

ACKNOWLEDGMENTS

Helpful discussions with Dr. Petr Chvosta and Dr. Reimer Kühn and valuable comments of Prof. Dan Voiculescu are gratefully acknowledged. We would particularly like to thank Prof. Franz Wegner for his insightful suggestions and his careful reading of the manuscript. This work was partly supported by the Deutsche Forschungsgemeinschaft (R.S.).

REFERENCES

1. P. W. Anderson, *Phys. Rev.* **109**:1492 (1958).
2. P. Lloyd, *J. Phys. C* **2**:1717 (1969).
3. E. N. Economou, *Green's Function in Quantum Physics* (Springer-Verlag, Berlin, 1983).
4. I. M. Lifshitz, S. A. Gredeskul, and L. A. Pastur, *Introduction to the Theory of Disordered Systems* (Wiley, New York, 1988).
5. P. Soven, *Phys. Rev.* **156**:809 (1967).
6. D. V. Taylor, *Phys. Rev.* **156**:1017 (1967).
7. B. Velický, *Phys. Rev.* **184**:614 (1969).
8. F. Wegner, *Phys. Rev. B* **19**:783 (1979).
9. A. M. Khorunzhy and L. A. Pastur, *Commun. Math. Phys.* **153**:605 (1993).
10. E. P. Wigner, *Ann. Math.* **62**:548 (1955); **67**:325 (1958).
11. L. Arnold, *J. Math. Anal Appl.* **20**:262 (1967).
12. D. Voiculescu, in *Lecture Notes in Mathematics*, No. 1132 (Springer, Berlin, 1985), p. 556.
13. D. Voiculescu, *J. Funct Anal.* **66**:323 (1986).
14. D. Voiculescu, *Invent. Math.* **104**:201 (1991).
15. D. Voiculescu, K. Dykema, and A. Nica, *Free Random Variables* (American Mathematical Society, Providence, Rhode Island, 1992).
16. D. Voiculescu, *Commun. Math. Phys.* **155**:71 (1993); *Invent. Math.*, to appear.
17. R. Speicher, *Prob. Theory Related Fields* **84**:141 (1990).
18. B. Kümmerer and R. Speicher, *J. Funct. Anal.* **103**:372 (1992).
19. R. Speicher, *Math. Ann.* **298**:611 (1994).
20. R. Speicher, *RIMS* **29**:731 (1993).
21. P. Neu and R. Speicher, *J. Phys. A: Math. Gen.* **28**:L79 (1995).
22. P. Neu and R. Speicher, *Z. Phys. B* **92**:399 (1993).

23. H. Maassen, *J. Funct. Anal.* **106**:409 (1992).
24. H. Bercovici and D. Voiculescu, *Indiana U. Math. J.* **42**:733 (1993).
25. L. A. Pastur, *Teor. Mat. Fiz.* **10**:102 (1973).
26. P. Neu and R. Speicher, *Z. Phys. B* **95**:101 (1994).
27. R. L. Hudson and K. R. Parthasarathy, *Commun. Math. Phys.* **93**:301 (1984).
28. U. Frisch and R. Bourret, *J. Math. Phys.* **11**:364 (1970).