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LETTER TO THE EDITOR

Random matrix theory for CPA: generalization of Wegner's n-orbital model

Peter Neu† and Roland Speicher‡§

† Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 19, 69120 Heidelberg, Germany

‡ Institut für Angewandte Mathematik, Universität Heidelberg, Im Neuenheimer Feld 294, 69120 Heidelberg, Germany

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Abstract. We introduce a generalization of Wegner's n-orbital model for the description of randomly disordered systems by replacing his ensemble of Gaussian random matrices by an ensemble of randomly rotated matrices. We calculate the one- and two-particle Green functions and the conductivity exactly in the limit $n \to \infty$. Our solution solves the coherent potential approximation equation of the ($n = 1$) Anderson model for arbitrarily distributed disorder. We show how the Lloyd model is included in our model.

The treatment of physical systems with disorder presents one of the great challenges in statistical physics. Realistic multi-site models, like the Anderson model [1], are in general unsolvable. Exact calculations are only possible in one pathological special case—namely for the Lloyd model [2] with Cauchy distributed disorder. Otherwise one has to use approximation techniques which reduce the multi-site to single-site models and treat them self-consistently. The most prominent of these methods is the so-called coherent potential approximation (CPA), see, e.g., [3].

Wegner [4] introduced a generalization of the Anderson model by putting n electronic states at each site and describing the disorder by Gaussian random matrices in these electronic states. Whereas for $n = 1$ this reduces to the usual (unsolvable) Anderson model, the opposite limit $n \to \infty$ becomes exactly solvable. Interestingly, the solution of this multi-site model coincides with a special CPA solution.

In this letter we introduce a generalization of Wegner's model by replacing his ensemble of Gaussian random matrices by a more general ensemble of random matrices—thus allowing arbitrarily distributed disorder. Nevertheless, by using recent results from Voiculescu [5, 6] and Speicher [7, 8] on the mathematical concept of 'freeness', we are still able to calculate the Green functions of this model in the limit $n \to \infty$ exactly. Again our solution solves the CPA equation of the ($n = 1$) Anderson model. Hence our model can be regarded as a rigorous mean-field model for CPA for arbitrarily distributed disorder.

Let us first recall Wegner's model. He considers a d-dimensional lattice where at each site r there are n electronic levels $|r\alpha\rangle$ numbered by $\alpha = 1, \ldots, n$. The interaction is governed by a Hamiltonian of the form

$$H = H_0 + H_1 \tag{1}$$

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where H_0 is deterministic, translational-invariant and diagonal in the electronic levels,

$$H_0 = \sum_{r,r',\alpha} v_{r-r'} |r\alpha\rangle\langle r'\alpha| \tag{2}$$

and H_1 describes the site-diagonal disorder

$$H_1 = \sum_{r,\alpha,\beta} \frac{1}{\sqrt{n}} f_r^{\alpha\beta} |r\alpha\rangle\langle r\beta|. \tag{3}$$

There, $f_r = \left((1/\sqrt{n}) f_r^{\alpha\beta}\right)_{\alpha,\beta=1}^{n}$ are Gaussian random matrices and the entries of f_r and of $f_{r'}$ are independent for $r \neq r'$. (This is the site-diagonal model of Wegner, we will not treat his 'local gauge invariant' model here.) By using techniques for calculating moments of Gaussian random matrices [9, 10], Wegner was able to calculate the one- and two-particle Green function in the limit $n \to \infty$.

To explain our generalization let us diagonalize the random matrices f_r in the form $f_r = u_r \hat{f}_r u_r^*$. Thus the ensemble of the f_r is determined by an ensemble of diagonal matrices $\hat{f}_r$ and an ensemble of unitary matrices u_r. In the limit $n \to \infty$, Wegner's original formulation is recovered if the diagonal $\hat{f}_r$ are taken as deterministic matrices having Wigner's semi-circle [9] as the eigenvalue distribution and if the u_r are random unitary matrices, given by the canonical invariant or Haar measure on $U(n)$, such that u_r and $u_{r'}$ are chosen independently of $U(n)$ for $r \neq r'$. Since this ensemble is invariant under independent rotations at different sites we may also replace the different $\hat{f}_r$ by one single (not necessarily diagonal) f, i.e. we have $f_r = u_r f u_r^*$ with the ensemble of u_r as stated above.

The advantage of this reformulation of Wegner's model is that now a generalization is obvious: we are *a priori* totally free in the choice for f. Thus our model is given by the following Hamiltonian:

$$H = \sum_{r,r',\alpha} v_{r-r'} |r\alpha\rangle\langle r'\alpha| + \sum_{r,\alpha,\beta} (u_r f u_r^*)_{\alpha,\beta} |r\alpha\rangle\langle r\beta| \tag{4}$$

where f is a deterministic Hermitian $n \times n$ matrix and $u_r \in U(n)$ are random unitary matrices, chosen independently for different sites. This means that we act at each site r with a copy $f_r := u_r f u_r^*$ 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 $r \neq r'$.

The possibility of treating this model in the limit $n \to \infty$ arises from the important observation by Voiculescu [5] (see also [11]) that there is a connection with his concept of free random variables [12, 6, 13]. Denote by $\langle \ldots \rangle_{\text{ens}}$ the average over our ensemble of random unitary matrices and let

$$\langle \ldots \rangle := \left\langle \frac{1}{n} \sum_{\alpha=1}^{n} \langle\alpha| \ldots |\alpha\rangle \right\rangle_{\text{ens}} \tag{5}$$

count the averaged eigenvalue distribution of our $n \times n$ matrices. Then we have for all $m \in \mathbb{N}$ and for all polynomials $p_1, \ldots, p_m$ with $\langle p_i(f) \rangle = 0$ $(i = 1, \ldots, m)$ in the limit $n \to \infty$ that also

$$\langle p_1(f_{r(1)}) p_2(f_{r(2)}) \ldots p_m(f_{r(m)}) \rangle = 0 \tag{6}$$

for all sequences of indices $r(1), \ldots, r(m)$, where all consecutive indices are different, i.e. where $r(i) \neq r(i+1)$ for all $i = 1, \ldots, m-1$. An example of (6) is

$$\langle p_1(f_1) p_2(f_2) p_3(f_1) p_4(f_2) \rangle = 0 \tag{7}$$

whereas for sequences with coinciding neighbouring indices one gets non-vanishing results like

$$\begin{aligned}\langle p_1(f_1)p_2(f_2)p_3(f_2)p_4(f_1)\rangle &= \langle p_1(f_1)p_4(f_1)\rangle\langle p_2(f_2)p_3(f_2)\rangle \\ &= \langle p_1(f)p_4(f)\rangle\langle p_2(f)p_3(f)\rangle.\end{aligned} \tag{8}$$

The property (6), recently introduced by Voiculescu [13, 6] under the name of 'freeness' in the mathematical literature, allows, as in Wegner's case, all mixed moments of the matrices f_r to be calculated (as, e.g., in (8)) and thus exact expressions to be derived for the Green functions of our model in the limit $n \to \infty$. Whereas one usually finds an infinite hierarchy of equations for averaged quantities, it is exactly the property of freeness (6) which closes our equations. For an effective handling of the calculations one needs the R-transform machinery of Voiculescu [14, 6] and Speicher's concept of non-crossing cumulants [7, 8]. The concrete calculations will be published elsewhere, here we only want to give the results.

The most important quantity is (the diagonal part of) the one-particle Green's function (1PG)

$$G(z) := \left\langle \frac{1}{n}\sum_{\alpha=1}^{n}\left\langle r\alpha\left|\frac{1}{z-H}\right|r\alpha\right\rangle\right\rangle_{\text{ens}} \tag{9}$$

the spectral function of which yields the density of states. Note that, due to the translation invariance of our Hamiltonian, $G(z)$ is independent of r and hence the local and global density of states coincide. If we denote in the same way the 1PG of the deterministic and disorder parts of H by G_0 and G_1, respectively, i.e.

$$G_0(z) = \left\langle r\left|\frac{1}{z-H_0}\right|r\right\rangle \tag{10}$$

$$G_1(z) = \left\langle \frac{1}{n}\sum_{\alpha=1}^{n}\left\langle \alpha\left|\frac{1}{z-f_r}\right|\alpha\right\rangle\right\rangle_{\text{ens}} = \frac{1}{n}\sum_{\alpha=1}^{n}\left\langle \alpha\left|\frac{1}{z-f}\right|\alpha\right\rangle \tag{11}$$

then the crucial property (6) allows us to derive the following self-consistent equation for $G(z)$:

$$G(z) = G_0\Big(z - R_1\big(G(z)\big)\Big) \tag{12}$$

where $R_1(z)$ is a kind of self-consistent self-energy for H_1, namely it is defined by

$$G_1(z) = \frac{1}{z - R_1\big(G_1(z)\big)} \tag{13}$$

with $R_1(0) = 0$. In the special case of a semi-circle eigenvalue distribution for f, G_1 is given by

$$G_1(z) = \frac{z - \sqrt{z^2 - 4\sigma^2}}{2\sigma^2} = \frac{1}{z - \sigma^2 G_1(z)} \tag{14}$$

showing that $R_1(z) = \sigma^2 z$. In this case our formula (12) reduces to Wegner's result [4, 15]:

$$G(z) = G_0\Big(z - \sigma^2 G(z)\Big). \tag{15}$$

Given $G(z)$ and $R_1(z)$, one can derive linear self-consistent equations for the one-particle and two-particle Green's functions. Again, the freeness property (6) is the essential ingredient for closing the equations. For the Fourier transform of the 1PG one obtains

$$\tilde{G}(q;z) = \frac{1}{z - v(q) - R_1\big(G(z)\big)} \tag{16}$$

with $v_r = \int_q v(q)e^{iqr}$ where

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

$\mathcal{V}$ being the volume of the first Brillouin zone (1BZ). For $R_1(z) = \sigma^2 z$ this reduces again to Wegner's result [4, 15].

The 2PG determines the conductivity as a velocity–velocity correlation function. Although, in general, the 2PG contains an additional term, one obtains by the symmetry argument $v_{-r} = v_r$ that only the product of the 1PGs contributes. Thus one finds for zero temperature and in the dc-limit $\omega \to 0$

$$\sigma(\omega, 0) = \frac{2\pi e^2 B}{\mathcal{V}}\,\mu^2(R_1(G); E_F) \tag{17}$$

where

$$B := \int_q \frac{|\nabla v(q)|^2}{|v(q) - \zeta(E_F + \omega + i0^+)|^2 |v(q) - \zeta(E_F + i0^+)|^2}$$

with $\zeta(z) = z - R_1(G(z))$ and the spectral function

$$\mu(R_1(G); E) = -\frac{1}{\pi}\operatorname{Im} R_1\big(G(z = E + i0^+)\big). \tag{18}$$

For $R_1(z) = \sigma^2 z$ this reduces to Wegner's result in a form given by Khorunzhy and Pastur [15].

The generality of our solution may be seen from the fact that it also includes the Lloyd model as a special case: Namely, choose a Cauchy distribution with parameter γ as the eigenvalue distribution for f. Then

$$G_1(z) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\gamma}{\gamma^2 + t^2}\frac{1}{z - t}\,dt = \frac{1}{z - i\gamma} \tag{19}$$

hence $R_1(z) = i\gamma$. This shows that the Cauchy distribution behaves in all relevant aspects like an imaginary δ distribution. For δ distributions, however, there is no difference between our model and the original Anderson Hamiltonian (see also [16, 17]). Since the Anderson model with Cauchy distributed disorder is nothing other than the Lloyd model, the latter is included in our investigations. In particular we recover from (12) the 1PG of the Lloyd model [2]

$$G(z) = G_0\big(z - i\gamma\big). \tag{20}$$

One surprising feature of the Wegner model is that its solution coincides with a special CPA solution. This also generalizes to our model. In general, the CPA solution for the Anderson model with single-site random variable X is given by the two equations

$$G(z) = G_0\big(z - \Sigma(z)\big) \tag{21}$$

and

$$\left\langle \frac{X - \Sigma(z)}{1 - (X - \Sigma(z))G(z)} \right\rangle = 0. \tag{22}$$

The first of these equations coincides with our solution (12) if we identify $\Sigma(z) = R_1(G(z))$. By using the equivalent form of (13), namely

$$G_1\big(R_1(z) + z^{-1}\big) = z \tag{23}$$

it can be checked that our solution also fulfils (22) if we choose as distribution for X the eigenvalue distribution of f. Note that we rigorously specified our model in the beginning

and that we are able to calculate all quantities without any further approximation. Thus our multi-site model is a rigorous mean-field model for the usual single-site CPA. One should also note that our previous remarks about the Lloyd model can now be taken as an explanation for the well known fact that the CPA is exact for the Lloyd model.

As an instructive example of our formalism let us consider the one-dimensional lattice with nearest-neighbour interaction and binary site-diagonal disorder for the special case $v = \sigma = 1$, where $2v$ is the half-band-width and σ^2 is the variance of the disorder. Then we have $G_0(z) = 1/\sqrt{z^2-1}$ and $R_1(z) = (\sqrt{1+z^2}-1)/2z$, which yields as a solution of (12):

$$G(z) = \frac{8}{6\sqrt{z^2-2}+2z}. \tag{24}$$

This provides

$$\mu(R_1(G); E) = \frac{1}{4\pi}\sqrt{2-E^2}\,\Theta(\sqrt{2}-E) \tag{25}$$

i.e. together with (17) a finite conductivity everywhere inside the band $\left[-\sqrt{2},\sqrt{2}\right]$.

Since we can prescribe in our model an arbitrary distribution for f, or for X in the CPA formulation, it is clear that our formalism is capable of covering many quite different examples, e.g., a superposition of binary noise or, more generally, the recently investigated q-noise [18]. Furthermore, our description using the theory of free random variables and the notion of non-crossing 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.

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References

[1] Anderson P W 1958 *Phys. Rev.* **109** 1492
[2] Lloyd P 1969 *J. Phys. C: Solid State Phys.* **2** 1717
[3] Lifshitz I M, Gredeskul S A and Pastur L A 1988 *Introduction to the Theory of Disordered Systems* (New York: Wiley)
[4] Wegner F 1979 *Phys. Rev.* **B19** 783
[5] Voiculescu D 1991 *Invent. Math.* **104** 201
[6] Voiculescu D, Dykema K and Nica A 1992 *Free Random Variables* (Providence, RI: AMS)
[7] Speicher R 1994 *Math. Ann.* **298** 611
[8] Neu P andSpeicher R 1993 *Z. Phys.* B **92** 399
[9] Wigner E P 1955 *Ann. Math.* **62** 548; 1958 **67** 325
[10] Arnold L 1967 *J. Math. Anal. Appl.* **20** 262
[11] Speicher R 1993 *RIMS* **29** 731
[12] Speicher R 1990 *Prob. Theor. Rel. Fields* **84** 141
[13] Voiculescu D 1985 *Lecture Notes in Mathematics* **1132** 556
[14] Voiculescu D 1986 *J. Funct. Anal.* **66** 323
[15] Khorunzhy A M and Pastur L A 1993 *Commun. Math. Phys.* **153** 605
[16] Maassen H 1992 *J. Funct. Anal.* **106** 409
[17] Bercovici H and Voiculescu D 1993 *Indiana U. Math. J.* **42** 733
[18] Neu P and Speicher R 1994 *Z. Phys.* B **95** 101