Physical applications of freeness

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Introduction

The mathematical concept 'freeness' was introduced by Voiculescu about 15 years ago in order to get some insight into the structure of the von Neumann algebras of the free groups. The starting idea of Voiculescu was to separate the notion of freeness from that concrete problem and to consider it on its own sake.

One leading principle of his investigations was to consider freeness as a non-commutative analogue to the classical notion 'independence of random variables'

This approach was very successful. Gradually it became clear that freeness has indeed a very interesting structure of its own and that there exist a lot of links to other fields.

One of the main links of freeness to an apriori unrelated context is the description of random matrices via freeness. This has opened the possibility to use freeness as an exact mathematical concept for the description of physical models and approximations which build (explicitely or implicitly) on random matrices.

One model of this kind, which recently has attracted some interest, is the search for masterfields in the large N limit of matrix models or QCD_2.

Here, I will report on the occurrence of freeness in another physical context – namely the so-called *coherent potential approximation (CPA)* for the Anderson model (which models electron hopping in disordered solids). This CPA has apriori no connection with random matrices, thus the appearance of freeness is even more surprising.

Freeness and random matrices

Let me start by recalling the basic definitions of free probability theory (see, e.g., [VDN, V2]). Since we are led by analogy with classical probability theory (in particular with the notion of 'independence') we will use a probabilistic language. Following a physical tradition we will denote the expectation of some element a with respect to a given functional φ usually by $\langle a\rangle := \varphi(a)$.

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Definition: 1) A *non-commutative probability space* $(\mathcal{A}, \varphi)$ consists of a unital algebra $\mathcal{A}$ and a unital linear functional

$$\varphi : \mathcal{A} \to \mathbf{C}, \qquad \varphi[1] = 1.$$

2) A *random variable* X is an element of the given algebra $\mathcal{A}$.
3) We say that random variables $X_1, X_2, \ldots \in \mathcal{A}$ are *free* (with respect to φ) 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 the following implication:

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

whenever

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

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).

This definition of freeness should be seen as a rule for calculating mixed moments in the free variables in terms of moments of the single variables. For example, if X and Y are free then the calculation of the mixed moment $\langle XYXY \rangle$ is reduced to an expression which vanishes according to the above definition of freeness, namely

$$\langle (X - \langle X \rangle 1)(Y - \langle Y \rangle 1)(X - \langle X \rangle 1)(Y - \langle Y \rangle 1) \rangle = 0,$$

leading to

$$\langle XYXY \rangle = \langle X^2 \rangle \langle Y \rangle^2 + \langle X \rangle^2 \langle Y^2 \rangle - \langle X \rangle^2 \langle Y \rangle^2.$$

The above definition of freeness was introduced to model special situations which appear in the von Neumann algebras of free groups. These von Neumann algebras are related to creation and annihilation operators on the full Fock space (these operators generate the Cuntz algebras or their extensions by the compacts). So it is no surprise that free random variables can be modelled quite canonically with the help of creation and annihilation operators on the full Fock space. Much more surprising is the appearance of freeness in a quite different context, namely as a model for random matrices in the limit $n \to \infty$.

Such random matrices X_n are $n \times n$-matrices whose entries are classical random variables and usually one is interested in the averaged eigenvalue-distribution $\mathrm{distr}(X_n)$ of these matrices corresponding to a state given by the averaged normalized trace.

Theorem [V1]: 1) Gaussian random matrices
Let

$$X_n = (a_{ij}^{(n)})_{i,j=1}^n, \qquad Y_n = (b_{ij}^{(n)})_{i,j=1}^n$$

be symmetric random $n \times n$-matrices with

- $a_{ij}^{(n)}$ $(1 \leq i \leq j \leq n)$ are mutually independent and normally distributed with mean zero and variance $1/n$.

- $b_{ij}^{(n)}$ $(1 \le i \le j \le n)$ are mutually independent and normally distributed with mean zero and variance $1/n$.
- all $a_{ij}^{(n)}$ are independent from all $b_{kl}^{(n)}$.

Then X_n and Y_n become free in the limit $n \to \infty$ with respect to

$$\langle \cdot \rangle := \langle \mathrm{tr}(\cdot) \rangle_{ensemble}.$$

2) randomly rotated matrices
Let A_n and B_n be symmetric deterministic (e.g. diagonal) $n \times n$-matrices with

$$\lim_{n\to\infty} \mathrm{distr}(A_n) = \mu, \qquad \lim_{n\to\infty} \mathrm{distr}(B_n) = \nu$$

for some compactly supported probability measures μ and ν. Let U_n be a random unitary matrix from the ensemble

$$\Omega_n = (\mathcal{U}(n), \mathit{Haar\ measure}).$$

Consider now

$$X_n := A_n, \qquad Y_n := U_n B_n U_n^*.$$

Then X_n and Y_n become free in the limit $n \to \infty$ with respect to

$$\langle \cdot \rangle := \langle \mathrm{tr}(\cdot) \rangle_{\Omega_n}.$$

Note that the second part of the theorem is much more general than the first one because Gaussian random matrices have in the limit $n \to \infty$ always Wigner's semicircle as eigenvalue distribution. In the second part, however, we are free to choose any distribution μ and ν for the limiting eigenvalue distribution.

CPA and n-orbital models

The Anderson model for the description of the hopping of an electron in a d-dimensional disordered lattice is given by a Hamiltonian of the form

$$H = H_0 + H_1 = \sum_{r,r' \in \mathbf{Z}^d} v_{|r-r'|} |r\rangle\langle r'| + \sum_{r \in \mathbf{Z}^d} \epsilon_r |r\rangle\langle r|,$$

where H_0 describes the deterministic translation-invariant hopping of the electron between different sites r and r' and additional random disorder is introduced in the form of H_1. The $\{\epsilon_r \mid r \in \mathbf{Z}^d\}$ are assumed to be identically distributed, independent random variables.

One of the main quantities one is interested in is the one-particle Green function $G(z)$ of that model,

$$G(z) := \langle \langle r | \frac{1}{z - H} | r \rangle \rangle_{ensemble}$$

(which is independent of r because of the translation invariance of our Hamiltonian). If $G_0(z)$ and $G_1(z)$ are the one-particle Green functions of H_0 and H_1, respectively, then the problem one has to face is the following: Calculate $G(z)$ out of the knowledge of $G_0(z)$ and $G_1(z)$.

There exits no analytic solution to this problem. Therefore, in dealing with the Anderson model one often uses approximations. One of the most successful approximations is the so-called *coherent potential approximation (CPA)* (see, e.g., [CPA]).

Roughly, this approximation consists in the following steps:

- We construct a mean field approximation by replacing the inhomogenous medium by an effective homogenous medium with an effective potential Σ, thus we replace the Green function of our original problem by $\tilde{G}(z) = G_0(z - \Sigma(z))$.

- We connect the original problem with the new problem via $G = \tilde{G} + \tilde{G}\langle J\rangle\tilde{G}$, where J is the scattering operator with respect to Σ. We write this scattering operator in terms of local fluctuations t_r as

$$\langle J\rangle = \sum_r \langle J_r\rangle \qquad \text{where} \qquad \langle J_r\rangle = \langle t_r(1 + \tilde{G}\sum_{r'\neq r} J_{r'})\rangle.$$

  Up to this point, all equations are exact. But now, we make our (single-site) approximation by factorizing the expectation of the product $t_r J_{r'}$ into the product of the corresponding expectations, i.e. we continue with

$$\langle J_r\rangle = \langle t_r\rangle(1 + \tilde{G}\sum_{r'\neq r}\langle J_{r'}\rangle).$$

- In order to have $G = \tilde{G}$ we require that $\langle t_r\rangle = 0$ which gives the following self-consistent CPA-equation

$$\Big\langle \frac{\epsilon_r - \Sigma(z)}{1 - (\epsilon_r - \Sigma(z))\tilde{G}(z)} \Big\rangle_{ensemble} = 0.$$

Although this approximation was quite successful, its mathematical status remained unclear. In particular the following question was open: The approximation takes place on the level of the Green functions by some ad hoc factorization. Is it possible to describe CPA on the level of the Hamiltonian itself, i.e. is there a well-defined Hamiltonian $\tilde{H}$, such that the exact Green function of $\tilde{H}$ coincides with the CPA solution $\tilde{G}$?

In [NS1, NS2] we showed that this is indeed the case and that this Hamiltonian $\tilde{H}$ can be described in terms of freeness. This is quite surprising since there is no explicit appearance of random matrices in the above approximation.

But there was one hint in the literature on a possible connection between CPA and random matrices (and thus freeness) – the so-called n-orbital model of Wegner [Weg]. This is another kind of approximation for the Anderson model which apriori has no direct connection with CPA.

Wegner introduced additional degrees of freedom at each site – so-called orbitals $\alpha = 1, \ldots, n$ (where n is a fixed natural number which will be sent to ∞ in the end).

So instead of $|r\rangle$ he has $|r, \alpha\rangle$ as basis vectors and he replaced the original Anderson Hamiltonian by a new one, $H^{(n)}$, where the deterministic part is diagonal in the orbitals, and the random part is taken as diagonal in the sites, but totally random in the orbitals. Thus Wegner considered the Hamiltonian

$$H^{(n)} = \sum_{r,r',\alpha} v_{|r-r'|} |r, \alpha\rangle\langle r', \alpha| + \sum_{r,\alpha,\beta} f_r^{\alpha\beta} |r, \alpha\rangle\langle r, \beta|$$

where the following assumptions on the matrices $f_r = (f_r^{\alpha\beta})_{\alpha,\beta=1}^n$ are made:

- for fixed r, each f_r is a symmetric Gaussian random matrix, i.e. all entries $f_r^{\alpha\beta}$ for $1 \leq \alpha \leq \beta \leq n$ are independent and normally distributed (with mean 0 and variance $1/n$).
- for $r \neq r'$, all entries of f_r are independent from all entries of $f_{r'}$.

The main reason for introducing such a model was that, by properties of random matrices, this model becomes solvable in the limit $n \to \infty$. Wegner nocticed also that this solution has a surprising feature: it solves the CPA-equation for a special disorder, namely for Wigner's semi-circle distribution of the ϵ_r.

CPA and freeness

By comparing the above assumptions on the f_r with the mentioned theorem of Voiculescu we see that, in our mathematical language, Wegner's model can in the limit $n \to \infty$ be described by a Hamiltonian $\tilde{H}$ of the form

$$\tilde{H} = \sum_{r,r'} v_{|r-r'|} |r\rangle\langle r'| + \sum_r f_r |r\rangle\langle r|,$$

where $\{f_r \mid r \in \mathbf{Z}^d\}$ are free random variables which are identically distributed according to Wigner's semi-circle.

But in this reformulation there is now of course no need to restrict the distribution of the f_r to a semi-circle distribution. Thus we consider the following class of *generalized Wegner models*: the Hamiltionian $\tilde{H}$ is as above where the f_r are free and identically distributed according to an arbitrary distribution P.

Again, by using the quite developed theory of freeness – in particular the R-transform machinery [VDN, NS2] – we are able to solve this model (by deriving some implicit relations for the corresponding Green functions) and this can be used to prove the following generalization of Wegner's observation on the connection between his n-orbital model and CPA.

Theorem [NS2]: Let the Hamiltonian $\tilde{H}$ be given as above where the $\{f_r \mid r \in \mathbf{Z}^d\}$ are free and identically distributed according to some distribution P. Then the solution for the one-particle Green function (and also for the two-particle Green function) of that model is identical to the CPA-solution of the corresponding Anderson model where the $\{\epsilon_r \mid r \in \mathbf{Z}^d\}$ are independent and identically distributed according to the same P.

Thus the above Hamiltonian $\tilde{H}$ fulfills exactly what we were looking for in order to get a mathematically rigorous model of CPA and we can now describe CPA as the replacement of independent random variables by free random variables.

Furthermore, the hitherto not well understood connection between CPA and Wegner-like models gets clarified by the realization that, in view of Voiculescu's theorem, Wegner-like models are just a concrete realization of that abstract replacement. In particular, we can also write down a concrete realization of our generalized Wegner models (and thus of CPA) in terms of orbitals. Namely, $\tilde{H}$ can be seen as the limit $n \to \infty$ of the following Hamiltonian:

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

where f is a fixed symmetric $n \times n$-matrix with the given distribution P, and u_r are random unitary matrices, choosen independently for $r \neq r'$.

An application of our results to a mathematically rigorous calculation of diffusion exponents can be found in [SBB].

References

[CPA] P. Soven: Phys. Rev. 156 (1967), 809; D.V. Taylor: Phys. Rev. 156 (1967), 1017; B. Velicky: Phys. Rev. 184 (1969), 614.

[NS1] P. Neu and R. Speicher: Random matrix theory for CPA: generalization of Wegner's n-orbital model. J. Phys. A 28 (1995), L79-L83.

[NS2] P. Neu and R. Speicher: Rigorous mean-field model for coherent-potential approximation: Anderson model with free random variables. J. Stat. Phys. 80 (1995), 1279-1308.

[SBB] H. Schulz-Baldes and J. Bellissard: Anomalous transport: a mathematical framework. Preprint 1997

[V1] D. Voiculescu: Limit laws for random matrices and free products. Invent. Math. 104 (1991), 201-220.

[V2] D. Voiculescu: Free probability theory: random matrices and von Neumann algebras. (Proceedings of the International Congress of Mathematicians, Zürich, 1994) Birkhäuser, Boston, 1995, pp 227-241.

[VDN] D. Voiculescu, K. Dykema, and A. Nica: Free Random Variables. CRM Monograph Series, Vol. 1, AMS, 1992

[Weg] F. Wegner: Phys. Rev. B 19 (1979), 783