Dynamical and Quenched Random Matrices and Homolumo Gap

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Abstract

We consider a rather general type of matrix model, in which the fluctuations of the matrix are partly given by some fundamental randomness and partly dynamically, even quantum mechanically. We then study the homolumo-gap effect, which means that we study how the level density gets attenuated near the Fermi surface, while considering the matrix as the Hamiltonian matrix for a single fermion interacting with this matrix. In the case of the quenched randomness (the fundamental one) dominating the quantum mechanical one and not too small coupling to the fermions we calculate the homolumo gap that in the first approximation consists of there being essentially no levels for the a single fermion between two steep gap boundaries. The filled and empty level densities are in this first approximation just pushed, each to its side. In the next approximation these steep drops in the spectral density are smeared out to have an error-function shape. The studied model could be considered as a first step towards the more general case of considering a whole field of matrices - defined say on some phase space - rather than a single matrix.

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I. BASIC IDEA

The homolumo gap goes back to the Jahn-Teller effect [1], which describes spontaneous breaking of the molecular symmetry owing to the partial filling of degenerate electron states in the molecular “shell” at the Fermi energy. In general, it is not difficult to see that if some deformation of the molecule could lower the filled and raise the empty levels this would lower the energy of the electrons. Thus an attenuation of the density of electron levels near the Fermi level is expected, i.e. the interval from the highest occupied level (molecular orbit) “homo” up to the lowest unoccupied level (molecular orbit), “lumo”, would be increased. It is from these short hand notations "homo" and "lumo" that the effect has got the name homolumo effect and the spacing between the two levels neighbouring the Fermi level the name homolumo gap.

The point giving an interest to the homolumo effect is that it is so general that one might find in nature many systems expected to show such effect. For example, in the field of material sciences the study of the material-specific characteristics of the homolumo gap attracts a lot of attention, see Ref.[2] as an example. However, dependence of the homolumo gap on the relevant parameters in a specific system may be very complicated due to complexity of interactions involved. Therefore, to study development of the homolumo gap in a set up not so much dependent on the details of the interactions one would rather make some simplified model which captures the main features of such complex systems.

An obvious simplified system to think about is a molecule in which positions of the nuclei and the collective charge distribution of the electrons produce a Hamiltonian for a single electron. We assume that these complicated molecule interactions can be described by a matrix. We consider the matrix elements as dynamical variables due to their dependence on the positions of the nuclei and other dynamical degrees of freedom. Furthermore, we assume that there exists some suitable stable ground state of the molecule, such that the dynamics of the matrix elements can basically be described by a harmonic approximation. Finally, we subject the parameters determining the ground state to some distribution law. This last assumption could be justified in several ways. For example one can simply assume that there is some fundamental randomness in the system or one can argue that in this way one can describe some external influence. Moreover, the system which we consider might be so complicated that we do not want to or cannot treat it in detail. We rather make a statistical ansatz for the hard to compute properties of the system in order to obtain a good treatment of certain general features of the system. Since in any case the Hamiltonian for a single fermion is writable as a matrix it is natural to consider this matrix having a random distribution, but we must nevertheless consider it dynamical, so that it can be acted upon and pushed by forces from the fermions.

In this paper we build the model on these general assumptions. In its ground state the system can be viewed as a particular representative of the models known in the literature as the “random matrix models in an external field” [3, 4]. We believe that by considering various forms of randomness and dynamics in the model one should be able to approach close to specific realistic situations and describe some very general features like the homolumo gap reasonably correctly. In the previous works [5, 6] we had only the quantum mechanical dynamical matrix with the minimum in potential energy occurring for the matrix elements being zero before the fermion interaction term was switched on. We could only obtain a reliable homolumo gap in the limit of strong coupling of the fermions to the matrix., i.e., for \( g > \omega^{3/2} \). In the large-\( N \) limit this resulted in two well-separated semi-circle distributions...
for the matrix level density. Adding the quenched (fundamental) randomness (parametrized by a new parameter $\tilde{\omega}$) increases the spread of the level distribution allowing us to study the region $g \sim \omega^2/\sqrt{\tilde{\omega}}$. In this region the coupling of the fermions is still strong, but the level shift $g/\omega^2$ can be comparable or even smaller compared to the spread in levels given by $\sim 1/\sqrt{\tilde{\omega}}$. In this case we can put forward the picture of the homolumo gap as a gap in a potentially much broader distribution.

In the following section we shall set up our model at first w.r.t. the bosonic degrees of freedom, meaning the matrix $M$ as a dynamical and quenched random system. Then in section III we introduce the fermions and the interaction of the matrix with them, the matrix times a constant $g$ being the single fermion Hamiltonian. After that the spectrum for the filled states is studied and the effect of the fermions acting back on the matrix dynamics is considered in section IV so that a true homolumo gap can be derived. For the calculation the characteristic width of the fluctuations of the Fermi level $\mu_F$ is needed, and the estimation of it is given in Appendix. In section V we discuss the importance of the obtained results and some plans for further work.

II. SET UP OF A MODEL

In order to make an as realistic model as possible w.r.t. the way in which it is random and dynamical, but not so precise in details we want to set up a dynamical matrix, which get fluctuations/randomness in two ways:

- First we could have the randomness of a matrix that simply consists in that the matrix elements are put to random values. Assigning the probability distribution to matrix elements and choosing general symmetry properties (under transposition, such as the matrix being hermitian e.g.) of a matrix leads to a model which can be addressed within standard random matrix theory [7].

- Secondly we want the matrix to be dynamical in the sense that it can be influenced by interaction with fermions. These dynamical degrees of freedom can then be quantized, resulting in the fluctuations of the ground state.

For simplicity we take the random distribution to be Gaussian, and the dynamics to be that of harmonic oscillators, which happen to deliver Gaussian fluctuations too.

Let us explain how these proposals for distribution of the matrices lead to the following set up. We start with fundamental random numbers giving what we call the central values or bottom of potentials matrix element values. The simplest choice of a distribution is to let each real and imaginary part of the matrix elements have a Gaussian distribution with the same spread and with average zero. Furthermore, in this paper we work with hermitian matrices, but generalization to e.g. quaternionic hermitian ones is straightforward. Thus we get a random matrix, which we call $M_0$. For this random matrix $M_0$ the distribution is just of the type studied as the simplest case in [7]. It is well known that the eigenvalues have the famous semicircle distribution (in the large-N limit), see (9) below.

What would be the effect of introducing in addition to such a quenched randomness, dynamics of the matrix? Let us use the $N \times N$ random matrix $M_0$ to construct a potential energy for a dynamical $N \times N$ matrix $M$. We assume for our model the potential

$$V(M) = \frac{\omega^2}{2} \text{Tr}(M - M_0)^2.$$  (1)
Then the simplest is to supplement this potential energy with the kinetic energy that is usual in matrix models. This gives the Hamiltonian for our matrix model

\[ H = \frac{1}{2} \text{Tr} P_M^2 + \frac{\omega^2}{2} \text{Tr}(M - M_0)^2, \]  

(2)

where we defined

\[ \text{Tr} P_M^2 = -\sum_{i,j=1}^{N} \frac{\partial^2}{\partial M_{ij} \partial M_{ji}}. \]

The ground state wave-function of the system defined by the Hamiltonian (2) is

\[ \Psi_0(M) \propto \exp\left(-\frac{\omega}{2} \text{Tr}(M - M_0)^2\right), \]

(3)

Assuming that the probability distribution for random matrix \( M_0 \) is

\[ P(M_0) = N(\tilde{\omega}, N) \exp\left(-\tilde{\omega} \text{Tr}(M_0^2)\right), \]

(4)

with the normalization constant being

\[ N(\tilde{\omega}, N) = \frac{2N}{(N-1)!} \frac{1}{\pi^{N/2}} \]

the expectation value of the level density \( \rho(x) = \text{Tr}(x - M) \) in the ground state (3) is

\[ \langle\langle \rho(x) \rangle\rangle_0 = N \int dMdM_0 e^{-\tilde{\omega} \text{Tr}(M_0^2)} e^{-\omega \text{Tr}(M - M_0)^2} \text{Tr}(x - M), \]

(5)

with \( N = N(\omega, N) N(\tilde{\omega}, N) \). Note that we normalize the level density as

\[ \int \rho(x) dx = N, \]

(6)

where \( N \) is the number of levels, i.e. the order of the matrices \( M \) and \( M_0 \). Now we write the expectation value of the level density as

\[ \langle\langle \rho(x) \rangle\rangle_0 = N(\omega, N) N(\tilde{\omega}, N) \int dMdM_0 \rho(x) e^{-(\tilde{\omega} + \omega) \text{Tr}(M_0 - \frac{\omega}{\tilde{\omega}} M)^2} e^{-\frac{\omega}{\tilde{\omega}} \text{Tr}(M^2)} = \]

\[ = \left( \frac{\pi}{\omega + \tilde{\omega}} \right)^{N^2/2} 2^{-N(N-1)/2} N(\omega, N) N(\tilde{\omega}, N) \int dM \rho(x) e^{-\frac{\omega}{\tilde{\omega}} \text{Tr}(M^2)} = \]

\[ = 2^{N(N-1)/2} \left( \frac{\omega \tilde{\omega}}{\pi(\omega + \tilde{\omega})} \right)^{N^2/2} \int dM \rho(x) e^{-\frac{\omega}{\tilde{\omega}} \text{Tr}(M^2)} = \]

\[ = N \left( \frac{\omega \tilde{\omega}}{\omega + \tilde{\omega}}, N \right) \int dM \rho(x) e^{-\frac{\omega}{\tilde{\omega}} \text{Tr}(M^2)}. \]

(7)

The last expression is the standard matrix integral \[^7\] giving weighted sum of (squared) Hermite polynomials:

\[ \langle\langle \rho(x) \rangle\rangle_0 = e^{-\frac{\omega \tilde{\omega}}{\omega + \tilde{\omega}} x^2} \sum_{i=1}^{N} \frac{H_i^2 \left( \sqrt{\frac{\omega \tilde{\omega}}{\omega + \tilde{\omega}}} x \right)}{2^i i! \sqrt{\pi}}, \]

(8)
which in the large-$N$ limit reduces to the Wigner semicircle distribution:
\[
\langle \langle \rho(x) \rangle \rangle_0 \approx \frac{2}{\pi} \frac{\omega \tilde{\omega}}{\omega + \tilde{\omega}} \sqrt{N \frac{\omega + \tilde{\omega}}{\omega \tilde{\omega}}} - x^2,
\]
non-vanishing only for \( x \in [-\sqrt{N \frac{\omega + \tilde{\omega}}{\omega \tilde{\omega}}}, \sqrt{N \frac{\omega + \tilde{\omega}}{\omega \tilde{\omega}}}] \). We see that as a consequence of introducing the random part in the potential the width of the distribution grows, as \( \frac{\omega \tilde{\omega}}{\omega + \tilde{\omega}} < \omega \).

Further we shall introduce the interaction with fermions and these fermions shall simply interact with the dynamical matrix \( M \) functioning as the Hamiltonian for a single fermion. That means of course that the number of states in our model for the single fermion equals the number of rows (and thus also columns) of the matrix \( M \). We introduce a strength of coupling \( g \), so that we can by varying it vary the degree to which the matrix degrees of freedom get influenced by the interaction with the fermions. We can also vary the spread in the fundamental random distribution of the matrix \( M_0 \) which we used in generating the potential for \( M \). In this way we can put in more or less of the contribution to the matrix that is not dynamical and cannot be shifted by pressure from the interacting particles.

### III. ADDING THE FERMIONS

In this section we extend the above model \( (2) \) with \( M_0 \) being given to be quenched random according to \( (4) \) by introducing an interaction with the fermions already mentioned, so that the Hamiltonian becomes
\[
H = \frac{1}{2} \text{Tr} P_M^2 + \frac{\omega^2}{2} \text{Tr}(M - M_0)^2 + \frac{g}{2} \sum_{i,j=1}^{N} M_{ij} (f_i^\dagger f_j - f_j f_i^\dagger). \tag{10}
\]

Using the unitary matrix \( V \), we can diagonalize the matrix \( M_0 \) and write the Hamiltonian \( (10) \) in the form
\[
H = \frac{1}{2} \text{Tr} \tilde{P}_M^2 + \frac{\omega^2}{2} \text{Tr}(\tilde{M} - D)^2 + \frac{g}{2} \sum_{i,j=1}^{N} (\tilde{M} - D)_{ij} (\tilde{f}_i^\dagger \tilde{f}_j - \tilde{f}_j \tilde{f}_i^\dagger) + \frac{g}{2} \sum_{i=1}^{N} d_i (\tilde{f}_i^\dagger \tilde{f}_i - \tilde{f}_i \tilde{f}_i^\dagger), \tag{11}
\]
where we defined
\[
V^\dagger M_0 V = D = \text{diag}(d_1, \cdots, d_N),
\]
\[
f^\dagger V = \tilde{f}^\dagger, \ V^\dagger f = \tilde{f}, \ V^\dagger M V = \tilde{M}. \tag{12}
\]
The matrix \( V \) is undetermined up to permutation of eigenvalues of \( M_0 \) and we choose it to be such that eigenvalues are ordered\(^1\)
\[
d_i < d_j \text{ for } i < j. \tag{13}
\]

In the following we use an approximation in which filled and empty levels in the basis of Fock space spanned by \( \tilde{f} \) basically do not interact. This approximation assumes that \( g \) is large.

\(^1\) We always assume non-degeneracy of the eigenvalues.
enough so that ordering introduced by transforming with \( V \) is preserved. At the same time we need that in the basis of \( \tilde{f} \) interaction between filled and empty levels can be ignored:

\[
\tilde{M} - D \approx \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix}.
\] (14)

Ignoring the off-diagonal block elements may be justified by estimating the second order perturbation correction to eigenvalues of the matrix \( \tilde{M} \), which assume to be dominated by the \( M_0 \)-eigenvalues. An element of the off-diagonal block in (14), denoted by \( v \), is typically of the order \( 1/\sqrt{\omega} \). Then the second order perturbation of a level becomes (since the level difference in the denominator \( E_n - E_m \) must at least contain roughly the shifting \( \sim g/\omega^2 \) due to the fermions)

\[
\frac{|v|^2}{E_n - E_m} \approx \frac{1/\omega}{\# / \sqrt{\omega} + g/\omega^2} \leq \omega/g,
\] (15)

where \( \# \) stands for the relevant level number difference. Whether this can be ignored compared to the size of the shift due to the fermions \( g/\omega^2 \) or the typical quenched contribution \( \# / \sqrt{\omega} \) depends respectively on whether the dimensionless ratio \( \omega^3/g^2 \) or \( \sqrt{\omega} g/\omega \) are small compared to unity. To avoid the significant quantum fluctuations in the filling of the levels (so that they are in a superposition of being filled and empty) we need anyway that shift of the levels is large compared to the characteristic width of quantum fluctuations of the levels: \( g/\omega^2 >> 1/\sqrt{\omega} \), and we see that the first requirement is in this case automatically satisfied. The second is also fulfilled in the case we mainly think of that \( \omega > \tilde{\omega} \), namely that the quenched fluctuation dominates the quantum mechanical one. Therefore our main approximation \( g/\omega^{3/2} >> 1 \) means that the expected homolumo gap width \( g/\omega^2 \) (= the shift due to the fermions) is large compared to the quantum fluctuations \( \sim 1/\sqrt{\omega} \) and that is relevant for our ability to calculate. We may then use the scale of \( \tilde{\omega} \) to have the total spread of level distribution large compared to the displacement due to fermions.

Having this approximation in mind, the Hamiltonian (11) can be decomposed as

\[
H = H_1 + H_2 := \sum_{\sigma=1,2} H_\sigma,
\]

\[H_\sigma = \frac{1}{2} \text{Tr} P_{M_\sigma}^2 + \frac{\omega^2}{2} \text{Tr}(M_\sigma^2) + \frac{g}{2} \sum_{i,j=1}^N M_{\sigma,ij}(\bar{f}_i^\dagger \bar{f}_j - \bar{f}_j \bar{f}_i^\dagger) + \frac{g}{2} \sum_{i=1}^N d_{\sigma,i}(\bar{f}_i^\dagger \bar{f}_i - \bar{f}_i \bar{f}_i^\dagger), \] (16)

with the ground state given by

\[
\psi \approx e^{-\frac{1}{2} \text{Tr} \left[ M_1 + \frac{g}{2\omega^2} 0 \\ 0 & M_2 - \frac{g}{2\omega^2} \right]^2} \bar{f}_1^\dagger \cdots \bar{f}_{N_f}^\dagger |0\rangle,
\] (17)

where \( N_f \) is the number of filled levels.
IV. HOMOLUMO GAP

We are interested in the expectation value of the density of filled ($N_f$ lowest) levels in the ground state (17) given as:

$$\langle \langle \rho_{\text{filled}}(x) \rangle \rangle = \mathcal{N}(\bar{\omega}, N) \mathcal{N}(\omega, N) \sum_C \int dM_0 dM \times$$

$$\times e^{-\bar{\omega} \text{Tr}(M_0^2)} e^{-\omega \text{Tr}(M - M_0 + \frac{g}{2\omega^2}V \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} V^\dagger)} \prod_{i,\alpha} \theta(d_{C(\alpha)} - d_{C(i)}) \text{Tr} \delta(x - M_1 - D_1),$$

where sum over $\mathcal{C}$ means sum over all possible combinations of dividing $N$ levels into $N_f$ filled (denoted by indices $\{i\}$) and $N_e$ empty (denoted by indices $\{\alpha\}$). Matrix $D_1$ contains $N_f$ lowest eigenvalues of the matrix $M_0$ which are not ordered among themselves and similarly $D_2$ contains $N_e$ highest eigenvalues of $M_0$. In order to proceed we expand the Gaussian into powers of $1/\omega$ and use definition of ”matrix delta function” which could be thought of as an $N^2$-dimensional delta function

$$\delta(M) = \lim_{\omega \to -\infty} \mathcal{N}(\omega, N) e^{-\omega \text{Tr}(M^2)} = \Pi_{i \leq j} \delta(S_{ij}) \Pi_{k < l} \delta(A_{kl}),$$

where we introduced matrices $S = (M + M^t)/2$ and $A = (M - M^t)/2i$, so that $M = S + iA$. With this definition, one can easily show that we can expand the Gaussian in the following way:

$$\left(\frac{\omega}{\pi}\right)^{N^2/2} e^{-\omega \text{Tr}(M - M_0)^2} = \sum_k \frac{1}{k! \omega^k} \frac{\partial^k}{\partial \epsilon^k} \mathcal{N}(1/\epsilon, N_f) e^{-\frac{1}{\epsilon} \text{Tr}(M - M_0)^2} \bigg|_{\epsilon \to 0} = \sum_k \frac{1}{k! \omega^k} \Delta^k_{M_0} \delta(M - M_0).$$

Here $\Delta_{M_0} = \frac{1}{4} \sum_{ij} \frac{\partial^2}{\partial M_{ij} \partial M_{ji}}$ is the matrix Laplacian. Using (20) for the second Gaussian in (18) we obtain after integration by parts

$$\langle \langle \rho_{\text{filled}}(x) \rangle \rangle = \mathcal{N}(\bar{\omega}, N) \sum_C \sum_k \frac{1}{k! \omega^k} \int dM_0 dM \delta \left( M - M_0 + \frac{g}{2\omega^2}V \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} V^\dagger \right) \times$$

$$\times \Delta^k_{M_0} e^{-\bar{\omega} \text{Tr}(M_0^2)} \prod_{i,\alpha} \theta(d_{C(\alpha)} - d_{C(i)}) \text{Tr} \delta(x - M_1 - D_1) =$$

$$= \mathcal{N}(\bar{\omega}, N) \sum_C \sum_k \frac{1}{k! \omega^k} \int dM_0 dM \delta \left( M - M_0 + \frac{g}{2\omega^2}V \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} V^\dagger \right) \times$$

$$\times \Delta^k_{M_0} e^{-\bar{\omega} \text{Tr}(M_0^2)} \prod_{i,\alpha} \theta(d_{C(\alpha)} - d_{C(i)}) \text{Tr} \delta(x + g/2\omega^2 - D_1).$$

We now introduce fluctuating Fermi level $\mu(M_0)$ such that $d_{C(i)} < \mu(M_0) < d_{C(\alpha)}$. For example, we can choose $\mu(M_0) = (\max\{d_{C(\alpha)}\} + \min\{d_{C(i)}\})/2$. Therefore under the integral we can make the replacement

$$\prod_{i,\alpha} \theta(d_{C(\alpha)} - d_{C(i)}) = \prod_{i,\alpha} \theta(d_{C(\alpha)} - \mu(M_0)) \theta(\mu(M_0) - d_{C(i)}).$$
and we write:

\[
\langle \langle \rho_{\text{filled}}(x) \rangle \rangle = \mathcal{N}(\tilde{\omega}, N) \sum_c \sum_k \frac{1}{k! \omega^k} \int dM_0 dM \delta \left( M - M_0 + \frac{g}{2\omega^2} V \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} V^\dagger \right) \times \\
\times \Delta_{M_0}^k e^{-\tilde{\omega} \text{Tr}(M_0^2)} \prod_{i,\alpha} \theta(d_{\alpha}(\mu))\theta(\mu(M_0) - d_{\alpha}(\mu)) \text{Tr} \delta(x + g/2\omega^2 - D_1) = \\
= \mathcal{N}(\tilde{\omega}, N) \sum_c \sum_k \frac{1}{k! \omega^k} \int dM_0 dM \delta \left( M - M_0 + \frac{g}{2\omega^2} V \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} V^\dagger \right) \times \\
\times \Delta_{M_0}^k e^{-\tilde{\omega} \text{Tr}(M_0^2)} \prod_{i,\alpha} \theta(d_{\alpha}(\mu))\theta(\mu(M_0) - d_{\alpha}(\mu)) \theta(\mu(M_0) - x - g/2\omega^2) \times \\
\times \text{Tr} \delta(x + g/2\omega^2 - D_1).
\]

In the last step we inserted \( \theta(\mu(M_0) - x - g/2\omega^2) \), using the fact that the square of theta-function is again theta-function. Due to this theta-function we can include the density of empty levels under the integral and sum into full density:

\[
\langle \langle \rho_{\text{filled}}(x) \rangle \rangle = \mathcal{N}(\tilde{\omega}, N) \sum_c \sum_k \frac{1}{k! \omega^k} \int dM_0 dM \delta \left( M - M_0 + \frac{g}{2\omega^2} V \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} V^\dagger \right) \times \\
\times \Delta_{M_0}^k e^{-\tilde{\omega} \text{Tr}(M_0^2)} \prod_{i,\alpha} \theta(d_{\alpha}(\mu))\theta(\mu(M_0) - d_{\alpha}(\mu)) \theta(\mu(M_0) - x - g/2\omega^2) \times \\
\times \left( \text{Tr} \delta(x + g/2\omega^2 - D_1) + \text{Tr} \delta(x + g/2\omega^2 - D_2) \right) = \\
= \mathcal{N}(\tilde{\omega}, N) \mathcal{N}(\omega, N) \int dM_0 dM \theta(\mu(M_0) - x - g/2\omega^2) e^{-\tilde{\omega} \text{Tr}(M_0^2)} \times \\
\times e^{-\omega \text{Tr}(M_0^2)} \left( M - M_0 + \frac{g}{2\omega^2} V \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} V^\dagger \right)^2 \text{Tr} \delta \left( x + g/2\omega^2 - M - \frac{g}{2\omega^2} V \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} V^\dagger \right). 
\]

At this point we note that \( \mu(M_0) \) behaves as a typical eigenvalue, fluctuations of which are described by a Gaussian distribution. This means that the leading contribution to the integral (22) we obtain approximating \( \mu(M_0) \) by constant \( \mu_F \), where \( \mu_F \) is determined from the condition:

\[
\intdx \langle \langle \rho_{\text{filled}}(x) \rangle \rangle = N_f.
\]

In order to account for the fluctuations of \( \mu(M_0) \) around \( \mu_F \) we introduce a Gaussian distribution for \( \mu(M_0) \) with central value \( \mu_F \) and width \( \omega_F \), which is estimated in Appendix. Finally, after the redefinition

\[
M - \frac{g}{2\omega^2} V \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} V^\dagger \rightarrow M,
\]

8
we obtain:

\[
\langle\langle \rho_{\text{filled}}(x) \rangle \rangle \approx \sqrt{\frac{\omega_F}{\pi}} \int d\mu e^{-\omega_F(\mu-\mu_F)^2} \theta(\mu - x - g/2\omega^2)N(\tilde{\omega}, N)N(\omega, N) \times \\
\int dM_0 dM e^{-\omega \text{Tr}(M_0^2)} e^{-\omega \text{Tr}(M-M_0)^2} \text{Tr}\delta(x + g/2\omega^2 - M) = \\
\frac{1}{\sqrt{\pi}} \int_{\sqrt{\omega_F}(x + g/2\omega^2 - \mu_F)}^{\infty} dy e^{-y^2} \times \\
N(\tilde{\omega}, N)N(\omega, N) \int dM_0 dM e^{-\omega \text{Tr}(M_0^2)} e^{-\omega \text{Tr}(M-M_0)^2} \text{Tr}\delta(x + g/2\omega^2 - M) = \\
\frac{1}{2} \text{erfc}(\sqrt{\omega_F}(x + g/2\omega^2 - \mu_F)) \langle\langle \rho(x + g/2\omega^2) \rangle \rangle_0.
\]

(23)

In the final expression (24) we obtained the product of the density distribution (7) and the complementary error function \( \text{erfc}(z) = 1 - \text{erf}(z) \), for \( z = \sqrt{\omega_F(x + g/2\omega^2 - \mu_F)} \) in our case. We notice two effects appearing: displacement of the distribution, i.e. the opening of the gap, and smoothing-out of the edges of the distribution due to the (complementary) error function. The parameter \( \omega_F \) appearing in the error function, is estimated in Appendix to be

\[
\omega_F = \frac{1}{2\delta\mu_F} = \frac{(\pi \rho(\mu_F))^2}{\ln(N)}.
\]

(25)

In the limit \( \omega_F \to \infty \) we could ”freeze out” the fluctuations of the Fermi level and as the error-function goes to theta-function we would get sharp cut-offs at the edges of the homololumo gap, see figure [1].

FIG. 1: We sketched the filled levels density for \( \omega_F \to \infty \) (left) and \( \omega_F \) finite (right), for \( N = 28 \) and \( N_f = 14 \).

Note that the density of empty levels is similarly obtained as

\[
\langle\langle \rho_{\text{empty}}(x) \rangle \rangle = \frac{1}{2} \left(1 + \text{erf}(\sqrt{\omega_F(x - g/2\omega^2 - \mu_F)}) \right) \langle\langle \rho(x - g/2\omega^2) \rangle \rangle_0.
\]

It is easy to check that

\[
\int dx (\langle\langle \rho_{\text{filled}}(x) \rangle \rangle + \langle\langle \rho_{\text{empty}}(x) \rangle \rangle) = N,
\]

as it should according to normalization (6).
Moreover, we now can determine the effective Fermi level $\mu_F$ by taking $\omega_F \to \infty$ in (23) thus obtaining

$$\int^{\mu_F} dx \langle \langle \rho(x) \rangle \rangle_0 = N_f.$$  

In the large-N limit this leads to

$$\frac{2}{\pi} \int_{-1}^{\tilde{\mu}_F} dx \sqrt{1-x^2} = \frac{N_f}{N},$$

with $\tilde{\mu}_F = \mu_F \sqrt{N\frac{\omega+\tilde{\omega}}{\omega\tilde{\omega}}}$.

V. DISCUSSION AND OUTLOOK

In the previous works [5, 6] we introduced the model having the quantum mechanical dynamical matrix with the minimum in potential energy occurring for the matrix elements being zero before the fermion interaction term were switched on. We could only obtain a reliable homolumo gap in the limit of the coefficient $g$ for the coupling of the fermions to the matrix (basically same notation as in this article) was large, and then we got the spectrum to be two largely separated Wigner semicircles. For the calculation to be trustworthy and doable we had fermion states either filled or empty but not in superposition. That meant that we needed the quantum fluctuations going as $\delta_{qm} \sim \sqrt{1/\omega}$ to be small compared to the distance in the level energy $\sim g/\omega^2$, originating from the push by fermions. When we had all the separation of the levels due to quantum fluctuations, we could only get the push dominate over the quantum fluctuation by pulling the filled levels far away from the empty ones.

In the present work we, however, introduced yet another mechanism for spreading the levels before switching the fermion interaction on, namely the quenched (or fundamental) randomness of the levels. That means that the matrix elements are by their dynamical potential attracted to a value which is not zero but quenched random by a fluctuation given by the parameter $\tilde{\omega}$. Looking at the case of $\tilde{\omega}$ being small so that quenched fluctuations becomes the dominant fluctuations we can avoid that the push becomes larger than the size of the original distribution extension, because the distribution in eigenvalue space is made extensive by the quenched fluctuations. Nevertheless we could still keep the push large compared to the quantum fluctuations, so that we could calculate the homolumo gap in a trustable way. Thus we found in our type of matrix model with both quantum and quenched level fluctuation contributions - but in the case wherein the quenched fluctuations dominate - a homolumo-gap effect that meant that we

- Start from the no-fermion-interaction spectrum density $\rho$.
- Fill the lowest levels as high as needed to have the given $N_f$ fermions put in.
- Next we simply push respectively the filled sector and the empty sector down and up in level-energy by $g/2\omega^2$. This operation leaves (in the first approximation) an interval of length $g/\omega^2$ in between the filled and empty levels in which there are no levels at all. This is the homolumo gap.
• In the next approximation we then show that the boundaries of this level-empty interval are not completely sharp but rather smoothed out. The density of levels is rather given as the level density as before the fermion interaction displaced by the \( \pm \frac{g}{2\omega^2} \) multiplied by a (complementary) error function smoothing out the steep level density falls. Since an error function is very close to a theta function in our case, we effectively have very low level density in the gap as long as our approximations work. It might however be interesting to investigate further how the gap may be filled out by extending our calculation.

It should be understood that we consider the importance of calculations of the homolumo-gap effect as being due to fact that the model assumed occurs very generally: It is just some bosonic degrees of freedom interacting with fermions. We assume a specific statistical distribution and the model dynamics, but really we have in mind that practical cases of interactions of fermions with a system of boson degrees of freedom are usually too complicated for analytic analyses. Therefore it is of great significance, if one could obtain some information about such complicated systems - such as e.g. the homolumo-gap effect - even if one has modeled the complicated system by a random one. The standard example where such a procedure has been used and is relevant is the case of complex nuclei and molecules, as discussed in Introduction. We may also look at several well-known phenomena as being in reality homolumo-gap effects although not really always announced like that: Anderson localization leading to the transition from metals to insulators is the obvious example. 

One could also use the general model in the present article in cases, where there is in reality interaction between the fermions directly even though such interactions were not explicitly considered above. One should just think of using the Hartree-Fock approximation - replacing the mutual interactions of fermions by an effective interaction with a “background” that can easily be described by the dynamical matrix \( M \). In such a thinking we might even see superconductivity as an example of an effect of homolumo gap, namely the gap in the quasi-electron spectrum in the superconductor state is the homolumo gap.

Originally the motivation behind this work is the dream of Random Dynamics that the most fundamental laws of nature are so complicated that we should assume them to be basically random. In such a Random Dynamics philosophy, assuming at least existence of fermions and bosons, we are again set for application of a model like the present one and may speculate on the significance of the homolumo gap for the theory behind the Standard Model and behind special relativity etc.

One of the soon to be studied developments of the present model is to introduce a system of conserved or at least approximately conserved quantum numbers say for the fermions alone at first. We could think of such conserved quantum numbers to be e.g., the quasi-momentum components for the electrons in a crystal. We can then set up some distribution assumption and some dynamics for a whole set of matrices \( M(\vec{p}) \), one for each quasi-momentum vector. These matrices \( M(\vec{p}) \) should now be assumed random and dynamical in such a way that they preserve continuity w.r.t. the momentum vector \( \vec{p} \). In the approximation that the matrices \( M(\vec{p}) \) have dynamics and quenched randomness independent of each other for each \( \vec{p} \)-value separately it would be possible to apply the analysis done in present work. However, for such a field of matrices one should expect break-down of continuity which would reflect on underlying topology. In fact we plan to address the question of possible topological frustrations and hope to fulfill the old dream of Random Dynamics of deriving the unavoidability of Weyl fermions in the low energy limit i.e., near the Fermi surface.

Another direction in which we hope to develop the present work is to make the analogue of
the homolumo gap with the fermions replaced by bosons. Interestingly enough, the model
describing interaction of bosons with a dynamical matrix was discussed as a toy model
capable of shading some light on the black-hole information problem [10].

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Appendix: Mean square deviation of the fluctuating Fermi level

Here we would like to estimate the width of the fluctuations of the Fermi level. We are
going to use the results of Brézin and Zee [11] and therefore we adopt the following notations:

\[ M = \sqrt{N\tilde{M}}, \quad \rho(x) = \text{Tr}\delta(x - M) = \frac{1}{\sqrt{N}}\text{Tr}\delta(\tilde{x} - \tilde{M}) = \sqrt{N}\tilde{\rho}(\tilde{x}), \quad x = \sqrt{N}\tilde{x}, \]

where \( \tilde{\rho}(\tilde{\nu}) = \frac{1}{N}\text{Tr}\delta(\tilde{\nu} - \tilde{M}) \). The average number of particles in the interval \((\tilde{\nu}_1, \tilde{\nu}_2)\) is given by

\[ \tilde{N}(\tilde{\nu}_1, \tilde{\nu}_2) = N \int d\tilde{\nu}\tilde{\rho}(\tilde{\nu}) \]

and the mean square deviation of particles in the interval \((\tilde{\nu}_1, \tilde{\nu}_2)\) is given by

\[ \delta^2 \tilde{N}(\tilde{\nu}_1, \tilde{\nu}_2) = \langle \tilde{N}^2(\tilde{\nu}_1, \tilde{\nu}_2) \rangle - \langle \tilde{N}(\tilde{\nu}_1, \tilde{\nu}_2) \rangle^2 = N^2 \int_{\tilde{\nu}_1}^{\tilde{\nu}_2} \int_{\tilde{\nu}_1}^{\tilde{\nu}_2} d\mu d\nu \rho_c(\mu, \nu), \]

where the approximation

\[ \rho_c(\mu, \nu) \approx -\tilde{\rho}^2(\tilde{\mu}) \frac{\sin^2 z}{z^2} + \frac{1}{N}\tilde{\rho}(\tilde{\mu})\delta(\mu - \nu), \quad z = \pi N(\mu - \nu)\tilde{\rho}(\tilde{\mu}), \quad \tilde{\mu} = \frac{\mu + \nu}{2}, \]

is extracted from [11]. Changing the integration variables to \( \tilde{\mu} \) and \( \mu - \nu \) we can express the mean square deviation of the number of particles as a sum of two “triangle” contributions

\[ \int_{\tilde{\nu}_1}^{\tilde{\nu}_2} \int_{\tilde{\nu}_1}^{\tilde{\nu}_2} d\mu d\nu \rho_c(\mu, \nu) = \int_{\tilde{\nu}_1}^{\tilde{\nu}_2} d\tilde{\mu} \int_{2(\tilde{\mu} - \tilde{\nu}_2)}^{2(\tilde{\mu} - \tilde{\nu}_2)} d(\mu - \nu)\rho_c(\tilde{\mu}, \mu - \nu) + \]

\[ + \int_{\tilde{\nu}_1}^{\tilde{\nu}_1 + \tilde{\nu}_2} d\tilde{\mu} \int_{2(\tilde{\mu} - \tilde{\nu}_1)}^{2(\tilde{\mu} - \tilde{\nu}_1)} d(\mu - \nu)\rho_c(\tilde{\mu}, \mu - \nu). \]

For \( \tilde{\nu}_1 \to -\infty, \tilde{\nu}_2 \to \infty \) integration has to be performed over the whole plane and we can use following approximation for the leading term

\[ \frac{\sin^2 z}{z^2} \approx \frac{1}{N\tilde{\rho}(\tilde{\mu})}\delta(\mu - \nu). \]
We see that in this case the integral over \(d(\mu - \nu)\) vanishes. Rewriting this result in the following way:

\[
0 \approx \int_{-\infty}^{\infty} d(\mu - \nu)\rho_c(\mu, \nu) = \int_{(\mu-\nu)_{\text{min}}}^{(\mu-\nu)_{\text{max}}} d(\mu - \nu)\rho_c(\mu, \nu) + \int_{-\infty}^{(\mu-\nu)_{\text{min}}} d(\mu - \nu)\rho_c(\mu, \nu) + \int_{(\mu-\nu)_{\text{max}}}^{\infty} \rho_c(\mu, \nu),
\]

enables us to express the last term which we want to calculate:

\[
\int_{(\mu-\nu)_{\text{min}}}^{(\mu-\nu)_{\text{max}}} d(\mu - \nu)\rho_c(\mu, \nu) \approx - \int_{(\mu-\nu)_{\text{min}}}^{(\mu-\nu)_{\text{max}}} d(\mu - \nu)\rho_c(\mu, \nu) - \int_{-\infty}^{(\mu-\nu)_{\text{min}}} d(\mu - \nu)\rho_c(\mu, \nu).
\]

Then we proceed by using approximation:

\[
\frac{\sin^2 z}{z^2} \approx \frac{1}{2z^2},
\]

which is valid when the integral runs over a large range in \(z\) where thus \(\sin^2 z\) averages out to 1/2. Integral over \(d(\mu - \nu)\) for the first “triangle” gives

\[
\int_{(\mu-\nu)_{\text{min}}}^{(\mu-\nu)_{\text{max}}} d(\mu - \nu)\rho_c(\mu, \nu) = 2 \int_{(\mu-\nu)_{\text{min}}}^{(\mu-\nu)_{\text{max}}} d(\mu - \nu)\rho_c^2(\mu) \frac{1}{2z^2} \approx \frac{1}{|(\mu - \nu)_{\text{max}}|\pi^2 N^2} = \frac{1}{(\pi N)^2 2(\nu_2 - \bar{\mu})},
\]

and complete contribution of this “triangle” is given by:

\[
\int_{\nu_2}^{\nu_2} d\bar{\mu} \frac{1}{(\pi N)^2} \frac{1}{2(\nu_2 - \bar{\mu})}.
\]

The divergence at \(\bar{\mu} \to \nu_2\) has to be cut off for the integration area where the approximation \(\sin^2 z \to 1/2\) in no longer valid. Noting that if for example \(0 < z < \pi/4\) then \(\sin^2 z \leq 1/2\) and thus we can put say for \(z < \pi/8\) that \(\sin^2 z \approx 0\). Taking this into account our integral becomes

\[
\int_{\nu+\nu_2}^{\nu_2} d\bar{\mu} \frac{1}{(\pi N)^2} \frac{1}{2(\nu_2 - \bar{\mu})} \to - \frac{1}{2\pi^2 N^2} \int_{\nu+\nu_2}^{\Delta} \frac{1}{y} = \frac{1}{2\pi^2 N^2} \ln \frac{(\nu_2 - \nu_1)}{2\Delta},
\]

where \(\Delta\) is determined from the condition \(z > \pi/8\):

\[
z \to \frac{\pi}{8} \Rightarrow (\mu - \nu)_{\text{max}} = 2(\nu_2 - \bar{\mu}) > \frac{1}{8N\bar{\rho}(\bar{\mu})} \Rightarrow \nu_2 - \Delta > \bar{\mu}, \Delta = \frac{1}{16N\bar{\rho}(\bar{\mu})}.
\]

Assuming now that \(\nu_2 - \nu_3\) is typical distance we have that \((\nu_2 - \nu_1)\rho \approx 1/2\). Finally, taking also into account contribution from the other “triangle” we find the mean square deviation of the number of particles in the typical distance:

\[
\delta^2 \tilde{N}(\nu_1, \nu_2) \approx \frac{1}{\pi^2} \ln N.
\]
From another point of view we can look on the deviation of the number of particles in some interval as originating from the fluctuating edges of the interval. Since the number of levels per $d\tilde{\nu}$ is $N\tilde{\rho}(\tilde{\nu})d\tilde{\nu}$ we can write

$$\delta^2(\tilde{\nu}_1 - \tilde{\nu}_2) = \frac{\delta^2\tilde{N}(\tilde{\nu}_1, \tilde{\nu}_2)}{2(N\tilde{\rho})^2} \approx \frac{\ln N}{2(\pi \tilde{\nu} N)^2},$$

where the factor 2 is due to the two edges, and for the width of fluctuations of the level $\tilde{\nu}$ we find

$$\delta(\tilde{\nu}) = \frac{\sqrt{\ln N}}{\sqrt{2\pi \tilde{\rho}(\tilde{\nu})}N},$$

which is exactly the same result as the one obtained for the fluctuation of eigenvalues in the bulk for the Gaussian unitary ensemble \[12\]. Finally, specializing above result for the Fermi level, we estimate width of the fluctuations of the Fermi level:

$$\delta\mu_F = \frac{\sqrt{\ln N}}{\sqrt{2\pi \rho(\mu_F)}}.$$

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