Homolumo gap and matrix model

I. Andrić, L. Jonke, and D. Jurman
Theoretical Physics Division, Rudjer Bošković Institute, P.O. Box 180, 10002 Zagreb, Croatia

H. B. Nielsen
The Niels Bohr Institute, Copenhagen DK 2100, Denmark[*]
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We discuss a dynamical matrix model by which probability distribution is associated with Gaussian ensembles from random matrix theory. We interpret the matrix M as a Hamiltonian representing interaction of a bosonic system with a single fermion. We show that a system of second-quantized fermions influences the ground state of the whole system by producing a gap between the highest occupied eigenvalue and the lowest unoccupied eigenvalue.

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Introduction.—Random matrices [1] first studied by Wigner [2] have applications in many branches of (many-body) physics, e.g., nuclear and molecular physics. The matrix elements are considered statistical variables and take random values. On the other hand, one can consider a dynamical matrix model in which the matrix elements are dynamical variables so that the whole matrix has become a mechanical system, which may even be quantized and corresponding quantum field theory may be formulated. Such dynamical matrices have found use in description of disordered system and in string theory [3].

In the present work, we treat a dynamical matrix model by which probability distribution in the ground state is associated with Gaussian ensembles from random matrix theory. We interpret the matrix M as a Hamiltonian representing interaction of a "bosonic" system, such as, for example, the nuclei in a molecule, with a single fermion, e.g., a single electron in a molecule. In particular, an eigenvalue of the matrix corresponds to an eigenenergy of a fermion. Without going into a lot of detail about the single fermion interaction, we consider a backreaction from the system of the second-quantized fermions. A characteristic effect of such a backreaction is to drive the matrix in the direction of lowering the energy of the eigenstates occupied by fermions. In the case of a molecule, this backreaction is the force from the electrons pushing on the nuclei seeking to drive them into such a position so as to lower the filled single electronic orbit energy eigenvalues. Since a similar push to lower the unoccupied levels is absent, or even has the opposite sign, as will be argued later, hereby a gap can easily arise between the highest occupied eigenvalue (homo, where mo stands for molecular orbit) and the lowest unoccupied eigenvalue (lumo). The gap is what is called the homolumo gap [4]. The interest in the homolumo gap steams from the fact that the details of the model seem very unimportant. You should get it whenever you have a system of bosonic variables interacting with the fermions, provided that the bosonic variables are sufficiently soft as to yield to the pressure from the fermions.

The purpose of this paper is to evaluate how distribution of eigenvalues of the matrix adjust to produce a homolumo gap in a quite general setting. First, we formulate field theory corresponding to the large N limit of the random $(N \times N)$ matrix. Then, we introduce the dynamical matrix model by which the probability distribution in the ground state coincides with the large N limit of the "free" Gaussian ensemble from the random matrix theory. The notion of the dynamical model enables us to model the interaction potential, which arose as a consequence of the backreaction of the second-quantized fermions. Finally, exploring the effect of adding this interaction potential to the free matrix model, we obtain characteristic homolumo gap.

Field theory formulation of the random matrix model.—The field theory we discuss is defined by the following functional integral

$$Z[\rho] = \int \mathcal{D}\rho \exp\Big\{(\lambda-1)\int dx\rho(x)\ln\rho(x) + \lambda\int dxdy\rho(x)\ln(x-y)\rho(y) - \int dx\rho(x)P(x)\Big\}, \quad (1)$$

for some (polynomial) function $P(x)$ and a dimensionless parameter λ. The integral (1) corresponds to the large N limit of the matrix integral from random matrix theory

$$Z = \int dM e^{-\mathrm{Tr}P(M)}, \quad (2)$$

where $P(M)$ is a polynomial in $N \times N$ matrix M. In terms of eigenvalues x_i of the matrix M, the matrix integral (2) can be expressed as

$$Z = \int \prod_i dx_i \prod_{i<j} (x_i - x_j)^{2\lambda} e^{-\sum_i P(x_i)}. \quad (3)$$

Here, the parameter $\lambda = 1/2$, 1, 2 for real-symmetric, Hermitian and quaternionic-real matrix M, respectively.

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The origin of the first two terms in (1) is the new invariant measure resulting from changing the variables from x_i to $\rho(x)$ (see Refs. [5,6]),

$$\prod_{i<j}(x_i - x_j)^{2\lambda} \to \exp\Big\{\lambda \int dx\rho(x)\ln\rho(x) + \lambda \int dxdy\rho(x)\ln(x-y)\rho(y)\Big\}, \quad (4)$$

$$\int \prod_i^N dx_i \to \int \mathcal{D}\rho \exp\Big\{-\int dx\rho(x)\ln\rho(x)\Big\}. \quad (5)$$

While in (3) the statistical variables are the eigenvalues x_i, in the large N limit, one introduces the density field $\rho(x)$, which then by itself becomes a statistical variable. In parallel with Ref. [7], we interpret (1) as a quantum field theory describing statistical random matrix model (2). By varying (1) with respect to ρ and taking the derivative with respect to x, we find that the most probable configuration satisfies following equation:

$$(\lambda - 1)\frac{\partial_x \rho}{\rho} - 2\lambda\pi\rho^H = \partial_x P, \quad (6)$$

where f^H denotes the Hilbert transform of the function f. From (6), we obtain the Riccati differential equation for the new field $W = \rho^H + i\rho$ in analogy with [8]

$$(\lambda-1)\partial_x W - \lambda\pi W^2 - W\partial_x P = (\rho\partial_x P)^H - \rho^H\partial_x P \quad (7)$$

This equation corresponds to the usual Riccati equation for the resolvent function in the random matrix theory, except that here the first term vanishes *exactly* for the Hermitian matrix model ($\lambda = 1$). The difference comes from the additional term in measure (5).

Before introducing the matrix model that describes interaction of fermions and bosons, we need the notion of dynamical system to be able to define and model the potential, and also, to be able to interpret the integrand in (1) as a probability density functional in the ground state of this dynamical model. This requirement is satisfied by the following Hamiltonian (see [8] for details):

$$H = \frac{1}{2}\int dx\rho(x)A^\dagger(x)A(x) + E_0, \quad (8)$$

where $A(x)$ is given by

$$A(x) = \partial_x\pi(x) + i\partial_x\frac{\delta\ln\Phi}{\delta\rho(x)}, \quad (9)$$

for Φ being the ground-state functional [i.e., the square root of the integrand in (1)] and $\pi(x)$ the canonical momentum satisfying $[\partial_x\pi(x), \rho(y)] = -i\partial_x\delta(x-y)$. Now, we interpret Eq. (6) as a BPS equation of motion. Let us consider a simple example of the free Gaussian ensemble defined by (3) with $P(x) = x^2$. The operator $A(x)$ of the corresponding dynamical model is

$$A(x) = \partial_x\pi(x) + i\Big(\frac{\lambda-1}{2}\frac{\partial_x\rho(x)}{\rho(x)} - \lambda\pi\rho^H(x) - x\Big), \quad (10)$$

and the Hamiltonian can be written as

$$H = \frac{1}{2}\int dx\rho(x)(\partial_x\pi(x))^2 + \frac{1}{2}\int dx\rho(x) \times \Big(\frac{\lambda-1}{2}\frac{\partial_x\rho(x)}{\rho(x)} - \lambda\pi\rho^H(x) - x\Big)^2 + E_0, \quad (11)$$

The second term is called effective potential V_{eff} and represents the physical potential for the dynamical model in question. The ground-state functional satisfying $A(x)\Phi = 0$ is

$$\Phi = \exp\Big\{\frac{(\lambda-1)}{2}\int dx\rho(x)\ln\rho(x) + \frac{\lambda}{2}\int dxdy\rho(x) \times \ln(x-y)\rho(y) - \frac{1}{2}\int dx\rho(x)x^2\Big\}, \quad (12)$$

giving the integrand of the (1) as a probability density functional in the ground state. The semiclassical solution is given by the solution of the Eq. (6), which in the case of $\lambda = 1$ reads $-\pi\rho^H(x) = x$ and gives the usual Wigner semicircle law for the distribution of eigenvalues for the Hermitian Gaussian ensemble. In the rest of the paper, we restrict ourselves to the $\lambda = 1$ case.

Interaction with fermions.—It is simply the idea of the interaction of the already described dynamical matrix model with the system of fermions that we postulate that the dynamical matrix itself is the Hamiltonian for a single fermion. Then on top of that, we second quantize the fermions, so that it becomes possible to have filled or emptied all the (basis) states for this matrix. If we especially seek the ground state of the whole system—dynamical matrix plus fermions—we shall be interested in the case when the eigenstates of the dynamical matrix are filled below a certain value x_F, the Fermi surface (value), while the ones above x_F are empty. In the case where we can ignore that this Fermi surface (energy) depends on the (dynamical) state of the matrix, the interaction with the fermions simply gives an extra potential

$$V_{\text{fermion}}(x) = x\theta(x_F - x). \quad (13)$$

At this point, we introduce the zero-point energy for fermion modes. If we want to write a Hermitian Hamiltonian contribution from a single particle state as a bilinear expression in the annihilation a and creation $a^\dagger$ operators and symmetrized in taking the product, we must take the commutator expression

$$H = \frac{\omega}{2}[a^\dagger, a] = \omega a^\dagger a - \frac{\omega}{2}. \quad (14)$$

The extra term $-\omega/2$ compared to the pure number operator term, $\omega N = \omega a^\dagger a$, is analogous to the zero-point energy term $\omega/2$ for a boson model

$$H = \frac{\omega}{2}\{a^\dagger, a\} = \omega a^\dagger a + \frac{\omega}{2}. \quad (15)$$

With this analogy between bosons and fermions in mind, we can claim that there is a zero-point energy $-\omega/2$ for the fermion mode, meaning that the energy of an empty level is

indeed $-\omega/2$, rather than the naive zero. Then of course the energy of the filled level should be $\omega/2$.

The system which we consider is of a dynamical matrix M interacting with a system of second-quantized fermions described by annihilation a_i and creation $a_j^\dagger$ operators denoted by the same indices $\{i, j\}$ as the columns and rows in the dynamical matrix M. This means—with the convention of inclusion of the zero-point energy—that the energy term for the interaction of the dynamical matrix M with the fermions, and that includes actually all energy of the fermions, becomes

$$H_{\text{int.fermion}} = \frac{1}{2}\left[(a_1^\dagger, a_2^\dagger, , a_N^\dagger), M(t) \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} \right]. \quad (16)$$

If we let a_i and $a_i^\dagger$ be annihilation and creation operators for the eigenstate of matrix M instead of for the original basis vectors, Hamiltonian (16) would reduce to

$$H_{\text{int.fermion}} = \sum_i \frac{1}{2} x_i [a_i^\dagger, a_i] = \sum_i x_i \left(a_i^\dagger a_i - \frac{1}{2} \right). \quad (17)$$

In the following, it is understood that the energy eigenvalues have been enumerated in increasing order, so that $x_1 \leq x_2 \leq \ldots \leq x_{i-1} \leq x_i \leq x_{i+1} \leq \ldots \leq x_N$. We can of course consider any energy number x_F obeying $x_{n_f} \leq x_F \leq x_{n_f+1}$ the Fermi surface (energy), n_f being the number of fermions. Instead of keeping the number of fermions fixed to n_f, we include a chemical potential term in the Hamiltonian,

$$H_{\text{ch}} = -x_F \cdot \#\text{fermions} = -x_F \cdot n_f = -x_F \sum_i a_i^\dagger a_i. \quad (18)$$

With such a term one arranges the minimal energy situation to have precisely the (wanted) value x_F for the fermisurface. Analogously to the fermion interaction term (17), we shall also for this chemical potential term choose symmetrized expression $[a_i^\dagger, a_i]$ in the annihilation and creation operators. If we consider the situation in which the fermions for a given state of the dynamical matrix M had adjusted to lower the energy most possible (for fixed M), then we would have the n_f lowest eigenvalues x_i filled and remaining $N - n_f$ eigenenergy levels empty. Including zero-point energy the value of the $H_{\text{int.fermion}}$ part of the Hamiltonian would be

$$H_{\text{int.fermion}}|_{\text{minimal}} = \sum_{i=1}^{n_f} \frac{1}{2} x_i - \sum_{i=n_f+1}^{N} \frac{1}{2} x_i \to \frac{1}{2} \int dx \rho(x) x \,\text{sign}(x_F - x), \quad (19)$$

and the chemical potential term would give

$$H_{\text{ch}}|_{\text{minimal}} = -\sum_{i=1}^{n_f} \frac{1}{2} x_F + \sum_{i=n_f+1}^{N} \frac{1}{2} x_F \to -\frac{x_F}{2} \int dx \rho(x) \,\text{sign}(x_F - x). \quad (20)$$

Ground state and the spectrum distribution.—The full Hamiltonian for the system would contain additional terms coming from fermion interaction and chemical potential terms

$$H_{\text{full}} = H + H_{\text{int.fermion}}|_{\text{minimal}} + H_{\text{ch}}|_{\text{minimal}}. \quad (21)$$

Properly it should, however, be stressed that although we shall formally use this expression, it is in fact only physically justified when one seeks the ground state. If the system gets excited, we also expect the fermion part of it to get excited, and then one should in principle treat the fermionic part of the system as a properly second-quantized system.

In seeking the minimum of effective potential of our dynamical model

$$V_{\text{eff}} = \frac{1}{2} \int dx \left\{ \frac{\pi^2}{3} \rho^3(x) + \omega^2 x^2 \rho(x) - \mu \rho(x) - (x_F - x) \,\text{sign}(x_F - x) \rho(x) \right\}, \quad (22)$$

and in solving $\delta V_{\text{eff}}/\delta \rho = 0$, one obtains the semiclassical ground-state eigenvalue density

$$\rho(x) = \frac{1}{\pi} \sqrt{\mu + (x_F - x) \,\text{sign}(x_F - x) - \omega^2 x^2}. \quad (23)$$

For $x < x_F$, i.e., for filled states, we have

$$\rho(x) = \frac{\omega}{\pi} \sqrt{\frac{\tilde{\mu} + x_F}{\omega^2} - \left(x + \frac{1}{2\omega^2} \right)^2}, \quad (24)$$

and for empty states, $x > x_F$, we have

$$\rho(x) = \frac{\omega}{\pi} \sqrt{\frac{\tilde{\mu} - x_F}{\omega^2} - \left(x - \frac{1}{2\omega^2} \right)^2}. \quad (25)$$

Pictorially, we obtained semicircle law for both, filled and empty states, separated by the gap, when the chemical potential $\tilde{\mu} = \mu + (2\omega)^{-2}$ satisfies $x_F < \tilde{\mu} < x_F + 1/\omega^2$, and $0 < x_F < 1$ (see Fig. 1).

Notice that the term $(x - x_F)\text{sign}(x - x_F)$ in V_{eff} has a constant derivative, corresponding to a constant "electric field," on each side of the Fermi surface x_F. This electric field pulls the energy levels away from x_F, producing the homolumo gap. If we did not symmetrize the interaction with respect to filled and empty states, we would have $\theta(x - x_F)$ instead of $\text{sign}(x - x_F)$, i.e., we would still obtain the gap, only it would not be symmetric with respect to x_F.

A more intuitive physical picture could be, however, obtained in the following way. As we are interested only in the ground state, we approximate the fermionic interaction with a smooth polynomial expression, as depicted in Fig. 2. Choosing $f(x) = ax^6 - bx^4 - cx^2$, we obtain for

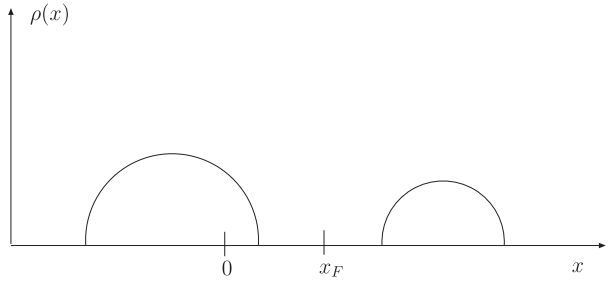

FIG. 1. On the left, we have filled levels, and on the right, empty ones.

the ground-state functional

$$\Phi = \exp\left\{\frac{1}{2}\int dxdy\rho(x)\ln(x-y)\rho(y) - \frac{1}{2}\int dx\rho(x)(fx^4 - gx^2)\right\}. \quad (26)$$

This corresponds to

$$Z = \int \prod_i dx_i \prod_{i<j}(x_i - x_j)^2 e^{-f\sum_i x_i^4 + g\sum_i x_i^2}, \quad (27)$$

giving, for deep enough wells, the two-cut solution. This shows that a homolumo gap can appear in a very generic system. Maybe even too generic, as it is basically just a two-cut solution of a Hermitean matrix model. However, the physical interpretation and field-theory formulation that we presented enables one to go beyond the ground state using rather standard techniques. Remember that it has been shown [1] that there are a few eigenvalues left outside of the semicircle, meaning that there are few states left in the gap. Thinking of our model as a field-theoretical model, one can look for the instanton contributions [9] that are expected to give strongly reduced but nonzero level density near the Fermi surface. Detailed analysis of these effects is left for further investigation.

One purpose of the presented studies in a very general setting is the application of the homolumo gap effect in the of Random Dynamics project [10]. There, one starts from the observation that at the present the energies at our disposal are extremely low, compared with the supposed

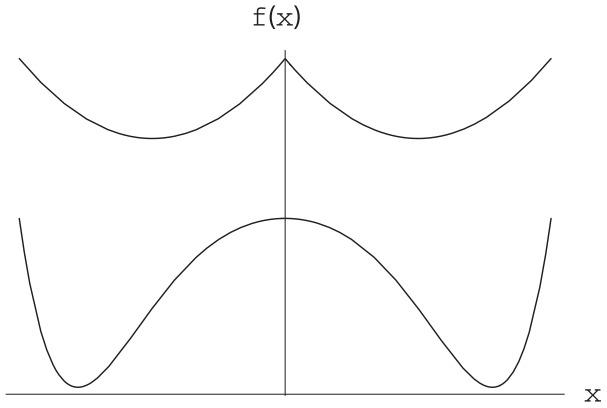

FIG. 2. Smoothing the potential: The upper graph is $f(x) = x^2 - |x|$, and the lower graph is $f(x) = -x^2 - x^4 + 2x^6$.

fundamental energy scale, presumably to be identified with the Planck scale. Thus, the ''poor physicist'' can only hope to bring say a fermion from just below the Fermi energy to just above it from the fundamental scale point of view. Obviously, the appearance of a homolumo gap of the fundamental energy scale order of magnitude would prevent creation of any fermion whatsoever. What we are really interested in is obtaining strong reduction of level density near the Fermi surface, instead of a genuine homolumo gap. Namely, if the level density in the energy range we consider is especially low, then whenever a potential scattering from one momentum eigenstate to one with a different eigen momentum should take place, there will be an especially small phase space available for it. That is to say there would be very few states to scatter into, and thus we expect much fewer such momentum violating scatterings would take place. This strong enhancement in the accuracy of momentum conservation would be interpreted as a random dynamics spirit derivation of momentum conservation.

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