Simulations of fluctuations of quantum statistical systems of electrons.

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1 Abstract

The random matrix ensembles (RMT) of quantum statistical Hamiltonian operators, e.g. Gaussian
random matrix ensembles (GRME) and Ginibre random matrix ensembles (Ginibre RME),
are applied to following quantum statistical systems: nuclear systems, molecular systems,
and two-dimensional electron systems (Wigner-Dyson’s electrostatic analogy). The Ginibre
ensemble of nonhermitean random Hamiltonian matrices $K$ is considered. Each quantum
system described by $K$ is a dissipative system and the eigenenergies $Z_i$ of the Hamiltonian
are complex-valued random variables. The second difference of complex eigenenergies is
viewed as discrete analog of Hessian with respect to labelling index. The results are consid-
ered in view of Wigner and Dyson’s electrostatic analogy. An extensio
n of space of dynamics
of random magnitudes is performed by introduction of discrete space of labeling indices.
The comparison with the Gaussian ensembles of random hermitean Hamiltonian matrices
$H$ is performed. Measures of quantum chaos and quantum integrability with respect to
eigenenergies of quantum systems are defined and they are calculated.

Quantum statistical information functional is defined as negentropy (opposite of von
Neumann’s entropy or minus entropy). The probability distribution functionals for the
random matrix ensembles (RMT) are derived from the maximum entropy principle.

2 Introduction

Random Matrix Theory (RMT) studies as an example random matrix variables correspond-
ing to random quantum Hamiltonian operators $H$. Their matrix elements $H_{ij}$ are independent random scalar variables [1, 2, 3, 4, 5, 6, 7, 8]. There were studied among others the
following Gaussian Random Matrix ensembles GRME: orthogonal GOE, unitary GUE, sym-
plectic GSE, as well as circular ensembles: orthogonal COE, unitary CUE, and symplectic
CSE. The choice of ensemble is based on quantum symmetries ascribed to the Hamiltonian
H. The Hamiltonian $H$ acts on quantum space $V$ of eigenfunctions. It is assumed that $V$ is $N$-dimensional Hilbert space $V = F^N$, where the real, complex, or quaternion field $F = \mathbb{R}, \mathbb{C}, \mathbb{H}$, corresponds to GOE, GUE, or GSE, respectively. If the Hamiltonian matrix $H$ is hermitean $H = H^\dagger$, then the probability density function of $H$ reads:

$$f_H(H) = C_H \beta \exp\left[-\beta \cdot \frac{1}{2} \cdot \text{Tr}(H^2)\right],$$

$$C_H = \left(\frac{\beta}{2\pi}\right)^{N_H \beta/2},$$

$$N_H = N + \frac{1}{2} N(N - 1),$$

$$\int f_H(H)dH = 1,$$

$$dH = \prod_{i=1}^{N} \prod_{j \geq i}^{D-1} \prod_{\gamma = 0}^{D-1} dH_{ij}^{(\gamma)},$$

$$H_{ij} = (H_{ij}^{(0)}, ..., H_{ij}^{(D-1)}) \in F,$$

where the parameter $\beta$ assume values $\beta = 1, 2, 4$, for GOE($N$), GUE($N$), GSE($N$), respectively, and $N_H$ is number of independent matrix elements of hermitean Hamiltonian $H$. The Hamiltonian $H$ belongs to Lie group of hermitean $N \times N F$-matrices, and the matrix Haar’s measure $dH$ is invariant under transformations from the unitary group $U(N, F)$. The eigenenergies $E_i, i = 1, ..., N, \text{ of } H,$ are real-valued random variables $E_i = E_i^*$. It was Eugene Wigner who firstly dealt with eigenenergy level repulsion phenomenon studying nuclear spectra [1, 2, 3]. RMT is applicable now in many branches of physics: nuclear physics (slow neutron resonances, highly excited complex nuclei), condensed phase physics (fine metallic particles, random Ising model [spin glasses]), quantum chaos (quantum billiards, quantum dots), disordered mesoscopic systems (transport phenomena), quantum chromodynamics, quantum gravity, field theory.

3 The Ginibre ensembles

Jean Ginibre considered another example of GRME dropping the assumption of hermiticity of Hamiltonians thus defining generic $F$-valued Hamiltonian $K$ [1, 2, 9, 10]. Hence, $K$ belong to general linear Lie group $GL(N, F)$, and the matrix Haar’s measure $dK$ is invariant under transformations form that group. The distribution of $K$ is given by:

$$f_K(K) = C_K \beta \exp\left[-\beta \cdot \frac{1}{2} \cdot \text{Tr}(K^\dagger K)\right],$$

$$C_K = \left(\frac{\beta}{2\pi}\right)^{N_K \beta/2},$$

$$N_K = N^2,\beta,$$

$$\int f_K(K)dK = 1.$$
\[
dK = \prod_{i=1}^{N} \prod_{j=1}^{N} \prod_{\gamma=0}^{D-1} dK_{ij}^{(\gamma)},
\]

\[
K_{ij} = (K_{ij}^{(0)}, ..., K_{ij}^{(D-1)}) \in F,
\]

where \( \beta = 1, 2, 4 \), stands for real, complex, and quaternion Ginibre ensembles, respectively. Therefore, the eigenenergies \( Z_i \) of quantum system ascribed to Ginibre ensemble are complex-valued random variables. The eigenenergies \( Z_i, i = 1, ..., N \), of nonhermitean Hamiltonian \( K \) are not real-valued random variables \( Z_i \neq Z_i^* \). Jean Ginibre postulated the following joint probability density function of random vector of complex eigenvalues \( Z_1, ..., Z_N \) for \( N \times N \) Hamiltonian matrices \( K \) for \( \beta = 2 \) [1, 2, 9, 10]:

\[
P(z_1, ..., z_N) = \prod_{j=1}^{N} \frac{1}{\pi \cdot j!} \prod_{i<j} |z_i - z_j|^2 \cdot \exp(-\sum_{j=1}^{N} |z_j|^2),
\]

where \( z_i \) are complex-valued sample points \( (z_i \in \mathbf{C}) \).

We emphasize here Wigner and Dyson’s electrostatic analogy. A Coulomb gas of \( N \) unit charges moving on complex plane (Gauss’s plane) \( \mathbf{C} \) is considered. The vectors of positions of charges are \( z_i \) and potential energy of the system is:

\[
U(z_1, ..., z_N) = -\sum_{i<j} \ln |z_i - z_j| + \frac{1}{2} \sum_i |z_i|^2.
\]

If gas is in thermodynamical equilibrium at temperature \( T = \frac{1}{2k_B} (\beta = \frac{1}{k_B} = 2, k_B \) is Boltzmann’s constant), then probability density function of vectors of positions is \( P(z_1, ..., z_N) \) Eq. (3). Therefore, complex eigenenergies \( Z_i \) of quantum system are analogous to vectors of positions of charges of Coulomb gas. Moreover, complex-valued spacings \( \Delta^1 Z_i \) of complex eigenenergies of quantum system:

\[
\Delta^1 Z_i = Z_{i+1} - Z_i, i = 1, ..., (N - 1),
\]

are analogous to vectors of relative positions of electric charges. Finally, complex-valued second differences \( \Delta^2 Z_i \) of complex eigenenergies:

\[
\Delta^2 Z_i = Z_{i+2} - 2Z_{i+1} + Z_i, i = 1, ..., (N - 2),
\]

are analogous to vectors of relative positions of vectors of relative positions of electric charges.

The eigenenergies \( Z_i = Z(i) \) can be treated as values of function \( Z \) of discrete parameter \( i = 1, ..., N \). The “Jacobian” of \( Z_i \) reads:

\[
\text{Jac} Z_i = \frac{\partial Z_i}{\partial i} \approx \frac{\Delta^1 Z_i}{\Delta^1 i} = \Delta^1 Z_i.
\]

We readily have, that the spacing is an discrete analog of Jacobian, since the indexing parameter \( i \) belongs to discrete space of indices \( i \in I = \{1, ..., N\} \). Therefore, the first derivative
with respect to $i$ reduces to the first differential quotient. The Hessian is a Jacobian applied to Jacobian. We immediately have the formula for discrete ”Hessian” for the eigenenergies $Z_i$:

$$
\text{Hess} Z_i = \frac{\partial^2 Z_i}{\partial i^2} \approx \frac{\Delta^2 Z_i}{\Delta^1 i^2} = \Delta^2 Z_i.
$$

(8)

Thus, the second difference of $Z$ is discrete analog of Hessian of $Z$. One emphasizes that both ”Jacobian” and ”Hessian” work on discrete index space $I$ of indices $i$. The spacing is also a discrete analog of energy slope whereas the second difference corresponds to energy curvature with respect to external parameter $\lambda$ describing parametric “evolution” of energy levels [11, 12]. The finite differences of order higher than two are discrete analogs of compositions of ”Jacobians” with ”Hessians” of $Z$.

The eigenenergies $E_i, i \in I$, of the hermitean Hamiltonian $H$ are ordered increasingly real-valued random variables. They are values of discrete function $E_i = E(i)$. The first difference of adjacent eigenenergies is:

$$
\Delta^1 E_i = E_{i+1} - E_i, \ i = 1, ..., (N - 1),
$$

(9)

are analogous to vectors of relative positions of electric charges of one-dimensional Coulomb gas. It is simply the spacing of two adjacent energies. Real-valued second differences $\Delta^2 E_i$ of eigenenergies:

$$
\Delta^2 E_i = E_{i+2} - 2E_{i+1} + E_i, \ i = 1, ..., (N - 2),
$$

(10)

are analogous to vectors of relative positions of vectors of relative positions of charges of one-dimensional Coulomb gas. The $\Delta^2 Z_i$ have their real parts $\text{Re} \Delta^2 Z_i$, and imaginary parts $\text{Im} \Delta^2 Z_i$, as well as radii (moduli) $|\Delta^2 Z_i|$, and main arguments (angles) $\text{Arg} \Delta^2 Z_i$. $\Delta^2 Z_i$ are extensions of real-valued second differences:

$$
\Delta^2 E_i = E_{i+2} - 2E_{i+1} + E_i, \ i = 1, ..., (N - 2),
$$

(11)

of adjacent ordered increasingly real-valued eigenenergies $E_i$ of Hamiltonian $H$ defined for GOE, GUE, GSE, and Poisson ensemble PE (where Poisson ensemble is composed of uncorrelated randomly distributed eigenenergies) [13, 14, 15, 16, 17, 18, 19, 20, 21]. The Jacobian and Hessian operators of energy function $E(i) = E_i$ for these ensembles read:

$$
\text{Jac} E_i = \frac{\partial E_i}{\partial i} \approx \frac{\Delta^1 E_i}{\Delta^1 i} = \Delta^1 E_i,
$$

(12)

and

$$
\text{Hess} E_i = \frac{\partial^2 E_i}{\partial i^2} \approx \frac{\Delta^2 E_i}{\Delta^1 i^2} = \Delta^2 E_i.
$$

(13)

The treatment of first and second differences of eigenenergies as discrete analogs of Jacobians and Hessians allows one to consider these eigenenergies as a magnitudes with statistical properties studied in discrete space of indices. The labelling index $i$ of the eigenenergies is an additional variable of ”motion”, hence the space of indices $I$ augments the space of dynamics of random magnitudes.
One may also study the finite expressions of random eigenenergies and their distributions. The finite expressions are more general than finite difference quotients and they represent the derivatives of eigenenergies with respect to labelling index $i$ more accurately [22, 23].

4 The Maximum Entropy Principle

In order to derive the probability distribution in matrix space we apply the maximum entropy principle:

$$\max \{ S_\beta(f_X) : \langle 1 \rangle = 1, \langle \mathcal{H}_X \rangle = U_\beta \},$$

which yields:

$$\max \{ S_\beta(f_X) : \int f_X(X) dX = 1, \int \mathcal{H}_X(X)f_X(X)dX = U_\beta \},$$  \hspace{1cm} (15)

where $X = H$ or $X = K$ for Gaussian or Ginibre ensembles, respectively, and $\mathcal{H}_X(X) = \frac{1}{2} \text{Tr}(X^\dagger X)$. The maximization of entropy $S_\beta(f_X) = \int (-k_B \ln f_X(X))f_X(X)dX$ under two additional constraints of normalization of the probability density function, and of equality of its first momentum and intrinsic energy, is equivalent to the minimization of the following functional $\mathcal{F}(f_X)$ with the use of Lagrange multipliers $\alpha_1, \beta_1$:

$$\min \{ \mathcal{F}(f_X) \}, \hspace{1cm} \text{where} \hspace{1cm} \mathcal{F}(f_X) = \int (k_B \ln f_X(X))f_X(X)dX + \alpha_1 \int f_X(X)dX + \beta_1 \int \mathcal{H}_X(X)f_X(X)dX.$$  \hspace{1cm} (16)

It follows, that the first variational derivative of $\mathcal{F}(f_X)$ must vanish:

$$\frac{\delta \mathcal{F}(f_X)}{\delta f_X} = 0,$$

which produces:

$$k_B(\ln f_X(X) + 1) + \alpha_1 + \beta_1 \mathcal{H}_X(X) = 0,$$  \hspace{1cm} (17)

and equivalently:

$$f_X(X) = C_{X,\beta} \cdot \exp[-\beta \cdot \mathcal{H}_X(X)]$$

$$C_{X,\beta} = \exp[-(\alpha_1 + 1) \cdot k_B^{-1}], \beta = \beta_1 \cdot k_B^{-1}.$$  \hspace{1cm} (18)

The variational principle of maximum entropy does not force additional condition on functional form of $\mathcal{H}_X(X)$. The quantum statistical information functional $I_\beta$ is the opposite of entropy:

$$I_\beta(f_X) = -S_\beta(f_X) = \int (+k_B \ln f_X(X))f_X(X)dX.$$  \hspace{1cm} (19)

Information is negentropy, and entropy is neginformation. The maximum entropy principle is equivalent to minimum information principle.
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