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Level statistics of Hessian matrices: random matrices with conservation constraints

W.-J. Ma[a,*], T.-M. Wu[b], J. Hsieh[c], S.-L. Chang[b]

[a] *Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan, ROC*
[b] *Institute of Physics, National Chiao-Tung University, Hsin-Chu, Taiwan, ROC*
[c] *Institute of Mathematics, Academia Sinica, Nankang, Taipei, Taiwan, ROC*

Abstract

We consider the Hessian matrices of simple liquid systems as a new type of random matrices. By numerically comparing the distribution of the nearest-neighbor level spacing of the eigenvalues with the Wigner's surmise, we found that the level statistics is akin to the generic Gaussian Orthogonal Ensemble (GOE), in spite of the constraints due to the summation rules and the presence of the correlation among the components inherited with the underlying spatial configuration. The distribution is in good agreement with the Wigner's prediction if only the extended eigenstates are considered. Indeed, our theoretical analysis shows that the ensemble of real symmetric matrices with full randomness, but constrained by the summation rules, is equivalent to the GOE with matrices of the rank lowered by the spatial dimension.

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Keywords: Hessian; Random matrices; GOE; Level statistics

In characterizing the spatially disordered condensed systems, such as the amorphous solids and the liquids, the methods of normal-mode analysis on the Hessian of the potential energy surface has attracted much attention recently [1–5]. The approach is analogous to its counterpart for the crystalline solid in that it traces the origin of the physical properties to the collective motion in the system. The spatial disorder, on the other hand, raises the issues on the level statistics [2,6] of the collections of random Hessian matrices. The matrices possess the correlations inherited from the underlying

* Corresponding author. Institute of Mathematics, Academia Sinica, Taipei, Taiwan, ROC. Fax: +886-2-2783-4187.
E-mail address: mwj@gate.sinica.edu.tw (W.-J. Ma).

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spatial configuration [5,7] and are also constrained by the summation rules, as the result of the conservation of momentum [8], which consequently produce zero eigenvales in number of the spatial dimension.

According to the theory of random matrices addressed by Wigner and Dyson [9], a collection of real symmetric matrices with full randomness can be modeled by the Gaussian Orthogonal Ensemble (GOE), where the only level correlation is imposed by the transformation symmetry within the ensemble. It is conjectured in various physical problems that the symmetry remains the dominant factor on the local properties such as the nearest-neighbor level spacing (LS) distribution in the presence of additional correlations. For random Hessian matrices, in recent numerical calculations of the LS distribution done for the frequency spectra [10], we have found the evidence for the type of GOE. Since the matrices are constrained by the summation rules, it deserves some clarification because the rules in general are not preserved under the similarity transformation applied by the orthogonal matrices. In this paper, we first present our numerical data for the LS distribution of the eigenvalue spectra for the Lennard Jones liquid, obtained from the molecular dynamics simulation [11]. The LS distribution for the levels in regions of extended states are shown to agree with Wigner's surmise. We, then, summarize our recent explanation [13] on how the summation rules can be released so that the conservation-constrained random matrices can be considered within the context of GOE.

The simplest version of the summation rules requires a vanishing total sum in each row of a real symmetric matrix. For the Hessian matrix H of a system of N pairwise-interacting identical particles, the summation rules are contained by the expression of its N^2 blocks of 3×3 matrices [1]

$$H_{ij} = -T(\vec{r}_{ij}) \text{ for the off-diagonal block } (i \neq j)\,,$$
$$\sum_{k \neq i} T(\vec{r}_{ik}) \text{ for the diagonal block } (i = j)\,, \tag{1}$$

$1 \leqslant i,\ j \leqslant N$, determined by the pair interaction potential $\phi(r)$ and varies with the relative position vector $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$ via the tensor $T(\vec{r})$ [1]. Eq. (1) states that the diagonal blocks of H compensate the total off-diagonal blocks in the same row of blocks.

Fig. 1 demonstrates the using of the quantity [11]

$$R_N^{\alpha} = \left(\sum_{j=1}^{N} |\, \vec{e}_j^{\,\alpha}|^4 \right)^{-1} \tag{2}$$

to estimate the participating particle number of the eigen state α by summing over the fourth power of the contribution by the individual particles to the unit eigenvector $(\vec{e}_1^{\,\alpha}, \ldots, \vec{e}_N^{\,\alpha})$. By analyzing R_N, averaged over states with the same eigenvalues, and considering its dependence on the size of the system [11,12], the region of extended states can be distinguished from the non-extended states (Figs. 1 and 2). We have carried out the LS calculation over the selected regions, equivalent to the selection of windows of specific length scales [2]. While the LS distribution of the whole spectrum

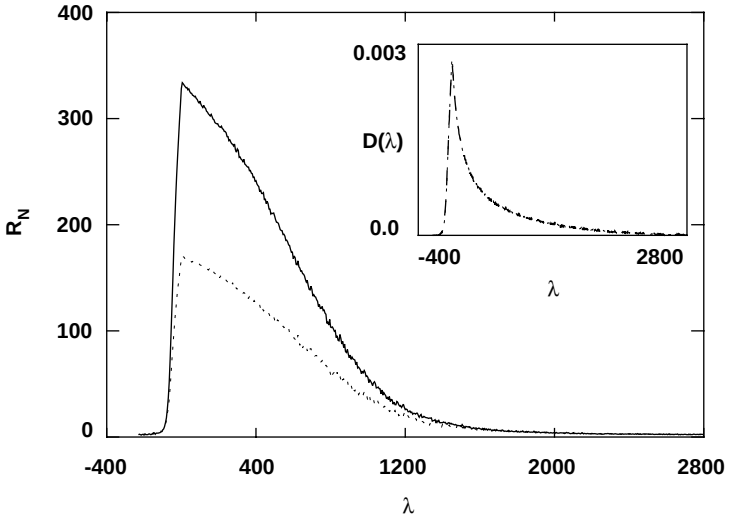

Fig. 1. The participating particle number R_N vs. eigenvalue λ averaged over 100 configurations for two Lennard Jones fluid systems with particle number $N = 750$ (—) and $N = 375$ ($\cdots$), respectively. Both systems are at the reduced temperature $T^* = 0.83$ and the reduced density $\rho^* = 0.972$. Their densities of states, plotted in the inset, are virtually identical. (Note that R_N is close to the size N of the systems in the regions not too far away from the zero eigenvalue, indicating the motion of each eigenstate in these regions is shared by most of the particles of the system.) It is in contrast to the situation in the region of localized states over the two ends of the eigenvalue axis, where R_N is basically independent of N.

greatly deviates from the Wigner's surmise, with the presence of an exponential tail in the larger separation regime, the LS distribution in the regions of extended states agrees with Wigner's distribution (Fig. 3). The LS considered in each latter region is locally scaled via the unfolding procedure [6,14]

$$s_i = \int_{\lambda_i}^{\lambda_{i+1}} D(\lambda)\,\mathrm{d}\lambda\,, \tag{3}$$

where the quantity $\int_{-\infty}^{\lambda} D(\lambda)\,\mathrm{d}\lambda$ is calculated by taking the smooth part of the cumulative spectrum obtained from the raw data.

Now, we turn to the explanation why the summation rules may not cause a fundamental change in local properties. For $3N \times 3N$ real symmetric matrix M, the condition of GOE allows its diagonalization matrix K in

$$M = K\,diag(\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_{3N})\,K^t \tag{4}$$

to possess the full $O(3N)$ symmetry. Taking into account the matrix properties of $T(\vec{r})$ in Eq. (1), the theoretical issue is addressed to consider those $3N \times 3N$ real symmetric matrices $M^{(C)}$ constrained by the 'block summation rules' [13]:

$$m^{(C)}_{(i,\mu)(i,\nu)} = -\sum_{j \neq i} m^{(C)}_{(i,\mu)(j,\nu)}\,, \tag{5}$$

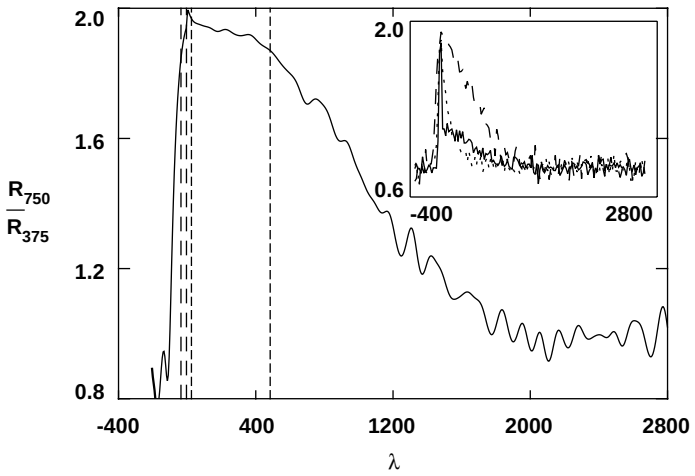

Fig. 2. The ratio between the participating particle number of the two systems depicted in Fig. 1. The ratio is close to that between the sizes of the systems for the extended states, which have their eigenvalues in between -36.0 and -4.0 (marked by the pair of vertical broken lines), and in between 25.0 and 484.0 (marked by the two dashed lines). The inset shows the plot for the systems at $T^* = 1.4$ and $\rho^* = 0.4$ (—), 0.6 ($\cdots$) and 0.8 (---), respectively. It indicates the extended states could become rare at low density.

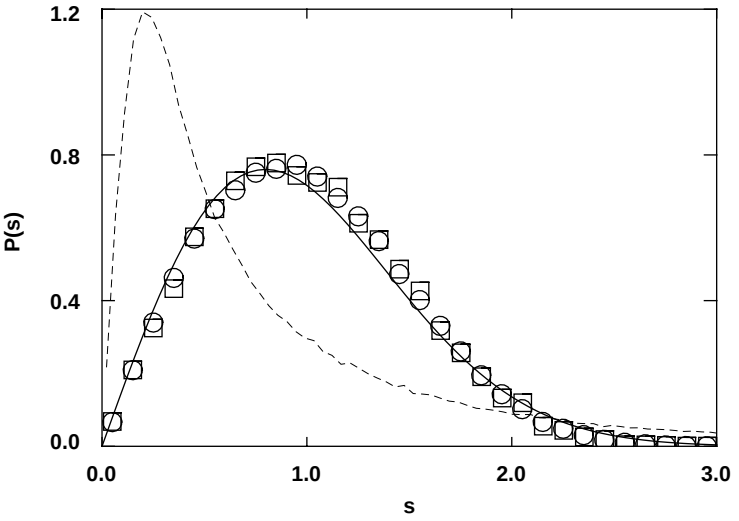

Fig. 3. Level spacing distributions with the unfolding procedure for the extended states with positive eigenvalues (◯) and that for the extended states with negative eigenvalues (□) at $T^* = 0.83$, $\rho^* = 0.972$ for $N = 750$. Both are very close to Wigner's surmise (—). The dashed line is the LS distribution for all states without unfolding the spectra. The three zero modes are excluded and 100 configurations are averaged in all cases.

where we adapt the notation $(i,\mu) \equiv 3(i-1)+\mu$ for $1 \leqslant i,j \leqslant N$ and $1 \leqslant \mu,\nu \leqslant 3$. It is apparent that the rules cannot be retained under the arbitrary symmetry operation over $SO(3N)$. But we are able to establish a one-to-one and onto mapping [13] between the constrained matrix $M^{(C)}$ and a unconstrained matrix $M^{(-)}$ with the same set of non-trivial eigenvalues but with a lowered rank $((3N-3))$ via the equality

$$K_0^{(C)^t} M^{(C)} K_0^{(C)} = \begin{pmatrix} M^{(-)} & & 000 \\ & & \vdots\vdots\vdots \\ 0 & \cdots & 000 \\ 0 & \cdots & 000 \\ 0 & \cdots & 000 \end{pmatrix}, \tag{6}$$

where $K_0^{(C)}$ is an orthogonal matrix taking up the constraint, (Eq. (5)). Thus, the full randomness of the ensemble of conservation constrained matrix $M^{(C)}$ is realized as the full $O(3N-3)$ symmetry possessed by the corresponding $M^{(-)}$. The ensemble of real symmetric matrices with full randomness, but constrained by the block summation rules, is equivalent to the GOE with matrices of the rank lowered by the block dimension.

From the numerical evidence and the theoretical analysis, we conclude that the local properties of the level statistics of Hessian matrices is still akin to the GOE, in spite of the presence of conservation constraints.

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References

[1] T. Keyes, J. Chem. Phys. 101 (1997) 2921.
[2] J.W. Kantelhardt, A. Bunde, L. Schweitzer, Phys. Rev. Lett. 81 (1998) 4907.
[3] S.N. Taraskin, S.R. Elliot, Phys. Rev. B 61 (2000) 12 017.
[4] W.J. Ma, T.M. Wu, Physica A 281 (2000) 393.
[5] T.S. Grigera, V. Martín-Mayor, G. Parisi, P. Verrocchio, Phys. Rev. Lett. 87 (2001) 85 502.
[6] S. Sastry, N. Deo, S. Franz, Phys. Rev. E 64 (2001) 16 305.
[7] M. Mézard, G. Parisi, A. Zee, Nucl. Phys. B 559 (1999) 689.
[8] Y. Wan, R.M. Stratt, J. Chem. Phys. 98 (1993) 3224.
[9] M.L. Mehta, Random Matrices, 2nd Edition, Academic Press, New York, 1991.
[10] T.M. Wu, W.J. Ma, S.L. Chang, unpublished data.
[11] T.M. Wu, W.J. Ma, S.F. Tsay, Physica A 254 (1998) 257.
[12] T.M. Wu, W.J. Ma, J. Chem. Phys. 110 (1999) 447.
[13] W.J. Ma, T.M. Wu, J. Hsieh, J. Phys. A Math. Gen. 36 (2003) 1451.
[14] T. Guhr, A. Müller-Groeling, H.A. Weidenmüller, Phys. Rep. 299 (1998) 189.