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Conservation constraints on random matrices

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Abstract

We study the random matrices constrained by the summation rules that are present in the Hessian of the potential energy surface in the instantaneous normal mode calculations, as a result of momentum conservation. In this paper, we analyse the properties related to such conservation constraints in two classes of real symmetric matrices: one with purely row-wise summation rules and the other with the constraints on the blocks of each matrix, which underscores partially the spatial dimension. We show explicitly that the constraints are removable by separating the degrees of freedom of the zero-eigenvalue modes. The non-spectral degrees of freedom under the constraints can be realized in terms of the ordinary constraint-free orthogonal symmetry but with the rank deducted by the block dimension. We propose that the ensemble of real symmetric matrices with full randomness, constrained by the summation rules, is equivalent to the Gaussian orthogonal ensemble (GOE) with lowered rank. Independent of the joint probability distribution, the Jacobian contributed by the transformation from the matrix coordinates to the spectral coordinates, possesses the same spectral-variable dependence in these two cases. We verify numerically that the small-separation asymptotic in the nearest-neighbour level spacing distribution is indeed governed by the same symmetry power factor, $\beta = 1$, as that of the GOE, under conservation constraints and other underlying spatial correlations.

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1. Introduction

The fascinating level statistics of random matrices has been explored in different physics problems. The accumulated numerical and theoretical studies continually reveal various examples [1–4], ranging from the spectra of collections of nuclei to the transport properties of

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solids, that comply with the prototypes of Gaussian ensembles addressed in the seminal works of Wigner and Dyson [5, 6]. One class of recent interesting problems is related to the Hessian matrices, the matrices characterizing the curvatures of the total potential energy surface. The problems involve the analysis of the normal modes for liquids or disordered solids. The eigenvalues and the corresponding eigenvectors of the Hessian matrices are calculated with the harmonic terms isolated from the expansion of potential energy, for the disordered and typically mechanically non-equilibrium configuration at each instantaneous moment. Such analysis of instantaneous normal modes (INMs) [7–9] has been shown to be informative for the characterization of the energy landscape for states with disordered configurations [10–12]. The evidence from the numerical data of the nearest-neighbour level-spacing distributions [13] suggests the validity of the Wigner–Dyson statistics for this new type of random matrix. The presence of the 'localized modes', however, causes deviation as is present in similar types of problems occurring in other contexts [13]. Under the constraints of the summation rules [8, 9] and other intrinsic interrelation among the matrix elements [14–16], one fundamental question is, then, how robust is the level statistics of random Hessian matrices? In this paper, we focus on the issue of summation rules.

The physical systems under our consideration are the systems of pairwise-interacting identical particles, where the Hessian matrices are constrained by the summation rules as a result of the conservation of linear momentum. The simplest version of the summation rules requires a real symmetric $N \times N$ matrix $\mathbf{M}^{(C)}$,[4] to have a vanishing total sum for its entries in each row (or equivalently in each column) $\sum_{j=1}^{N} m_{ij}^{(C)} = 0$, that is,

$$m_{ii}^{(C)} = -\sum_{j \neq i} m_{ij}^{(C)} \qquad \text{for} \quad i = 1, 2, \ldots, N. \tag{1}$$

The rules are present as the results of conservation laws, in various contexts such as the transition matrix describing the probability flow [17, 18] or the Laplacian matrix characterizing the connectivity of a random graph [18–20]. For three-dimensional systems, the summation rules on the Hessian matrices are imposed among the 3×3 tensor blocks (see section 3), which are more restrictive than those described by equation (1). Nevertheless, the analysis of this simple version of summation rules is sufficient to reveal the answers to the questions of how the summation rules modify the algebraic properties of the matrices and whether they introduce any additional correlations into the level statistics.

The random matrix theory (RMT) pioneered by Wigner and Dyson addresses the level statistics of the matrices with full randomness. According to the theory, the statistical distribution for the eigenvalues of the matrices in a Gaussian ensemble is described by a Boltzmann distribution e^{-E} with E consisting of two parts [1, 6]: a quadratic confining potential part, which is contributed by a Gaussian probability distribution, and a level repulsion part, characterizing the inherent level correlation. The latter carries the contribution by the product of differences of the eigenvalues,

$$\prod_{i<j} (\lambda_i - \lambda_j)^{\beta} \tag{2}$$

with the symmetry power factor β counting the number of degrees of freedom allowed for each matrix element [1]. For an ensemble of real symmetric matrices, we have $\beta = 1$. The presence of equation (2) provides an indispensable source of level correlation and is independent of the assumptions made for the part of the confining potential.

[4] We use the superscript '(C)' as the label of the matrix and its related quantities to highlight the presence of the rules.

For real symmetric matrices with the matrix elements constrained by the summation rules (1), it seems unclear from first sight what their effects are, on the inter-relation among the spectral variables λ_i in equation (2), aside from the fact that zero is a common eigenvalue to all matrices. The numerical evidence from the level spacing properties of the INM spectra [13] seems to suggest generally no deviation from the statistics governed by equation (2), in spite of the presence of the conservation constraints and other inter-relations among the matrix elements of a Hessian [14–16]. To provide a theoretical verification of the validity of the form (2) under the constraints of the summation rules and to find out whether any new level correlation could be introduced by the rules, we carry out a detailed examination on the assumptions and the mathematical formulation for the Gaussian orthogonal ensemble (GOE) to see how the constraints can be fitted into the framework. The key issue is that, for the ensemble of real symmetric matrices with full randomness, the probability distribution is invariant under the similarity transformation on the matrices by any orthogonal matrix. Such a property could not, however, hold for an ensemble of matrices constrained by the summation rules, because the rules are not preserved under an arbitrary orthogonal similarity transformation. We resolve the problem by mapping the constrained matrices to matrices without constraints but with the rank lowered by one. It is shown that the presence of a factor in the form of equation (2), related to the diagonalization procedure, is still valid under the linear constraints imposed by the summation rules (1) and an ensemble with full randomness constrained by the rules is the GOE with the lowered rank.

In this paper, we consider two types of conservation constraints: the ordinary type described by equation (1) and its mathematical generalization to the rules on the blocks of submatrices. While the latter states the conservation constraints present in a Hessian matrix, the former describes the physical circumstance replacing each block of tensor in the Hessian by a scalar. In section 2, we review the assumptions and the mathematical formulation for the Gaussian ensemble of real symmetric matrices. We then explain, in section 3, the type of summation rules present in the Hessian matrix. In section 4, the diagonalization procedures of the real symmetric matrices with the constraints by the scalar summation rules (1) are analysed and we establish a one-to-one correspondence between the constrained and unconstrained matrices with the latter of rank lowered by one. The origin of the factor (2), with $\beta = 1$, in the transformation Jacobian for the constrained matrices is also examined. In section 5, we extend the analysis to matrices subject to the blocked summation rules. The one-to-one correspondence between the conservation-constrained matrices and the constraint-free matrices is established with the latter having the rank lowered by the block dimension. In the final section, we discuss the implication of the results obtained in the previous sections. For a few simulated liquid systems, we verify numerically the linear small-value asymptote in the nearest-neighbour level spacing distribution predicted by equation (2) for the spectra of the Hessian matrices with each tensor block replaced by a scalar. We discuss the conditions required for the conservation-constrained ensemble with Gaussian or other types of probability distribution. Parts of the detailed derivations and proofs omitted in the main text are included in appendices A–C.

2. Gaussian orthogonal ensemble

The GOE [1] is an idealized ensemble defined for the set $S(N)$ of all $N \times N$ real symmetric matrices where the probability distributions for the matrix elements satisfy the following assumptions:

Assumption I, the matrix elements are statistically independent;
Assumption II, the overall probability distribution is invariant under the similarity transformation by any orthogonal matrix.

While the ensemble was originally designed to describe the Hamiltonian matrices, assumption II requires the invariance under the state-norm preserving (symmetry) operations. In $S(N)$, any such operation is described by an $N \times N$ matrix $\mathbf{K}$ satisfying the orthogonality condition $\mathbf{K}^t\mathbf{K} = 1$ (the superscript 't' denotes the transpose of the matrix). One such operation is the diagonalization of a matrix $\mathbf{M} = [m_{ij}] \in S(N)$, $1 \leqslant i, j \leqslant N$,

$$\mathbf{K}^t\mathbf{M}\mathbf{K} = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N) \equiv \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ & & \vdots & \\ 0 & \cdots & 0 & \lambda_N \end{pmatrix} \tag{3}$$

or conversely,

$$\mathbf{M} = \mathbf{K} \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N)\mathbf{K}^t. \tag{4}$$

The probability function is assumed to be invariant under any of the 'left-group translation' $\mathbf{L}$ of $\mathbf{K}$

$$\mathbf{L}\mathbf{M}\mathbf{L}^t = \mathbf{K}_1 \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N)\mathbf{K}_1^t \qquad \text{with} \quad \mathbf{K}_1 = \mathbf{L}\mathbf{K}$$

over the $\frac{N(N-1)}{2}$ degree-of-freedom topological group $SO(N)$ (we adapt the convention requiring the unity determinant here), to which $\mathbf{L}$, $\mathbf{K}$ and $\mathbf{K}_1$ belong [21]. Consider $S(N)$ as a manifold extended by the matrix elements m_{ij}, on which the probability distribution of the ensemble is defined. Equations (3) and (4) describe the transformation between two coordinate systems: the system m of matrix coordinates, taking the $\frac{N(N+1)}{2}$ independent matrix elements, say, $\{m_{ij}, 1 \leqslant i \leqslant j \leqslant N\}$ as its components; and the system (q, λ) of spectral coordinates, containing the N spectral variables $\lambda \equiv (\lambda_1, \lambda_2, \ldots, \lambda_N)$ and the $l = N^2 - \frac{N(N+1)}{2} = \frac{N(N-1)}{2}$ non-spectral parameters $q \equiv (q_1, q_2, \ldots, q_l)$ which control the matrix $\mathbf{K}$ in equation (4). Assumption II states the independence of the probability distribution on the non-spectral parameters q. Indeed, according to assumption I, the joint probability distribution F is a product of the individual distribution functions of the $\frac{N(N+1)}{2}$ independent matrix elements,

$$F = \prod_{\langle ij \rangle} f_{ij}(m_{ij}). \tag{5}$$

The invariance property required by assumption II reduces it further to an exponential function of the trace of a sum, over the powers of the matrix up to the second order [1, 22],

$$F = \mathrm{e}^{-a \operatorname{Tr}(M^2) + b \operatorname{Tr}(M) + c} \tag{6}$$

i.e. a Gaussian function of the eigenvalues.

In addition to the Gaussian probability distribution (6), the level statistics of the GOE is determined decisively by the Jacobian $\left|\frac{\partial m}{\partial(q,\lambda)}\right|$ of the transformation from the matrix coordinates m to the spectral coordinates (q, λ), the spectral dependence of which is the product of differences between spectra variables

$$\prod_{i<j} (\lambda_i - \lambda_j). \tag{7}$$

The presence of the factor (7) is purely from the coordinate transformation on the manifold $S(N)$ and is not a consequence of the assumptions I or II. The correlation introduced by the factor (7), termed as a 'geometric correlation' by some authors [3], is always present whether the probability distribution F is a Gaussian, or whether it has q-dependence or not.

3. Summation rules in Hessian matrices

To examine explicitly the constraints on the Hessian matrix, we write down the matrix for a system of N identical particles interacting via the same central-force pairwise potential in three-dimensional space, in terms of the submatrices

$$\begin{aligned} \mathbf{H}_{ij} &= -\mathbf{T}(\vec{r}_{ij}) \qquad \text{for the off-diagonal block} \quad (i \neq j) \\ &\sum_{k\neq i} \mathbf{T}(\vec{r}_{ik}) \qquad \text{for the diagonal block} \qquad (i = j) \end{aligned} \tag{8}$$

for $1 \leqslant i, j \leqslant N$, where the 3×3 symmetric matrix $\mathbf{T}(\vec{r}_{ij})$ is determined by the pair interaction potential and varies with the relative position vector $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$ [8, 9]. The Hessian matrix $\mathbf{H}$ is the $3N \times 3N$ matrix composed of $N \times N$ blocks of submatrices $\mathbf{H}_{ij}$. Equation (8) states the important property that the diagonal blocks of $\mathbf{H}$ compensate the total off-diagonal blocks in the same row (of blocks), that is, the summation rules for the blocks. In terms of the matrix elements of the blocks, the rules are written as[5]

$$h_{(i,\mu)(i,\nu)} = -\sum_{j\neq i} h_{(i,\mu)(j,\nu)} \tag{9}$$

for the nine entries $1 \leqslant \mu, \nu \leqslant d = 3$.

To fit the summation rules into the framework of RMT, we need to consider the symmetric properties of the Hessian matrix. For systems with central-force interaction, we have $\mathbf{T}(\vec{r}_{ij}) = \mathbf{T}(\vec{r}_{ji})$ (see appendix A). $\mathbf{H}$ is thus symmetric block-wise

$$\mathbf{H}_{ij} = \mathbf{H}_{ji}. \tag{10}$$

Since T is itself symmetric (see appendix A), $\mathbf{H}$ is also symmetric within each block $\mathbf{H}_{ij}$, that is,

$$h_{(i,\mu)(j,\nu)} = h_{(i,\nu)(j,\mu)}. \tag{11}$$

The two properties (11) and (10) imply that the matrix $\mathbf{H}$ is overall symmetric

$$h_{(i,\mu)(j,\nu)} = h_{(j,\nu)(i,\mu)}. \tag{12}$$

To simplify the analysis, we leave out in our analysis the constriction addressed by equations (10) and (11) and we consider only the matrices with the overall symmetric property described by equation (12) under the constraints (9). We show in section 5 that such constraints are the mathematically reasonable extension of the summation rules (1). It is, however, worth noting that the spatial dimension of the system is only partially underscored. In order to reflect the physical dimension of the space, the tensor properties possessed by the matrix $\mathbf{T}$ and the underlying correlations [8, 15, 16] inherited with the position vector in $\mathbf{T}$ should be included. These issues are beyond the scope of this paper.

The two classes of matrices under consideration in this paper are thus: the set $S^{(C)}(N)$ of the real symmetric matrices constrained by equation (1), which is the physical equivalence of the case with the blocks in a Hessian matrix reduced to scalar values; and $S^{(C)}(N, 3)$, a subset of $S^{(C)}(3N)$ with the entries in each member matrix $\mathbf{M}^{(C)}$ obeying the blocked summation rules:

$$m^{(C)}_{(i,\mu)(i,\nu)} = -\sum_{j\neq i} m^{(C)}_{(i,\mu)(j,\nu)} \tag{13}$$

[5] Using the notation $(i, \mu) \equiv d \times (i-1) + \mu$, the matrix element $h_{(i,\mu)(j,\nu)}$ is the entry $\mu\nu$ in the block of submatrix $\mathbf{H}_{ij}$. (We use the dummy indices of small Latin letters range from 1 to N and the Greek letters from 1 to d.)

for $1 \leqslant \mu, \nu \leqslant 3$. Equation (13) implies (1), which justifies the remark that[6] $S^{(C)}(N, 3) \subset S^{(C)}(3N)$. For the convenience of comparison, we highlight the matrices and all the related quantities subject to the conservation constraints with the superscript '(C)'.

In the following, whenever we mention one set of matrices as a 'manifold', we refer to the set equipped with the two systems of Euclidean coordinates: the matrix coordinates, consisting of the independent matrix elements; and the spectral coordinates, which contain the spectral variables and the non-spectral diagonalization parameters. The local transformation between these two types of coordinate systems [1, 23] on the manifold $S(N)$ is well defined because they are related by the analytical algebraic expressions. The consideration involves the properties of the infinitesimal neighbourhood (the topology) of each entity in $S(N)$ [24] and there is no need to evoke the concept of 'distance' (metric) between two entities on the manifold [25]. For the same reason, such local transformation is also well defined on $S^{(C)}(N)$, in spite of the presence of the conservation constraints (section 4).

4. Real symmetric matrices with conservation constraint

As a subset of measure zero in $S(N)$, the manifold $S^{(C)}(N)$ cannot inherit the topological properties directly from $S(N)$. The linear constraints (1), nevertheless, allow the $\frac{N(N-1)}{2}$ independent variables, $\left\{m_{ij}^{(C)}, 1 \leqslant i < j \leqslant N\right\}$, as the components for the system of matrix coordinates $m^{(C)}$, to fill the whole subspace $\mathbf{R}^{\frac{N(N-1)}{2}}$ in the Euclidean space $\mathbf{R}^{\frac{N(N+1)}{2}}$. Our task here is to find the equivalence of the constraints (1) on the spectral coordinates and find out whether or how their effects can be simply described as the reduction of dimension. The trick is to track and match the numbers of degrees of freedom between the two systems on the two sides of (4).

4.1. Conservation constraints on spectral coordinates

Since the summation rules require zero as a common eigenvalue, corresponding to the mode of centre-of-mass translation, for all matrices in $S^{(C)}(N)$, we have only $N-1$ spectral variables $\lambda_1^{(C)}, \lambda_2^{(C)}, \ldots, \lambda_{N-1}^{(C)}$, with $\lambda_N^{(C)} \equiv 0$ excluded. We express the diagonalization matrix $\mathbf{K} = \mathbf{K}^{(C)}$ of equations (3) and (4) in terms of a row of orthonormal column vectors $\mathbf{K}^{(C)} = \left(\vec{a}_1^{(C)}, \vec{a}_2^{(C)}, \ldots, \vec{a}_N^{(C)}\right)$, with[7]

$$K_{ji}^{(C)} = a_{ij}^{(C)} \qquad \text{and} \qquad \vec{a}_i^{(C)} = \begin{pmatrix} a_{i1}^{(C)} \\ a_{i2}^{(C)} \\ \vdots \\ a_{iN}^{(C)} \end{pmatrix}$$

corresponding to the eigenvalue $\lambda_i^{(C)}$ for $1 \leqslant i \leqslant N$. The rules described by equation (1) state

$$\sum_{j=1}^{N} \sum_{k=1}^{N} a_{ki}^{(C)} \lambda_k^{(C)} a_{kj}^{(C)} = 0 \tag{14}$$

[6] According to such notation, we have $S^{(C)}(N) \equiv S^{(C)}(N, 1)$.

[7] Note the interchanged order in the indices between the matrix element and the component of the column vector.

which is equivalent to requiring that the column vector

$$\begin{pmatrix} \lambda_1^{(C)} \sum_{j=1}^{N} a_{1j}^{(C)} \\ \lambda_2^{(C)} \sum_{j=1}^{N} a_{2j}^{(C)} \\ \vdots \\ \lambda_N^{(C)} \sum_{j=1}^{N} a_{Nj}^{(C)} \end{pmatrix}$$

be perpendicular to a set of orthonormal basis composing of matrix $\mathbf{K}$ (see appendix B). The only such vector is the null vector. Thus, we must have

$$\sum_{k=1}^{N} a_{ik}^{(C)} = 0 \tag{15}$$

for $\lambda_i^{(C)} \neq 0$. Since $a_{ik}^{(C)}$ describes the eigen amplitude of the particle k, the result says that the total momentum for each individual mode $\lambda_i^{(C)}$ is zero except for the mode characterizing the translation motion of the centre of mass. We have the following lemma.

Lemma 1. *Under equation (4), the necessary and sufficient condition for a matrix* $\mathbf{M} = \mathbf{M}^{(C)}$ *to satisfy the summation rules (1) is that each column of the transformation matrix* $\mathbf{K} = \mathbf{K}^{(C)}$ *corresponding to a nonzero eigenvalue, obeys the rules (15).*

Thus, the number of independent constraint equations on the transformation matrix $\mathbf{K}^{(C)}$ is $N - 1$. We have $\bar{l} = l - (N - 1) = \frac{(N-1)(N-2)}{2}$ remaining degrees of freedom for $\mathbf{K}_I^{(C)}$. $\bar{l}$ is also the number of degrees of freedom allowed for a set of orthonormal bases composing the transformation matrix $\mathbf{K}^{(-)}$ that generates matrices $\mathbf{M}^{(-)}$ in $S(N-1)$ via the equation $\mathbf{M}^{(-)} = \mathbf{K}^{(-)} \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{N-1}) \mathbf{K}^{(-)t}$.[8] Let $q^{(C)} \equiv \left(q_1^{(C)}, q_2^{(C)}, \ldots, q_{\bar{l}}^{(C)}\right)$ and $q^{(-)} \equiv \left(q_1^{(-)}, q_2^{(-)}, \ldots, q_{\bar{l}}^{(-)}\right)$ be the sets of the $\bar{l}$ independent parameters of $\mathbf{K}^{(C)}$ (for $\mathbf{M}^{(C)}$ in $S^{(C)}(N)$) and $\mathbf{K}^{(-)}$ (for $\mathbf{M}^{(-)}$ in $S(N-1)$), respectively. The correspondence between the matrices in $S^{(C)}(N)$ and those in $S(N-1)$ is established by identifying the common set of eigenvalues

$$\lambda^{(-)} \equiv (\lambda_1, \ldots, \lambda_{N-1}) = \lambda^{(C)} \equiv \left(\lambda_1^{(C)}, \ldots, \lambda_{N-1}^{(C)}\right)$$

and by appropriately relating the parameters $q^{(C)} \leftrightarrow q^{(-)}$. Indeed, any given orthogonal transformation matrix $\mathbf{K}_0^{(C)}$ satisfying the conservation constraints (15) stated in lemma 1 can be used to establish a one-to-one correspondence between the matrices $\mathbf{M}^{(C)} \in S^{(C)}(N)$ and $\mathbf{M}^{(-)} \in S(N-1)$ with identical spectral variables, by applying the similarity transformation to $\mathbf{M}^{(C)}$,

$$\mathbf{K}_0^{(C)t} \mathbf{M}^{(C)} \mathbf{K}_0^{(C)} = \begin{pmatrix} & & 0 \\ & \mathbf{M}^{(-)} & \vdots \\ 0 & \cdots & 0 \end{pmatrix} \tag{16}$$

where the matrix elements of the Nth row and the Nth column on the right-hand side are zeros (see appendix C for the derivation). A set of $SO(N-1)$-symmetry operations can be defined correspondingly for the $\frac{(N-1)(N-2)}{2}$ degrees of freedom in the non-spectral parameters on the manifold $S^{(C)}(N)$ by the following lemma:

[8] We use superscript '$(-)$' here to highlight the quantities related to matrices with the rank lowered by one.

Lemma 2. *Under the mapping (16), the diagonalization transformation matrices* $\mathbf{K}^{(C)}$ *and* $\mathbf{K}^{(-)}$*, for* $\mathbf{M}^{(C)}$ *and* $\mathbf{M}^{(-)}$ *respectively, are related by*

$$\mathbf{K}^{(C)} = \mathbf{K}_0^{(C)} \begin{pmatrix} & & 0 \\ & \mathbf{K}^{(-)} & \vdots \\ 0 & \cdots & 01 \end{pmatrix} \tag{17}$$

Unlike the random Hamiltonian matrices described by $S(N)$, where the group operations in $SO(N)$ are related to the symmetry operations allowed for the Hamiltonian, the exact meaning of the group operations over $SO(N-1)$ for conservation-constrained manifold $S^{(C)}(N)$, however, requires filling more physical content from the real systems.

4.2. Transformation to spectral coordinates

The derivation of the Jacobian, which leads to the presence of the factor (2) for Gaussian ensembles (or (7) for GOE), can be found in the standard books on random matrices [1, 23]. The key ideas are as follows. Firstly, the Jacobian is factorized into a product of two functions, each depending exclusively on the spectral variables λ or non-spectral parameters q only. This is a result of repeatedly applying orthogonality condition for the matrix $\mathbf{K}$ in equation (4). The matrix of which the determinant defines the Jacobian can be expressed as the transformed result by the same $\mathbf{K}$ on a blocked matrix with two subblocks. One is a unity submatrix, contributed by the differentiations of those spectral variables λ_i, before the transformation to matrix coordinates, with respect to themselves. The other contains the entries of the commutators, each between one matrix exclusively depending on non-spectral parameters q and the other the diagonal matrix $\mathrm{diag}(\lambda_1, \lambda_2, \ldots)$, originated from the differentiations with respect to q under the orthogonality condition on $\mathbf{K}$. These commutators contribute to the factorized Jacobian and the presence of the differences of spectral variables. From the mapping defined by the similarity transformation (16), it is not difficult to see that the presence of the conservation constraints would still make the corresponding derivation valid in leading to similar results.

We, therefore, have the factorized expression for the Jacobian[9]

$$\left| \frac{\partial m^{(C)}}{\partial (q^{(C)}, \lambda^{(C)})} \right| = G^{(C)}(q^{(C)}) \prod_{1 \leqslant i < j \leqslant N-1} \left(\lambda_i^{(C)} - \lambda_j^{(C)}\right). \tag{18}$$

With equation (18), the probability of finding a matrix in a volume $\mathrm{d}m^{(C)} \equiv \mathrm{d}m_{12}^{(C)}\, \mathrm{d}m_{13}^{(C)} \ldots \mathrm{d}m_{(N-1)N}^{(C)}$ can be expressed as

$$\begin{aligned} F(m^{(C)})\, \mathrm{d}m^{(C)} &= F(m^{(C)}(q^{(C)}, \lambda^{(C)})) \left| \frac{\partial m^{(C)}}{\partial (q^{(C)}, \lambda^{(C)})} \right| \mathrm{d}q^{(C)}\, \mathrm{d}\lambda^{(C)} \\ &= g(q^{(C)}, \lambda^{(C)}) \prod_{1 \leqslant i < j \leqslant N-1} \left(\lambda_i^{(C)} - \lambda_j^{(C)}\right) \mathrm{d}q^{(C)}\, \mathrm{d}\lambda^{(C)} \end{aligned} \tag{19}$$

[9] Following the notation for partitioned matrices introduced in chapter 3 of [1], the detailed and straightforward derivation leads to the expression

$$G^{(C)}(q^{(C)}) = \det\left[\left(S_h^{(C)}\right)_{tu}\right] \det\left[a_{tv}^{(C)} a_{uw}^{(C)} + a_{uv}^{(C)} a_{tw}^{(C)} - a_{tv}^{(C)} a_{uv}^{(C)} - a_{tw}^{(C)} a_{uw}^{(C)}\right]^{-1}$$

where $1 \leqslant t < u \leqslant N$, $1 \leqslant v < w \leqslant N$ and $\mathbf{S}_k^{(C)} \equiv \mathbf{K}^{(C)t} \frac{\partial \mathbf{K}^{(C)}}{\partial q_k^{(C)}}$.

where the probability distribution $F(m^{(C)})$, as a function of the off-diagonal elements $m^{(C)}$ defined on $S^{(C)}(N)$, is expressed in terms of the new coordinates $(q^{(C)}, \lambda^{(C)})$. The level statistics is thus described by the distribution

$$P^{(C)}(\lambda^{(C)}) = f^{(C)}(\lambda^{(C)}) \prod_{i<j} \left(\lambda_i^{(C)} - \lambda_j^{(C)}\right) \tag{20}$$

after the ensemble averaging over the non-spectral parameters $q^{(C)}$ in equation (19).

5. Blocked conservation constraint

In this section, we show that the blocked summation rules (13) are a generalization of the scalar rules (1), in the sense that the correspondence (16) between $S^{(C)}(N)$ and $S(N-1)$ can be extended between $S^{(C)}(N,3)$ and $S(3N-3)$. For the convenience of comparison, we extend the previous convention to highlight the matrices and their related quantities in $S^{(C)}(N,3)$ by the superscript '(C)'; and those in $S(3N-3)$ by '$(-)$'.

Our starting point is the pair of similarity transformations, the diagonalization transformation on the $3N \times 3N$ real symmetric matrix $\mathbf{M} \in S(3N)$, by the orthogonal matrix $\mathbf{K}$

$$\mathbf{K}^t\mathbf{M}\mathbf{K} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_{3N}) \equiv \begin{pmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & 0 & \lambda_3 & \cdots & 0 \\ & & \vdots & & \\ 0 & \cdots & & 0 & \lambda_{3N} \end{pmatrix} \tag{21}$$

and its converse (cf equations (3) and (4))

$$\mathbf{M} = \mathbf{K}\,\mathrm{diag}(\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_{3N})\mathbf{K}^t. \tag{22}$$

In order to simplify the expression of matrix multiplication in terms of the summation of products of matrix elements, we adapt the duplex of indices used in section 3, to denote the subscript for matrix element in matrix $\mathbf{M}$ composed of N^2 3×3 blocks, with $m_{(i,\mu)(j,\nu)}$ representing the $\mu\nu$ element in the ij block. Correspondingly we denote the eigenvalues $\lambda_{(i,\mu)} \equiv \lambda_{3(i-1)+\mu}$, with $1 \leqslant i \leqslant N$ and $1 \leqslant \mu \leqslant 3$. For real symmetric matrix $\mathbf{M}$, the diagonalization transformation matrix $\mathbf{K}$ in equation (21) can be expressed in terms of the orthonormal basis vectors

$$\vec{a}_{(i,\mu)} = \begin{pmatrix} a_{(i,\mu)(1,1)} \\ a_{(i,\mu)(1,2)} \\ a_{(i,\mu)(1,3)} \\ \vdots \\ a_{(i,\mu)(N,3)} \end{pmatrix}$$

corresponding to the eigenvalue $\lambda_{(i,\mu)}$, with

$$\mathbf{K} = (\vec{a}_{(1,1)}, \vec{a}_{(1,2)}, \vec{a}_{(1,3)}, \ldots, \vec{a}_{(N,3)}) \tag{23}$$

or $\mathbf{K}_{(j,\nu)(i,\mu)} = a_{(i,\mu)(j,\nu)}$. Conversely, any orthonormal basis defines an orthogonal transformation matrix $\mathbf{K}$, that produces a real symmetric matrix $\mathbf{M}$ with the given eigenvalues via equation (22). The latter equation, therefore, generates the whole set $S(3N)$ of real symmetric matrices of rank $3N$.

We now impose the block summation rules (13) on the $3N \times 3N$ real symmetric matrix $\mathbf{M}^{(C)} \in S^{(C)}(N,3)$, composed of N^2 blocks of 3×3 matrices $\mathbf{M}^{(C)}_{ij} = \left[\left(M^{(C)}_{ij}\right)_{\mu\nu}\right] \equiv \left[m^{(C)}_{(i,\mu)(j,\nu)}\right]$, with $1 \leqslant i, j \leqslant N$ and $1 \leqslant \mu, \nu \leqslant 3$. There are three zero eigenvalues shared by all matrices in $S^{(C)}(N,3)$, we have only $3N-3$ spectral variables $\lambda_{(i,\mu)}$, for $1 \leqslant i \leqslant N-1$ and $1 \leqslant \mu \leqslant 3$, with $\lambda^{(C)}_{(N,1)} = \lambda^{(C)}_{(N,2)} = \lambda^{(C)}_{(N,3)} = 0$ excluded. Similar to the case of scalar version of summation rules, we can show that the necessary and sufficient condition for matrix $\mathbf{M}^{(C)}$ to satisfy the block summation rules is that (see appendix B),

$$\sum_{j=1}^{N} a^{(C)}_{(i,\mu)(j,\nu)} = 0 \tag{24}$$

for all $1 \leqslant \mu, \nu \leqslant 3$ and $i \neq N$. As in section 4, we can establish a one-to-one correspondence between the matrices $\mathbf{M}^{(C)} \in S^{(C)}(N,3)$ and $\mathbf{M}^{(-)} \in S(3N-3)$, with the same set of eigenvalues excluding $\lambda^{(C)}_{(N,\mu)}$ ($\mu = 1, 2, 3$), via

$$\mathbf{K}_0^{(C)^t}\mathbf{M}^{(C)}\mathbf{K}_0^{(C)} = \begin{pmatrix} & & 0 & 0 & 0 \\ & \mathbf{M}^{(-)} & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 \end{pmatrix} \tag{25}$$

by any orthonormal matrix $\mathbf{K}^{(C)}_0$ satisfying the condition (24), and an additional constriction

$$\sum_{j} a^{(C)}_{(N,\mu)(j,\nu)} \neq 0 \qquad \text{for} \quad \mu, \nu = 1, 2, 3 \tag{26}$$

on the rows (columns) of components for each of the three basis vectors of $\mathbf{K}^{(C)}_0$ with zero eigenvalue (see appendix C).

In a comparison with the case for matrices with scalar conservation constraint discussed in section 4.1, we can see the role played by the block dimension. Firstly, for d dimension system, $\frac{d(d-1)}{2}$ of the blocked summation rules are dependent on the rest of the rules. Next, the degrees of freedom corresponding to zero eigenvalues are inactive in the diagonalized expression for $\mathbf{M}^{(C)}$ and contribute only to the $d \times d$ null submatrix in the mapping as described by equation (25). It is understood that these zero-eigenvalue modes describe the translational motion of the whole system, which is irrelevant for the spectral properties. This explains why they do not participate the transformation between the matrix coordinates and the spectral coordinates. To establish the one-to-one correspondence (25), the additional condition (26) for the matrix $\mathbf{K}^{C}_0$ is, however, required.

6. Discussion

6.1. Level-spacing distribution in the zero separation limit

It is expected from equation (20) that a linear asymptotic behaviour in the small level-separation regime in the nearest-neighbour level spacing distribution. We have carried out the numerical calculation for the distribution of the nearest-neighbour level spacing s, in the spectra of the matrices with conservation constraints obtained by collecting the instantaneous configurations in the molecular dynamic simulations. We consider the liquid systems [26, 27] of the Lennard–Jones, truncated Lennard–Jones, sodium and gallium atoms, respectively. In figure 1, we

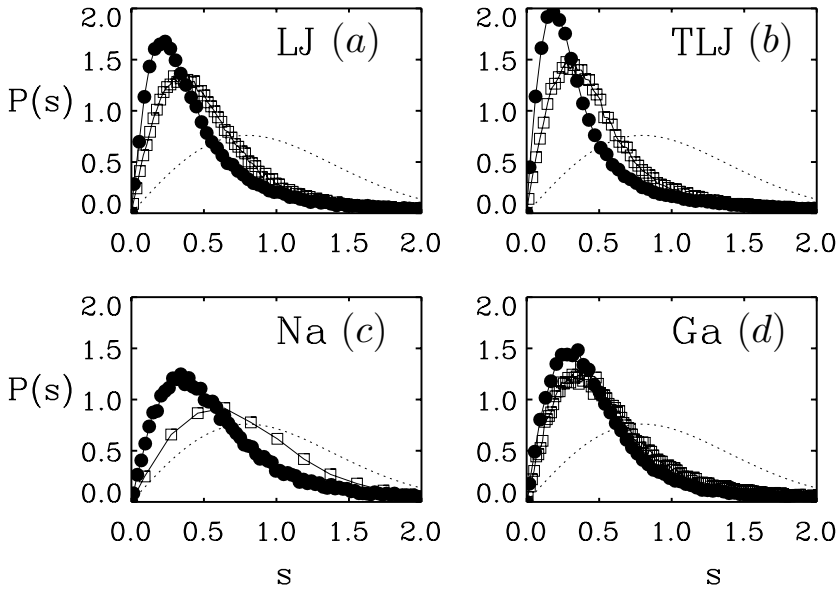

Figure 1. The distributions of the nearest-neighbour level spacings for the spectra of the Hessian matrices with each 3×3 block (8) replaced by a scalar value, either its scalar transverse component (filled circles) or the longitudinal component (squares), as compared with the Wigner's surmise (dotted line). The configurations are obtained in molecular dynamic simulations for fluid systems with the Lennard–Jones (*a*), truncated Lennard–Jones (*b*), sodium (*c*) and gallium (*d*) atoms, respectively. In all cases, the level-spacing distributions are numerically rescaled so that their first moments are unity [1].

present the data for the Hessian matrices with each 3×3 block $\mathbf{T}(\vec{r})$ in equation (8) replaced by a scalar value, either its scalar transverse component or the longitudinal component (appendix A) for the four systems of liquid. In spite of the overall diversified deviations from the Wigner's surmise [1], the results agree with the linear s-dependence in the small s regime, for all four systems in either of the two cases. For the original Hessian matrices described by equation (8), which are constrained by the summation rules for block matrix elements (section 5), a similar theoretical analysis can still lead to the expression (19). Indeed, we found the same linear asymptotic behaviour in the level-spacing distribution over the small spacing regime in both the eigenvalue spectra of INM [13], for the systems of liquid considered in figure 1.

6.2. Conditions for Gaussian ensemble with conservation constraint

Any ensemble of matrices defined on $S^{(C)}(N)$ has a corresponding ensemble on $S(N-1)$, related by the mapping (16). We show that an ensemble defined on $S^{(C)}(N)$ with full randomness is a Gaussian ensemble, if the two basic assumptions for GOE are adjusted compatibly with the conservation constraints.

We examine here the contents of the two assumptions stated in section 2, in applying to the conservation-constrained probability functions defined on $S^{(C)}(N)$. Firstly, since the linear relation stated in equation (16) preserves the statistical independence of the matrix elements, the content of assumption I can be equivalently stated for an ensemble on $S^{(C)}(N)$ and its correspondence defined on $S(N-1)$. Next, while assumption II for GOE has the well-established physical basis for the case of random Hamiltonian matrices, where the group translation carried out over $SO(N-1)$ for the non-spectral parameters q is related to the

symmetry operations allowed for the real symmetric Hamiltonian matrix, such physical basis is lacking for the conservation-constrained ensemble, because the group translation over $SO(N-1)$ for the non-spectral parameters may not be a symmetry operation. Nevertheless, assumption II can be rephrased as the independence of the probability distribution on the non-spectral variables (section 2), which seems a reasonable assumption for systems where only the spectral-dependent physical properties are considered. It is, therefore, natural to consider the prototypical ensemble of real symmetric matrices constrained by summation rules under the assumptions:

> *Assumption I′*, the matrix elements are statistically independent (to the extent allowed by the conservation constraints and the symmetric requirement;
>
> *Assumption II′*, their joint probability distribution can be expressed as a function with the spectral variables the only variables.

This is an ensemble with full randomness and possesses the Gaussian distribution. Thus, the correspondence (16) establishes the equivalence between the ensemble defined by assumptions I′ and II′ for matrices in $S^{(C)}(N)$ and the GOE, defined by assumptions I and II, for matrices in $S(N-1)$.

In constructing the equivalence relationship between the two ensembles, we have used the fact that, for the unconstrained ensemble, the only type of probability distribution invariant under the full orthogonal symmetry is the Gaussian function of the trace of the random matrix [1] (section 2). In the absence of the orthogonality symmetry, we will have a deformed distribution under the mapping (16) in removing the conservation constraints by reducing the rank, for the case of a non-Gaussian ensemble.

6.3. Relevance of conservation constraint

Our analysis, motivated by the Hessian matrices constrained by momentum conservation, is applicable to any family of real symmetric matrices constrained by the conservation laws. In reality, physical systems rarely possess full randomness, especially on account of the fact that the $SO(N-1)$ degrees of freedom for the non-spectral parameters implied by assumption II′ are not inherited directly from a physical principle in a conservation-constrained ensemble (sections 4 and 6.2). Nevertheless, there are conjectures [1, 23] supported by numerical data that certain local properties, such as the nearest-neighbour level-spacing distribution in the large N limit, are dominated by the factor (7). Our analysis suggests that the GOE is the prototypical ensemble addressed in RMT to be related to the collections of real symmetric matrices constrained by the summation rules [13]. It is worth noting that the results are applied to the statistical properties of the eigenlevels without referring to the details of the eigenvectors. The latter usually contain information on the physical origin of the presence of the specific eigenmodes. There are still issues for level statistics to be clarified for non-ideal situations encountered in real physical problems where matrices constrained by conservation laws are present. More numerical results from the realization of various types of conservation-constrained systems [13, 19, 28] may provide the motivation for such issues.

In summary, we have revealed with the theoretical analysis supported by some numerical evidence, the connection between the conservation-constrained ensembles and the generic GOE, in their local level statistical properties. We have also clarified the identical relationship between the ensemble of constrained matrices with full randomness and the GOE with the rank lowered by the spatial dimension, by establishing a one-to-one correspondence between the matrices in the two ensembles. The analysis may be suggestive for issues concerning the conservation constraints in the more complicated situation.

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Appendix A. *T*-matrix in the Hessian matrix

For identical particles with central-force pairwise interaction $\phi(r)$, $\mathbf{T}(\vec{r})$ is written as [8, 9],

$$\mathbf{T}(\vec{r}) = A(r)(\mathbf{1} - \hat{\mathbf{r}}\hat{\mathbf{r}}) + B(r)\hat{\mathbf{r}}\hat{\mathbf{r}}$$

with the transverse component $A(r) = \frac{\phi'(r)}{r}$ and the longitudinal component $B(r) = \phi''(r)$. $\hat{\mathbf{r}} = \vec{r}/r = (\bar{x}, \bar{y}, \bar{z})$ is a unit vector and the dyadic $\hat{\mathbf{r}}\hat{\mathbf{r}}$ corresponds to the 3×3 matrix $\begin{pmatrix} \bar{x}\bar{x} & \bar{x}\bar{y} & \bar{x}\bar{z} \\ \bar{y}\bar{x} & \bar{y}\bar{y} & \bar{y}\bar{z} \\ \bar{z}\bar{x} & \bar{z}\bar{y} & \bar{z}\bar{z} \end{pmatrix}$. Thus, each $\mathbf{T}(\vec{r})$ carries three degrees of freedom, determined by the relative position vector $\vec{r}$.

Appendix B. Summation rules on non-spectral parameters

The summation rules (1) are expressed in terms of new coordinates $(q^{(C)}, \lambda^{(C)})$ in equation (14). The condition can be rewritten as

$$\begin{pmatrix} a_{11}^{(C)} & a_{21}^{(C)} & \cdots & a_{N1}^{(C)} \\ a_{12}^{(C)} & a_{22}^{(C)} & \cdots & a_{N2}^{(C)} \\ & & \vdots & \\ a_{1N}^{(C)} & a_{2N}^{(C)} & \cdots & a_{NN}^{(C)} \end{pmatrix} \begin{pmatrix} \lambda_1^{(C)} \sum_{j=1}^{N} a_{1j}^{(C)} \\ \lambda_2^{(C)} \sum_{j=1}^{N} a_{2j}^{(C)} \\ \vdots \\ \lambda_N^{(C)} \sum_{j=1}^{N} a_{Nj}^{(C)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

The row vectors $\left\{ \left(a_{1i}^{(C)}, a_{2i}^{(C)}, \ldots, a_{Ni}^{(C)} \right) / i = 1, 2, \ldots, N \right\}$ form a set of orthonormal bases as a result of the closure condition, $\sum_{k=1}^{N} a_{ki}^{(C)} a_{kj}^{(C)} = \delta_{ij}$ for the basis formed by the orthonormal column vectors $\left\{ \vec{a}_i^{(C)} / i = 1, 2, \ldots, N \right\}$ discussed in the main text.

Similarly, we can show that the blocked summation rules (13) are equivalent to the perpendicular of the vector

$$\begin{pmatrix} \lambda_{(1,1)}^{(C)} \sum_{j=1}^{N} a_{(1,1)(j,\nu)}^{(C)} \\ \lambda_{(1,2)}^{(C)} \sum_{j=1}^{N} a_{(1,2)(j,\nu)}^{(C)} \\ \lambda_{(1,3)}^{(C)} \sum_{j=1}^{N} a_{(1,3)(j,\nu)}^{(C)} \\ \lambda_{(2,1)}^{(C)} \sum_{j=1}^{N} a_{(2,1)(j,\nu)}^{(C)} \\ \vdots \\ \lambda_{(N,3)}^{(C)} \sum_{j=1}^{N} a_{(N,3)(j,\nu)}^{(C)} \end{pmatrix}$$

to a set of ON basis vectors for each ν, $1 \leqslant \nu \leqslant 3$, which must be a null vector.

Appendix C. One-to-one correspondence between $S^{(C)}(N)$ and $S(N-1)$, and that between $S^{(C)}(N, 3)$ and $S(3N-3)$

Here, we give the derivation of the one-to-one correspondence between a matrix subject to the scalar constraints (1) and another matrix possessing the same set of eigenvalues in lowered rank without the constraints via (16).

Suppose $\mathbf{K}^{(C)}$ is the diagonalization transformation matrix for $\mathbf{M}^{(C)}$

$$\mathbf{M}^{(C)} = \mathbf{K}^{(C)}\,\mathrm{diag}\big(\lambda_1^{(C)}, \lambda_2^{(C)}, \ldots, \lambda_{N-1}^{(C)}, \lambda_N^{(C)} = 0\big)\mathbf{K}^{(C)t}. \tag{C.1}$$

Since $\mathbf{K}^{(C)}$ corresponds to an ON basis consists of column vectors, say,

$$\vec{b}_i^{(C)} = \begin{pmatrix} b_{i1}^{(C)} \\ b_{\mathrm{i2}}^{(C)} \\ \vdots \\ b_{iN}^{(C)} \end{pmatrix} \qquad 1 \leqslant i \leqslant N$$

there must exist another ON matrix $\mathbf{E}$ transforming the set of ON basis $\big\{\vec{a}_i^{(C)} \big/ 1 \leqslant i \leqslant N\big\}$ corresponding to $\mathbf{K}_0^{(C)}$, into $\big\{\vec{b}_i^{(C)} \big/ 1 \leqslant i \leqslant N\big\}$:

$$\mathbf{K}^{(C)} = \mathbf{K}_0^{(C)}\mathbf{E}. \tag{C.2}$$

That is, $\vec{b}_i^{(C)} = \sum_k e_{ik}\vec{a}_k^{(C)}$, or, in terms of the components, $b_{ij}^{(C)} = \sum_k e_{ik}a_{kj}^{(C)}$, with $e_{ji} = E_{ij}, a_{ji}^{(C)} = \big(K_0^{(C)}\big)_{ij}$ and $b_{ji}^{(C)} = K_{ij}^{(C)}$. On applying the summation rules (15) to the diagonalization transformation matrix $\mathbf{K}^{(C)}$, we have $\sum_{j=1}^N b_{ij}^{(C)} = \sum_{j=1}^N \sum_{k=1}^N e_{ik}a_{kj}^{(C)} = 0$ for $i \neq N$, which reduces to $e_{iN}\sum_j a_{Nj}^{(C)} = 0$ under the corresponding constraints on the matrix $\mathbf{K}_0^{(C)}$. We must have $e_{iN} = 0$ for $i \neq N$. Furthermore, taking into account of the orthogonality conditions for the vectors composing $\mathbf{E}$, the necessary and sufficient condition for $\mathbf{M}^{(C)}$ to obey the conservation constraints is

$$\mathbf{E} = \begin{pmatrix} & & 0 \\ & \mathbf{K}^{(-)} & \vdots \\ 0 & \cdots & 01 \end{pmatrix} \tag{C.3}$$

where $\mathbf{K}^{(-)}$ is an $(N-1)\times(N-1)$ ON matrix. Substituting equations (C.2) and (C.3) into equation (C.1), we obtain equation (17). Equation (16) is then true with

$$\mathbf{M}^{(-)} = \mathbf{K}^{(-)}\,\mathrm{diag}\big(\lambda_1^{(C)}, \lambda_2^{(C)}, \ldots, \lambda_{N-1}^{(C)}\big)\mathbf{K}^{(-)t}. \tag{C.4}$$

Conversely, for any $\mathbf{M}^{(-)} \in S(N-1)$, $\mathbf{K}^{(C)}$ obtained from its diagonalization transformation matrix $\mathbf{K}^{(-)}$ by equation (17) can be considered as the diagonalization transformation matrix for a matrix $\mathbf{M}^{(C)}$ in $S^{(C)}(N)$ with the same set of eigenvalues excluding the zero eigenvalue. The two matrices $\mathbf{M}^{(-)}$ and $\mathbf{M}^{(C)}$ are then related by equation (16). Thus, equation (16) defines a one-to-one correspondence between $S^{(C)}(N)$ and $S(N-1)$. It can also be shown that equation (17) is the only possible relation between $\mathbf{K}^{(C)}$ in (C.1) and $\mathbf{K}^{(-)}$ in (C.4) under the mapping defined by equation (16).

For the case with blocked constraints (13), the establishing of the one-to-one mapping from $S^{(C)}(N,3)$ on to $S(3N-3)$ follows basically the same route of derivation. We can show that, with any orthonormal matrix $\mathbf{K}_0^{(C)}$ satisfying the conditions (24) and (26), the diagonalization transformation matrix $\mathbf{K} = \mathbf{K}^{(C)}$ in equation (22), with $\lambda_{3N-2}^{(C)} = \lambda_{3N-1}^{(C)} = \lambda_{3N}^{(C)} = 0$, for any matrix $\mathbf{M}^{(C)} \in S^{(C)}(N,3)$ must be related to $\mathbf{K}_0^{(C)}$ by

$$\mathbf{K}^{(C)} = \mathbf{K}_0^{(C)}\mathbf{E} \tag{C.5}$$

with

$$\mathbf{E} = \begin{pmatrix} \mathbf{K}^{(-)} & 0 \\ 0 & \mathbf{K}' \end{pmatrix} \tag{C.6}$$

where $\mathbf{K}^{(-)} \in SO(3N-3)$ and $\mathbf{K}' \in SO(3)$, comprises all possible $\mathbf{K} = \mathbf{K}^{(C)}$ in equation (22), to generate the whole family $S^{(C)}(N, 3)$.

We can see the role played by the block dimension. The rotation $\mathbf{K}'$ in the three-dimensional subspace extended for the zero-eigenvalue is inactive in generating the matrix $\mathbf{M}^{(C)}$. To generate $S^{(C)}(N, 3)$ by equation (22) with $\mathbf{K} = \mathbf{K}^{(C)}$ defined by equations (C.5) and (C.6), only the $(3N-3) \times (3N-3)$ orthogonal transformations $\mathbf{K}^{(-)}$ on the non-translational degrees of freedom is effective. The similarity transformation carried by $\mathbf{K}^{(-)}$ over the $3N-3$ subspace generates all $\mathbf{M}^{(-)}$ in $S(3N-3)$. In addition to this, in the derivation of equation (C.6), the condition (26) is required in the reasoning. Such a requirement is automatically fulfilled for the scalar case (C.3), because the summations of the components of individual basis vectors for an ON basis cannot vanish simultaneously.

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