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Application of the Sherman-Morisson formula to scattering problems by multi-component systems

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Abstract. The scattering matrix for multi-component systems is recalculated using the extended form of the Sherman-Morisson formula. The matrix elements are given explicitly in closed form. The Gibbs-Duhem relation separates the density and composition contributions.

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1 Introduction

The classical method for the evaluation of the scattering at zero angle by multi-component systems starts with the following formulation of the scattered intensity:

$$I = \sum_{i,j=1..p} b_i b_j S_{ij} \,,$$

where the b_j's are the scattering length of the p species and the S_{ij} are the elements of the scattering matrix $\mathbf{S}$. It has been shown [1] that $\mathbf{S}^{-1}$ can be decomposed into two terms: a density and a composition fluctuation,

$$\mathbf{S}^{-1} = \left[\mathbf{A} + \Gamma^{-1}\mathbf{v}\mathbf{v}^{\mathrm{T}}\right] \,, \tag{1}$$

where $\mathbf{A}$ is the matrix of the chemical potential gradients $(\partial\mu_i/\partial n_j)_{p,T,n_k \neq i,j}$, $\Gamma = V\chi_T$, V being the total volume of the system, χ_T the isothermal compressibility, n_j the number of molecules in the i-th component, and $\mathbf{v}$ the column vector of the partial volumes of the components and $\mathbf{v}^{\mathrm{T}}$ its transpose.

The problem is to invert $\mathbf{S}^{-1}$. Recently, Benoît and Jannink [1] proposed a new method for this inversion. In this paper we present a more general derivation based on the Sherman-Morisson [2] formula (SMF), *i.e.*, which, assuming $\mathbf{A}$ to be a non-singular matrix, reads as

$$\mathbf{S} = \mathbf{A}^{-1} - \frac{\mathbf{A}^{-1}\mathbf{v}\mathbf{v}^{\mathrm{T}}\mathbf{A}^{-1}}{\Gamma + \mathbf{v}^{\mathrm{T}}\mathbf{A}^{-1}\mathbf{v}} \,. \tag{2}$$

This identity can be verified by direct matrix multiplication. This formula was used, generically, in the field of multi-component polymer dynamics in the early nineties to obtain an expression for the mobility matrix in the mean-field approximation [3,4]. In these applications, the matrix $\mathbf{A}$ was not singular, and the application of the SMF was straightforward. In the present application, the matrix $\mathbf{A}$ of equation (1) is singular due to the Gibbs-Duhem rule and hence the SMF rule cannot be used directly. The purpose of this communication is thus to extend SMF to allow $\mathbf{A}$ to be singular, so that the expression of the static structure factor in the thermodynamic limit can be calculated in closed form even when the Gibbs-Duhem rule is implemented. The first part of this paper is therefore devoted to the extension of the SMF, and the second part to its application to the scattering problem.

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2 The derivation of the extended version of the SMF

We first calculate the determinant of the matrix $\mathbf{A} + \Gamma^{-1}\mathbf{v}\mathbf{v}^{\mathrm{T}}$ (see App. A) as

$$\left|\mathbf{S}^{-1}\right| = \left|\mathbf{A} + \Gamma^{-1}\mathbf{v}\mathbf{v}^{\mathrm{T}}\right| = |\mathbf{A}| + \Gamma^{-1}\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v} \,, \tag{3}$$

where $\mathbf{A}^{\mathrm{ad}}$ is the adjoint of $\mathbf{A}$, *i.e.*, the transpose of the cofactor matrix of $\mathbf{A}$, and related to the inverse of $\mathbf{A}$ as

$$\mathbf{A}^{-1} = \frac{\mathbf{A}^{\mathrm{ad}}}{|\mathbf{A}|} \,. \tag{4a}$$

The elements of $\mathbf{A}^{\mathrm{ad}}$ are expressed as

$$A^{\mathrm{ad}}_{ij} = \frac{\partial\,|\mathbf{A}|}{\partial a_{ji}} \,. \tag{4b}$$

The second term in equation (3) can be expressed explicitly in terms of the elements a_{ij} of $\mathbf{A}$ as

$$\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v} = \sum_{\mu=1}^{p} |\mathbf{C}_\mu| \ , \qquad (5a)$$

where

$$\mathbf{C}_\mu = \begin{bmatrix} a_{11} .. \ v_1 v_\mu .. \ a_{1p} \\ : \quad : \quad : \\ a_{s1} .. \ v_s v_\mu .. \ a_{sp} \\ : \quad : \quad : \\ a_{p1} .. \ v_p v_\mu .. \ a_{pp} \end{bmatrix} , \qquad (5b)$$

v_s being the partial volumes of the components at constant pressure. The matrix $\mathbf{C}_\mu$ is obtained by replacing elements $a_{s\mu}$ in the μ-th column of $\mathbf{A}$ by $v_s v_\mu$ for $s = 1 \ldots p$ as explained in Appendix A.

We then express the right-hand side of equation (1) in terms of the adjoint of $[\mathbf{A} + \Gamma^{-1}\mathbf{v}\mathbf{v}^{\mathrm{T}}]$ and its determinant using equation (4a):

$$\mathbf{S} = \frac{1}{|\mathbf{A} + \Gamma^{-1}\mathbf{v}\mathbf{v}^{\mathrm{T}}|} \left[\mathbf{A} + \Gamma^{-1}\mathbf{v}\mathbf{v}^{\mathrm{T}}\right]^{\mathrm{ad}} . \qquad (6a)$$

Clearly, the front factor is just the determinant of $\mathbf{S}$ according to equation (3):

$$|\mathbf{S}| = \frac{1}{|\mathbf{A}| + \Gamma^{-1}\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v}} . \qquad (6b)$$

The elements of the second factor in equation (6a) can be expressed as the partial derivatives of the determinant of $|\mathbf{A} + \Gamma^{-1}\mathbf{v}\mathbf{v}^{\mathrm{T}}|$ with respect to its elements $x_{ji} = a_{ji} + \Gamma^{-1}v_j v_i$ according to equation (4b). Since the second term in x_{ji} is independent of a_{ji}, the differentiation can be performed with respect to a_{ji} only. Hence, we obtain

$$S_{ij} = |\mathbf{S}| \frac{\partial}{\partial a_{ji}} \left(|\mathbf{A}| + \Gamma^{-1}\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v}\right) . \qquad (7a)$$

This is the desired extension of the SMF which is valid even when the matrix $\mathbf{A}$ is singular. The first term in equation (7a) is just the adjoint matrix $\mathbf{A}^{\mathrm{ad}}$ according to equation (4b). Hence, $\mathbf{S}$ can be written as

$$\mathbf{S} = |\mathbf{S}| \left(\mathbf{A}^{\mathrm{ad}} + \Gamma^{-1}\mathbf{Z}\right) , \qquad (7b)$$

where we have introduced the matrix $\mathbf{Z}$ to denote

$$Z_{ij} = \frac{\partial}{\partial a_{ji}} \left(\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v}\right) . \qquad (8)$$

We mention in passing that the right-hand side of equation (7a) can be written more compactly, and interestingly, by using equation (6b) as

$$S_{ij} = |\mathbf{S}| \frac{\partial}{\partial a_{ji}} \frac{1}{|\mathbf{S}|} .$$

In order to express the elements Z_{ij} in terms of the elements of $\mathbf{A}$ and $\mathbf{v}$, we substitute $\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v}$ from equations (5) into (8), and obtain

$$Z_{ij} = \sum_{\mu=1}^{p} \frac{\partial |\mathbf{C}_\mu|}{\partial a_{ji}} . \qquad (9)$$

We present the expression of Z_{ij} explicitly for $p = 2$ and 3 to illustrate the implementation of this formula.

For p (number of constituents) $= 2$,

$$Z_{ij} = \frac{\partial}{\partial a_{ji}} \begin{vmatrix} v_1^2 & a_{12} \\ v_1 v_2 & a_{22} \end{vmatrix} + \frac{\partial}{\partial a_{ji}} \begin{vmatrix} a_{11} & v_1 v_2 \\ a_{21} & v_2^2 \end{vmatrix} \quad (i, j = 1, 2)$$

or

$$\mathbf{Z} = \begin{bmatrix} v_2^2 & -v_1 v_2 \\ -v_1 v_2 & v_1^2 \end{bmatrix} . \qquad (10)$$

For $p = 3$,

$$Z_{ij} = \frac{\partial}{\partial a_{ji}} \begin{vmatrix} v_1^2 & a_{12} & a_{13} \\ v_2 v_1 & a_{22} & a_{23} \\ v_3 v_1 & a_{32} & a_{33} \end{vmatrix} + \frac{\partial}{\partial a_{ji}} \begin{vmatrix} a_{11} & v_1 v_2 & a_{13} \\ a_{21} & v_2^2 & a_{23} \\ a_{31} & v_3 v_2 & a_{33} \end{vmatrix} + \frac{\partial}{\partial a_{ji}} \begin{vmatrix} a_{11} & a_{12} & v_1 v_3 \\ a_{21} & a_{22} & v_2 v_3 \\ a_{31} & a_{32} & v_3^2 \end{vmatrix} ,$$

or

$$\begin{aligned}
Z_{11} &= a_{33}v_2^2 + a_{22}v_3^2 - (a_{23} + a_{32})v_2 v_3 , \\
Z_{22} &= a_{11}v_3^2 + a_{33}v_1^2 - (a_{13} + a_{31})v_1 v_3 , \\
Z_{33} &= a_{11}v_2^2 + a_{22}v_1^2 - (a_{12} + a_{21})v_1 v_2 , \\
Z_{12} &= a_{13}v_2 v_3 - a_{12}v_3^2 - a_{33}v_1 v_2 + a_{32}v_1 v_3 , \\
Z_{21} &= a_{31}v_2 v_3 - a_{21}v_3^2 - a_{33}v_1 v_2 + a_{23}v_1 v_3 , \\
Z_{13} &= a_{12}v_2 v_3 - a_{13}v_2^2 - a_{22}v_1 v_3 + a_{23}v_1 v_2 , \\
Z_{31} &= a_{21}v_2 v_3 - a_{31}v_2^2 - a_{22}v_1 v_3 + a_{32}v_1 v_2 , \\
Z_{23} &= a_{13}v_1 v_2 + a_{21}v_1 v_3 - a_{11}v_2 v_3 + a_{23}v_1^2 , \\
Z_{32} &= a_{31}v_1 v_2 + a_{12}v_1 v_3 - a_{11}v_2 v_3 + a_{32}v_1^2 . \qquad (11)
\end{aligned}$$

We note that the matrix $\mathbf{A}$ is not assumed to be symmetric in the derivation of the above results. When $\mathbf{A} = \mathbf{A}^{\mathrm{T}}$, we also have $\mathbf{Z} = \mathbf{Z}^{\mathrm{T}}$ so that the calculation of Z_{ij} is simplified.

In conclusion, equation (9) provides a simple algorithm to calculate the elements of $\mathbf{Z}$ for any number of components.

3 Application to scattering by multi-component systems

3.1 The thermodynamic modelling

The scattering by multi-component systems has aroused great interest [1,5–7], because of the information that it contains, and because of a certain degree of freedom in the interpretation. The modelling is based on thermodynamics: There are p species, characterised by abundance's n_i, partial volumes v_i, chemical potentials μ_i, $i = 1, \ldots, p$. The scattering matrix $\mathbf{S}$, of order p, is defined by its elements

$$S_{ij} = \langle \delta n_i \delta n_j \rangle = \delta\mu_i / \delta n_j \mid_{V,T} \ . \tag{12}$$

The derivatives are taken at constant volume and temperature. Thermodynamics allows to obtain a decomposition for the inverse scattering matrix, as in equation (1):

$$\mathbf{S}^{-1} = \mathbf{A} + \mathbf{P}_v \,, \tag{13}$$

where the elements a_{ij} of $\mathbf{A}$ are the increments $\delta\mu_i/\delta n_j \mid_{P,T}$ taken at constant pressure and temperature. The symbol $\mathbf{P}_v$ means the projector on vector $\mathbf{v}$:

$$\mathbf{P}_v \mid_{ij} = v_i v_j / \chi_T V \,. \tag{14}$$

The Gibbs-Duhem rule writes

$$\mathbf{An} = 0 \,, \tag{15}$$

where $\mathbf{n}$ = column $(n_1, n_2, \ldots, n_p)$. It has been shown [1,6] that the inverse of (13), *i.e.*, the scattering matrix, takes the form

$$\mathbf{S} = \mathbf{P}_n + \mathbf{B} \,, \tag{16}$$

where $\mathbf{P}_n$ is the projector on vector $\mathbf{n}$,

$$\mathbf{P}_n \mid_{ij} = n_i n_j \chi_T / V \tag{17}$$

and $\mathbf{B}$ is the composition fluctuation contribution. It has the property

$$\mathbf{Bv} = 0 \,, \tag{18}$$

a relation conjugated to the Gibbs-Duhem rule. The problem is to determine the elements of $\mathbf{B}$. Several solutions [1,7] have been proposed which are complementary. Here we propose a new approach based on the extended-version Sherman-Morisson formula derived in Section 2. This approach has the advantage to give explicit results, and it helps to gain some new insight into the problem.

3.2 The Sherman-Morisson inversion: A re-normalized formulation

The problem which arises in modelling the scattering experiment is to obtain equation (16) from equation (13). The extended SMF in equation (7b) gives $\mathbf{S} = |\mathbf{S}|(\mathbf{A}^{\mathrm{ad}} + \mathit{\Gamma}^{-1}\mathbf{Z})$ which we reproduce here as

$$\mathbf{S}(\alpha) = \mathbf{S}_0(\alpha) + \mathbf{S}_1(\alpha) \,, \tag{19}$$

where

$$\mathbf{S}_0(\alpha) = \frac{\mathit{\Gamma}\mathbf{A}^{\mathrm{ad}}}{\mathit{\Gamma}\alpha + \mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v}} \,, \tag{20a}$$

$$\mathbf{S}_1(\alpha) = \frac{\mathbf{Z}}{\mathit{\Gamma}\alpha + \mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v}} \,, \tag{20b}$$

where $\alpha = |\mathbf{A}|$. In these equation the square matrix $\mathbf{A}$ is completely arbitrary in the sense that the elements a_{ij} are all independent variables. When the Gibbs-Duhem(G-D) rule is invoked, the determinant $\alpha = 0$, and equations (20) reduce to

$$\mathbf{S}_0(0) = \frac{\mathit{\Gamma}\mathbf{A}^{\mathrm{ad}}}{\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v}} \,, \tag{21}$$

$$\mathbf{S}_1(0) = \frac{\mathbf{Z}}{\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v}} \,. \tag{22}$$

In order to reproduce the thermodynamic results based on the G-D rule as reported in reference [1], we have to make full use of the consequences of the G-D constraints:

$$a_{i1}n_1 + a_{i2}n_2 + \ldots + a_{ip}n_p = 0 \qquad (i = 1, 2, \ldots, p) \,, \tag{23}$$

as well as the fact that in scattering problems the matrix $\mathbf{A}$ is symmetric. It is shown in Appendix B that, when it is done, the adjoint matrix $\mathbf{A}^{\mathrm{ad}}$ acquires the following delightfully simple form:

$$\mathbf{A}^{\mathrm{ad}} = \frac{A_{11}^{\mathrm{ad}}}{n_1^2}\mathbf{nn}^{\mathrm{T}} \,, \tag{24}$$

where $\mathbf{n}$ is the column vector $(n_1, n_2, \ldots, n_p)$. This result was obtained in reference [1] in the case of $p = 3$. Substituting equation (24) into equation (21), and using $V = \mathbf{n}^{\mathrm{T}}\mathbf{v}$, where V is the volume of the system, we obtain

$$\mathbf{S}_0(0) = \frac{\mathit{\Gamma}}{V^2}\mathbf{nn}^{\mathrm{T}} \,, \tag{25}$$

which is identical to the projector $\mathbf{P}_n$ defined in equation (17), with $\mathit{\Gamma} = V\chi_T$.

The other contribution $\mathbf{B}$ in equation (16), which is related to the composition fluctuations, is identical to $\mathbf{S}_1(0)$ in equation (22). Hence, using $\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v} = (V^2/n_1^2)A_{11}^{\mathrm{ad}}$, we get

$$B_{ij} = \frac{n_1^2}{V^2 A_{11}^{\mathrm{ad}}} Z_{ij} \,, \tag{26}$$

where Z_{ij} are given by equation (9) in general. The use of G-D constraints in the calculation of B_{ij} does not lead to any simplification. We present explicit results only for $p = 2$ and $p = 3$ as an illustration. For $p = 2$, $A_{11}^{\mathrm{ad}} = a_{22}$, and Z_{ij} are given in equation (10):

$$\mathbf{B} = \frac{n_1^2}{V^2 a_{22}} \begin{bmatrix} v_2^2 & -v_1 v_2 \\ -v_1 v_2 & v_1^2 \end{bmatrix} ,$$

which is a standard result.

For $p = 3$, $A_{11}^{\mathrm{ad}} = a_{22}a_{33} - a_{12}^2$, and Z_{ij} are given in equation (11). We present only B_{11} as an example:

$$B_{11} = \frac{n_1^2}{V^2(a_{22}a_{33} - a_{23}^2)}(a_{33}v_2^2 + a_{22}v_3^2 - 2a_{23}v_2v_3) \,,$$

which was also obtained in reference [1].

We note that the property in equation (18), *i.e.*, $\mathbf{Bv} = 0$, is easily verified in the case of $p = 2$. The proof

$\mathbf{Bv} = 0$, or, equivalently, $\mathbf{Zv} = 0$, for an arbitrary number of components is based on the following identity:

$$\frac{\partial^2|\mathbf{A}|}{\partial a_{ji} a_{\nu\mu}} = -\frac{\partial^2|\mathbf{A}|}{\partial a_{\nu i} a_{j\mu}},$$

which follows from the fact that the simultaneous interchange of the indices j and ν, and the interchange of the j-th and ν-th rows of $|\mathbf{A}|$ implies differentiation with respect to the same elements. The minus sign comes from the interchange of two rows in a determinant. The following steps are now self-explanatory:

$$Z_{ij} v_j = v_j v_\nu v_\mu \frac{\partial^2|\mathbf{A}|}{\partial a_{ji} a_{\nu\mu}} = v_j v_\mu v_\nu \frac{\partial^2|\mathbf{A}|}{\partial a_{\nu i} a_{j\mu}} = -v_j v_\mu v_\nu \frac{\partial^2|\mathbf{A}|}{\partial a_{ji} a_{\nu\mu}} = -Z_{ij} v_j .$$

A general method of computation of the scattering by multi-component, compressible systems has been presented. It assumes that the chemical potential gradients at constant pressure are known.

3.3 Discussions

The decomposition of the scattering matrix $\mathbf{S}$, re-derived with a new method in the preceding sections, calls for the following comments:

1) This decomposition is given for any value of $\alpha = \text{Det}\ \mathbf{A}$. The case $\alpha = 0$ corresponds to constant pressure and temperature conditions. The case $\alpha \neq 0$ is not yet fully interpreted but could correspond to an adiabatic situation.
The condition $\alpha = 0$ is a necessary condition for the rule to be obeyed: It produces a separation into a density fluctuation matrix and a composition fluctuation matrix. On the contrary, when $\alpha \neq 0$, the rule is not obeyed, and it is not possible to partition $\mathbf{S}$ into density and composition contributions.
2) The fact that the scattering matrix $\mathbf{S}$ may be decomposed into a density and a composition fluctuation sub-matrices does not automatically imply that density and composition fluctuations are uncorrelated. For this to occur it is necessary that $\mathbf{S}$ be represented as a direct sum [8]:
$$\mathbf{S} = \mathbf{B} \oplus \mathbf{P}_n . \tag{27}$$
Such a situation exists, when, for instance, $\mathbf{B}$ is the inverse of the restriction of $\mathbf{A}$ to the subspace orthogonal to vector "n" [7]. The matrix $\mathbf{P}_n$ being the projector on "$\mathbf{n}$", there is no intersection between the respective subspaces. This representation allows uncorrelated fluctuations [9], which could perhaps be observed experimentally.
3) The property $\mathbf{Bv} = 0$ is a key relation for the introduction of contrasts. It is however not the only one, if one considers the fact that the scattered intensity is a quadratic form of the scattering matrices: One can imagine many transformations which would leave the intensity unchanged.

Appendix A. Calculation of the determinant of $\mathbf{S}^{-1}$

We start with the expansion of $|\mathbf{S}^{-1}|$:

$$|\mathbf{S}^{-1}| = \sum_P (-1)^P (a_{1k_1} + \Gamma^{-1} v_1 v_{k_1}) \times (a_{2k_2} + \Gamma^{-1} v_2 v_{k_2}) \dots (a_{pk_p} + \Gamma^{-1} v_p v_{k_p}),$$

where the symbols have their usual meanings. Upon expansion we get

$$|\mathbf{S}^{-1}| = |\mathbf{A}| + \frac{1}{\Gamma} v_1 \sum_P (-1)^P v_{k_1} a_{2k_2} \dots a_{p,k_p} + \dots + \frac{1}{\Gamma} v_p \sum_P (-1)^P a_{1k_1} \dots a_{p-1,k_{p-1}} v_{k_p} + \frac{1}{\Gamma^2} \left\{ v_1 v_2 \sum_p (-1)^P v_{k_1} v_{k_2} a_{3k_3} \dots a_{pk_p} + \dots \right\}.$$

The terms involving $(1/\Gamma)^2$ and the higher powers are zero because they involve determinants with two identical rows. The sum of the terms involving $1/\Gamma$ is equal to $(1/\Gamma)\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v}$. Hence equation (3) follows.

To calculate $\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v}$ in terms of the elements a_{ij} and v_s, we start with the matrix identity $a_{\nu\mu} A^{\mathrm{ad}}_{\mu\nu} = |\mathbf{A}|$ for any given μ with summation on ν. This is the expansion of the determinant $|\mathbf{A}|$ into the elements of the μ-th column. Thus, $v_\nu A^{\mathrm{ad}}_{\mu\nu} = |\mathbf{X}_\mu|$ is the determinant of a matrix $\mathbf{X}_\mu$ which is obtained by replacing the elements $a_{\nu\mu}$ in the μ-th column of $|\mathbf{A}|$ by v_ν, $\nu = 1, 2, \dots p$. Consider now the summation $v_\mu |\mathbf{X}_\mu|$ for $\mu = 1, 2 \dots p$. Each term in this summation, say the μ-th term, is the determinant of a matrix $\mathbf{C}_\mu$, which is obtained by replacing the elements $a_{\nu\mu}$ in the μ-th column of $|\mathbf{A}|$ by $v_\mu v_\nu$, $\nu = 1, 2, \dots p$. Hence, $\mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{ad}}\mathbf{v} = v_\mu A^{\mathrm{ad}}_{\mu\nu} v_\nu = \sum_{s=1}^{p} |\mathbf{C}_s|$ has been established, proving equations (5) in the text.

Appendix B. Implementation of the Gibbs-Duhem relation in the SMF

The G-D relations are expressed as $a_{ij} n_j = 0$, $i = 1, 2, \dots, p$, where summation on j is implied. For a given set of values of n_j, we can solve these equations for the diagonal terms as

$$a_{ii} = -\frac{1}{n_i} \sum_{j \neq i} a_{ij} n_j ,$$

where we treat a_{ij} as $p(p-1)$ independent variables for $i \neq j$. Since $\mathbf{An} = 0$ implies $|\mathbf{A}| = 0$, we have

$$\sum_{j=1}^{p} a_{ij} A^{\mathrm{ad}}_{ji} = 0, \quad i = 1, 2, \dots, p,$$

where $A^{\rm ad}_{ji}$ does not depend on a_{ik} or a_{kj} for any k by its definition as adjoint. The diagonal term is given by

$$a_{ii}A^{\rm ad}_{ii} = -\sum_{j=1\neq i}^{p} a_{ij}A^{\rm ad}_{ji}\,.$$

Substituting a_{ii} from above, we find

$$\sum_{j=1\neq i}^{n} a_{ij}\left[\frac{n_j}{n_i}A^{\rm ad}_{ii} - A^{\rm ad}_{ji}\right] = 0\,.$$

Since a_{ij} are independent variables and the coefficients do not depend on them, we obtain

$$\frac{A^{\rm ad}_{ji}}{n_j} = \frac{A^{\rm ad}_{ii}}{n_i}\,, \qquad \text{for any } i \text{ and } j\,, \tag{B1}$$

which can also be written as $A^{\rm ad}_{ji}/n_j = A^{\rm ad}_{ki}/n_k$ for any j and k for a given i. Expressing the off-diagonal elements in terms of the diagonal elements using equation (B1), we can express the elements of the adjoint matrix $\mathbf{A}^{\rm ad}$ as

$$\left[\mathbf{A}^{\rm ad}\right]_{\mu\nu} = \frac{n_\mu}{n_\nu}\,A^{\rm ad}_{\nu\nu}\,. \tag{B2}$$

So far, we have not assumed that the matrix $\mathbf{A}$ is symmetric. When $\mathbf{A} = \mathbf{A}^{\rm T}$, we also have $A^{\rm ad}_{ji} = A^{\rm ad}_{ij}$. When substituted into equation (B1), the latter yields

$$A^{\rm ad}_{ji} = (n_j/n_i)A^{\rm ad}_{ii} = A^{\rm ad}_{ij} = (n_i/n_j)A^{\rm ad}_{jj}\,.$$

So, the diagonal elements satisfy $A^{\rm ad}_{ii} = (n_i/n_j)^2 A^{\rm ad}_{jj}$ or $A^{\rm ad}_{ii} = (n_i/n_1)^2 A^{\rm ad}_{11}$, *i.e.*, they can be expressed only in terms of one of them. Using this result in equation (B2), we find

$$\left[\mathbf{A}^{\rm ad}\right]_{\mu\nu} = \frac{n_\mu n_\nu}{n_1^2}\,A^{\rm ad}_{11}\,,$$

which leads to equation (24) in the text.

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