Onsager symmetry relations and the maximum number of propagating hydrodynamic modes

H. N. W. Lekkerkerker
Fakulteit van de Wetenschappen, Vrije Universiteit Brussel, 1050 Brussels, Belgium

W. G. Laidlaw
Department of Chemistry, The University of Calgary, Calgary, Alberta, Canada T2N 1N4
(Received 20 August 1973)

A relation between the maximum number of propagating hydrodynamic modes and the number of variables that are odd under time reversal and which are coupled to variables that are even under time reversal, is obtained using the Onsager symmetry relations.

I. INTRODUCTION

The question of the maximum number of propagating hydrodynamic modes has been raised in the recent literature.[1,2] Martin, Parodi, and Pershan[2] note that time-reversal invariance has, as a consequence, that the propagating modes must occur in pairs. The purpose of this paper is to show, using the Onsager symmetry relations, that one can go further. Indeed, it is possible to show that a system in which m variables that are odd under time reversal and that are coupled to n variables ($n \geq m$) that are even under time reversal exhibits at most $2m$ propagating modes. The proof is in fact an extension of an earlier demonstration[3] that, in an isotropic system in which one odd variable is coupled to n even variables, there are at most two propagating modes.

II. ONSAGER SYMMETRY RELATIONS

The spatially Fourier-transformed linearized hydrodynamic equations are denoted as follows

$$\frac{\partial}{\partial t}\, \underline{\alpha}(\vec{q}, t) = -\underline{M}(\vec{q})\underline{\alpha}(\vec{q}, t)\,. \tag{1}$$

Here $\underline{\alpha}(\vec{q}, t)$ is a column vector containing the $\vec{q}$th spatial Fourier components of the perturbations in the state variables $\underline{A}$:

$$\alpha_j(\vec{q}, t) = \int [A_j(\vec{r}, t) - \langle A_j\rangle] e^{-i\vec{q}\cdot\vec{r}}\, d\vec{r}\,, \tag{2}$$

where $\langle A_j\rangle$ is the average value of the variable A_j. The matrix $\underline{M}(\vec{q})$ is commonly referred to as the hydrodynamic matrix. The Onsager symmetry relations can be written as[4,5]

$$(\underline{M}(\vec{q})\underline{\chi}(\vec{q}))^\dagger = \underline{E}\underline{M}(\vec{q})\underline{\chi}(\vec{q})\underline{E}\,. \tag{3}$$

Here $\underline{E}$, the so-called signature matrix, is a diagonal matrix with elements E_j equal to $+1$, when A_j is even under time reversal, and equal to -1, when A_j is odd under time reversal, and the matrix $\underline{\chi}(\vec{q})$ describes the mean squares of the thermal fluctuations $\underline{\alpha}(\vec{q}, t)$:

$$\underline{\chi}(\vec{q}) = \langle \underline{\alpha}(\vec{q})\underline{\alpha}^\dagger(\vec{q})\rangle\,. \tag{4}$$

From its definition it is immediately apparent that $\underline{\chi}(\vec{q})$ is a Hermitian, positive definite matrix, and from time-reversal invariance it follows[4] that $\underline{\chi}(\vec{q})$ commutes with $\underline{E}$.

In order to utilize the Onsager symmetry relations to determine the distribution of the roots of $\underline{M}(\vec{q})$, it is convenient to work with a matrix $\underline{K}(\vec{q})$ related to $\underline{M}(\vec{q})$ by a similarity transformation, which, as we shall see, displays the Onsager symmetry relations in a more direct way. The transformation is written

$$\underline{K}(\vec{q}) \equiv \underline{U}^\dagger \underline{\chi}^{-1/2}(\vec{q})\underline{M}(\vec{q})\underline{\chi}^{1/2}(\vec{q})\underline{U}\,. \tag{5}$$

Here $\underline{U}$ is an unitary matrix that commutes with $\underline{E}$, and will specified in more detail in Sec. III. Using the fact that both $\underline{\chi}(\vec{q})$ and $\underline{U}$ commute with $\underline{E}$, it follows from the Onsager symmetry relations (3) that $\underline{K}(\vec{q})$, defined by Eq. (5), has the symmetry

$$\underline{K}^\dagger(\vec{q}) = \underline{E}\underline{K}(\vec{q})\underline{E}\,. \tag{6}$$

The symmetry relation of Eq. (6) implies that the characteristic polynomial of $\underline{K}(\vec{q})$, which is equal to the characteristic polynomial of $\underline{M}(\vec{q})$, that is,

$$p(\lambda) = \det(\underline{K}(\vec{q}) - \lambda\underline{I}) = \det(\underline{M}(\vec{q}) - \lambda\underline{I})$$

is a real polynomial and thus the complex roots (if any) appear in pairs, which are each others complex conjugate. The symmetry relation of Eq. (6) also implies a relation between the diagonalizing matrices of $\underline{K}(\vec{q})$. The similarity transformation[6] that diagonalizes $\underline{K}(\vec{q})$ is written

$$\underline{V}^{-1}\underline{K}(\vec{q})\underline{V}=\underline{\Lambda}\,, \tag{7}$$

where $\underline{\Lambda}$ is a diagonal matrix with elements λ_j, which are the eigenvalues of $\underline{K}(\vec{q})$. Following the same arguments that were used in Sec. V of Ref. 3, it can be shown that

$$\underline{V}^{-1}=\underline{P}\underline{V}^{\dagger}\underline{E}\,. \tag{8}$$

The matrix $\underline{P}$ has the following form: In the case where λ_i is real, the only nonzero element in the ith row is $P_{ii}=1$, and in the case where λ_i is complex and $\lambda_j=\lambda_i^*$, the only nonzero elements in the ith and jth rows are $P_{ij}=P_{ji}=1$. The relation between $\underline{V}$ and $\underline{V}^{-1}$ given by Eq. (8) will be used in Sec. III, where the eigenvalues of the hydrodynamic matrix are considered. One may remark that Eq. (8), together with the definition of $\underline{K}(\vec{q})$ given by Eq. (5), implies the symmetry relation of Eq. (9), between the diagonalizing matrices of $\underline{M}(\vec{q})$ (which are denoted by $\underline{S}$ and $\underline{S}^{-1}$):

$$\underline{S}^{-1}=\underline{P}\underline{S}^{\dagger}\underline{\chi}^{-1}(\vec{q})\underline{E}\,. \tag{9}$$

As in the case of isotropic systems[3,7] with one odd variable coupled to n even variables, this relation would appear to be generally useful in the calculation of the intensities of the hydrodynamic normal modes.

III. EIGENVALUES OF THE HYDRODYNAMIC MATRIX

Assuming that the system can be described by n variables that are even under time reversal, and m variables that are odd under time reversal, we denote the even ones by $A_1\cdots A_n$ and the odd ones by $A_{n+1}\cdots A_{n+m}$. Since

$$\underline{E}=\text{diag}(1,\ldots,1,-1,\ldots,-1)\,, \tag{10}$$

where there are n entries in $1,\ldots,1$, and m entries in $-1,\ldots,-1$, both the upper-left $n\times n$ block and lower-right $m\times m$ block of $\underline{K}(\vec{q})$ are readily seen to be Hermitian matrices. It is convenient to choose $\underline{U}$, introduced in Eq. (5), such that these blocks are diagonalized; i.e., one takes

$$U=\begin{bmatrix}\underline{U}_1 & \underline{0}\\ \underline{0} & \underline{U}_2\end{bmatrix},$$

where $\underline{U}_1$ and $\underline{U}_2$ are n- and m-dimensional unitary matrices that, respectively, diagonalize the upper-left $n\times n$ block and lower-right $m\times m$ block of the matrix $\underline{\chi}^{-1/2}(\vec{q})\underline{M}(\vec{q})\underline{\chi}^{1/2}(\vec{q})$. Then $K(\vec{q})$ takes the form

$$\underline{K}(\vec{q})=\left[\begin{array}{ccc|ccc} K_{11} & & 0 & K_{1,n+1} & \cdots & K_{1,n+m}\\ & \ddots & & \vdots & & \vdots\\ 0 & & K_{nn} & K_{n,n+1} & \cdots & K_{n,n+m}\\ \hline -K^*_{1,n+1} & \cdots & -K^*_{n,n+1} & K_{n+1,n+1} & & 0\\ \vdots & & \vdots & & \ddots & \\ -K^*_{1,n+m} & \cdots & -K^*_{n,n+m} & 0 & & K_{n+m,n+m}\end{array}\right], \tag{11}$$

where the diagonal elements are real.

Consider first the case of one odd variable coupled to n even variables. (We have already treated[3] this situation for the special case of isotropic systems where the hydrodynamic matrix is real). The characteristic polynomial of $\underline{K}(\vec{q})$ given by Eq. (11) with $m=1$ can be written

$$p(\lambda)=\det(\underline{K}(\vec{q})-\lambda\underline{I})=\prod_{i=1}^{n+1}(K_{ii}-\lambda)+\sum_{j=1}^{n}|K_{j,n+1}|^2\prod_{i\neq j}^{n}(K_{ii}-\lambda)\,. \tag{12}$$

For the sake of convenience it will be assumed that the elements K_{ii}, $i=1\cdots n$ are all distinct,[8] and without loss of generality one may take them to be ordered such that $K_{11}<K_{22}<\cdots<K_{nn}$. It then follows directly from the expression for the characteristic polynomial (12) that $p(K_{ii})$, $i=1\cdots n$, is positive for i odd and negative for i even. Thus $p(\lambda)$ changes sign at least $n-1$ times for real values of λ, and since $p(\lambda)$ is a real polynomial it has at least $n-1$ real roots. Consequently there are at most two complex eigenvalues, or, in other words, there are at most two propagating hydrodynamic modes. The $n-1$ real roots $\lambda_1\cdots\lambda_{n-1}$ lie between K_{11} and K_{nn}, indeed $K_{ii}<\lambda_i<K_{i+1,i+1}$, $i=1\cdots n-1$.

Consider now the case of two odd variables coupled to n even variables ($n\geq 2$). The matrix $\underline{K}(\vec{q})$ is first partitioned as

$$\underline{K}(\vec{q})=\begin{bmatrix}\underline{A} & \underline{B}\\ \underline{C} & \underline{D}\end{bmatrix},$$

where $\underline{A}$ and $\underline{D}$ are square matrices of dimension $n+1$ and 1, respectively. From the form of $\underline{K}(\vec{q})$ given by Eq. (11) with $m=2$, it follows that $\underline{A}$ involves only one odd variable [cf. Eq. (12)], and hence has at most two complex eigenvalues, and it can be shown that

$$\underline{B}^{\dagger}=-\underline{C}\,.$$

Now define a matrix $\underline{K}'(\vec{q})$ related to $\underline{K}(\vec{q})$ by a similarity transformation

$$\underline{K}'(\vec{q}) = \underline{T}^{-1}\underline{K}(\vec{q})\underline{T}. \tag{13}$$

Here

$$\underline{T} = \begin{bmatrix} \underline{Q} & \underline{0} \\ \underline{0} & 1 \end{bmatrix}, \tag{14}$$

where $\underline{Q}$ is the diagonalizing matrix of $\underline{A}$.

It will be assumed that $\underline{A}$ has indeed the maximum number (i.e., two) of complex eigenvalues and the elements of $\underline{K}'(q)$ are then arranged such that $K'_{11} \cdots K'_{n-1,n-1}$ are real and $K'^{*}_{nn} = K'_{n+1,n+1}$. The matrix $\underline{Q}$ can be normalized such that it has the symmetry given by Eq. (8):

$$\underline{Q}^{-1} = \underline{P}\underline{Q}^{\dagger}\underline{E}, \tag{15}$$

where

$$\underline{P} = \begin{bmatrix} 1 & & & & \\ & \ddots & \begin{matrix} n-1 \\ \text{entries} \end{matrix} & 0 & \\ 0 & & \ddots & & \\ & & & 1 & \\ & & & & \begin{matrix} 0 & 1 \\ 1 & 0 \end{matrix} \end{bmatrix}$$

and $\underline{E} = \text{diag}(1, \ldots, 1, -1)$, where there are n entries in $1, \ldots, 1$. Using the relation of Eq. (15) between $\underline{Q}$ and $\underline{Q}^{-1}$, it follows that $\underline{K}'(\vec{q})$, defined by Eq. (13), has the form

$$\underline{K}'(\vec{q}) = \left[\begin{array}{ccc|cc|c} K'_{11} & & 0 & & & K'_{1,n+2} \\ & \ddots & & & 0 & \vdots \\ 0 & & K'_{n-1,n-1} & & & K'_{n-1,n+2} \\ \hline & & & K'_{n,n} & 0 & K'_{n,n+2} \\ & 0 & & 0 & K'_{n+1,n+1} & K'_{n+1,n+2} \\ \hline -K'^{*}_{1,n+2} & \cdots & -K'^{*}_{n-1,n+2} & -K'^{*}_{n+1,n+2} & -K'^{*}_{n,n+2} & K'_{n+2,n+2} \end{array}\right], \tag{16}$$

where $K'_{n+2,n+2} = K_{n+2,n+2}$ and is thus real.

The characteristic polynomial of $\underline{K}(\vec{q})$ can now be written

$$p(\lambda) = \det(\underline{K}(\vec{q}) - \lambda\underline{I}) = \det(\underline{K}'(\vec{q}) - \lambda\underline{I}) = \prod_{i=1}^{n+2}(K'_{ii} - \lambda) + \sum_{j=1}^{n-1}|K'_{j,n+2}|^2 \prod_{i\neq j}^{n+1}(K'_{ii} - \lambda)$$
$$+ K'_{n,n+2}K'^{*}_{n+1,n+2}\prod_{i\neq n}^{n+1}(K'_{ii} - \lambda) + K'_{n+1,n+2}K'^{*}_{n,n+2}\prod_{i=1}^{n}(K'_{ii} - \lambda). \tag{17}$$

Again for convenience, it will be assumed that the elements $K'_{11} \cdots K'_{n-1,n-1}$ are all distinct, and without loss of generality one may take them to be ordered such that $K'_{11} < K'_{22} < \cdots < K'_{n-1,n-1}$. It then follows directly from the expression for the characteristic polynomial (17) that $p(K'_{ii})$, $i = 1 \cdots n-1$ is positive for i odd and is negative for i even. Thus $p(\lambda)$ changes sign at least $n-2$ times for real values of λ, and since $p(\lambda)$ is a real polynomial, it follows that it has at least $n-2$ real roots. Consequently, there are at most four complex eigenvalues, or, in other words, there are at most four propagating modes. The $n-2$ real roots $\lambda_1 \cdots \lambda_{n-2}$ lie between K'_{11} and $K'_{n-1,n-1}$ (which in turn lie between K_{11} and $K_{n,n}$), indeed $K'_{ii} < \lambda_i < K'_{i+1,i+1}$, $i = 1 \cdots n-2$.

Starting from the above result, it can be shown, following the same steps as in the extension of one odd variable to two odd variables, that, in the case of three odd variables coupled to n even variables ($n \geq 3$), there are at most six propagating modes. Continuing this way, one arrives at the result stated in Sec. I, that a coupled set of m odd variables and n even variables ($n \geq m$) exhibits at most $2m$ propagating modes.

IV. CONCLUDING REMARKS

The Onsager symmetry relations allow one, without making actual calculations, to determine characteristics of the distribution of the roots of the hydrodynamic matrix. The results obtained here should be useful in the study of the mode structure of systems with a complicated hydrodynamics. Furthermore, the symmetry relation between the diagonalizing matrices of the hydrodynamic matrix obtained here should be useful in the calculation of the intensities of the hydrodynamic normal modes.

ACKNOWLEDGMENTS

This research has been sponsored in part by the Internationale Instituten voor Fysica en Chemie, gesticht door E. Solvay. The support of the National Research Council of Canada is also acknowledged.

---

[1]L. Blum and Z. W. Salsburg, J. Chem. Phys. 50, 1654 (1969).

[2]P. C. Martin, O. Parodi, and P. S. Pershan, Phys. Rev. A 6, 2401 (1972).

[3]H. N. W. Lekkerkerker and W. G. Laidlaw, Phys. Rev. A 5, 1604 (1972).

[4]See, e.g., B. U. Felderhof, J. Chem. Phys. 44, 602 (1966).

[5]The superscript † indicates the Hermitian conjugate.

[6]It is assumed that by a similarity transformation a diagonal matrix can be obtained from the hydrodynamic matrix.

[7]H. N. W. Lekkerkerker and W. G. Laidlaw, Phys. Rev. A 7, 1332 (1973).

[8]The proof for the case for two or more K_{ii} equal to one another follows the same general lines with the same result.