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CALCULATION OF FUNCTIONALS OF MATRICES ARISING IN SOLID STATE PHYSICS AND QUANTUM CHEMISTRY

BY

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ABSTRACT

A large variety of physical and chemical systems are characterized by the repetition of identical units. The periodic structure of these systems allow their handling by similar mathematical methods. It is the purpose of this thesis to present certain techniques for the evaluation of analytic functions of matrices associated with such systems. The method consists of Poisson-type transformations of finite sums, which lead to rapidly converging expressions for the problems considered. Examples related to lattice dynamics and molecular orbital theory are discussed. Certain restricted sums of perturbation theory are calculated exactly by a method of independent interest. An extensive list of matrices arising from diverse periodic systems, together with their eigenvalues and eigenvectors, is presented. This extends and generalizes results in the literature.

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INTRODUCTION

There are a large variety of phenomena in physics and theoretical chemistry which are characterized by the repetition of identical units. This type of model arises in the study of lattice structure as in lattice dynamics, exciton theory, polymer chains and other similar situations. Many of the equations which appear in the analysis of such periodic systems have similar features, and allow simplifications due to the periodicities involved.

The first one to call attention to the class of mathematical problems which arise from periodic phenomena was Rutherford [1,2], who calculated the eigenvectors and eigenvalues of particular continuant and circulant matrices useful mainly in the solution of one dimensional problems. Some of this work was continued in a mathematical context by Egervary [3]. Of course, particular problems involving periodic structures have been solved from Bernouilli onwards. A good deal of this work is summarized in the books by Brillouin [4] and by Parodi and Brillouin [5]. Recently there has been some interest in this genre of problems, as it arises from the analysis of molecular systems, [6,7].

It is the purpose of this thesis to present certain techniques for calculating analytic functions of circulant and continuant matrices, appropriate to the solution of one- and higher-dimensional problems. In doing so we shall also extend some of the results of Rutherford, particularly in regards to matrices characteristic of multi-atomic problems and lattices with defects.

In Chapter I we introduce the basic equations describing the vibrational motion of crystal lattices in the harmonic approximation and the matrices associated with particular atomic configurations are derived. These are a good example of the type of problem arising in studies of the physics of periodic units. The main model employed is that of a rectangular lattice with a variety of boundary conditions. The ground work needed for the elaboration of these systems can be useful for the treatment of models with other symmetries. The statistical mechanics of lattices is shown to lead naturally to the concept of function of a matrix and the need for an explicit evaluation of its elements.

Chapter II describes problems selected from several fields (theoretical chemistry, molecular physics, etc.) which give rise to types of matrices similar to those discussed in Chapter I.

Chapter III presents a technique for calculating analytic functions of the particular matrices introduced in the previous chapters. The task at hand is shown to be the evaluation of certain finite sums. This is accomplished by a summation method somewhat similar to the Poisson sum formula. The formalism thus developed is then applied to several examples in one-, two- and three-dimensions which lead to specific analytic results. The method provides a scheme for numerical work in cases which are analytically intractable.

The systems dealt with in foregoing chapters possessed unperturbed periodicities. When perturbations are introduced (such as isotopic impurities, holes, etc.) the treatment has to be modified. Montroll and coworkers have shown [8,9] how to evaluate sums of analytic functions of the unknown eigenfrequencies of such systems by using matric Green's functions of the unperturbed systems. While the same approach could be adopted here by employing the results of Chapter III, one can instead find approximate eigenfrequencies and then evaluate the appropriate sums of these. This procedure is illustrated in Chapter IV where closed form expressions are found for the restricted sums of ordinary perturbation theory, by using a method of some intrinsic interest.

In order to increase the coherence of presentation some of the lengthier derivations have been relegated to appendices. In addition, a special appendix is devoted to the listing of matrices which appear most frequently in applications. This appendix contains generalizations and extensions of Rutherford's work [1,2] and each matrix listed in it is accompanied, whenever possible, by its eigenvalues, eigenvectors and the closed form of its characteristic polynomial.

CHAPTER I

DYNAMICS OF A CRYSTAL LATTICE

A solid is by definition a group of atoms arranged in a regular array (lattice), which perform small oscillations about their equilibrium positions. It is usually assumed that the forces acting on each particle in the lattice can be derived from a potential.

In most cases the exact form of this potential is not known and arbitrary constants have to be introduced in the theory. On the other hand, stability considerations show that the potential energy of the lattice can be expanded in a Taylor series about the equilibrium positions, at least for temperatures below those at which a state transition takes place. If only the first non-zero term is retained in this expansion, the potential energy becomes a quadratic form in the displacements of the atoms. This procedure is known as the harmonic approximation, the nomenclature referring to the fact that here the solid is regarded as a set of coupled harmonic oscillators. The harmonic approximation describes adequately many of the vibrational properties of a solid although it cannot explain characteristics such as thermal expansion, temperature variation of the elastic constants, etc. For the treatment of these phenomena higher order terms in the series expansion have to be included in the potential energy. In this work all the systems considered will be treated in the harmonic approximation.

The general theory of lattice vibrations is discussed in detail in several books [10, 11]; here only an outline of the theory will be given and specialization will be made to those models for which the methods of calculation described in Chapter III apply.

To write down the Hamiltonian for the lattice we assume for definiteness that there are N unit cells each containing n particles. We define $\mathbf{r}^0\binom{\ell}{\kappa}$ and $\mathbf{r}\binom{\ell}{\kappa}$ to be the position vector at equilibrium and the actual position vector, respectively, of the κ-th particle in the ℓ-th unit cell, both related to a suitable origin of co-ordinates. The vectors $\mathbf{r}^0\binom{\ell}{\kappa}$ represent the lattice sites and can be written also in the form

$$\mathbf{r}^0\begin{pmatrix}\ell\\ \kappa\end{pmatrix} = \mathbf{r}^0(\ell) + \mathbf{r}^0(\kappa) \tag{1}$$

with

$$\mathbf{r}^0(\ell) = \ell_1\,\mathbf{a}_1 + \ell_2\,\mathbf{a}_2 + \ell_3\,\mathbf{a}_3 \tag{2}$$

where the $\mathbf{a}_j$ are three noncoplanar vectors called the primitive translation vectors of the crystal and the ℓ_j are three integers, positive, negative or zero. The position vector of the κ-th particle in the unit cell with respect to some origin there, is denoted above by $\mathbf{r}^0(\kappa)$. All crystals the unit cells of which contain only one particle are called Bravais crystals – other crystals are called nonprimitive.

In the harmonic approximation the potential energy of the lattice is given by

$$\Phi = \Phi_0 + \sum_{\ell,\kappa} \nabla_{\mathbf{r}\binom{\ell}{\kappa}}\,\Phi\Big|_0 \cdot \left(\mathbf{r}\begin{pmatrix}\ell\\ \kappa\end{pmatrix} - \mathbf{r}^0\begin{pmatrix}\ell\\ \kappa\end{pmatrix}\right)$$

$$+\frac{1}{2}\sum_{\substack{\ell,\kappa\\ \ell',\kappa'}} \left(\mathbf{r}\begin{pmatrix}\ell\\ \kappa\end{pmatrix} - \mathbf{r}^0\begin{pmatrix}\ell\\ \kappa\end{pmatrix}\right)\cdot \nabla_{\mathbf{r}\binom{\ell}{\kappa}}\,\nabla_{\mathbf{r}\binom{\ell'}{\kappa'}}\,\Phi\Big|_0 \cdot \left(\mathbf{r}\begin{pmatrix}\ell'\\ \kappa'\end{pmatrix} - \mathbf{r}^0\begin{pmatrix}\ell'\\ \kappa'\end{pmatrix}\right) \tag{3}$$

The zero subscript above denotes evaluation at the appropriate equilibrium position. By definition

$$\nabla_{\mathbf{r}\binom{\ell}{\varkappa}} \Phi \Big|_0 = 0 \tag{4}$$

If we define the displacements from equilibrium by

$$\mathbf{u}\binom{\ell}{\varkappa} = \mathbf{r}\binom{\ell}{\varkappa} - \mathbf{r}^0\binom{\ell}{\varkappa} \tag{5}$$

and the (α, β) component of the tensor $\nabla\nabla\Phi\,|_0$ by

$$\Phi_{\alpha\beta}\begin{pmatrix}\ell & \ell' \\ \varkappa & \varkappa'\end{pmatrix} = \nabla_{x_\alpha\binom{\ell}{\varkappa}} \nabla_{x_\beta\binom{\ell'}{\varkappa'}} \Phi \Big|_0 \; ; \quad \alpha, \beta = 1, 2, 3 \tag{6}$$

then the potential energy can be written as follows:

$$\Phi = \Phi_0 + \frac{1}{2} \sum_{\substack{\ell\varkappa\alpha \\ \ell'\varkappa'\beta}} \Phi_{\alpha\beta}\begin{pmatrix}\ell & \ell' \\ \varkappa & \varkappa'\end{pmatrix} u_\alpha\binom{\ell}{\varkappa} u_\beta\binom{\ell'}{\varkappa'} \tag{7}$$

This is a quadratic surface in 3Nn dimensions and one can investigate its invariance properties under a variety of transformations. This will not be done here as it is excellently presented in [11]. We want to remark that while important, these invariance properties pertain mostly to infinite lattices and lattices with boundaries which have been removed by use of the Born-von Karman cyclic constraints.

The coefficient of $\Phi_{\alpha\beta}\begin{pmatrix}\ell & \ell' \\ \varkappa & \varkappa'\end{pmatrix}$ is the force exerted in the α-direction on the particle at $\mathbf{r}^0\binom{\ell}{\varkappa}$ when the particle at $\mathbf{r}^0\binom{\ell'}{\varkappa'}$ is displaced a unit distance in the β-direction, and from eq. (6) we see that

$$\Phi_{\alpha\beta}\begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa' \end{pmatrix} = \Phi_{\beta\alpha}\begin{pmatrix} \ell' & \ell \\ \varkappa' & \varkappa \end{pmatrix} \tag{8}$$

If the potential energy consists only of two-body interactions, with each pair of particles interacting via a potential function $\phi_{\varkappa\varkappa'}(\mathbf{r})$ which depends only on the magnitude of their separation, the atomic force constants will take the form:

$$\Phi_{\alpha\beta}\begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa' \end{pmatrix} = -\frac{\partial^2}{\partial x_\alpha \, \partial x_\beta} \phi_{\varkappa\varkappa'} \Bigg|_{\mathbf{r}=\mathbf{r}\begin{pmatrix} \ell \\ \varkappa \end{pmatrix} - \mathbf{r}\begin{pmatrix} \ell' \\ \varkappa' \end{pmatrix}} \tag{9}$$

The number of particle species is at most equal to the number of particles in the unit cell. Therefore $M_\varkappa$, $\varkappa = 1, \ldots, n$, will denote the mass of the $\varkappa$-th particle in the unit cell, and we can write the equations of motion

$$M_\varkappa \ddot{u}_\alpha\begin{pmatrix} \ell \\ \varkappa \end{pmatrix} = -\sum_{\ell' \varkappa' \beta} \Phi_{\alpha\beta}\begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa' \end{pmatrix} u_\beta\begin{pmatrix} \ell' \\ \varkappa' \end{pmatrix} \tag{10}$$

There are two different approaches usually adopted for solving these equations:

1. <u>The Plane-Wave Method</u>

If in eqs.(10) one proceeds to the limit of an elastic continuum, one obtains a wave equation for the displacement vector of an arbitrary point in the medium. An expansion of the displacement in plane waves of the type $\exp\{2\pi i \mathbf{k}\cdot\mathbf{r} - i\omega t\}$ leads in most cases to a solution of the problem, the amplitudes being determined from the boundary conditions.

This treatment of the wave equation suggests a similar procedure for the discrete crystal lattice. If we make the substitution

$$u_\alpha\begin{pmatrix} \ell \\ \varkappa \end{pmatrix} = \frac{1}{\sqrt{M_\varkappa}} v_\alpha(\varkappa) \exp\left[-i\omega t + 2\pi i \, \mathbf{k}\cdot\mathbf{r}^0(\ell)\right] \tag{11}$$

where $\mathbf{r}^0(\ell)$ is as in eq. (2), $\mathbf{k}$ is a three-dimensional vector to be subsequently determined from boundary conditions, and $v_\alpha(\varkappa)$ is independent of ℓ, we find

$$\omega^2 v_\alpha(\varkappa) = \sum_{\varkappa'\beta} D^{\ell}_{\alpha\beta}\begin{pmatrix} \mathbf{k} \\ \varkappa\varkappa' \end{pmatrix} v_\beta(\varkappa') \tag{12}$$

where

$$D^{\ell}_{\alpha\beta}\begin{pmatrix} \mathbf{k} \\ \varkappa\varkappa' \end{pmatrix} = \frac{1}{\sqrt{M_\varkappa M_{\varkappa'}}} \sum_{\ell'} \Phi_{\alpha\beta}\begin{pmatrix} \ell\ \ell' \\ \varkappa\ \varkappa' \end{pmatrix} \exp\{2\pi i\mathbf{k}\cdot[\mathbf{r}^0(\ell') - \mathbf{r}^0(\ell)]\} \tag{13}$$

If one can at this point make the quantities D defined in eq. (13) independent of ℓ, then a considerable reduction of the problem is achieved. To this end specific assumptions about the second order force constants have to be made: either the lattice is infinite and its periodicity insures invariance under rigid body translations produced by a lattice vector $\mathbf{r}^0(\ell)$, or it is finite with periodic boundary conditions. Both cases lead to the relations

$$\Phi_{\alpha\beta}\begin{pmatrix} \ell\ \ell' \\ \varkappa\ \varkappa' \end{pmatrix} = \Phi_{\alpha\beta}\begin{pmatrix} \ell - \ell' \\ \varkappa\quad \varkappa' \end{pmatrix} \tag{14}$$

i.e., the atomic force constants depend only on the difference $\ell - \ell'$.

This being the case the superscript ℓ can be suppressed in eqs. (12) and (13). Thus eq. (12) can be rewritten

$$\omega^2 v_\alpha(\varkappa) = \sum_{\varkappa'\beta} D_{\alpha\beta}\begin{pmatrix} \mathbf{k} \\ \varkappa\varkappa' \end{pmatrix} v_\beta(\varkappa') \tag{15}$$

with

$$D_{\alpha\beta}\begin{pmatrix} \mathbf{k} \\ \varkappa\varkappa' \end{pmatrix} = \sum_{\ell} \Phi_{\alpha\beta}\begin{pmatrix} \ell \\ \varkappa\varkappa' \end{pmatrix} \exp[-2\pi i\,\mathbf{k}\cdot\mathbf{r}^0(\ell)] \tag{16}$$

Therefore there are only 3n equations instead of 3Nn or an infinite number of them. The set of equations (15) will have a solution if the determinant of the coefficients will vanish

$$\left| D_{\alpha\beta}\begin{pmatrix} \mathbf{k} \\ \varkappa\,\varkappa' \end{pmatrix} - \omega^2\,\delta_{\alpha\beta}\,\delta_{\varkappa\varkappa'} \right| = 0 \qquad (17)$$

It is easily seen from the definition (16) that the matrix of the coefficients D is Hermitian. The 3n solutions $\omega_j^2(\mathbf{k})$ are then real and the stability of the lattice requires that these be positive.

To a certain extent the reduction effected above is illusory since the vectors $\mathbf{k}$ which satisfy the boundary conditions for a finite lattice have still to be found. This brings us back to the original problem. For an infinite lattice the 3r functions $\omega_j^2(\mathbf{k})$ can be regarded as the branches of a multivalued function $\omega^2(\mathbf{k})$.

The plane-wave method is indispensable in all those cases for which the normal mode frequencies cannot be explicitly found. Moreover it is the starting point of the quantum-mechanical treatment of solids, scattering of waves and particles, etc.

2. <u>The Normal Mode Method</u>

In this method the following substitution

$$u_\alpha\begin{pmatrix} \ell \\ \varkappa \end{pmatrix} = U_\alpha\begin{pmatrix} \ell \\ \varkappa \end{pmatrix} e^{-i\omega t} \qquad (18)$$

is used in eq. (10) to yield

$$M_\varkappa\,\omega^2\,U_\alpha\begin{pmatrix} \ell \\ \varkappa \end{pmatrix} - \sum_{\ell'\varkappa'\beta} \Phi_{\alpha\beta}\begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa' \end{pmatrix} U_\beta\begin{pmatrix} \ell' \\ \varkappa' \end{pmatrix} = 0 \qquad (19)$$

The condition that the set of equations (19) have a nontrivial solution is

$$\left| \Phi_{\alpha\beta} \begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa \end{pmatrix} - M_{\varkappa}\, \omega^2\, \delta_{\ell\ell'}\, \delta_{\varkappa\varkappa'}\, \delta_{\alpha\beta} \right| = 0 \tag{20}$$

The roots of this equation are the normal mode frequencies of the crystal. The $3Nn \times 3Nn$ symmetric matrix in eq. (20) is known as the dynamical matrix of the system, usually denoted by $\Delta(\omega^2)$ or simply Δ. The boundary conditions are automatically introduced through the specific form of the dynamical matrix. Generally, if the roots of eq. (20) cannot be found analytically, the numerical solution is more complicated that that of the reduced eq. (17) and this approach is not useful. But if one considers short-range interactions (i.e., interactions between distant neighbors can be neglected) and certain simple boundary conditions, there exist several models which possess explicit analytic solutions.

It is this latter aspect of the normal mode method which will be utilized exclusively in the sequel. We wish to emphasize that the application of the plane wave method to these soluble models, though possible, is much less convenient than that of the present method.

Before we proceed to the actual models, a further question has to be answered: how to connect the atomic force constants with the geometrical and physical structure of a given lattice. It readily appears that knowledge of the invariance properties of Φ is not sufficient for this purpose. If we restrict the discussion to two-body interactions, a more physical approach is through the forces acting between pairs of particles. This approach has been used by Born [10] and subsequently amplified by de Launay [12], whose treatment we follow.

Let $\vec{\mathfrak{F}}\begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa' \end{pmatrix}$ be the force exerted on the particle located at $(\ell, \varkappa)$ by the particle located at $(\ell', \varkappa')$. Then by definition

$$\vec{\mathfrak{F}}\begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa' \end{pmatrix} = \Phi\begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa' \end{pmatrix} \cdot \left[\mathbf{u}\begin{pmatrix} \ell' \\ \varkappa' \end{pmatrix} - \mathbf{u}\begin{pmatrix} \ell \\ \varkappa \end{pmatrix}\right] \tag{21}$$

where Φ is the 3×3 matrix with elements given by eq. (9), and we see that Φ is also a force density tensor possessing only 6 independent components.

The procedure of de Launay is essentially to write for Φ a linear combination of dyadics

$$\Phi\begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa' \end{pmatrix} = \alpha\, \boldsymbol{\varepsilon\varepsilon} + \alpha'\, \boldsymbol{\xi\xi} + \alpha''\, \boldsymbol{\eta\eta} \tag{22}$$

where

$$\alpha,\ \alpha',\ \alpha'' = \alpha,\ \alpha',\ \alpha'' \begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa' \end{pmatrix}$$

and

$$\boldsymbol{\varepsilon},\ \boldsymbol{\xi},\ \boldsymbol{\eta} = \boldsymbol{\varepsilon},\ \boldsymbol{\xi},\ \boldsymbol{\eta} \begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa' \end{pmatrix}$$

One of the three unit vectors, say $\boldsymbol{\varepsilon}$, is chosen as follows

$$\boldsymbol{\varepsilon}\begin{pmatrix} \ell & \ell' \\ \varkappa & \varkappa' \end{pmatrix} = \frac{\mathbf{r}^0\begin{pmatrix} \ell' \\ \varkappa' \end{pmatrix} - \mathbf{r}^0\begin{pmatrix} \ell \\ \varkappa \end{pmatrix}}{\left|\mathbf{r}^0\begin{pmatrix} \ell' \\ \varkappa' \end{pmatrix} - \mathbf{r}^0\begin{pmatrix} \ell \\ \varkappa \end{pmatrix}\right|} \tag{23}$$

while the remaining two are taken to form with $\boldsymbol{\varepsilon}$ a right-handed orthogonal triad. There are not enough conditions to make the choice of these two unique and therefore a certain degree of arbitrariness remains. Despite this fact, it is not difficult to choose these vectors for actual models, as will be described below.

The coefficients α and α', α'' are known as the central force and non-central force constants, respectively. These depend on the type of the two-body interaction and also on the separation distance – the constants will vary for different neighbors even when the same type of interaction is involved.

In the following we present the equations of motion and the dynamical matrices for several models of finite lattices in one, two, and three dimensions.

1.1 One-Dimensional Lattices

In this section we shall discuss finite linear chains and classify these according to their symmetries and the boundary conditions imposed.

The model assumed is that of N particles $M_1, M_2, \ldots, M_N$ arranged on a line and constrained to vibrate longitudinally, as in Fig. 1. The equilibrium positions x_j^o obey the conditions

$$x_{j+1}^o - x_j^o = a_j \, ; \quad j = 1, \ldots, N-1 \tag{24}$$

Figure 1

where the a_j's denote the spacing constants of the linear lattice. If none of the a_j's coincide there will be $N(N-1)/2$ independent force constants. This case is of no interest here since no periodicity is involved. We consider below the case where the two-body interactions are independent of the particle masses and assume that the particles, at equilibrium, are equidistantly spaced. Then the number of independent force constants reduces to $N - 1$. According to our model the tensor Φ of eq. (22) reduces in this case to one constant $\alpha(\ell, \ell')$ since $\epsilon\epsilon$ becomes 1. Moreover the properties of the two-body interaction assumed lead to force constants α with the property

$$\alpha(\ell, \ell') = \alpha(|\ell - \ell'|) \equiv \alpha_j; \quad j = 1, \ldots, N-1 \tag{25}$$

In order to write down the dynamical matrix the boundary conditions have to be explicitly introduced. This is done below.

1.1.1 Linear Chains with Free Ends

The forces acting on the two end particles M_1 and M_2, according to eqs. (21) and (25) are respectively:

$$\left.\begin{aligned} F_1 &= \sum_{j=1}^{N-1} \alpha_j (u_{j+1} - u_1) \\ F_N &= \sum_{j=1}^{N-1} \alpha_{N-j} (u_j - u_N) \end{aligned}\right\} \tag{26}$$

Then the dynamical matrix is

$$\Delta_N(\omega^2) = \begin{pmatrix} A_1 - M_1\omega^2, & -\alpha_1, & \cdots & , -\alpha_{N-1} \\ -\alpha_1, & A_2 - M_2\omega^2, & \ddots & \vdots \\ \vdots & \ddots & \ddots & \\ & & A_{N-1} - M_{N-1}\omega^2, & -\alpha_1 \\ \alpha_{N-1} & \cdots & -\alpha_1, & A_1 - M_N\omega^2 \end{pmatrix} \tag{27}$$

in which

$$\left.\begin{aligned} A_j &= \sum_{r=1}^{N-j} \alpha_r + \sum_{r=1}^{j-1} \alpha_r; \quad j = 2, \ldots, N-1 \\ A_1 &= \sum_{r=1}^{N-1} \alpha_r \end{aligned}\right\} \tag{28}$$

The eigenvalues and eigenvectors of the matrix (27) are in general unknown. But if the chain is monatomic $M_j = M$, $j = 1, \ldots, N$, one eigenvalue is zero and its associated eigenvector is

$$U_0 = \begin{pmatrix} 1 \\ 1 \\ \cdot \\ \cdot \\ 1 \end{pmatrix} \tag{29}$$

This of course reflects the invariance of the lattice against rigid translations and as a result in matrix theory it is a particular case of the somewhat more general theorem: If the sums of the elements in each row (column) of a matrix coincide, the matrix has one eigenvalue equal to this sum and the associated eigenvector is that of eq. (29).

A monatomic chain for which all interactions can be neglected except those between nearest neighbors yields a matrix Δ of the form

$$\Delta_N(\omega^2) = \begin{pmatrix} a+b & b & & & 0 \\ b & a & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & a & b \\ 0 & & & b & a+b \end{pmatrix} \tag{30}$$

with

$$a = 2\alpha_1 - M\omega^2 ; \quad b = -\alpha_1 \tag{31}$$

This matrix appears in eq. (63) of Appendix E and is discussed there. Use of eq. (31) above gives then the frequencies

$$\omega_r^2 = \frac{4\alpha_1}{M} \sin^2 \frac{\pi r}{2N}; \quad r = 0, 1, \ldots, N-1 \tag{32}$$

The eigenvectors are presented in the same Appendix.

A monatomic chain with two distinct spacing constants a_1 and a_2 regularly alternating is characterized, for nearest neighbor interactions, by two different force constants β, γ and leads to the matrix

$$\Delta_N(\omega^2) = \begin{pmatrix} a+c & b & & & & 0 \\ b & a & c & & & \\ & c & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & a & b \\ 0 & & & & b & a+b \end{pmatrix} \tag{33}$$

in which

$$a = \beta + \gamma - M\omega^2; \quad b = -\beta; \quad c = -\gamma \tag{34}$$

and b, c alternate regularly along the minor diagonals in eq. (33).

This type of matrix is treated in the section following eq. (79') of Appendix E. It is shown there that if $N = 2n$ then the eigenvalues and eigenvectors can be found explicitly. Using eq. (34) we obtain the frequencies

$$\left.\begin{aligned} \omega_r^2 &= \frac{\beta + \gamma \pm \sqrt{\beta^2 + 2\beta\gamma \cos\frac{\pi k}{n} + \gamma^2}}{M}; \quad r = 1, \ldots, n-1 \\ \omega_0^2 &= 0 \\ \omega_{2n}^2 &= \frac{2\beta}{M} \end{aligned}\right\} \tag{35}$$

The frequencies ω_0^2 and ω_{2n}^2 coincide, for $\beta, \gamma \to \alpha_1$, with the two frequencies of eq. (32) obtained by the substitution of $r = 0$ and $r = N/2$, respectively. We note also that the frequency ω_{2n}^2 is independent of the number of particles. As such it is called a "surface" frequency, a term borrowed from the theory of an elastic continuum with free boundaries. At present no analytic results are available for the odd case $N = 2n + 1$.

The diatomic chain with nearest neighbor interactions and masses alternating regularly along the chain has the dynamical matrix

$$\Delta_N(\omega^2) = \begin{pmatrix} u+b & b & & & 0 \\ b & v & \ddots & & \\ & \ddots & u & \ddots & \\ & & \ddots & \ddots & b \\ 0 & & & b & * \end{pmatrix} \tag{36}$$

in which

$$u = 2\alpha_1 - M_1\omega^2; \quad v = 2\alpha_1 - M_2\omega^2; \quad b = -\alpha_1 \tag{37}$$

and the last term on the main diagonal is either $u + b$ (for N odd) or $v + b$ (for N even). As the odd case does not possess at present analytic solutions, we consider only $N = 2n$. Then the eigenvalues and eigenvectors are given in eqs. (99), (101) and (102), (103) of Appendix E and we can write the frequencies

$$\left.\begin{aligned} \omega_k^2 &= \alpha_1 \frac{M_1 + M_2 \pm \sqrt{(M_1 - M_2)^2 + 4M_1M_2\cos^2\frac{\pi k}{2n}}}{M_1 M_2} \\ k &= 1, \ldots, n-1 \\ \omega_0^2 &= 0 \\ \omega_{2n}^2 &= \frac{\alpha_1(M_1 + M_2)}{M_1 M_2} \end{aligned}\right\} \tag{38}$$

Again ω_{2n}^2 is the "surface" frequency and as in the previous case there are two frequency branches or bands corresponding to the $\pm$ signs in eq. (38).

For odd N, $N = 2n + 1$, the only information available is the dispersion relation

$$\frac{u \sin(2n+2)\,\theta + 2\sqrt{uv}\,\sin(2n+1)\,\theta + v \sin 2n\,\theta}{\sin 2\theta} = 0 \qquad (39)$$

in which $\sqrt{uv} = 2b \cos\theta$. This is of course the characteristic equation of the matrix in eq. (36) and can be put in the form

$$\{\sqrt{u}\,\sin(n+1)\,\theta + \sqrt{v}\,\sin(n\theta)\}\,\{\sqrt{u}\,\cos(n+1)\,\theta + \sqrt{v}\,\cos n\theta\} = 0 \qquad (40)$$

which exhibits the existence of two frequency branches also in this case.

1.1.2 Linear Chain with Fixed Ends

Here again we assume mass-independent interactions and equidistant spacing of the equilibrium sites (unless specified otherwise). The two end particles are supposed to interact with rigid walls via the same force constants employed throughout the chain. Though more realistic, the inclusion of different force constants for the end particles will render the problem tractable only be perturbation methods. We restrict therefore the discussion to the former situation.

The dynamical matrix for the polyatomic case is

$$\Delta_N(\omega^2) = \begin{pmatrix} A_1 - M_1\omega^2, & -\alpha_1, & \cdots & -\alpha_{N-1} \\ -\alpha_1 & A_2 - M_2\omega^2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & -\alpha_1 \\ -\alpha_{N-1}, & \cdots & -\alpha_1, & A_N - M_N\omega^2 \end{pmatrix} \qquad (41)$$

in which

$$
A_r = \begin{cases} \sum_{j=1}^{N-1} \alpha_j + \alpha_1; & r = 1, N \\ \\ \sum_{j=1}^{N-r} \alpha_j + \sum_{j=1}^{r-1} \alpha_j; & r = 2, \ldots, N-1 \end{cases} \tag{42}
$$

As for a chain with free ends, the polyatomic case cannot be treated analytically. The cases for which closed analytic expressions of the eigenfrequencies are available will be listed below.

The monatomic chain with nearest neighbor interactions only, has the dynamical matrix

$$
\Delta_N(\omega^2) = \begin{pmatrix} a & b & & & 0 \\ b & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & b \\ 0 & & & b & a \end{pmatrix} \tag{43}
$$

with

$$
a = 2\alpha_1 - M\omega^2; \quad b = -\alpha_1 \tag{44}
$$

Using eq. (44) and the result (10) of Appendix E, we obtain the frequencies

$$
\omega_r^2 = \frac{4\alpha_1}{M} \sin^2 \frac{\pi r}{2(N+1)}, \quad r = 1, \ldots, N
$$

The eigenvectors are exhibited in eq. (12) of the Appendix.

The inclusion of interactions among more distant neighbors in the dynamical matrix makes the problem of calculating the eigenvalues analytically extremely difficult, and all efforts in this direction have been so far unsuccessful.

The diatomic chain, with particles M_1 and M_2 alternating regularly along the chain, can be regarded for $N = 2n$ as a lattice with a basis the unit cell of which contains two particles of different species. Because of the simplicity of the situation, one can disregard this feature and proceed directly.

For equidistant spacing and mass-independent interactions, the dynamical matrix is

$$\Delta_N(\omega^2) = \begin{pmatrix} u & b & & & 0 \\ b & v & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & b \\ 0 & & & b & * \end{pmatrix} \tag{45}$$

in which

$$u = 2\alpha_1 - M_1\,\omega^2; \qquad v = 2\alpha_1 - M_2\,\omega^2 \tag{46}$$

and the last element on the main diagonal is either u (for N odd) or v (for N even). The eqs. (36) and (42) of Appendix E show, on using eq. (46) above, that the frequencies for these two cases are given by:

$N = 2n$

$$\omega_k^2 = \frac{\alpha_1}{M_1 M_2}\left[M_1 + M_2 \pm \sqrt{(M_1 - M_2)^2 + 4 M_1 M_2 \cos^2 \frac{\pi k}{2n+1}} \right]$$

$$k = 1, \ldots, n \tag{47}$$

$\underline{N = 2n + 1}$

$$\left.\begin{aligned}
\omega_k^2 &= \frac{\alpha_1}{M_1 M_2}\left[M_1 + M_2 \pm \sqrt{(M_1 - M_2)^2 + 4M_1 M_2 \cos^2 \frac{\pi k}{2n+2}}\,\right] \\
k &= 1, \ldots, n \\
\omega_{2n+1}^2 &= \frac{2\alpha_1}{M_1}
\end{aligned}\right\} \tag{48}$$

The dynamical matrix for a diatomic chain with two different spacing constants similarly alternating is

$$\Delta_{2n+1}(\omega^2) = \begin{pmatrix} u & b & & & 0 \\ b & v & c & & \\ & c & \ddots & \ddots & \\ & & \ddots b & v & c \\ 0 & & & c & u \end{pmatrix} \tag{49}$$

in which

$$u = \beta + \gamma - M_1 \omega^2; \quad v = \beta + \gamma - M_2 \omega^2; \quad b = -\beta; \quad c = -\gamma \tag{50}$$

and β, γ are the two different force constants between nearest neighbors. Eqs. (56) and (59) of Appendix E show the frequencies to be

$$\left.\begin{aligned}
\omega_k^2 &= \frac{1}{2M_1 M_2}\left[(\beta + \gamma)(M_1 + M_2) \pm \sqrt{(\beta+\gamma)^2 (M_1 + M_2)^2 - 16\beta\gamma M_1 M_2 \sin^2 \frac{\pi k}{2n+2}}\,\right] \\
k &= 1, \ldots, n \\
\omega_{2n+1}^2 &= \frac{\beta + \gamma}{M_1}
\end{aligned}\right\} \tag{51}$$

Here again we observe the separation of the frequencies into two distinct branches. If this type of diatomic chain consists of an even number of particles, $N = 2n$, exact results are no longer available.

1.1.3 Linear Chain with Periodic Boundary Conditions

The chain is assumed here to form a closed loop. This means that there are no end particles and the interactions proceed along the shorter separation distances on the loop. Use of the forces defined in eq. (21) with mass independence and the assumption of equidistant spacing, yield for the polyatomic case the dynamical matrix

$$\Delta_N(\omega^2) = \begin{cases} \mathrm{diag}\,(A - M_1\omega^2,\ A - M_2\omega^2,\ \ldots,\ A - M_N\omega^2) - (\alpha_1\,\alpha_2\cdots\alpha_n\,\alpha_{n-1}\cdots\alpha_1)_{\mathrm{cyc.}} \\ \qquad N = 2n \\ \mathrm{diag}\,(A - M_1\omega^2,\ A - M_2\omega^2,\ \ldots,\ A - M_N\omega^2) - (\alpha_1\,\alpha_2\cdots\alpha_n\,\alpha_n\,\alpha_{n-1}\cdots\alpha_1)_{\mathrm{cyc.}} \\ \qquad N = 2n + 1 \end{cases} \tag{52}$$

in which diag (** . . . *) denotes a diagonal matrix with the elements specified in parantheses, and $(**\ldots *)_{\mathrm{cyc.}}$ denotes a matrix the first row of which consists of the specified elements *, the other rows being obtained from the first by (counter-clockwise) cyclic permutations. Also

$$A = \begin{cases} 2\displaystyle\sum_{j=1}^{n-1} \alpha_j + \alpha_N; & N = 2n \\ 2\displaystyle\sum_{j=1}^{n} \alpha_j; & N = 2n + 1 \end{cases} \tag{53}$$

We note that the number of independent force constants is here reduced to either $N/2$ or $(N - 1)/2$.

In contrast to previous cases, the frequencies and eigenvectors of the monatomic chain are known explicitly for the general case and can be given from eqs. (153) and (154) of Appendix E as follows:

$$\omega_k^2 = \begin{cases} \dfrac{4}{M} \displaystyle\sum_{j=1}^{n-1} \alpha_j \sin^2 \dfrac{\pi k j}{2n} + \dfrac{\alpha_n}{M} [1 - (-1)^k] \\ \qquad k = 0, 1, \cdots, 2n - 1 \; ; \; N = 2n \\ \dfrac{4}{M} \displaystyle\sum_{j=1}^{n} \alpha_j \sin^2 \dfrac{\pi k j}{2n+1} \\ \qquad k = 0, 1, \cdots, 2n \; ; \; N = 2n + 1 \end{cases} \tag{54}$$

It is seen that one frequency ($k = 0$) vanishes just as for a chain with free ends.

The frequencies and eigenvectors of a diatomic chain with an even number of particles can also be found. Using the eqs. (135) and (140) of Appendix E, we find the frequencies

$$\omega_k^2 = \frac{(M_1 + M_2)^2}{8 M_1 M_2} \left[\Omega_k^2 + \Omega_{k+n}^2 \pm \sqrt{(\Omega_k^2 - \Omega_{k+n}^2)^2 + 4 \left(\frac{M_1 - M_2}{M_1 + M_2} \right)^2 \Omega_k^2 \, \Omega_{k+n}^2} \right]^*$$

$$k = 0, \cdots, n - 1 \tag{55}$$

*The corresponding result in the literature is given only for nearest neighbors interactions and is not as transparent as the above.

in which

$$\Omega_r^2 = \frac{2}{M_1 + M_2} \left\{ 4 \sum_{j=1}^{n-1} \alpha_j \sin^2 \frac{\pi r j}{2n} + \alpha_n \left[1 - (-1)^r \right] \right\}^*$$

$$r = 0, \cdots, 2n - 1 \tag{56}$$

It is of interest to note that when the odd-indexed α's vanish, the radical in eq. (55) disappears and a decoupling of the motion takes place, i.e., the resulting frequencies are those of two separate loops with particles M_1 and M_2 respectively.

Here also the diatomic chain with an odd number of particles cannot be solved analytically.

Other situations can be also treated exactly. For instance if, everything being as before, we introduce two distinct spacing constants, as in Fig. 2, the dynamical matrix for a chain with only nearest neighbor interactions, will be

$$\mathbf{\Delta}_{2n}(\omega^2) = \begin{pmatrix} u & b & 0 & \cdots & 0 & c \\ b & v & c & & & 0 \\ 0 & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ \vdots & & & \ddots & \ddots & c \\ 0 & 0 & & c & u & b \\ c & 0 & \cdots & 0 & b & v \end{pmatrix} \tag{57}$$

in which

$$u = \beta + \gamma - M_1 \omega^2 ; \; v = \beta + \gamma - M_2 \omega^2 ; \; b = -\beta ; \; c = -\gamma \tag{58}$$

---

*These are just the frequencies for a <u>monatomic</u> chain with particle mass $(M_1 + M_2)/2$.

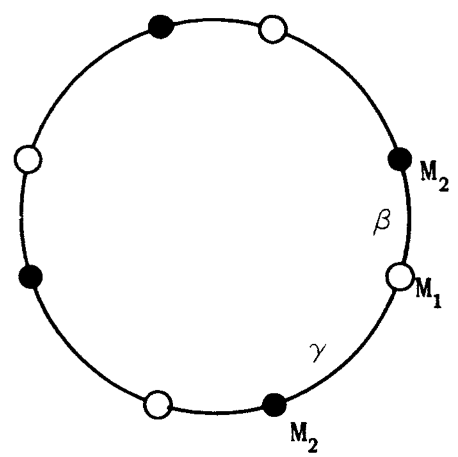

Figure 2

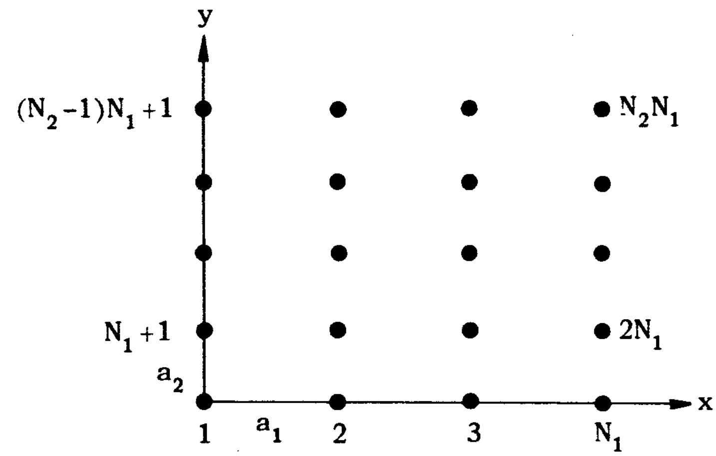

Figure 3

On using (58) above and eq. (161) of Appendix E we find the frequencies

$$\omega_k^2 = \frac{1}{2M_1M_2}\left[(\beta+\gamma)\,(M_1+M_2) \pm \sqrt{(\beta+\gamma)^2\,(M_1+M_2)^2 - 16\,\beta\gamma M_1 M_2 \sin^2\frac{\pi k}{n}}\,\right]$$

$$k = 0, \cdots, n-1 \tag{59}$$

1.2 Two-Dimensional Lattices

The plane lattices to be considered in this section will be rectangular. The model assumed is shown in Fig. 3: the unit cell is based on the vectors $\mathbf{a}_1 = a_1\,\mathbf{i}$; $\mathbf{a}_2 = a_2\,\mathbf{j}$, where $\mathbf{i}, \mathbf{j}$ are the unit vectors in the x- and y- directions, respectively. We assume the lattice to consist of N_2 horizontal rows equidistantly separated, with N_1 particles equidistantly spaced in each row.

The discussion will be restricted here to at most eight neighbors (for particles not on the boundary). For instance, the particle located at the site $\mathbf{a}_1 + \mathbf{a}_2$ is assumed to interact via two-body forces only with the particles at the sites

0 (this is labeled 1 in Fig. 3), $\mathbf{a}_1$, $2\mathbf{a}_1$, $\mathbf{a}_2$, $2\mathbf{a}_2$, $2\mathbf{a}_1 + \mathbf{a}_2$, $\mathbf{a}_1 + 2\mathbf{a}_2$ and $2(\mathbf{a}_1 + \mathbf{a}_2)$. For these sites to represent indeed the first, second and third neighbors, we have to assume

$$a_1,\ a_2 > \frac{1}{2}\sqrt{a_1^2 + a_2^2}\ .$$

The particles will be constrained to vibrate only in the plane of the lattice. The force density tensor $\boldsymbol{\Phi}$ will then be that of eq. (22), with α'' suppressed. The eight unit vectors $\boldsymbol{\varepsilon}$ needed in eq. (22), and their counterparts $\boldsymbol{\xi}$, are given here by

$$\left.\begin{array}{ll}
\boldsymbol{\varepsilon}_1 = -\boldsymbol{\varepsilon}_2 = \mathbf{i} & \boldsymbol{\xi}_1 = -\boldsymbol{\xi}_2 = \mathbf{j} \\
\boldsymbol{\varepsilon}_3 = -\boldsymbol{\varepsilon}_4 = \mathbf{j} & \boldsymbol{\xi}_3 = -\boldsymbol{\xi}_4 = -\mathbf{i} \\
\boldsymbol{\varepsilon}_5 = -\boldsymbol{\varepsilon}_6 = \dfrac{\mathbf{a}_1 + \mathbf{a}_2}{\sqrt{a_1^2 + a_2^2}}\ ; & \boldsymbol{\xi}_5 = -\boldsymbol{\xi}_6 = \dfrac{-\mathbf{a}_1 + \mathbf{a}_2}{\sqrt{a_1^2 + a_2^2}} \\
\boldsymbol{\varepsilon}_7 = -\boldsymbol{\varepsilon}_8 = \dfrac{-\mathbf{a}_1 + \mathbf{a}_2}{\sqrt{a_1^2 + a_2^2}} & \boldsymbol{\xi}_7 = -\boldsymbol{\xi}_8 = -\dfrac{\mathbf{a}_1 + \mathbf{a}_2}{\sqrt{a_1^2 + a_2^2}}
\end{array}\right\} \qquad (60)$$

Though immaterial in the two-dimensional case, we have used here the convention that angles between unit vectors are measured counter-clockwise from $\boldsymbol{\varepsilon}$ to $\boldsymbol{\xi}$.

There are three central and three noncentral force constants associated with the unit vectors of (60), in the following manner

$$\{\boldsymbol{\varepsilon}_1, \boldsymbol{\varepsilon}_2\} \leftrightarrow \alpha_1\ ;\ \{\boldsymbol{\varepsilon}_3, \boldsymbol{\varepsilon}_4\} \leftrightarrow \alpha_2\ ;\ \{\boldsymbol{\varepsilon}_5, \boldsymbol{\varepsilon}_6, \boldsymbol{\varepsilon}_7, \boldsymbol{\varepsilon}_8\} \leftrightarrow \alpha_3 \qquad (61)$$

and similar relations for $\boldsymbol{\xi}$ with α'.

We consider below different boundary conditions.

1.2.1 Plane Lattice with Free Boundaries

The equations of motion and the dynamical matrix are found in Appendix A. Here we quote the results.

A monatomic lattice has the dynamical matrix

$$\Delta\,(\omega^2) = \begin{pmatrix} F' & G & & & & \\ \tilde{G} & F & \ddots & & 0 & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & 0 & & \ddots & F & G \\ & & & & \tilde{G} & F'' \end{pmatrix} \tag{62}$$

in which

$$F' = \begin{pmatrix} A_3 & B & & & \\ B & A_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & A_2 & B \\ & & & B & A_4 \end{pmatrix}_{N_1 \times N_1} ; \quad F'' = \begin{pmatrix} A_4 & B & & & \\ B & A_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & A_2 & B \\ & & & B & A_3 \end{pmatrix}_{N_1 \times N_1}$$

$$F = \begin{pmatrix} A_1 & B & & & \\ B & A & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & A & B \\ & & & B & A_1 \end{pmatrix}_{N_1 \times N_1} ; \quad G = \begin{pmatrix} C & D & & & \\ E & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & D \\ & & & E & C \end{pmatrix}_{N_1 \times N_1}$$

where $\tilde{G}$ denotes the transpose of G, and $A_1, A_2, \ldots, E$ are defined in eqs. (6) and (7) of Appendix A.

Two eigenfrequencies can be seen from the equations of motion to vanish, corresponding of course to a rigid translation of the lattice. The two independent eigenvectors for this case are obtained when putting in turn

$$\mathbf{U}_{\ell,m} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}; \quad \mathbf{U}_{\ell,m} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{64}$$

for all (ℓ, m), with $\mathbf{U}$ defined in eq. (4) of Appendix A.

The remaining eigenfrequencies cannot be found analytically in the general case. But if next-nearest neighbor interactions are neglected, then the following simplifications take place

$$\mathbf{D} = \mathbf{E} = \mathbf{0}; \ \mathbf{A}_1 = \mathbf{A} + \mathbf{B}; \ \mathbf{A}_2 = \mathbf{A} + \mathbf{C}; \ \mathbf{A}_3 = \mathbf{A}_4 = \mathbf{A} + \mathbf{B} + \mathbf{C} \tag{65}$$

and

$$\tilde{\mathbf{G}} = \mathbf{G}; \ \mathbf{F}' = \mathbf{F}'' = \mathbf{F} + \mathbf{G} \tag{66}$$

Note that for this case the motions of the atoms in the x- and y-direction are independent.

Using (65), the dynamical matrix simplifies to

$$\mathbf{\Delta}_{2N_1 N_2}(\omega^2) = \begin{pmatrix} \mathbf{F}+\mathbf{G} & \mathbf{G} & & & \\ \mathbf{G} & \mathbf{F} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \mathbf{F} & \mathbf{G} \\ & & & \mathbf{G} & \mathbf{F}+\mathbf{G} \end{pmatrix} \tag{67}$$

As $\mathbf{F}$ and $\mathbf{G}$ are now commuting matrices, we can use eq. (203) of Appendix E and the definitions of the 2×2 matrices $\mathbf{A}, \mathbf{B}, \mathbf{C}$ to write the frequencies:

$$\left.\begin{aligned} \left[\omega^{(1)}_{kj}\right]^2 &= \frac{4\alpha}{M}\sin^2 k\theta + \frac{4\beta'}{M}\sin^2 j\varphi \\ \left[\omega^{(2)}_{kj}\right]^2 &= \frac{4\alpha'}{M}\sin^2 k\theta + \frac{4\beta}{M}\sin^2 j\varphi \end{aligned}\right\} \begin{aligned} k &= 0, \cdots, N_1 - 1 \\ j &= 0, \cdots, N_2 - 1 \end{aligned} \tag{68}$$

in which $\theta = \pi/2N_1$; $\varphi = \pi/2N_2$.

It is seen therefore that a rectangular plane lattice, in this model, has $2N_1 N_2 - 1$ distinct normal frequencies. This property persists even for the case $N_1 = N_2$ or when the unit cell is a square (for which $\alpha = \beta$ and $\alpha' = \beta'$). On the other hand, if $N_1 = N_2$ and the unit cell is square, the number of distinct frequencies is reduced to $N_1 N_2$, each being doubly degenerate.

It is not difficult now to write down the dynamical matrix for the diatomic lattice. In addition to the two masses one has to take into account the three types of interaction possible:

$$M_1 \leftrightarrow M_1 \; ; \; M_1 \leftrightarrow M_2 \; ; \; M_2 \leftrightarrow M_2$$

The case $M_1 \leftrightarrow M_2$ corresponds here to nearest neighbors and the other two to next nearest neighbors. Since we cannot find the eigenvalues for more distant neighbors even in the monatomic case, we shall restrict the discussion to nearest neighbors interactions. The dynamical matrix for this case is given then essentially by eq. (67), with the following modifications: 1. The 2×2-$\mathbf{A}$ matrices alternate regularly along the main diagonal of $\mathbf{F}^{(\ )}$:

$$\mathbf{F}^{(1)} = \begin{pmatrix} \mathbf{A}^{(1)} + \mathbf{B} & & \mathbf{B} & & \\ \mathbf{B} & \mathbf{A}^{(2)} & & \ddots & 0 \\ & \ddots & \ddots & & \ddots \\ & & \ddots & \ddots & \mathbf{B} \\ 0 & & & \mathbf{B} & \mathbf{A}^{(\ )} + \mathbf{B} \end{pmatrix} \tag{69}$$

in which

$$\left.\begin{aligned} \mathbf{A}^{(1)} &= \begin{pmatrix} 2(\alpha + \beta') - M_1 \omega^2 & 0 \\ 0 & 2(\alpha' + \beta) - M_1 \omega^2 \end{pmatrix} \\ \mathbf{A}^{(2)} &= \begin{pmatrix} 2(\alpha + \beta') - M_2 \omega^2 & 0 \\ 0 & 2(\alpha' + \beta) - M_2 \omega^2 \end{pmatrix} \end{aligned}\right\}$$

and

$$F^{(2)} = \begin{pmatrix} A^{(2)} + B & B & & & 0 \\ B & A^{(1)} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & B \\ 0 & & & B & A^{(\ )} + B \end{pmatrix} \tag{71}$$

The dynamical matrix has the form

$$\Delta(\omega^2) = \begin{pmatrix} F^{(1)} + G & G & & & 0 \\ G & F^{(2)} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & G \\ 0 & & & G & F^{(\ )} + G \end{pmatrix} \tag{72}$$

where the matrices $F^{(1)}$, $F^{(2)}$ alternate regularly along the main diagonal.

Though certain reductions of the dynamical matrix in eq. (72) are possible, analytic expressions for the frequencies cannot be found.

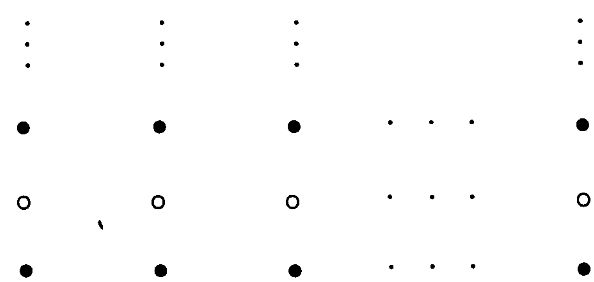

Figure 4. $\bullet \rightarrow M_1$; $\circ \rightarrow M_2$

On the otherhand if we consider the lattice shown in Fig. 4, which consists of alternating rows of two types of particles M_1, M_2, and assume $N_2 = 2n_2$, the dynamical matrix will have the form

$$\boldsymbol{\Delta}(\omega^2) = \begin{pmatrix} \mathbf{F}^{(1)}+\mathbf{G} & \mathbf{G} & & 0 \\ \mathbf{G} & \mathbf{F}^{(2)} & \ddots & \\ & \ddots & \ddots & \mathbf{G} \\ 0 & & \mathbf{G} & \mathbf{F}^{(2)}+\mathbf{G} \end{pmatrix} \tag{73}$$

in which $\mathbf{F}^{(1)}$ and $\mathbf{F}^{(2)}$ alternate along the main diagonal of $\boldsymbol{\Delta}$ and

$$\mathbf{F}^{(j)} = \begin{pmatrix} \mathbf{A}^{(j)}+\mathbf{B} & \mathbf{B} & & 0 \\ \mathbf{B} & \mathbf{A}^{(j)} & \ddots & \\ & \ddots & \ddots & \mathbf{B} \\ 0 & & \mathbf{B} & \mathbf{A}^{(j)}+\mathbf{B} \end{pmatrix} \quad j = 1,2 \tag{74}$$

The matrices $\mathbf{A}^{(1)}$, $\mathbf{A}^{(2)}$, $\mathbf{B}$ and $\mathbf{G}$ are as defined previously. As $\mathbf{F}^{(1)}$, $\mathbf{F}^{(1)}$ and $\mathbf{G}$ are commuting in pairs, it is shown in Appendix E that the eigenvalues of $\boldsymbol{\Delta}$ can be found. Using then eq. (209) of that Appendix, we obtain two groups of frequencies, each group consisting of four branches:

Group 1

$$\omega_{kj}^2 = \frac{1}{M_1 M_2}\left\{(M_1 + M_2)(\beta' + 2\alpha \sin^2 j\theta) \pm \sqrt{(M_1 - M_2)^2 (\beta' + 2\alpha \sin^2 j\theta)^2 + 4 M_1 M_2 \beta'^2 \cos^2 k\varphi}\right\}$$

$$\omega_{kj}^2 = \frac{1}{M_1 M_2}\left\{(M_1 + M_2)(\beta + 2\alpha' \sin^2 j\theta) \pm \sqrt{(M_1 - M_2)^2 (\beta + 2\alpha' \sin^2 j\theta)^2 + 4 M_1 M_2 \beta^2 \cos^2 k\varphi}\right\} \tag{75}$$

in which

$$j = 0, \cdots, N_1 - 1 \; ; \; k = 1, \cdots, n_2 - 1 \; ; \; \theta = \frac{\pi}{2N_1} \; ; \; \varphi = \frac{\pi}{2n_2} \tag{76}$$

Group 2

$$\omega_j^2 = \frac{1}{M_1 M_2}\left\{(M_1 + M_2)\left(\frac{\beta'}{2} + 2\alpha \sin^2 j\theta\right) \pm \sqrt{(M_1 - M_2)^2\left(\frac{\beta'}{2} + 2\alpha \sin^2 j\theta\right)^2 + M_1 M_2 \beta'^2}\right\}$$

$$\omega_j^2 = \frac{1}{M_1 M_2}\left\{(M_1 + M_2)\left(\frac{\beta}{2} + 2\alpha' \sin^2 j\theta\right) \pm \sqrt{(M_1 - M_2)^2\left(\frac{\beta}{2} + 2\alpha' \sin^2 j\theta\right)^2 + M_1 M_2 \beta^2}\right\} \tag{77}$$

with θ as in eq. (76) and $j = 0, \ldots, N_1 - 1$.

The frequencies in the last group are those associated with the surface modes. Two of these vanish (for $j = 0$), corresponding to rigid translations of the lattice.

1.2.2 Plane Lattice with Rigid Boundaries

Here we assume the marginal particles to interact with the rigid boundaries via the same two-body forces operating inside the lattice. Therefore using the same notation as before, the only equations of motion that change are those for the marginal particles. Proceeding as in § 1.2 of Appendix A we find the dynamical matrix for a monatomic lattice to be of the form:

$$\boldsymbol{\Delta}(\omega^2) = \begin{pmatrix} \mathbf{F} & \mathbf{G} & & \\ \tilde{\mathbf{G}} & \ddots & \ddots & \\ & \ddots & \ddots & \mathbf{G} \\ & & \tilde{\mathbf{G}} & \mathbf{F} \end{pmatrix}_{N_2 \times N_2} \tag{78}$$

in which

$$\mathbf{F} = \begin{pmatrix} \mathbf{A} & \mathbf{B} & & & \\ \mathbf{B} & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \mathbf{B} \\ & & & \mathbf{B} & \mathbf{A} \end{pmatrix}_{N_1 \times N_1} ; \quad \mathbf{G} = \begin{pmatrix} \mathbf{C} & \mathbf{D} & & & \\ \mathbf{E} & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \mathbf{D} \\ & & & \mathbf{E} & \mathbf{C} \end{pmatrix}_{N_1 \times N_1} \tag{79}$$

and $\mathbf{A}, \mathbf{B}, \ldots, \mathbf{E}$ are as defined in eq. (6) of Appendix A.

Again we note that $\mathbf{F}$, $\mathbf{G}, \tilde{\mathbf{G}}$ do not commute. This stems from the fact that $\mathbf{D}$ and $\mathbf{E}$ do not commute with one another or with $\mathbf{A}$, $\mathbf{B}$. The coupling between the motions in the x- and y-directions is given by $\mathbf{D}$ and $\mathbf{E}$, more specifically by the matrix element δ. It is clear therefore, from the expression defining δ, that if $\alpha_3' \sim \alpha_3$, then $\delta \sim 0$ and all the 2×2 matrices involved become diagonal, with

$$\mathbf{D} = \mathbf{E} = \begin{pmatrix} -\gamma & 0 \\ 0 & -\gamma \end{pmatrix} ; \quad \tilde{\mathbf{G}} = \mathbf{G} \tag{80}$$

Assuming the condition $\delta \sim 0$ to be satisfied, the motions in the x- and y-directions become independent and the frequencies will be obtained by equating to zero the λ_{kj} given in eq. (175) of Appendix E, namely

$$\left.\begin{aligned} &\left[\mathbf{A} + 2\,\mathbf{C}\cos\frac{\pi j}{N_2+1}\right] + 2\left[\mathbf{B} + 2\,\mathbf{D}\cos\frac{\pi j}{N_2+1}\right]\cos\frac{\pi k}{N_1+1} = 0 \\ &k = 1, \cdots, N_1 ; \quad j = 1, \cdots, N_2 \end{aligned}\right\} \tag{81}$$

Finally two groups of frequencies are obtained

$$\omega_{kj}^2 = \frac{2\alpha}{M}\left(1 - \cos\frac{\pi k}{N_1+1}\right) + \frac{2\beta'}{M}\left(1 - \cos\frac{\pi j}{N_2+1}\right) + \frac{4\gamma}{M}\left(1 - \cos\frac{\pi k}{N_1+1}\cos\frac{\pi j}{N_2+1}\right) \tag{82}$$

and

$$\omega^2_{kj} = \frac{2\alpha'}{M}\left(1-\cos\frac{\pi k}{N_1+1}\right) + \frac{2\beta}{M}\left(1-\cos\frac{\pi j}{N_2+1}\right) + \frac{4\gamma}{M}\left(1-\cos\frac{\pi k}{N_1+1}\cos\frac{\pi j}{N_2+1}\right) \quad (83)$$

with k and j as in eq. (81).

We remark that the boundary conditions under consideration do not lead to degeneracies in the spectrum, even for a lattice with a square unit cell (in which case $\alpha = \beta$; $\alpha' = \beta'$). The degeneracy that exists for a square lattice ($N_1 = N_2$) with square unit cell, is removed by the introduction of the next-nearest neighbor interactions, represented here by γ.

For the diatomic lattice with regular alternation of M_1 and M_2, the changes in the dynamical matrix are likewise obvious and we can write:

$$\Delta(\omega^2) = \begin{pmatrix} F_1 & G & & & 0 \\ G & F_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & G \\ 0 & & & G & F \end{pmatrix} \quad (84)$$

in which F_1 and F_2 alternate regularly along the main diagonal and

$$\left.\begin{aligned} F_1 = \begin{pmatrix} A^{(1)} & B & & & 0 \\ B & A^{(2)} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & B \\ 0 & & & B & A^{(\ )} \end{pmatrix} ; \quad F_2 = \begin{pmatrix} A^{(2)} & B & & & 0 \\ B & A^{(1)} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & B \\ 0 & & & B & A^{(\ )} \end{pmatrix} \end{aligned}\right\}$$

The matrices $\mathbf{A}^{(1)}$, $\mathbf{A}^{(2)}$ which alternate regularly in $\mathbf{F}_1, \mathbf{F}_2$ are as defined in eq. (70), $\mathbf{D}$ and $\mathbf{E}$ as in eq. (80), $\mathbf{G}$ as in eq. (79), and $\mathbf{B}, \mathbf{C}$ as in eq. (6) of Appendix A.

The eigenvalues of $\mathbf{\Delta}(\omega^2)$ can be found explicitly, for all parities of N_1, N_2, as shown in the treatment following eq. (177) of Appendix E. Here we quote results only for the case $N_2 = 2n_2$, and use eq. (195) in Appendix E (with A_r replaced by $\mathbf{A}^{(r)}$, $r = 1, 2$) to write down the frequencies. These appear in four distinct branches:

$$\omega^2_{jk} = \frac{1}{M_1 M_2} \Big\{ (M_1 + M_2)\ [\alpha + \beta' + 2\gamma(1 - \cos j\theta \cos k\varphi]\ \pm$$
$$\pm \sqrt{(M_1 - M_2)^2\ [\alpha + \beta' + 2\gamma(1 - \cos j\theta \cos k\varphi]^2 + 4M_1M_2\,[\alpha \cos j\theta + \beta' \cos k\varphi]^2} \Big\} \tag{86}$$

$$\omega^2_{jk} = \frac{1}{M_1 M_2} \Big\{ (M_1 + M_2)\ [\alpha' + \beta + 2\gamma\ (1 - \cos j\theta \cos k\varphi)]\ \pm$$
$$\pm \sqrt{(M_1 - M_2)^2\ [\alpha' + \beta + 2\gamma\ (1 - \cos j\theta \cos k\varphi)]^2 + 4M_1M_2\,[\alpha' \cos j\theta + \beta \cos k\varphi]^2} \Big\}$$

with

$$k = 1, \cdots, n_2\ ;\ j = 1, \cdots, N_1\ ;\ \theta = \frac{\pi}{N_1 + 1}\ ;\ \varphi = \frac{\pi}{2n_2 + 1}$$

It is of interest to compare the frequency spectrum of this model with the one obtained when a rearrangement of the particles has taken place. The rearrangement envisaged is the one already considered in Fig. 4 of the previous section, namely alternating rows of two types of particles, each row consisting of identical particles.

The dynamical matrix is (where for simplicity we assume $N_2 = 2n_2$):

$$\mathbf{\Delta}(\omega^2) = \begin{pmatrix} \mathbf{F}_1 & \mathbf{G} & & & 0 \\ \mathbf{G} & \mathbf{F}_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \mathbf{G} \\ 0 & & & \mathbf{G} & \mathbf{F}_2 \end{pmatrix} \tag{87}$$

in which

$$\mathbf{F}_1 = \begin{pmatrix} \mathbf{A}^{(1)} & \mathbf{B} & & & 0 \\ \mathbf{B} & \mathbf{A}^{(1)} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \mathbf{B} \\ 0 & & & \mathbf{B} & \mathbf{A}^{(1)} \end{pmatrix} ; \; \mathbf{F}_2 = \begin{pmatrix} \mathbf{A}^{(2)} & \mathbf{B} & & & 0 \\ \mathbf{B} & \mathbf{A}^{(2)} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \mathbf{B} \\ 0 & & & \mathbf{B} & \mathbf{A}^{(2)} \end{pmatrix} \tag{89}$$

and $\mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \mathbf{B}, \mathbf{G}$ are as in eq. (84).

The matrices $\mathbf{F}_1, \mathbf{F}_2$ and $\mathbf{G}$ commute in pairs, and so do all the 2×2 matrices involved. This being the case, eq. (183) of Appendix E shows the frequencies to be the roots of the matric equations

$$\omega^4 \left(\frac{M_1 - M_2}{2}\right)^2 \mathbf{I}_2 - \left\{\frac{\mathbf{A}^{(1)} + \mathbf{A}^{(2)}}{2} + 2\mathbf{B}\cos j\theta + 2\,[\mathbf{C} + 2\,\mathbf{D}\cos j\theta]\cos k\varphi\right\} \times$$

$$\times \left\{\frac{\mathbf{A}^{(1)} + \mathbf{A}^{(2)}}{2} + 2\mathbf{B}\cos j\theta - 2\,[\mathbf{C} + 2\mathbf{D}\cos j\theta]\cos k\varphi\right\} = 0 \tag{90}$$

in which

$$\theta = \frac{\pi}{N_1 + 1} ; \; \varphi = \frac{\pi}{2n_2 + 1} ; \; j = 1, \cdots, N_1 ; \; k = 1, \cdots, n_2 \tag{91}$$

Finally, the frequencies we obtain, appear in four distinct branches:

$$\omega_{kj}^2 = \frac{1}{M_1 M_2}\left\{(M_1+M_2)\ [\alpha(1-\cos j\theta)+\beta'+2\gamma] \pm\right.$$

$$\left.\pm\ \sqrt{(M_1-M_2)^2\ [\alpha(1-\cos j\theta)+\beta'+2\gamma]^2+4M_1M_2\ [\beta'+2\gamma\cos j\theta]^2\cos^2 k\varphi}\right\}$$

$$\omega_{kj}^2 = \frac{1}{M_1 M_2}\left\{(M_1+M_2)\ \ [\alpha'(1-\cos j\theta)+\beta+2\gamma\ ] \pm\right.$$

$$\left.\pm\ \sqrt{(M_1-M_2)^2\ [\alpha'\ (1-\cos j\theta)+\beta+2\gamma\ ]^2+4M_1M_2\ [\beta+2\gamma\cos j\theta]^2\cos^2 k\varphi}\right\} \tag{92}$$

with k, j, θ and φ as in eq. (91).

Similar expressions can be easily found also in case N_2 is odd.

1.2.3 Plane Lattice with Periodic Boundary Conditions

Here particles on opposite boundaries interact with one another and therefore we can envisage the lattice particles as being located on the surface of a torus. This means that there are no marginal particles.

One can write down the dynamical matrix taking account of all possible interactions, since in fact the eigenfrequencies can be explicitly exhibited for this general case. For the sake of simplicity and comparison with preceding results, we consider below only nearest and next-nearest neighbor interactions.

It is not difficult to show that the dynamical matrix for the monatomic lattice is

$$\Delta(\omega^2) = \begin{pmatrix} F & G & & \tilde{G} \\ \tilde{G} & \ddots & \ddots & 0 \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & G \\ G & & \tilde{G} & F \end{pmatrix}_{N_2\times N_2} \tag{93}$$

where

$$\mathbf{F} = \begin{pmatrix} \mathbf{A} & \mathbf{B} & & & \mathbf{B} \\ \mathbf{B} & \ddots & \ddots & & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & & \ddots & \ddots & \mathbf{B} \\ \mathbf{B} & & & \mathbf{B} & \mathbf{A} \end{pmatrix}_{N_1 \times N_1} ; \quad \mathbf{G} = \begin{pmatrix} \mathbf{C} & \mathbf{D} & & & \mathbf{E} \\ \mathbf{E} & \ddots & \ddots & & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & & \ddots & \ddots & \mathbf{D} \\ \mathbf{D} & & & \mathbf{E} & \mathbf{C} \end{pmatrix}_{N_1 \times N_1} ; \quad \tilde{\mathbf{G}} = \begin{pmatrix} \mathbf{C} & \mathbf{E} & & & \mathbf{D} \\ \mathbf{D} & \ddots & \ddots & & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & & \ddots & \ddots & \mathbf{E} \\ \mathbf{E} & & & \mathbf{D} & \mathbf{C} \end{pmatrix} \qquad (94)$$

The matrices $\mathbf{A}, \ldots, \mathbf{E}$ are as defined in eq. (6) of Appendix A.

It is seen that $\Delta(\omega^2)$ is a two-dimensional circulant matrix and that $\mathbf{F}$, $\mathbf{G}$ and $\tilde{\mathbf{G}}$ are circulant in their elements. Then we can use eq. (216) of Appendix E to write down the following matric equation the roots of which are the frequencies of the system:

$$0 = \mathbf{A} + 2\mathbf{B}\cos j\theta + 2\mathbf{C}\cos k\varphi + 2\mathbf{D}\cos(k\varphi + j\theta) +$$

$$+ 2\mathbf{E}\cos(k\varphi - j\theta) \equiv \Lambda_{kj} \; ; \; k = 0, \cdots, N_2 - 1 \; ; \; j = 0, \cdots, N_1 - 1 \qquad (95)$$

in which $\theta = 2\pi/N_1$; $\varphi = 2\pi/N_2$.

The explicit form of the 2×2 matrix Λ_{kj} is

$$\Lambda_{kj} = \begin{pmatrix} 4\alpha\sin^2(j\theta/2) + 4\beta'\sin^2(k\varphi/2) + 4\gamma(1 - \cos j\theta\cos k\varphi) - M\omega^2; & 4\delta\sin j\theta\sin k\varphi \\ \\ 4\delta\sin j\theta\sin k\varphi\; ; & 4\alpha'\sin^2(j\theta/2) + 4\beta\sin^2(k\varphi/2) + 4\gamma'(1 - \cos j\theta\cos k\varphi) - M\omega^2 \end{pmatrix}$$

(96)

Finally the frequencies are given by

$$\omega_{kj}^2 = \frac{2}{M}\Big\{(\alpha + \alpha')\sin^2(j\theta/2) + (\beta + \beta')\sin^2(k\varphi/2) + (\gamma + \gamma')(1 - \cos j\theta\cos k\varphi) \pm$$

$$\pm \sqrt{[(\alpha - \alpha')\sin^2(j\theta/2) + (\beta' - \beta)\sin^2(k\varphi/2) + (\gamma - \gamma')(1 - \cos j\theta\cos k\varphi)]^2 + (2\delta\sin j\theta\sin k\varphi)^2}\Big\}$$

$$j = 0, \cdots, N_1 - 1 \; ; \; k = 0, \cdots, N_2 - 1, \; \theta = 2\pi/N_1 ; \; \varphi = 2\pi/N_2 \qquad (97)$$

We note that here we obtain two branches, a result to be expected from the inclusion of next-nearest neighbor interactions. If δ is negligible, then the x- and y-motions are independent and the frequency spectrum reduces to one branch only. We observe that for $j = k = 0$ we obtain a vanishing, doubly degenerate frequency.

When we consider the <u>diatomic</u> lattice the only solvable case is when both N_1 and N_2 are even. Then, if $N_1 = 2n_1$, $N_2 = 2n_2$, the dynamical matrix takes the form:

$$\mathbf{\Delta}(\omega^2) = \begin{pmatrix} \mathbf{F}_1 & \mathbf{G} & & \tilde{\mathbf{G}} \\ \tilde{\mathbf{G}} & \mathbf{F}_2 & \ddots & 0 \\ & \ddots & \ddots & \ddots \\ 0 & \ddots & \mathbf{F}_1 & \mathbf{G} \\ \mathbf{G} & & \tilde{\mathbf{G}} & \mathbf{F}_2 \end{pmatrix}_{N_2 \times N_2} \tag{98}$$

in which $\mathbf{G}$ and $\tilde{\mathbf{G}}$ are as for the monatomic case, while

$$\mathbf{F}_1 = \begin{pmatrix} \mathbf{A}^{(1)} & \mathbf{B} & & \mathbf{B} \\ \mathbf{B} & \mathbf{A}^{(2)} & \ddots & 0 \\ & \ddots & \ddots & \ddots \\ 0 & \ddots & \mathbf{A}^{(1)} & \mathbf{B} \\ \mathbf{B} & & \mathbf{B} & \mathbf{A}^{(2)} \end{pmatrix} ; \quad \mathbf{F}_2 = \begin{pmatrix} \mathbf{A}^{(2)} & \mathbf{B} & & \mathbf{B} \\ \mathbf{B} & \mathbf{A}^{(1)} & \ddots & 0 \\ & \ddots & \ddots & \ddots \\ 0 & \ddots & \mathbf{A}^{(2)} & \mathbf{B} \\ \mathbf{B} & & \mathbf{B} & \mathbf{A}^{(1)} \end{pmatrix} \tag{99}$$

and $\mathbf{A}^{(1)}$, $\mathbf{A}^{(2)}$ as in eq. (84).

The matrices $\mathbf{F}_1$, $\mathbf{F}_2$ and $\mathbf{G}$ do not commute. Therefore the appropriate treatment is that preceding eq. (241) of Appendix E where it is shown that $\mathbf{\Delta}(\omega^2)$ is reducible to two types of block matrices on the main diagonal. These matrices denoted $\mathbf{K}^{(0)}$ and $\mathbf{K}^{(1)}$ in eq. (241), become here 4×4 matrices. These matrices cannot be further simplified and the resulting equations are of the fourth degree in ω^2. Hence, for this model, we obtain eight frequency branches. Analytic expressions for the frequencies can be found only for $4(N_1 + N_2 - 2)$ of them – corresponding to the cases for which the coefficients of the coupling parameter δ vanish, making all the 2×2 matrices diagonal. Below we exhibit the $2N_1N_2$ frequencies obtained when δ is dropped from the start:

$$\omega_{kj}^2 = \frac{1}{M_1 M_2} \Big\{ (M_1 + M_2) \left[\alpha + \beta' + 2\gamma (1 - \cos j\theta \cos k\varphi)\right] \pm$$
$$\pm \sqrt{(M_1 - M_2)^2 \left[\alpha + \beta' + 2\gamma(1 - \cos j\theta \cos k\varphi)\right]^2 + 4M_1M_2 \left[\alpha \cos j\theta + \beta' \cos k\varphi)\right]^2} \Big\} \tag{100}$$

$$\omega_{kj}^2 = \frac{1}{M_1 M_2} \Big\{ (M_1 + M_2) \left[\alpha' + \beta + 2\gamma (1 - \cos j\theta \cos k\varphi)\right] \pm$$
$$\pm \sqrt{(M_1 - M_2)^2 \left[\alpha' + \beta + 2\gamma (1 - \cos j\theta \cos k\varphi)\right]^2 + 4M_1M_2 \left[\alpha' \cos j\theta + \beta \cos k\varphi\right]^2} \Big\} \tag{101}$$

$$\omega_{kj}^2 = \frac{1}{M_1 M_2} \Big\{ (M_1 + M_2) \left[\alpha + \beta' + 2\gamma (1 + \cos j\theta \cos k\varphi)\right] \pm$$
$$\pm \sqrt{(M_1 - M_2)^2 \left[\alpha + \beta' + 2\gamma (1 + \cos j\theta \cos k\varphi)\right]^2 + 4M_1M_2 \left[\alpha \cos j\theta - \beta' \cos k\varphi\right]^2} \Big\} \tag{102}$$

$$\omega_{kj}^2 = \frac{1}{M_1 M_2} \Big\{ (M_1 + M_2) \left[\alpha' + \beta + 2\gamma (1 + \cos j\theta \cos k\varphi)\right] \pm$$
$$\pm \sqrt{(M_1 - M_2)^2 \left[\alpha' + \beta + 2\gamma (1 + \cos j\theta \cos k\varphi)\right]^2 + 4M_1M_2 \left[\alpha' \cos j\theta - \beta \cos k\varphi\right]^2} \Big\} \tag{103}$$

In the last four expressions we have

$$j = 0, \ldots, n_1 - 1; \quad k = 0, \ldots, n_2 - 1; \quad \theta = \pi/n_1; \quad \varphi = \pi/n_2 \tag{104}$$

The $4(N_1 + N_2 - 2)$ frequencies mentioned previously can be obtained from eq. (100) - (102) by letting j and k take in turn the value 0. Two frequencies, obtained from eqs. (100) and (101) for $k = j = 0$, vanish.

1.3 Three-Dimensional Lattices

In this section we consider a rectangular space lattice. The model assumed is shown in Fig. 5. The unit cell is based on the vectors $\mathbf{a}_1 = a_1\mathbf{i}$, $\mathbf{a}_2 = a_2\mathbf{j}$; $\mathbf{a}_3 = a_3\mathbf{k}$, where $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$ are unit vectors in the x-, y- and z-directions, respectively. We further assume the lattice to consist of N_1 particles in each row parallel to the x-axis, N_2 and N_3 particles in rows parallel to the y- and z-axes, respectively.

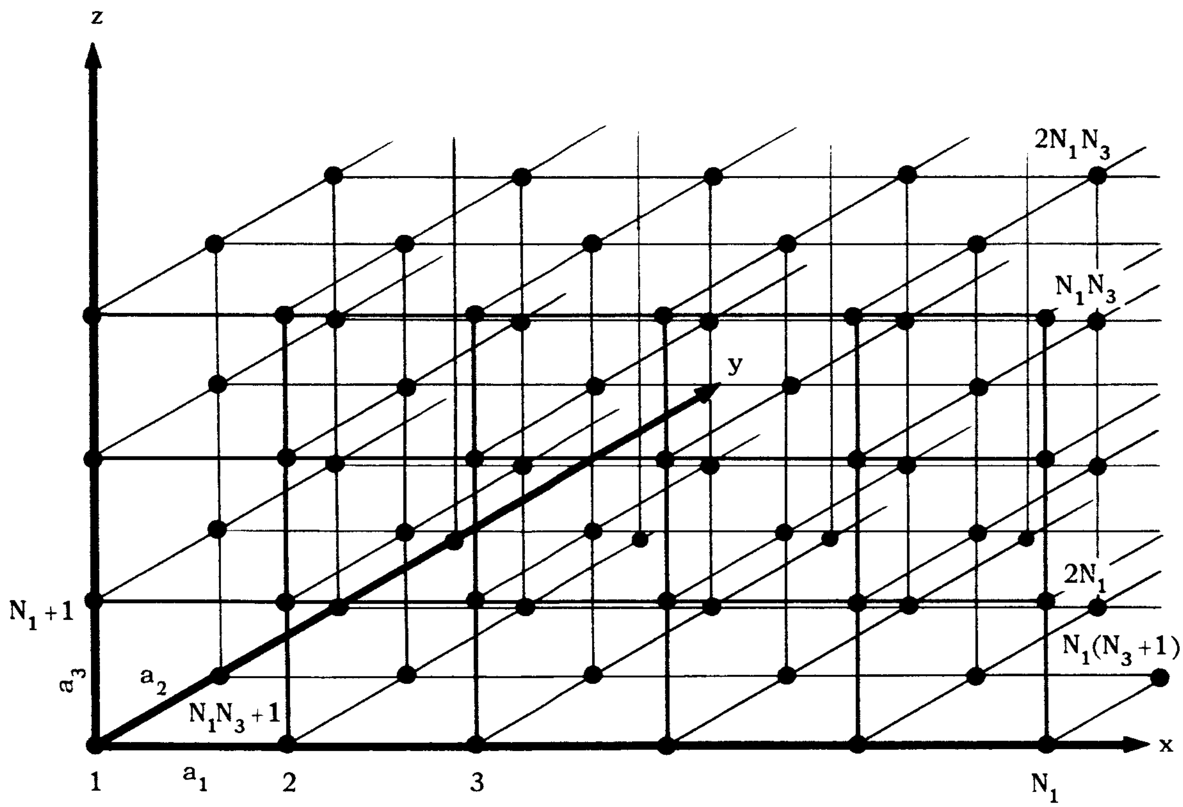

Figure 5

No constraints are imposed here on the vibrations of the particles and hence the force tensor Φ will be used in the form given by eq. (22). The discussion will include 26 immediate neighbors, located at the vertices of 8 unit cells. For these to represent first, second and third neighbors, certain not too stringent conditions have to be imposed on the relative values of a_1, a_2 and a_3.

As before, the two-body interactions considered are assumed to be mass-independent.

The unit vectors ε, ξ, η and the force constants associated with the twenty-six neighbors are exhibited in section 2 of Appendix A.

1.3.1 Lattice with Free Boundaries

Following the procedure described in Appendix A, the dynamical matrix for the monatomic lattice could be written down so as to include all the neighbors considered in the present model. Since such generality precludes an exact solution for the frequencies, the discussion below will be restricted to the case of nearest neighbors interactions. The dynamical matrix for this case is:

$$\boldsymbol{\Delta}(\omega^2) = \begin{pmatrix} \mathbf{S}+\mathbf{T} & \mathbf{T} & & & 0 \\ \mathbf{T} & \mathbf{S} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \mathbf{S} & \mathbf{T} \\ 0 & & & \mathbf{T} & \mathbf{S}+\mathbf{T} \end{pmatrix}_{N_2 \times N_2} \tag{105}$$

in which

$$\mathbf{S} = \begin{pmatrix} \mathbf{F}+\mathbf{G} & \mathbf{G} & & & 0 \\ \mathbf{G} & \mathbf{F} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \mathbf{F} & \mathbf{G} \\ 0 & & & \mathbf{G} & \mathbf{F}+\mathbf{G} \end{pmatrix}_{N_3 \times N_3} ; \quad \mathbf{T} = \begin{pmatrix} \mathbf{H} & & 0 \\ & \ddots & \\ 0 & & \mathbf{H} \end{pmatrix}_{N_3 \times N_3} \tag{106}$$

and

$$
\mathbf{F} = \begin{pmatrix} \mathbf{A}+\mathbf{B}_1 & \mathbf{B}_1 & & & 0 \\ \mathbf{B}_1 & \mathbf{A} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \mathbf{A} & \mathbf{B}_1 \\ 0 & & & \mathbf{B}_1 & \mathbf{A}+\mathbf{B}_1 \end{pmatrix}_{N_1 \times N_1} ; \quad \mathbf{G} = \begin{pmatrix} \mathbf{B}_3 & & 0 \\ & \ddots & \\ 0 & & \mathbf{B}_3 \end{pmatrix}_{N_1 \times N_1} \quad \mathbf{H} = \begin{pmatrix} \mathbf{B}_2 & & 0 \\ & \ddots & \\ 0 & & \mathbf{B}_2 \end{pmatrix}_{N_1 \times N_1} \tag{107}
$$

The matrices $\mathbf{B}_r$ are as in eqs. (12) of Appendix A and $\mathbf{A}$ as in eq. (18) of the same, with all $\mathbf{C}_r$ and $\mathbf{D}_r$ suppressed. All the 3×3 matrices involved are now diagonal.

The frequencies can be found immediately on using eq. (268) of Appendix E:

$$
\omega^2_{jkr} = \frac{4}{M} \begin{cases} \alpha_1 \sin^2 j\theta + \alpha''_2 \sin^2 k\varphi + \alpha'_3 \sin^2 r\psi \\ \alpha'_1 \sin^2 j\theta + \alpha_2 \sin^2 k\varphi + \alpha''_3 \sin^2 r\psi \\ \alpha''_1 \sin^2 j\theta + \alpha'_2 \sin^2 k\varphi + \alpha_3 \sin^2 r\psi \end{cases} \tag{108}
$$

in which

$$
\left.\begin{array}{l} j = 0, \ldots, N_1 - 1; \quad k = 0, \ldots, N_2 - 1; \quad r = 0, \ldots, N_3 - 1 \\ \theta = \pi/2N_1; \quad \varphi = \pi/2N_2; \quad \psi = \pi/2N_3 \end{array}\right\} \tag{109}
$$

The zero frequency ω_{000} is triply degenerate, while the rest are distinct. These frequencies will remain distinct even for a cubic unit cell, if at least one dimension (N_i) of the lattice is different from the other two. For a cubic lattice with a cubic unit cell all the frequencies (108) become triply degenerate in this approximation.

The dynamical matrix for the diatomic lattice can be readily written down, but as in the corresponding plane lattice the frequencies cannot be found exactly. Here we mention only that exact solutions exist for a lattice composed of alternating planes of two particle-species, each plane containing like particles. In the approximation of nearest neighbors, this type of lattice possesses twelve distinct frequency branches.

1.3.2 Lattice with Rigid Boundaries

The dynamical matrix for the monatomic lattice can be written down when interactions up to third neighbors are included, but the frequencies of the system cannot be found analytically. Therefore we restrict the discussion to the following soluble case: 1. Third order neighbors are neglected; 2. The off-diagonal elements of the matrices C_r defined in Appendix A are dropped. This last requirement is equivalent to assuming $\beta_j \approx \beta_j'$; $j = 1, 2, 3$.

Assuming these conditions to be satisfied, the dynamical matrix becomes

$$\Delta(\omega^2) = \begin{pmatrix} S & T & & & \\ T & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & T \\ & & & T & S \end{pmatrix}_{N_2 \times N_2} \tag{110}$$

with

$$S = \begin{pmatrix} F & G & & & 0 \\ G & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & G \\ 0 & & & G & F \end{pmatrix}; \quad T = \begin{pmatrix} H & K & & & 0 \\ K & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & K \\ 0 & & & K & H \end{pmatrix} \tag{111}$$

$$
\mathbf{G} = \begin{pmatrix} \mathbf{B}_3 & \mathbf{C}_3 & & 0 \\ \mathbf{C}_3 & \ddots & \ddots & \\ & \ddots & \ddots & \mathbf{C}_3 \\ 0 & & \mathbf{C}_3 & \mathbf{B}_3 \end{pmatrix}; \quad
\mathbf{H} = \begin{pmatrix} \mathbf{B}_2 & \mathbf{C}_1 & & 0 \\ \mathbf{C}_1 & \ddots & \ddots & \\ & \ddots & \ddots & \mathbf{C}_1 \\ 0 & & \mathbf{C}_1 & \mathbf{B}_2 \end{pmatrix}; \quad
\mathbf{K} = \begin{pmatrix} \mathbf{C}_5 & & 0 \\ & \ddots & \\ 0 & & \mathbf{C}_5 \end{pmatrix}
$$

and

$$
\mathbf{F} = \begin{pmatrix} \mathbf{A} & \mathbf{B}_1 & & 0 \\ \mathbf{B}_1 & \ddots & \ddots & \\ & \ddots & \ddots & \mathbf{B}_1 \\ 0 & & \mathbf{B}_1 & \mathbf{A} \end{pmatrix} \tag{112}
$$

Here the matrices $\mathbf{B}_i$ are as in eq. (12) of Appendix A while according to requirement (2) above we obtain

$$
\left.\begin{aligned}
\mathbf{C}_1 &= \mathbf{C}_2 = -\operatorname{diag}(\beta_1\ \beta_1\ \beta_1'') \\
\mathbf{C}_3 &= \mathbf{C}_4 = -\operatorname{diag}(\beta_2\ \beta_2''\ \beta_2) \\
\mathbf{C}_5 &= \mathbf{C}_6 = -\operatorname{diag}(\beta_3''\ \beta_3\ \beta_3)
\end{aligned}\right\} \tag{113}
$$

and

$$
\begin{aligned}
\mathbf{A} = \operatorname{diag}\{&2[\alpha_1 + \alpha_2'' + \alpha_3' + 2(\beta_1 + \beta_2 + \beta_3'')] - M\omega^2;\quad 2[\alpha_1' + \alpha_2 + \alpha_3'' + 2(\beta_1 + \beta_2'' + \beta_3)] - M\omega^2; \\
&2[\alpha_1'' + \alpha_2' + \alpha_3 + 2(\beta_1'' + \beta_2 + \beta_3)] - M\omega^2\}
\end{aligned} \tag{114}
$$

On using eq. (244) of Appendix E the frequencies can be written down immediately:

$$
\omega^2_{jkr} = \frac{4}{M}\begin{cases} \alpha_1 \sin^2 j\theta + \alpha_2'' \sin^2 k\varphi + \alpha_3' \sin^2 r\psi + \beta_1(1 - \cos 2j\theta \cos 2k\varphi) \\ \qquad + \beta_2(1 - \cos 2j\theta \cos 2r\psi) + \beta_3''(1 - \cos 2k\varphi \cos 2r\psi) \\ \alpha_1' \sin^2 j\theta + \alpha_2 \sin^2 k\varphi + \alpha_3'' \sin^2 r\psi + \beta_1(1 - \cos 2j\theta \cos 2k\varphi) \\ \qquad + \beta_2''(1 - \cos 2j\theta \cos 2r\psi) + \beta_3(1 - \cos 2k\varphi \cos r\psi) \\ \alpha_1'' \sin^2 j\theta + \alpha_2' \sin^2 k\varphi + \alpha_3 \sin^2 r\psi + \beta_1''(1 - \cos 2j\theta \cos 2k\varphi) \\ \qquad + \beta_2(1 - \cos 2j\theta \cos 2r\psi) + \beta_3(1 - \cos 2k\varphi \cos 2r\psi) \end{cases} \tag{115}
$$

in which

$$
j = 1,\ldots, N_1;\ k = 1,\ldots,N_2;\ r = 1,\ldots, N_3;\ \theta = \frac{\pi}{2(N_1+1)}\ ;\ \varphi = \frac{\pi}{2(N_2+1)}\ ;\ \psi = \frac{\pi}{2(N_3+1)}\ . \tag{116}
$$

If instead of neglecting the third neighbors interactions entirely we assume the force constants to be nearly equal,

$$
\gamma \sim \gamma' \sim \gamma'' \tag{117}
$$

then all the matrices $\mathbf{D}$ defined in Appendix A become equal to $-\gamma\mathbf{I}$. The frequencies for this case can again be found and will be as given in eq. (115), to each being added the term

$$
2\gamma(1 - \cos 2j\theta \cos 2k\varphi \cos 2r\psi). \tag{118}
$$

Whether this term is added or not, we see that this model posses three distinct frequency branches, a property that persists for a lattice with cubic unit cell. On the other hand if such a lattice is cubic (i.e., $N_1 = N_2 = N_3$) the frequencies become triply degenerate.

We consider now a diatomic lattice and shall assume the arrangement to be such that no two adjacent particles are alike. Then the dynamical matrix reads:

$$
\Delta(\omega^2) = \begin{pmatrix} S_1 & T & & & \\ T & S_2 & \ddots & & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & & \ddots & \ddots & T \\ & & & T & S_2 \end{pmatrix}_{N_2 \times N_2} \quad ; \; N_2 = 2n_2 \tag{119}
$$

in which

$$
\left.
\begin{aligned}
S_1 &= \begin{pmatrix} F_1 & G & & & \\ G & F_2 & \ddots & & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & & \ddots & \ddots & G \\ & & & G & F_2 \end{pmatrix}_{N_3 \times N_3} ; \; S_2 = \begin{pmatrix} F_2 & G & & & \\ G & F_1 & \ddots & & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & & \ddots & \ddots & G \\ & & & G & F_1 \end{pmatrix}_{N_3 \times N_3} ; \; N_3 = 2n_3 \\
F_1 &= \begin{pmatrix} A_1 & B_1 & & & \\ B_1 & A_2 & \ddots & & \\ & \ddots & \ddots & \ddots & 0 \\ 0 & & \ddots & \ddots & B_1 \\ & & & B_1 & A_2 \end{pmatrix}_{N_1 \times N_1} ; \; F_2 = \begin{pmatrix} A_2 & B_1 & & & \\ B_1 & A_1 & \ddots & & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & & \ddots & \ddots & B_1 \\ & & & B_1 & A_1 \end{pmatrix}_{N_1 \times N_1} ; \; N_1 = 2n_1
\end{aligned}
\right\} \tag{120}
$$

The matrices S_i , F_i , A_i ($i = 1, 2$) alternate regularly along the main diagonals of the appropriate matrices. G and T are as in eq. (111), while A_i is as given in eq. (114) with M replaced by M_i, $i = 1, 2$. We have chosen N_1 , N_2 , N_3, to be all even only to simplify the presentation, but in fact all possible choices lead, in this model, to exact solutions.

The frequencies of the system can be obtained by equating to zero the $\lambda^{\pm}_{jkr}$ in eq. (265) of Appendix E and solving for ω^2. Here we make use from the start of eq. (117) to include the third neighbors interactions. For brevity, we present the frequencies ω^2 as elements of a 3×3 diagonal matrix $\mathbf{\Omega}^{\pm}_{jkr}$,

$$\mathbf{\Omega}^{\pm}_{jkr} = \frac{1}{M_1 M_2}\left\{-(M_1 + M_2)\,\mathbf{P}_{jkr} \pm \sqrt{(M_1 - M_2)^2\,\mathbf{P}^2_{jkr} + 4 M_1 M_2\,\mathbf{Q}^2_{jkr}}\right\} \tag{121}$$

in which

$$\mathbf{P}_{jkr} = \mathbf{B}_1 + \mathbf{B}_2 + \mathbf{B}_3 + 2\mathbf{C}_1(1 - \cos j\theta \cos k\varphi) + 2\mathbf{C}_3(1 - \cos j\theta \cos r\psi)$$
$$+ 2\mathbf{C}_5(1 - \cos k\varphi \cos r\psi) - \gamma\mathbf{I}(1 - \cos j\theta \cos k\varphi \cos r\psi) \tag{122}$$

$$\mathbf{Q}_{jkr} = \mathbf{B}_1 \cos j\theta + \mathbf{B}_2 \cos k\varphi + \mathbf{B}_3 \cos r\psi\,. \tag{123}$$

All of the matrices appearing above are as in the monatomic case. On the other hand, we have here

$$j = 1, \dots, 2n_1;\ k = 1, \dots, n_2;\ r = 1, \dots, 2n_3;\ \theta = \frac{\pi}{N_1 + 1};\ \varphi = \frac{\pi}{N_2 + 1};\ \psi = \frac{\pi}{N_3 + 1}\,.$$

Eq. (122) shows the existence in this model, of six distinct frequency branches.

1.3.3 Lattice With Periodic Boundaries

The dynamical matrix for the monatomic lattice to be displayed here contains all the interactions assumed in the model.

$$\mathbf{\Delta}(\omega^2) = \begin{pmatrix} \mathbf{S} & \mathbf{T} & & \tilde{\mathbf{T}} \\ \tilde{\mathbf{T}} & \ddots & \ddots & 0 \\ & \ddots & \ddots & \mathbf{T} \\ \mathbf{T} & & \tilde{\mathbf{T}} & \mathbf{S} \end{pmatrix}_{N_2} \tag{123}$$

in which

$$
\left.
\begin{aligned}
&S = \begin{pmatrix} F & G & & \tilde{G} \\ G & \ddots & \ddots & 0 \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & G \\ G & & G & F \end{pmatrix}_{N_3} ; \quad T = \begin{pmatrix} H & K & & L \\ L & \ddots & \ddots & 0 \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & K \\ K & & L & H \end{pmatrix}_{N_3} \\
&F = \begin{pmatrix} A & B_1 & & B_1 \\ B_1 & \ddots & \ddots & 0 \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & B_1 \\ B_1 & & B_1 & A \end{pmatrix}_{N_1} ; \quad G = \begin{pmatrix} B_3 & C_3 & & C_4 \\ C_4 & \ddots & \ddots & 0 \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & C_3 \\ C_3 & & C_4 & B_3 \end{pmatrix}_{N_1} \\
&H = \begin{pmatrix} B_2 & C_1 & & C_2 \\ C_2 & \ddots & \ddots & 0 \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & C_1 \\ C_1 & & C_2 & B_2 \end{pmatrix}_{N_1} ; \quad K = \begin{pmatrix} C_5 & D_1 & & D_3 \\ D_3 & \ddots & \ddots & 0 \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & D_1 \\ D_1 & & D_3 & C_5 \end{pmatrix}_{N_1} ; \quad L = \begin{pmatrix} C_6 & D_4 & & D_2 \\ D_2 & \ddots & \ddots & 0 \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & D_4 \\ D_4 & & D_2 & C_6 \end{pmatrix}_{N_1}
\end{aligned}
\right\} \tag{124}
$$

All of the matrices $A, B_1, \ldots, D_4$ are as defined in § 2 of Appendix A.

The frequencies are obtained by equating to zero the determinant of the matrix in eq. (274) of Appendix E, thus leading to a third degree equation for ω^2. Explicit expressions can be derived if we assume the validity of the simplified conditions exhibited in eqs. (113) and (117), for which all the 3×3 matrices become diagonal.

For this case the frequencies ω^2 are the elements of the 3×3 diagonal matrix Ω_{jkr} given by

$$\Omega_{jkr} = -\frac{2}{M}\Big\{ \mathbf{B}_1 (1 - \cos j\theta) + \mathbf{B}_2 (1 - \cos k\varphi) + \mathbf{B}_3 (1 - \cos r\psi) +$$

$$+ 2\mathbf{C}_1 (1 - \cos j\theta \cos k\varphi) + 2\mathbf{C}_3 (1 - \cos j\theta \cos r\psi) + 2\mathbf{C}_5 (1 - \cos k\varphi \cos r\psi)$$

$$- 4\gamma \mathbf{I} (1 - \cos j\theta \cos k\varphi \cos r\psi)\Big\} \tag{125}$$

in which

$$j = 0, \cdots, N_1 - 1;\ k = 0, \cdots, N_2 - 1;\ r = 0, \cdots, N_3 - 1;\ \theta = 2\pi/N_1;\ \varphi = 2\pi/N_2;\ \psi = 2\pi/N_3 \tag{126}$$

and the matrices $\mathbf{B}_i$ are as in eq. (12) of Appendix A, while $\mathbf{C}_i$ as in eq. (113) above.

Three distinct frequency branches appear also here.

The only soluble case for a <u>diatomic</u> lattice is when N_1, N_2, N_3 are all even. This is in contrast to the diatomic lattice with rigid boundaries. The changes in the dynamical matrix of eq. (123) are as follows: instead of the $\mathbf{S}$ given in eq. (124) there are $\mathbf{S}_1$ and $\mathbf{S}_2$ alternating on the main diagonal of $\Delta(\omega^2)$, each one with alternating $\mathbf{F}_1$ and $\mathbf{F}_2$ on their main diagonals,

$$\mathbf{S}_1 = \begin{pmatrix} \mathbf{F}_1 & \mathbf{G} & & \tilde{\mathbf{G}} \\ \mathbf{G} & \mathbf{F}_2 & \ddots & 0 \\ & \ddots & \ddots & \mathbf{G} \\ \mathbf{G} & 0 & \tilde{\mathbf{G}} & \mathbf{F}_2 \end{pmatrix};\quad \mathbf{S}_2 = \begin{pmatrix} \mathbf{F}_2 & \mathbf{G} & & \tilde{\mathbf{G}} \\ \mathbf{G} & \mathbf{F}_1 & \ddots & 0 \\ & \ddots & \ddots & \mathbf{G} \\ \mathbf{G} & 0 & \tilde{\mathbf{G}} & \mathbf{F}_1 \end{pmatrix} \tag{127}$$

$$\mathbf{F}_1 = \begin{pmatrix} \mathbf{A}_1 & \mathbf{B}_1 & & \mathbf{B}_1 \\ \mathbf{B}_1 & \mathbf{A}_2 & \ddots & 0 \\ & \ddots & \ddots & \mathbf{B}_1 \\ \mathbf{B}_1 & 0 & \mathbf{B}_1 & \mathbf{A}_2 \end{pmatrix};\quad \mathbf{F}_2 = \begin{pmatrix} \mathbf{A}_2 & \mathbf{B}_1 & & \mathbf{B}_1 \\ \mathbf{B}_1 & \mathbf{A}_1 & \ddots & 0 \\ & \ddots & \ddots & \mathbf{B}_1 \\ \mathbf{B}_1 & 0 & \mathbf{B}_1 & \mathbf{A}_1 \end{pmatrix} \tag{128}$$

in which again $\mathbf{A}_i$ is as given in eq. (114) with M replaced by M_i, $i = 1, 2$.

Once more we assume the conditions given in eqs. (113) and (117), and make use of the results (306) and (307) in Appendix E to solve for the frequencies. It is seen that there are 24 distinct branches and we exhibit below six typical frequencies as the elements of a 3×3 diagonal matrix $\Omega^{\pm}_{jkr}$,

$$\Omega^{\pm}_{jkr} = \frac{1}{M_1 M_2} \left\{ -(M_1 + M_2) P_{jkr} \pm \sqrt{(M_1 - M_2)^2 P^2_{kjr} + 4M_1 M_2 Q^2_{jkr}} \right\} \quad (129)$$

in which P_{jkr} and Q_{jkr} are as defined in eqs. (122), (123), and

$$j = 0, \cdots, n_1 - 1;\ k = 0, \cdots, n_2 - 1;\ r = 0, \cdots, n_3 - 1;\ \theta = \pi/n_1;\ \varphi = \pi/n_2;\ \psi = \pi/n_3 \quad (130)$$

Three additional matrices of the same type as in eq. (129) but with different signs accompanying the cosines, complete the frequency spectrum of $\Delta(\omega^2)$. We note that the functional form of the frequencies for periodic boundary conditions coincides with that for rigid boundaries.

We conclude this chapter with two remarks: First, the treatment of harmonic lattices described in the opening section is fully adequate for attacking lattices with symmetries different from the rectangular model considered here. Second, although the linear chain and the plane lattice particles have been assumed to vibrate longitudinally and in the plane respectively, it is readily seen that these limitations can be dropped if certain simple reductions are carried out in the three-dimensional lattice.

CHAPTER II

OTHER APPLICATIONS

The physics of periodic units is by no means restricted to lattice-dynamical problems. In this chapter we shall present also situations which are unrelated to calculations with normal mode frequencies, yet require handling by similar mathematical techniques. The functions of matrices that arise and the finite sums associated with these, are not necessarily connected with the statistical mechanics of the systems. The functions appear naturally in most of the situations considered. The examples below, selected from diverse fields, will illustrate these ideas.

The theory of electrical lines is entirely analogous to lattice dynamics theory, and one can indeed set up a one-to-one correspondence between the quantities of interest in both theories. An example of this is given by Brillouin [4] in the treatment of an electrical line analogous to a diatomic linear chain with two distinct spacing constants.

A different example from classical physics was discussed by G. N. Watson [27]. He became interested in the evaluation of sums of the form:

$$S_N(r) = \sum_{k=1}^{N-1} [\operatorname{cosec}(k\theta/2)]^{-r}; \ \theta = 2\pi/N; \ r = 1, 3, \cdots \tag{1}$$

Apparently, these sums occur in a classical treatment of a Bohr type atom: electrons, equidistantly spaced, are assumed to move in the same circular orbit, with the positive nucleus at the center. The small oscillations of the system are found under the assumption of Coulomb interactions and the sums enter the resulting frequencies. The analogous gravitational problem is the motion of satellites rotating in a circle about a planet. This is a simplified form of the problem of Saturn's rings considered by Maxwell.

The sum above, laboriously evaluated by Watson, can be immediately brought to the form of a trace of a known matrix, on using the identity

$$2 \sin^2 (k\,\theta/2) = 1 - \cos k\,\theta \tag{2}$$

Introducing a parameter ϵ, which is ultimately made to vanish, we can write

$$S_N(r) = \lim_{\epsilon \to 0} \sum_{k=1}^{N-1} \left[\epsilon + \frac{1}{2} - \frac{1}{2} \cos k\,\theta \right]^{-r/2} \tag{3}$$

This sum is treated in eq. (90) of Chapter III.

The statistical mechanics of a finite plane lattice fully packed with rigid <u>dimers</u> (these are pairs of particles connected by bonds) provides an example of a situation where normal mode vibrations do not appear. The problem which has been treated independently by Fisher [28] and Kasteleyn [29], is to evaluate the configurational grand partition function of the system

$$Z_{MN} = \sum_{\substack{m,n \\ m+n=\frac{1}{2}MN}} g_{mn}(x, y)\, x^m y^n \tag{4}$$

in which g_{mn} (x, y) represents the number of ways of placing m horizontal (or x-dimers) and n vertical (or y-dimers) on a lattice with square unit cell and MN sites. Thermodynamically x, y are the activities of the x-, y -dimers respectively. Physically this problem is a simplified version of a model, including also monomers, considered in the thermodynamics of adsorbed films and mixed solutions [30, 31]. Fig. 1 shows a simple situation.

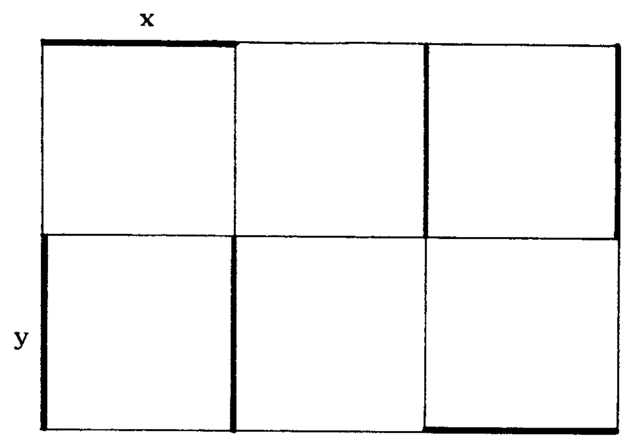

Figure 1

Using topological methods to enumerate the possible configurations, Fisher and Kasteleyn succeeded in showing that Z^2_{MN} is equal to the determinant of a two-dimensional continuant matrix (or a two-dimensional circulant matrix if the dimers are placed on the surface of a torus), as follows:

$$Z^2_{MN} = 2^{MN} \prod_{m=1}^{\frac{1}{2}M} \prod_{h=1}^{N} \{x^2 \cos^2 m\theta + y^2 \cos^2 n\varphi\} \tag{5}$$

$$\theta = \pi/(M+1); \ \varphi = \pi/(N+1)$$

A simple transformation brings this to the form

$$Z_{MN}^2 = \lim_{\epsilon \to 0} \prod_{m=1}^{\frac{1}{2}M} \prod_{n=1}^{N} \{\epsilon + \alpha^2 + x^2 \cos 2m\theta + y^2 \cos 2n\varphi\} \tag{6}$$

in which

$$\alpha^2 = x^2 + y^2$$

If we denote by $Z(\epsilon)$ the expression following the limit sign in eq. (6), we can write

$$\frac{\partial}{\partial \epsilon} \log Z(\epsilon) = \sum_{m=1}^{\frac{1}{2}M} \sum_{n=1}^{N} \frac{1}{\epsilon + \alpha^2 + x^2 \cos 2m\theta + y^2 \cos 2n\varphi} \tag{7}$$

This is a sum which can be readily approximated by using the techniques of Chapter III.

In the two-dimensional Ising model of a ferromagnet, the traces of certain matrices represent the thermodynamic functions associated with the system. The fundamental paper by Onsager [32] exhibits several such sums, the simplest being similar to that in eq. (1),

$$S_N(1) = \frac{1}{N} \sum_{k=1}^{N} \operatorname{cosec}(k - 1/2)\,\theta; \; \theta = \pi/N \tag{8}$$

in which N is the number of parallel chains (or rows). This sum enters the specific heat expression for the lattice of spins. The sum can be treated in a fashion analogous to that described for eq. (1).

A more complicated type of sum arises in this model when correlations between spins located at different sites are considered. Bruria Kaufman and Onsager [33] show the appropriate ensemble averages to yield sums of the form

$$\sum_{a} = \frac{1}{N} \sum_{k=1}^{N} \cos\left[2\pi a k/N + \delta'_{2k}\right]; \quad a = 0, 1, 2, \cdots \tag{9}$$

in which δ'_{2k} is given, for a quadratic lattice, by

$$\delta'_{2k} = \cot^{-1} \left\{ \frac{\cosh 2H \left[1 - \sinh 2H \cos (2\pi k/N)\right]}{\sin (2\pi k/N)} \right\} \tag{10}$$

where $H = J/kT$ and J is the interaction energy between nearest neighbors.

Similar sums appear also in the spherical model of a ferromagnet proposed by Berlin and Kac [34].

The theory of random walks on multidimensional lattices has lately attracted attention because of their mathematical equivalence with certain physical situations, notably the motion of defects in crystals and the theory of spin-wave interactions [35]. Extensive use is made there of Green's functions, which appear as multidimensional sums of the type shown in eqs. (163) and (207) of Chapter III.

In a study on the electronic states of a one-dimensional crystal under an applied electric field, P. Feuer [36] is led to sums of the type

$$S_N(n) = \frac{2}{N} \sum_{k=0}^{N} \frac{\cos nk\theta}{\sqrt{1 + 2\delta \cos k\theta}}; \quad \theta = 2\pi/N \tag{11}$$

These sums represent the coefficients needed to construct the localized Wannier functions from Bloch orbitals. This is a slightly more general sum than the one in eq. (1) (for $r = 1$).

The reverse problem of constructing Bloch orbitals from atomic orbitals, i.e., from localized functions centered around the lattice sites, leads to the important concept of overlap matrix $\boldsymbol{\Delta}$ [37]. If $\phi_\ell = \phi(\mathbf{r} - \mathbf{r}(\ell))$ is the normalized atomic orbital connected with the nucleus at the lattice point $\mathbf{r}(\ell) = \ell_1 \mathbf{a}_1 + \ell_2 \mathbf{a}_2 + \ell_2 \mathbf{a}_3$, then $\boldsymbol{\Delta}$ is defined as follows

$$\Delta_{\ell \ell'} = \int \phi^*_\ell \phi_{\ell'} \, d\mathbf{r} \tag{12}$$

The Born-von Karman cyclic conditions imply here that $\boldsymbol{\Delta}$ is a circulant matrix. If instead of the original set $\{\phi_\ell\}$, one requires a new set $\{\varphi_\mu\}$ of orthonormalized atomic orbitals, the transformation is

$$\varphi = \phi \, \boldsymbol{\Delta}^{-1/2} \tag{13}$$

Lowdin and al. [6] have evaluated $\boldsymbol{\Delta}^{-1/2}$ for a linear chain by using a Chebishev expansion method. This approach of linear combinations of atomic orbitals (LCAO) is known also as the tight-binding method.

Molecular theory abounds in systems characterized by repeated units. First, the problem of calculating the normal mode frequencies of molecules possessing periodicities: e.g., linear and zig-zag chains of atoms [5] lead to matrices (continuant and circulant) already considered. More interesting are the calculations of the electronic structure of polyenes and aromatic molecules. Lennard-Jones and al. [38] have treated these extensively by use of the molecular orbital (MO) method, and were lead to continuant and circulant type matrices, the eigenvalues of which gave the π -electron energies. Moreover, these authors encountered sums of the form

$$S_N = 2 \sum_{k=1}^{N} \sqrt{\alpha^2 + 2\alpha\beta \cos k\theta + \beta^2} \; ; \; \theta = 2\pi/(2N+1) \tag{14}$$

representing the total orbital energy.

Work along this line has been carried on by several authors [39], while more recently Salem [40], in a study of bond alternation in long polyenes obtains sums of the type

$$S_{2N+1}(r) = \frac{1}{2N+1} \sum_{k=-N}^{N} \frac{\cos rk\theta}{\sqrt{1 + 2t^2 \cos k\theta + t^4}} \; ; \; \theta = 2\pi/(2N+1) \tag{15}$$

In conclusion we remark that most of the authors mentioned above evaluate the sums they obtain by passing to the limit $N \to \infty$ and calculating the resulting integral. Lowdin [6] and Gilbert [7] are the exception – they evaluate their sums exactly. Salem uses a technique of changing the order of summations, but then expands in powers of t^2 and stops with the first term. A generalization of this technique is the basis of the mode of calculation presented in Chapter III.

It is to be remarked further that while the conversion of the sums into integrals is not critical for large N, for moderate or small number of particles this is no longer so. It is therefore important to be able to assess the corrections stemming from finite N. Our method has precisely this advantage.

CHAPTER III

METHOD OF CALCULATION AND SPECIFIC RESULTS

In the preceding chapters we have presented several physical and chemical problems that lead to the classes of matrices exhibited there. In this chapter we discuss functions of these matrices, in particular analytic functions. Such functions appear naturally in the statistical mechanics of the systems previously discussed and in perturbation treatments of chemical systems. One matrix function that already appears in classical physics is the inverse of $\boldsymbol{\Delta}(\omega^2)$: when external forces act on the system, knowledge of $\boldsymbol{\Delta}^{-1}(\omega^2)$ is necessary for the complete solution of the dynamical problem. The inverse of $\boldsymbol{\Delta}(\omega^2)$ (or the Green's function of $\boldsymbol{\Delta}$) is essential also in the method developed by Montroll et al. [8,9] for the calculation of characteristic frequencies of lattices with defects. On the other hand all of the thermodynamic functions of the systems previously discussed are essentially traces of analytic functions of the dynamical matrix $\boldsymbol{\Delta}(\omega^2)$: e.g., the partition function from which all thermodynamic functions can be deduced, is defined by:

$$- \log Z = \frac{\Phi_0}{kT} + \sum_{j=1}^{N} \left\{ \frac{1}{2} \frac{\hbar \omega_j}{kT} + \log\left(1 - e^{-\frac{\hbar\omega_j}{kT}}\right) \right\} \tag{1}$$

or in trace form

$$- \log Z = \frac{\Phi_0}{kT} + \mathfrak{T}r \left\{ \frac{1}{2} \frac{\hbar}{kT} \boldsymbol{\Delta}^{1/2}(\omega^2) + \right.$$

$$\left. + \log\left(1 - \exp\left(-\frac{\hbar}{kT} \boldsymbol{\Delta}^{1/2}(\omega^2)\right)\right) \right\} \tag{2}$$

where Φ_0 is the electronic ground state energy of the system.

The vibrational zero-point energy is just

$$E_0 = \frac{1}{2} \frac{\hbar}{kT} \mathfrak{Tr} \left\{ \Delta^{1/2} (\omega^2) \right\} \cdot \tag{3}$$

We note that to find the elements of the function of a matrix it is necessary to calculate certain finite sums involving the same function of its eigenvalues. Let us assume that $F(z)$ is a function defined on the spectrum of Δ and analytic in some neighborhood of the origin, and let λ_k, $k = 1, \ldots, N$, the eigenvalues of the matrix Δ be all contained in the circle of convergence of $F(z)$. Then if $\mathbf{T}$ is the matrix diagonalizing Δ, we can write

$$F(\Delta) = \sum_{n=0}^{\infty} \frac{F^{(n)}(0)}{n!} \Delta^h$$

$$= \sum_{n=0}^{\infty} \frac{F^{(n)}(0)}{n!} \mathbf{T} \Lambda^n \mathbf{T}^{-1} = \mathbf{T} F(\Lambda) \mathbf{T}^{-1} \tag{4}$$

where

$$\Lambda_{kj} = \lambda_k \delta_{kj} \cdot \tag{5}$$

Hence

$$[F(\Delta)]_{kr} = \sum_{j=1}^{N} F(\lambda_j) T_{kj} T_{jr}^{-1} . \tag{6}$$

Sums of this type are somewhat more general than the trace-type sums associated with the thermodynamic functions,

$$\sum_{j=1}^{N} F(\lambda_j) \equiv \mathfrak{Tr} \{F(\Delta)\} \cdot \tag{7}$$

It is of interest at this point to present alternative expressions for finite sums of the type discussed. First the contour integral representation based on the Cauchy residue theorem

$$\sum_{j=1}^{N} F(\lambda_j) = \frac{1}{2\pi i} \int_C F(z) \frac{d}{dz} \log \mathcal{D}_N(z)\, dz \tag{8}$$

in which

$$\mathcal{D}_N(z) \equiv \det(\mathbf{\Delta}_N - z\mathbf{I}) \tag{9}$$

if the λ_j are eigenvalues of a known matrix $\mathbf{\Delta}_N$, or $\mathcal{D}_N(z)$ a polynomial with λ_j for roots if no such matrix is known. The contour C has all λ_j in its interior.

The representation (8) is useful more for asymptotic approximations than for exact calculation of the sums.

A different representation arises when the sum is converted into an integral. Let the λ_j's be real numbers, then one can write for sufficiently well-behaved functions $F(\lambda)$

$$F(\lambda_j) = \int_{-\infty}^{\infty} F(\lambda)\, \delta(\lambda - \lambda_j)\, d\lambda \tag{10}$$

where δ is the Dirac δ-function.

Assume now that interchange of summation and integration is permissible. Then we obtain

$$\sum_{j=1}^{N} F(\lambda_j) = \int_{-\infty}^{\infty} F(\lambda) \left\{ \sum_{j=1}^{N} \delta(\lambda - \lambda_j) \right\} d\lambda . \tag{11}$$

We define now

$$\mathcal{G}(\lambda) \equiv \frac{1}{N} \sum_{j=1}^{N} \delta(\lambda - \lambda_j) \tag{12}$$

and hence

$$\sum_{j=1}^{N} F(\lambda_j) = N \int_{-\infty}^{\infty} F(\lambda)\, \mathcal{G}(\lambda)\, d\lambda . \tag{13}$$

If we denote by $\mathfrak{n}(\lambda)$ the number of λ_j's which are less than or equal to λ, it can be shown that

$$\mathfrak{n}(\lambda) = \sum_{j=1}^{N} H(\lambda - \lambda_j) \tag{14}$$

where $H(x)$ is the Heaviside unit function, and

$$\mathcal{G}(\lambda) = \frac{1}{N} \frac{d}{d\lambda} \mathfrak{n}(\lambda). \tag{15}$$

The function $\mathcal{G}(\lambda)$ is called the eigenvalue distribution function. It is not difficult to show also that

$$\mathcal{G}(|\lambda|) = 2|\lambda|\, \mathcal{G}(\lambda^2). \tag{16}$$

Later on in this Chapter we shall evaluate $\mathcal{G}(\lambda^2)$ for certain special forms of λ_j. The above formalism will be useful also for the conversion into integrals of sums other than the trace-type ones. In the following we shall treat both types of sums by a method which is different from both the complex and real integral representations. Although, for the sake of continuity, explicit reference is given to the matrices from which the eigenvalues arise, it will be apparent that the treatment is independent of this knowledge.

3.1 One-Dimensional Sums

In this paragraph general results regarding circulant and continuant matrices will be presented. We have seen that these matrices are associated with problems where periodic and rigid boundary condition, respectively, prevail. It is not difficult to write down formulas for the matrix connected with free boundaries, and also for more general situations — the only requirement being that the eigenvalues have the same functional form. We shall not do this here as the method is sufficiently well represented for the cases mentioned.

(i) Periodic Boundary Conditions

Instead of treating the symmetric case alone we shall consider here the more general case of an asymmetric circulant matrix, defined as in eq. (116) of Appendix E

$$\Delta = (s_0\ s_1\ \cdots\ s_{N-1})_{cyc.} \tag{17}$$

with eigenvalues

$$\lambda_k = \sum_{j=0}^{N-1} s_j\, e^{i\frac{2\pi jk}{N}}\ ;\ k = 0, \ldots, N-1. \tag{18}$$

As shown in eq. (124) of Appendix E, the diagonalizing matrix U is such as to reduce the (m, n)-element of $F(\Delta)$, to the form:

$$[F(\Delta)]_{mn} = \frac{1}{N}\sum_{k=0}^{N-1} F(\lambda_k)\exp\left[\frac{2\pi i\,(m-n)\,k}{N}\right]. \tag{19}$$

Therefore we consider in the remainder of this paragraph sums of the type

$$S_N = \frac{1}{N}\sum_{k=0}^{N-1} F(\lambda_k)\exp\left[-\frac{2\pi i\, r k}{N}\right] \tag{20}$$

where r is an integer. Without loss of generality we can restrict r to the range $0 \leq r \leq N-1$, as all other cases reduce to the form (20) by periodicity. When $r = 0$, S_N reduces to the simpler trace-type sum of eq. (7).

As it stands, the sum (20) cannot be computed unless N is small or unless $F(\lambda_k)$ has special features that enable the sum to be evaluated in closed form. Using a technique which is the generalization of a method quoted in [6], we shall convert this sum into a form which is more convenient for accurate calculation or for approximate evaluation.

Our technique is based on the fact that the λ_k's have the same functional dependence, namely, there exists a function $\lambda(\theta)$, which generates the eigenfrequencies under discussion

$$\lambda_k = \lambda(\theta_k). \tag{21}$$

Here we define

$$\lambda(\theta) = \sum_{j=0}^{N-1} s_j \exp(i j \theta). \tag{22}$$

Then clearly

$$\lambda_k = \lambda\left(\frac{2\pi k}{N}\right). \tag{23}$$

The form of $\lambda(\theta)$ suggests a Fourier series expansion for the function $F\{\lambda(\theta)\}$. Therefore we shall assume that such an expansion exists and write

$$F\{\lambda(\theta)\} = \sum_{j=0}^{\infty} A_j \exp(i j \theta) \tag{24}$$

with

$$A_j = \frac{1}{2\pi} \int_0^{2\pi} F\{\lambda(\theta)\} \exp(-i j \theta)\, d\theta . \tag{25}$$

In eq. (24) only positive j 's are required since $\lambda(\theta)$ contains only positive powers of $\exp(i\theta)$ and $F(z)$ only positive powers of z.

Using the expansion (24), we can write

$$F(\lambda_k) = \sum_{j=0}^{\infty} A_j \exp\left[\frac{2\pi i j k}{N}\right]$$

$$= \sum_{j=0}^{N-1} A_j^* \exp\left\{\frac{2\pi i jk}{N}\right\} \tag{26}$$

where the A_j^* are expressible in terms of the A's:

$$A_j^* = \sum_{\ell=0}^{\infty} A_{j+\ell N}. \tag{27}$$

The result in eq. (26) is a consequence of the periodicity of the trigonometric function $\exp(ij\theta)$. We note that the rearrangement of the series is legitimate since the analytic character of $F(z)$ guarantees uniform convergence within the circle of convergence.

Insertion of (17) into (11) leads to

$$S_N = \frac{1}{N} \sum_{k=0}^{N-1} \sum_{j=0}^{N-1} A_j^* \exp\left(\frac{2\pi i k(j-r)}{N}\right)$$

$$= A_r^*. \tag{28}$$

This result shows that a finite summation of this type acts like a filter on the Fourier coefficients of $F\{\lambda(\theta)\}$, "sifting" out an infinite number of them. In this connection a historical note is of interest: the British mathematician Thomas Simpson discovered in 1758 [13] that if a function $f(x)$ has the Taylor series expansion

$$f(x) = \sum_{n=0}^{\infty} f_n x^n$$

and if

$$S_N(r>0) \equiv \frac{1}{N} \sum_{k=0}^{N-1} f\left(e^{i\frac{2\pi k}{N}} x\right) e^{-\frac{2\pi i r k}{N}}$$

then

$$S_N = x^r \sum_{n=0}^{\infty} f_{r+nN} (x^N)^n.$$

This is a consequence of the fact that the sum of the roots of unity vanishes. Later on, De Morgan [13] extended this result to the roots of $x^N = -1$.

It is obvious that for $\lambda_k = e^{i\frac{2\pi k}{N}} z$, a Fourier expansion of $F(z)$ will not be needed in our treatment.

Returning now to the result (28) we see that the evaluation of the finite sum is reduced to the evaluation of the Fourier coefficients and the infinite summation of eq. (27). While this may seem to complicate matters, it must be remembered that Fourier coefficients decrease with increasing index, by virtue of the Riemann-Lebesgue lemma, and the convergence of the series can be quite rapid. Frequently the approximation

$$S_N \sim A_r \tag{29}$$

will be sufficient for computational purposes since when $F(z)$ is analytic, the Fourier coefficients will fall off exponentially with the index. Moreover the approximation of eq. (29) is precisely the conversion of the sum (20) into an integral (i.e., passage to the limit $N \to \infty$). This will be a particularly effective approximation when N is large. For those problems in which N is not large enough to warrant the approximation by an integral, the formula (28) allows one in principle to estimate the correction terms successively.

Procedures similar to those given above suffice to discuss the important special case when Δ is a symmetric matrix. We can write in this case

$$\Delta = \begin{cases} (s_0\ s_1\ \cdots\ s_M\ s_{M-1}\ \cdots\ s_1)_{\text{cycl.}} & N = 2M \\ (s_0\ s_1\ \cdots\ s_M\ s_M\ s_{M-1}\ \cdots\ s_1)_{\text{cycl.}} & N = 2M+1. \end{cases} \tag{30}$$

The eigenvalues can be written then

$$\lambda_k = s_0 + 2\sum_{j=1}^{M-1} s_j \cos\left(\frac{2\pi k j}{N}\right) + 2\epsilon\, s_M \cos\left(\frac{2\pi M k}{N}\right) \tag{31}$$

where

$$\epsilon = \begin{cases} \frac{1}{2} & \text{for} \quad N = 2M \\ 1 & \text{for} \quad N = 2M + 1 \,. \end{cases} \tag{32}$$

The function $\lambda(\theta)$ defined in eq. (21) is replaced in the present case by

$$\lambda(\theta) = s_0 + 2 \sum_{j=1}^{M-1} s_j \cos j\theta + 2\epsilon s_M \cos M\theta. \tag{33}$$

Then $\lambda(\theta)$ being an even function of θ, so is also $F\{\lambda(\theta)\}$ and we can assume the Fourier expansion:

$$F\{\lambda(\theta)\} = \frac{1}{2} A_0 + \sum_{n=1}^{\infty} A_n \cos n\theta \tag{34}$$

where

$$A_n = \frac{1}{\pi} \int_0^{2\pi} F\{\lambda(\theta)\} \cos n\theta. \tag{35}$$

As for the asymmetric circulant matrices, a rearrangement of the series for $F(\lambda_k)$ leads to

$$F(\lambda_k) = \sum_{j=0}^{N-1} A_j^* \cos \frac{2\pi j k}{N} \tag{36}$$

with

$$A_0^* = \frac{1}{2} A_0 + \sum_{\ell=1}^{\infty} A_{\ell N} \tag{37}$$

and

$$A_{j>0}^* = \sum_{\ell=0}^{\infty} A_{j+\ell N} \tag{38}$$

Then the sum (20) for the λ_k of eq. (31) becomes

$$S_N = \frac{1}{2} A_r^* . \tag{39}$$

If the exponential in eq. (20) is replaced by the cosine term cos $2\pi rk/N$, eq. (39) will be replaced by

$$S_N = \frac{1}{2} \left\{ A_r^* + A_{N-r}^* \right\} . \tag{40}$$

In both cases $r = 0$ leads to the formula for the trace-type sum,

$$S_N = A_0^* . \tag{41}$$

The results of the preceding analysis can be easily generalized to the calculation of sums of the form

$$S_N = \frac{1}{N} \sum_{k=0}^{N-1} F(\lambda_k) \exp\left[- \frac{i\pi(2k+1)r}{N} \right] \tag{42}$$

with r as in eq. (20) and

$$\lambda_k = \sum_{j=0}^{N-1} s_j \exp\left[\frac{i\pi(2k+1)j}{N} \right] \tag{43}$$

are the eigenvalues of the matrix Δ^+, called a skew-circulant in eq. (164) of Appendix E.

The argument leading from eq. (22) to eq. (27) can be repeated with a slight modification to yield in this case the result:

$$S_N = A_r^* \tag{44}$$

in which

$$A_r^* = \sum_{j=0}^{\infty} (-1)^j A_{r+jN} . \tag{45}$$

Similar results can be obtained for other values of r in eq. (42). If on the other hand the first row of Δ^+ can be written as

$$\Delta^+ = \begin{cases} (s_0 \; s_1 \; \cdots \; s_M, \; - s_{M-1} \; \cdots \; - s_1)_{\text{skew-cycl.}} & N = 2M \\ (s_0 \; s_1 \; \cdots \; s_M, \; - s_M \; \cdots \; - s_1)_{\text{skew-cycl.}} & N = 2M + 1 \end{cases} \tag{46}$$

then the eigenvalues are

$$\lambda_k = s_0 + 2 \sum_{j=1}^{M-1} s_j \cos \frac{\pi(2k+1)\,j}{N} + 2\,\epsilon\, s_M \cos \frac{\pi(2k+1)\,M}{N} \tag{47}$$

where

$$\epsilon = \begin{cases} \frac{i}{2} & N = 2M \\ 1 & N = 2M + 1 \; . \end{cases} \tag{48}$$

The Fourier expansion then contains only cosine terms

$$A_n = \frac{1}{\pi} \int_0^{2\pi} F\{\lambda(\theta)\} \cos n\theta \; d\theta \tag{49}$$

and the sum

$$S_N \equiv \frac{1}{N} \sum_{k=0}^{N-1} F(\lambda_k) \cos \frac{\pi(2k+1)r}{N} \tag{50}$$

with r as in eq. (20), can be represented by the expression:

$$S_N = \frac{1}{2} \left[A_r^* + A_{N-r}^* \right] \tag{51}$$

in which

$$\left.\begin{aligned} A_0^* &= \frac{1}{2} A_0 + \sum_{j=1}^{\infty} (-1)^j A_{jN} \\ A_{\ell>0}^* &= \sum_{j=0}^{\infty} (-1)^j A_{\ell+jN} \end{aligned}\right\} . \qquad (52)$$

An analysis of the preceding exposition shows clearly that the following general result can be stated:

From a given eigenvalue-generating function $\lambda(\theta)$ and a given analytic function $F(z)$—which is defined on and its domain of convergence contains the set of values $\{\lambda(\theta),\ 0 \le \theta \le 2\pi\}$— one can construct a whole class of finite sums by choosing N values θ_k, such that $e^{i\theta k}$ be the roots of an algebraic equation of the N^{th} degree. Since the set of Fourier coefficients for this class of sums is unique, the values of these sums will depend solely upon the filtering properties of the θ_k's.

We proceed now to apply the formulas developed above to cases of general interest. The discussion will be restricted to the asymmetric and symmetric circulants.

(i) <u>The Inverse Δ^{-1}</u>

The function $F(z) = z^{-1}$, strictly speaking, is not analytic in the neighborhood of the origin, yet the formulas developed above can still be applied if the integrals associated with the Fourier coefficients are taken as principal value integrals, whenever needed.

In the asymmetric case the integrals to be evaluated are

$$A_j = \frac{1}{2\pi} \int_0^{2\pi} \frac{e^{-ij\theta}\, d\theta}{s_0 + s_1 e^{i\theta} + s_2 e^{i2\theta} + \dots + s_{N-1} e^{i(N-1)\theta}}$$

$$= \frac{1}{2\pi i} \int_C \frac{dz}{z^{j+1} (s_0 + s_1 z + \dots + s_{N-1} z^{N-1})} \tag{53}$$

where C is the unit circle. The contribution to the integral from the pole at the origin is the coefficient of z^j in the Taylor expansion of

$$[P(z)]^{-1} \equiv [s_0 + s_1 z + \dots + s_{N-1} z^{N-1}]^{-1} = \sum_{j=0}^{\infty} A_j^{(P)} z^j \tag{54}$$

In the form of a determinant this contribution is

$$A_j^{(P)} = \frac{(-1)^j}{(s_0)^{j+1}} \times \begin{vmatrix} s_1 & s_0 & & & 0 \\ s_2 & s_1 & s_0 & & \\ \vdots & \ddots & \ddots & \ddots & \\ \vdots & & \ddots & \ddots & s_0 \\ s_j & \cdots & \cdots & s_2 & s_1 \end{vmatrix}_j ; \quad A_0^{(P)} = \frac{1}{s_0} \tag{55}$$

Unless a computer is used for the numerical evaluation of the determinant, this expression for $A_j^{(P)}$ is not very practical. An equivalent form can be found for $A_j^{(P)}$ provided the roots z_k of P (z) are known. Suppose that P (z) has no multiple roots (the extension to the more general case is trivial). Then we can write

$$P(z) = s_0 \prod_{k=1}^{N-1} (1 + \sigma_k z) \tag{56}$$

with $\sigma_k = -1/z_k$. In terms of the σ_k, the value of A_j is calculated to be

$$A_j = (-1)^j \sum_{k=1}^{N-1} \frac{\sigma_k^{j+1}}{P'\left(-\frac{1}{\sigma_k}\right)} . \tag{57}$$

Since the only dependence on j is through the term σ_k^{j+1} we may find an explicit expression for the $A_r^{*(p)}$:

$$A_r^{*(p)} = (-1)^r \sum_{k=1}^{N-1} \frac{1}{P'\left(-\frac{1}{\sigma_k}\right)} \cdot \frac{\sigma_k^{r+1}}{1 - (-\sigma_k)^N} \tag{58}$$

where we have summed the geometric series involved under the assumption that $|\sigma_k| < 1$.

In particular, $A_r^{(p)*}$ will coincide with A_r^* whenever P (z) has no roots inside or on the unit circle. There exist several sufficiency conditions for this to happen. One condition given by Landau [14], is

$$s_1' > s_2' > \ldots > s_{N-1}' > 0 ; \; s_k' = s_k / s_0 . \tag{59}$$

A second simple condition can be obtained by using Rouche's theorem*. For example if

$$|s_1'| + |s_2'| + \ldots + |s_e'| < 1 \tag{60}$$

then the roots of P(z) will lie outside of the unit circle provided

$$(1 + s_1' + s_2' + \ldots s_e') > (s_{e+1}' + \ldots + s_{N-1}') . \tag{61}$$

In particular this is true if

$$\sum_{j=1}^{N-1} |s_j'| < 1 \tag{62}$$

*Rouche's theorem states that if f(z) and g(z) are analytic within and on a closed curve C, and if $|f(z)| > |g(z)|$ on C, then f(z) and g(z) + f(z) have the same number of zeros inside the region bounded by C.

An exact result can be written down immediately for the case $s_k = 0, \; k \geq 3$ if it is assumed that only the pole at the origin contributes. Then the easiest way to evaluate the A_j's is to use their determinantal expression of eq. (54). Using the value of this determinant given for the appropriate form of eq. (15) in Appendix E, we find

$$A_j = \frac{(-1)^j}{s_0^{j+1}} \frac{1}{\sqrt{s_1^2 - 4s_0 s_2}} \left[\left(\frac{s_1 + \sqrt{s_1^2 - 4s_0 s_2}}{2} \right)^{j+1} - \left(\frac{s_1 - \sqrt{s_1^2 - 4s_0 s_2}}{2} \right)^{j+1} \right] . \tag{63}$$

Therefore the sum

$$S_N = \sum_{k=0}^{N-1} \frac{e^{-\frac{2\pi i r k}{N}}}{s_0 + s_1 e^{\frac{2\pi i k}{N}} + s_2 e^{\frac{4\pi i k}{N}}} \tag{64}$$

on evaluating A_r^* of eq. (28) with the A_j's of eq. (63), becomes

$$S_N = \frac{(-1)^r}{\sqrt{s_1^2 - 4s_0 s_2}} \left\{ \left(\frac{s_1 + \sqrt{s_1^2 - 4s_0 s_2}}{2s_0} \right)^{r+1} \frac{1}{1 - \left(\frac{s_1 + \sqrt{s_1^2 - 4s_0 s_2}}{2s_0} \right)^N} - \left(\frac{s_1 - \sqrt{s_1^2 - 4s_0 s_2}}{2s_0} \right)^{r+1} \frac{1}{1 - \left(\frac{-s_1 + \sqrt{s_1^2 - 4s_0 s_2}}{2s_0} \right)^N} \right\} \tag{65}$$

This expression has a finite, well-defined limit when $N \to \infty$.

The elements of the first row of Δ^{-1} are obtained from eq. (65) by letting r take the values $0, 1, \cdots, N-1$. These elements characterize Δ^{-1} completely since a function of a circulant matrix is also circulant.

It is clear that if all the s_k's vanish with the exception of (any) two of them, the sum again is easily evaluated in a closed form. In some instances it is more convenient to use a full Fourier expansion. For example if the λ_k's are of the form:

$$\left.\begin{aligned} \lambda_k &= s_0 + s_1\, e^{i\frac{2\pi k}{N}} + s_{N-1}\, e^{\frac{2\pi(N-1)k}{N}} \\ &= s_0 + s_1 e^{i\frac{2\pi k}{N}} + s_{N-1}\, e^{-i\frac{2\pi k}{N}} \end{aligned} \quad k = 0, \ldots, N-1 \right\} . \tag{66}$$

Then the appropriate $\lambda(\theta)$ is

$$\lambda(\theta) = s_0 + s_1\, e^{i\theta} + s_{N-1}\, e^{-i\theta} \tag{67}$$

and the Fourier coefficients associated with the sum

$$s_N = \frac{1}{N} \sum_{k=0}^{N-1} \frac{e^{-i\frac{2\pi rk}{N}}}{\lambda_k}$$

are

$$A_n = \frac{1}{2\pi} \int_0^{2\pi} \frac{e^{-in\theta}\, d\theta}{s_0 + s_1\, e^{i\theta} + s_{N-1}\, e^{-i\theta}} = \frac{1}{2\pi i} \int_c \frac{dz}{z^n(s_1\, z^2 + s_0\, z + s_{N-1})} \tag{68}$$

$n \geq 0$

$$A_{-n} = \frac{1}{2\pi} \int_0^{2\pi} \frac{e^{in\theta}\, d\theta}{s_0 + s_1\, e^{i\theta} + s_{N-1}\, e^{-i\theta}} = \frac{1}{2\pi i} \int_c \frac{z^n\, dz}{s_1\, z^2 + s_0\, z + s_{N-1}} . \tag{69}$$

$n > 0$

The values of these coefficients, which can be calculated exactly, depend on the location of the zeros of the denominators with respect to the unit circle. Since in Appendix D we exhibit an alternative way of computing such simple sums exactly, we shall neither calculate here the integrals (68) and (69), nor perform subsequently the summation for S_N.

Similar expressions will be obtained now for the symmetric case. Let us start with the expression (35) for

$$A_n = \frac{1}{\pi} \int_0^{2\pi} \frac{\cos n\theta\, d\theta}{s_0 + 2 \sum_{j=1}^{M-1} s_j \cos j\theta + 2\epsilon \cos M\theta} = \frac{1}{\pi} \int_0^{2\pi} \frac{\cos n\theta\, d\theta}{P_M(\cos\theta)} \tag{70}$$

The polynomial $P_M(\cos\theta)$ can be factorized such that

$$P_M(\cos\theta) = s_0 \prod_{j=1}^{M} (1 + \sigma_j \cos\theta) \tag{71}$$

where again σ_j are the reciprocals of the roots of $P_M(z)$. If we restrict the discussion to the previously investigated case of

$$\sum_{j=1}^{M} |s_j| < |s_0| \tag{72}$$

which means $|\sigma_j| < 1$ for all j, then the integrals A_n can be evaluated by partial fraction decomposition:

$$A_n = \frac{1}{\pi} \int_0^{2\pi} \cos n\theta \sum_{j=1}^{M} \frac{\sigma_j}{P'\left(-\frac{1}{\sigma_j}\right)} \frac{d\theta}{1 + \sigma_j \cos\theta} {}^{*}$$

$$= 2 \sum_{j=1}^{M} \frac{\sigma_j}{P'\left(-\frac{1}{\sigma_j}\right)} \left(\frac{(1-\sigma_j^2)^{1/2} - 1}{\sigma_j}\right)^n . \tag{73}$$

Hence the appropriate sum of eq. (40) can be summed explicitly

$$S_N = \sum_{j=1}^{M} \frac{\sigma_j}{(1-\sigma_j^2)^{1/2}} \frac{1}{P'\left(-\frac{1}{\sigma_j}\right)} \frac{1}{1 - \{[(1-\sigma_j^2)^{1/2} - 1]/\sigma_j\}^M}$$

$$\times \left[\left(\frac{(1-\sigma_j^2)^{1/2} - 1}{\sigma_j}\right)^r + \left(\frac{(1-\sigma_j^2)^{1/2} - 1}{\sigma_j}\right)^{M-r}\right]. \tag{74}$$

A number of exact results are available also in this case. For example if $\lambda(\theta)$ is of the form

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*The value of this integral is exhibited in Appendix B

$$\lambda(\theta) = s_0 + 2s_1 \cos\theta \tag{75}$$

then again using the integral (4) of Appendix B, we can write

$$A_n = \frac{1}{\pi}\int_0^{2\pi} \frac{\cos n\theta \, d\theta}{s_0 + 2s_1 \cos\theta}$$

$$= \begin{cases} \dfrac{1}{\sqrt{s_0^2 - 4s_1^2}} \left(\dfrac{\sqrt{s_0^2 - 4s_1^2} - s_0}{2s_1}\right)^n ; & \left|\dfrac{\sqrt{s_0^2 - 4s_1^2} - s_0}{2s_1}\right| < 1 \\[2ex] -\dfrac{(-1)^n}{\sqrt{s_0^2 - 4s_1^2}} \left(\dfrac{\sqrt{s_0^2 - 4s_1^2} + s_0}{2s_1}\right)^n ; & \left|\dfrac{\sqrt{s_0^2 - 4s_1^2} + s_0}{2s_1}\right| < 1 . \end{cases} \tag{76}$$

Then the first case in (76) leads to

$$S_N = \frac{1}{2}\frac{1}{\sqrt{s_0^2 - 4s_1^2}} \frac{\left(\dfrac{\sqrt{s_0^2 - 4s_1^2} - s_0}{2s_1}\right)^r + \left(\dfrac{\sqrt{s_0^2 - 4s_1^2} - s_0}{2s_1}\right)^{N-r}}{1 - \left(\dfrac{\sqrt{s_0^2 - 4s_1^2} - s_0}{2s_1}\right)^N} . \tag{77}$$

The second case leads to an identical form since the value of a finite sum is independent of the mode of summation as long as no terms are neglected.

Another case which admits of an exact treatment is the following:

$$\lambda_k = s_0 + 2s_1 \cos\frac{2\pi k}{N} + 2s_2 \cos\frac{4\pi k}{N} . \tag{78}$$

Instead of evaluating the Fourier coefficients it is simpler in this case to relate the sum associated with (78) to the sums associated with the eigenvalues $\lambda_k^{\pm}$ given by

$$\lambda_k^{\pm} = -2\sqrt{s_2}\, x^{\pm} + 2\sqrt{s_2} \cos\frac{2\pi k}{N} \tag{79}$$

where

$$x^{\pm} = \frac{-s_1 \pm \sqrt{s_1^2 - 4s_0 s_2 + 8 s_2^2}}{4s_2} \tag{80}$$

and $\lambda_k^+ \lambda_k^- = \lambda_k$. It is easy to see then that

$$S_N = \frac{1}{x^+ - x^-} [S_N^+ - S_N^-]. \tag{81}$$

(2) Other Functions of Δ

We have seen that the calculation of the inverse of the general circulant matrix already presents great difficulties. It is therefore not surprising that the evaluation of more involved functions complicates the computation considerably. Hence such cases will be best treated by numerical methods (assuming of course the elements s_j to be known). But even for numerical treatments the general discussion above is of value, since it exhibits clearly what are the dominant terms and therefore provides a practical scheme of computation.

For certain special cases some results can nevertheless be given in terms of known functions. These special cases are treated below.

(i) Δ^ν, $\nu \neq 0, 1, 2, \cdots$

The elements of Δ^ν give rise to the sums

$$S_N = \sum_{k=0}^{N-1} \left(s_0 + s_1 e^{\frac{2\pi i k}{N}} + s_2 e^{\frac{4\pi i k}{N}}\right)^\nu e^{-\frac{2\pi i r k}{N}} \tag{82}$$

where we have assumed

$$\lambda(\theta) = s_0 + s_1 e^{i\theta} + s_2 e^{i2\theta}. \tag{83}$$

The Fourier expansion of $[\lambda(\theta)]^\nu$ can be effected as follows:

$$(s_0 + s_1 e^{i\theta} + s_2 e^{i2\theta})^\nu = s_0^\nu [1 - 2xz + z^2]^\nu \tag{84}$$

where

$$x = -\frac{s_1}{2\sqrt{s_0 s_2}}; \quad z = \sqrt{\frac{s_2}{s_0}} e^{i\theta} \tag{85}$$

If it is true that $|s_2/s_0| < 1$ and $|s_1/s_0| < 1$, the following expansion is known [15] to exist

$$(1 - 2xz + z^2)^\nu = \sum_{h=0}^{\infty} C_n^{-\nu}(x)\, z^n \tag{86}$$

where $C_n^\mu(x)$ are Gegenbauer polynomials with the explicit representation

$$C_n^\mu(x) = (-1)^n \sum_{m=0}^{\left[\frac{n}{2}\right]} \binom{-\mu}{n-m}\binom{n-m}{m} (2x)^{n-2m}. \tag{87}$$

Therefore the Fourier coefficients of eq. (84) are

$$A_n \equiv \frac{1}{2\pi} \int_0^{2\pi} (s_0 + s_1 e^{i\theta} + s_2 e^{i2\theta})^\nu \; e^{-in\theta}\, d\theta$$

$$= s_0^\nu \left(\frac{s_2}{s_0}\right)^{n/2} C_n^{-\nu}\left(-\frac{s_1}{2\sqrt{s_0 s_2}}\right). \tag{88}$$

Inserting these values in previous formulas we obtain the sum S_N of eq. (82).

When Δ is <u>symmetric</u> the pertinent sums are of the form

$$S_N = \frac{1}{N} \sum_{k=0}^{N-1} \left(s_0 + 2s_1 \cos\frac{2\pi k}{N}\right)^\nu \cos\frac{2\pi r k}{N}. \tag{89}$$

The evaluation of this sum proceeds as follows: we write

$$(s_0 + 2s_1 \cos\theta)^\nu = (s_0)^\nu \frac{(1 - 2\beta\cos\theta + \beta^2)^\nu}{(1+\beta^2)^\nu} \tag{90}$$

where β is that root of the equation $s_1 x^2 + s_0 x + s_1 = 0$ which stays finite for $s_1 \to 0$,

$$\beta = -\frac{s_0}{2s_1} + \sqrt{\left(\frac{s_0}{2s_1}\right)^2 - 1}. \tag{91}$$

To find the Fourier expansion we require $|\beta| < 1$. Assuming this condition to be satisfied, we can use tables [16] to write down the result

$$A_n = \frac{1}{\pi} \int_0^{2\pi} (s_0 + 2s_1 \cos\theta)^\nu \cos n\theta \, d\theta$$

$$= \left(\frac{s_0}{1+\beta^2}\right)^\nu \frac{2\,\beta^n \Gamma(-\nu+n)}{\Gamma(-\nu)\,\Gamma(n+1)} F(-\nu, \ -\nu+n, \ n+1: \ \beta^2) \tag{92}$$

where F denotes the ordinary hypergeometric function. Then

$$\underset{r \neq 0}{S_N} = \left(\frac{s_0}{1+\beta^2}\right)^\nu \frac{1}{\Gamma(-\nu)} \sum_{n=0}^{\infty} \left\{ \frac{\beta^{r+nN}\Gamma(-\nu+r+nN)}{\Gamma(r+nN+1)} F(-\nu; \ -\nu+r+nN; \ r+nN+1; \ \beta^2) \right.$$

$$\left. + \frac{\beta^{(n+1)N-r}\Gamma(-\nu+(n+1)N-r)}{\Gamma((n+1)N-r+1)} F(-\nu; -\nu+(n+1)N-r; (n+1)N-r+1; \beta^2) \right\} \tag{93}$$

$$\underset{r = 0}{S_N} = \left(\frac{s_0}{1+\beta^2}\right)^\nu \left\{ F(-\nu, \ -\nu, \ 1; \ \beta^2) + \right.$$

$$\left. + \frac{2}{\Gamma(-\nu)} \sum_{n=1}^{\infty} \frac{\beta^{nN}\Gamma(-\nu+nN)}{\Gamma(nN+1)} F(-\nu; \ -\nu+nN; \ nN+1; \ \beta^2) \right\}. \tag{94}$$

For $\nu = \pm 1/2$, these results are somewhat analogous to those obtained by Löwdin, Pauncz, and de Heer [6] .

(ii) Exp $(\tau\Delta)$

The sums involved for the asymmetric case are of the form:

$$S_N = \frac{1}{N} \sum_{k=0}^{N-1} \exp\left(\tau\left[s_0 + s_1 e^{\frac{2\pi i k}{N}}\right]\right) e^{-\frac{2\pi i k r}{N}} \tag{95}$$

The Fourier coefficients are found by using the well-known expansion:

$$e^{\alpha e^{i\theta}} = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} e^{in\theta} \tag{96}$$

Hence

$$A_n \equiv \frac{1}{2\pi} e^{\tau s_0} \int_0^{2\pi} e^{-in\theta} \exp(\tau s_1 e^{i\theta})\, d\theta$$

$$= \frac{(\tau s_1)^n}{n!} e^{\tau s_0} \tag{97}$$

Therefore

$$S_N = e^{\tau s_0} \sum_{n=0}^{\infty} \frac{(\tau s_1)^{r+nN}}{(r + nN)!} \tag{98}$$

Similar results can be easily derived from the above for sin $(\tau\Delta)$, cos $(\tau\Delta)$ and $c^{\tau\Delta}$ (c a constant). For the symmetric case the pertinent sums are of the form:

$$S_N = \frac{1}{N} \sum_{k=0}^{N-1} \exp\left\{\tau\left(s_0 + 2s_1 \cos\frac{2\pi k}{N}\right)\right\} \cos\frac{2\pi rk}{N} \tag{99}$$

The Fourier coefficients are

$$A_n = \frac{1}{\pi} \int_0^{2\pi} e^{\tau s_0} \exp\{2s_1 \tau \cos\theta\} \cos n\theta\, d\theta$$

$$= e^{\tau s_0} \frac{1}{\pi} \int_0^{2\pi} \exp\{i(-2s_1 i\tau)\cos\theta\} \cos n\theta\, d\theta \tag{100}$$

Using the expansion [16]

$$\exp(iz\cos\theta) = J_0(z) + 2 \sum_{n=1}^{\infty} i^n J_n(z) \cos n\theta \tag{101}$$

we immediately obtain

$$A_n = 2e^{\tau s_0} I_n(2s_1 \tau); \quad n = 0, 1, \ldots \tag{102}$$

where $I_n(x)$ is the modified Bessel function of the first kind. Then

$$\underset{r\neq 0}{S_N} = e^{\tau s_0} \sum_{n=0}^{\infty} \left\{(-1)^{r+nN} I_{r+nN}(2s_1 t) + (-1)^{(n+1)N-r} I_{(n+1)N-r}(2s_1 \tau)\right\} \tag{103}$$

$$\underset{r=0}{S_N} = e^{\tau s_0}\left\{I_0(2s_1\tau) + 2\sum_{n=1}^{\infty}(-1)^{nN} I_{nN}(2s_1\tau)\right\} \tag{104}$$

Again the functions $\cos(\tau\Delta)$, $\sin(\tau\Delta)$ and $c^{\tau\Delta}$ can be evaluated by using the results above.

4. Calculation of the Eigenvalue Distribution Function

Here we want to evaluate the function $\mathcal{G}(\omega^2)$ defined in eq. (12) for two cases. For a monatomic linear chain the eigenvalues are

$$\omega_j^2 = a + 2b\cos\frac{2\pi j}{N}; \quad j = 0, \ldots, N-1 \tag{105}$$

We need therefore the Fourier expansion of the function $\delta(\omega^2 - a + 2b\cos\theta)$. Following the procedure of Lighthill [17] for generalized functions, it is easy to show, by making use of the transformation properties of the δ-function, that

$$\delta(\omega^2 - a - 2b\cos\theta) = \begin{cases} \dfrac{1}{2\pi\,|b|\,|\sin\varphi|}\left\{1 + 2\displaystyle\sum_{m=1}^{\infty}\cos m\varphi\cos m\theta\right\} \\ \qquad a - 2|b| \le \omega^2 < a + 2|b| \\ 0 \qquad \text{elsewhere} \end{cases} \tag{106}$$

In the above we have assumed for definiteness that $a \geq 2|b|$ and $b < 0$, the case most frequently met in practice.* Then φ is given as the principal branch of the function

*Other cases can be treated with similar ease.

$$\varphi = \arc\cos \frac{\omega^2 - a}{2b} \tag{107}$$

i.e., $0 \leq \varphi \leq \pi$.

Writing

$$\omega_s^2 = a - 2|b|; \quad \omega_L^2 = a + 2|b| \tag{108}$$

the above can be rewritten as follows:

$$\delta(\omega^2 - a - 2b\cos\theta) = \begin{cases} \dfrac{1}{\pi\sqrt{(\omega^2 - \omega_s^2)(\omega_L^2 - \omega^2)}} \left\{1 + 2\sum_{m=1}^{\infty} \cos m\varphi \cos m\theta\right\} \\ \qquad \omega_s^2 \leq \omega^2 \leq \omega_L^2 \\ 0 \qquad \text{elsewhere} \end{cases} \tag{109}$$

Performing the finite summation over j, we finally find:

$$\mathcal{G}(\omega^2) = \begin{cases} \dfrac{1}{\pi\sqrt{(\omega^2 - \omega_s^2)(\omega_L^2 - \omega^2)}} \left\{1 + 2\sum_{m=1}^{\infty} \cos mN\varphi\right\}; \quad \omega_s^2 \leq \omega^2 \leq \omega_L^2 \\ 0 \qquad \text{elsewhere} \end{cases} \tag{110}$$

On comparing this result (for $\omega_s = 0$) with that of Montroll et al. [11], we see that the infinite sum represents the correction terms* which depend explicitly on N, the number of particles in the chain.

It is of interest to note that $\mathcal{G}(\omega^2)$ can be also written in the form

$$\mathcal{G}(\omega^2) = \begin{cases} \dfrac{2}{\sqrt{(\omega^2 - \omega_s^2)(\omega_L^2 - \omega^2)}} \sum_{k=-\infty}^{\infty} \delta(N\varphi - 2\pi k) \\ 0 \qquad \text{elsewhere} \end{cases} \tag{111}$$

*When used as the kernel of an integral.

We note that the first term in the eigenvalue distribution function depends solely on the form of the eigenvalue generating function, while the correction terms depend also on the particular set of θ_k's associated with given boundary conditions. Since the first term is the more important one we do not explicitly exhibit correction terms for other boundary conditions.

We quote below the corresponding results for a <u>diatomic</u> chain the eigen-frequency generating function of which can be written as

$$\lambda_{\pm}(\theta) = \omega^2 - \alpha \pm \sqrt{\beta^2 + \gamma^2 \cos^2 \theta} \tag{112}$$

Then the Fourier expansion of the function

$$F(\theta) \equiv \delta\{\lambda_+(\theta)\} + \delta\{\lambda_-(\theta)\} \tag{113}$$

is given by

$$F(\theta) = \begin{cases} \dfrac{2}{\pi} \dfrac{|\omega^2 - \alpha|}{|(\omega^2 - \alpha)^2 - \beta^2|^{1/2} \, |\beta^2 + \gamma^2 - (\omega^2 - \alpha)^2|^{1/2}} \left\{1 + 2 \displaystyle\sum_{m=1}^{\infty} \cos 2m\varphi \cos 2m\theta \right\} \\ \qquad \text{for} \quad \alpha - |\beta^2 + \gamma^2|^{1/2} \leq \omega^2 \leq \alpha + |\beta^2 + \gamma^2|^{1/2} \\ 0 \qquad \text{elsewhere} \end{cases} \tag{114}$$

with φ given as the principal branch of

$$\varphi = \arc\cos \sqrt{\frac{(\omega^2 - \alpha)^2 - \beta^2}{\gamma^2}} \tag{115}$$

Then the frequency distribution function $\mathcal{G}(\omega^2)$

$$\mathcal{G}(\omega^2) = \frac{1}{2N} \sum_{j=0}^{2N-1} [\delta\{\lambda_+(\theta_j)\} + \delta\{\lambda_-(\theta_j)\}] \tag{116}$$

is given by

$$\mathcal{G}(\omega^2) = \begin{cases} \dfrac{2}{\pi} \dfrac{|\omega^2 - \alpha|}{|(\omega^2-\alpha)^2 - \beta^2|^{1/2}\;|\beta^2+\gamma^2-(\omega^2+\alpha)^2|^{1/2}} \left\{1 + 2\displaystyle\sum_{m=1}^{\infty} \cos 2mN\varphi\right\} \\ \qquad \text{for} \quad \alpha - |\beta^2+\gamma^2|^{1/2} \le \omega^2 \le \alpha + |\beta^2+\gamma^2|^{1/2} \\ 0 \qquad \text{elsewhere} \end{cases} \tag{117}$$

It is apparent that these results can be extended to more general situations, the sole requirement of this method being explicit knowledge of the real roots of the eigenvalue generating function (if such a one exists).

We conclude this section by noting that if the function $F\{\lambda(\theta)\}$ can be expressed as a sum of products of simpler functions whose Fourier coefficients are known, then repeated use of Parseval formula will lead to the desired Fourier expansion, and subsequently to the required sums.

(ii) Rigid Boundary Conditions

In this section we treat sums associated with the matrix

$$\boldsymbol{\Delta} = \begin{pmatrix} a & b & & & 0 \\ b & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & b \\ 0 & & & b & a \end{pmatrix} \tag{118}$$

shown in eq. (2) of Appendix E.

Before proceeding to the actual calculations we extend somewhat the scope of this discussion by including matrices (not necessarily symmetric) of the type

$$\boldsymbol{\Delta}' = \begin{pmatrix} a & b_1 & & & 0 \\ c_1 & a & b_2 & & \\ & c_2 & \ddots & \ddots & \\ & & \ddots & \ddots & b_{N-1} \\ 0 & & & c_{N-1} & a \end{pmatrix} \tag{119}$$

where it is assumed that for all $i = 1, \ldots, N-1$

$$b_i\, c_i = \text{const} = b^2. \tag{120}$$

In Appendix E the discussion following eq. (15) shows that Δ' and Δ are connected by a similarity transformation. Because of this property we will work henceforth with Δ exclusively. It can also be verified that the elements of an arbitrary analytic function $F(\Delta')$ are related to those of Δ as follows:

$$[F(\Delta')]_{mn} = \begin{cases} \left[\dfrac{c_n\, c_{n+1} \cdots c_{m-1}}{b_n\, b_{n+1} \cdots b_{m-1}}\right]^{1/2} \times [F(\Delta)]_{mn} & m > n+1 \\[2ex] [F(\Delta)]_{mn} & m = n \\[2ex] \left[\dfrac{b_m\, b_{m+1} \cdots b_{n-1}}{c_m\, c_{m+1} \cdots c_{n-1}}\right]^{1/2} \times [F(\Delta)]_{mn} & n \geq m+1 \end{cases} \tag{121}$$

Since the eigenvalues of Δ are

$$\lambda_k = a + 2b \cos \frac{\pi k}{N+1} \quad ; \; k = 1, \ldots, N \tag{122}$$

their generating function will be

$$\lambda(\theta) = a + 2b\cos\theta. \tag{123}$$

The elements of an analytic function $F(\Delta)$ can be written as

$$[F(\Delta)]_{mn} = \frac{1}{N+1} \sum_{k=1}^{N} F(\lambda_k) \left\{\cos\frac{\pi(m-n)k}{N+1} - \cos\frac{\pi(m+n)k}{N+1}\right\} \tag{124}$$

where use was made of eq. (6) and the form of T shown in eq. (12) of Appendix E. Assuming as before that $F\{\lambda(\theta)\}$ can be represented by a Fourier series

$$F\{\lambda(\theta)\} = \frac{A_0}{2} + \sum_{n=1}^{\infty} A_n \cos n\theta \tag{125}$$

where

$$A_n = \frac{1}{\pi} \int_0^{2\pi} F\{\lambda(\theta)\} \cos n\theta \, d\theta \tag{126}$$

it is seen that the $F(\lambda_k)$ result when θ is set equal to $\pi k/(N+1)$. Substituting the value of $F(\lambda_k)$ from eq. (125) into eq. (124), we obtain

$$[F(\Delta)]_{mn} = \frac{A_0}{2(N+1)} \sum_{k=1}^{N} \left\{ \cos \frac{\pi(m-n)k}{N+1} - \cos \frac{\pi(m+n)k}{N+1} \right\} +$$

$$+ \frac{1}{2(N+1)} \sum_{j=1}^{\infty} A_j \times \sum_{k=1}^{N} \left\{ \cos \frac{\pi(m-n-j)k}{N+1} - \cos \frac{\pi(m-n+j)k}{N+1} \right.$$

$$\left. - \cos \frac{\pi(m+n-j)k}{N+1} - \cos \frac{\pi(m+n+j)k}{N+1} \right\} \tag{127}$$

To evaluate the finite sums appearing in this equation we note that they are all special cases of the prototype sum

$$\sum_{k=1}^{N} \cos\frac{\pi s k}{N+1} = N\delta_{s,\pm 2r(N+1)}$$

$$+\frac{1}{2}\left[(-1)^N - 1\right]\left[1 - \delta_{s,\pm 2r(N+1)}\right]\delta_{s,\pm(2r+1)(N+1)}$$

$$-\left(1 - \delta_{s,\pm 2r(N+1)} - \delta_{s,\pm(2r+1)(N+1)}\right)\delta_{s,\pm 2r} \qquad (128)$$

where $r = 0, 1, 2, \ldots$. The use of this formula in eq. (127) results in

$$\underset{m \geq n}{[F(\mathbf{\Delta})]_{mn}} = \frac{1}{2}\left[B_{m-n} + B_{-(m-n)} - B_{m+n} - B_{-(m+n)}\right] \qquad (129)$$

where

$$B_j = \sum_{r=0}^{\infty} A_{j+2r(N+1)} \qquad (130)$$

and a coefficient A_ℓ is zero if ℓ is negative. The restriction $m \geq n$ is dictated by the symmetry of $\mathbf{\Delta}$ (which in turn implies the symmetry of $F(\mathbf{\Delta})$).

In the following paragraphs we shall give some specific applications of the formula of eq. (129).

1. Calculation of $\mathbf{\Delta}^{-1}$

We have already found the Fourier coefficients needed here in eq. (4) of Appendix B. When their expressions are inserted into the definition of the B's, the resulting series are geometric and the matrix elements can be written in closed form as

$$(\Delta^{-1})_{mn} = \frac{V^{2n}-1}{UV^{m+n}} \cdot \frac{V^{2(N+1)} - V^{2m}}{1 - V^{2(N+1)}} \qquad m \geq n \tag{131}$$

where

$$V = \frac{\sqrt{a^2 - 4b^2} - a}{2b} \; ; \; U = \sqrt{a^2 - 4b^2} \tag{132}$$

2. Calculation of Δ^{ν}, $\nu \neq 0, 1, 2, \ldots$

If V as obtained in eq. (132) satisfies

$$|V| < 1 \tag{133}$$

then the Fourier coefficients are given by eq. (92), on identifying V with β, s_0 with a and s_1 with b:

$$A_n = \left(\frac{a}{1 + V^2}\right)^{\nu} \frac{2V^n \, \Gamma(-\nu + n)}{\Gamma(-\nu)\,\Gamma(n+1)} \; F(-\nu, \; -\nu + n, \; n+1; \; V^2)$$

$$= 2(-b)^{\nu} \, V^{n-\nu} \frac{\Gamma(-\nu + n)}{\Gamma(-\nu)\,\Gamma(n+1)} \; F(-\nu, \; -\nu + n, \; n+1; V^2) \; ; \; n \geq 0 \, . \tag{134}$$

Then

$$[\Delta^{\nu}]_{mn} = \left(-\frac{b}{V}\right)^{\nu} \frac{1}{\Gamma(-\nu)} \left\{ \sum_{r=0}^{\infty} F(-\nu, -\nu + m - n + 2r(N+1), \; m - n + 2r(N+1) + 1; V^2) \times \right.$$

$$\times \frac{\Gamma(-\nu + m - n + 2r(N+1)}{\Gamma(m - n + 2r(N+1) + 1)} \quad V^{m-n+2r(N+1)} +$$

$$+\sum_{r=1}^{\infty} F(-\nu, -\nu+2r(N+1)-m+n, 2r(N+1)-m+n+1; V^2)\frac{\Gamma(-\nu-m+n+2r(N+1))}{\Gamma(n-m+2r(N+1)+1)} V^{-m+n+2r(N+1)}$$

$$-\sum_{r=0}^{\infty} F(-\nu, -\nu+m+n+2r(N+1), m+n+2r(N+1)+1; V^2)\frac{\Gamma(-\nu+m+n+2r(N+1)}{\Gamma(m+n+2r(N+1)+1)} V^{m+n+2r(N+1)}$$

$$\left.-\sum_{r=1}^{\infty} F(-\nu, -\nu+2r(N+1)-m-n, 2r(N+1)-m-n+1; V^2)\frac{\Gamma(-\nu+2r(N+1)-m-n)}{\Gamma(2r(N+1)-m-n+1)} V^{2r(N+1)-m-n}\right\}$$

(135)

3. Calculation of $\exp(\tau\boldsymbol{\Delta})$

The Fourier coefficients are given by

$$A_n = 2e^{\tau a} I_n(2b\tau)\ ;\ n = 0,\ 1,\ 2,\ \ldots \tag{136}$$

Then

$$\underset{m \geq n}{[e^{\tau\boldsymbol{\Delta}}]_{mn}} = e^{\tau a}\left\{\sum_{r=0}^{\infty} I_{m-n+2r(N+1)}(2b\tau) + \right.$$

$$+\sum_{r=1}^{\infty} I_{2r(N+1)-(m-n)}(2b\tau) - \sum_{r=0}^{\infty} I_{m+n+2r(N+1)}(2b\tau)$$

$$\left.-\sum_{r=1}^{\infty} I_{2r(N+1)-(m+n)}(2b\tau)\right\} \tag{137}$$

We can write down also the following result for the sum

$$S_N = \frac{1}{N+1}\sum_{k=1}^{N} e^{\tau\left(a+2b\cos\frac{\pi k}{N+1}\right)}\cos\frac{\pi mk}{N+1} \tag{138}$$

We can restrict m (because of periodicity) to the range $0 \leq m < 2(N+1)$. Then

$$S_N^m = e^{\tau a} \left\{ I_0(2b\tau) + \sum_{\ell=1}^{\infty} I_{2\ell(N+1)-m}(2b\tau) \right.$$

$$\left. + \sum_{\ell=1}^{\infty} I_{2\ell(N+1)+m}(2b\tau) \right\} -$$

$$-\frac{e^{\tau a}}{N+1} \left\{ I_0(2b\tau)\, \delta_{m,\,\text{even}} + \sum_{\ell=\left[\frac{m}{2}\right]+1}^{\infty} I_{2\ell-m}(2b\tau) \right.$$

$$\left. + \sum_{\ell=1}^{\infty} I_{m+2\ell}(2b\tau) + \underset{m \neq 0}{\sum_{\ell=1}^{\left[\frac{m}{2}\right]}} I_{m-2\ell}(2b\tau) \right\} \tag{139}$$

This result simplifies for $m = 0$ to:

$$S_{N,0} = e^{\tau a} \left\{ I_0(2b\tau) + 2 \sum_{\ell=1}^{\infty} I_{2\ell(N+1)}(2b\tau) \right\} -$$

$$-\frac{e^{\tau a}}{N+1} \cosh(2b\tau) \tag{140}$$

3.2 Two-Dimensional Sums

In this section we present results relating to sums arising only from periodic and rigid boundary conditions. Other cases, whenever tractable, can be treated in a similar fashion.

It is clear that as we proceed to higher dimensions, the computational difficulties multiply. Therefore fewer specific results will be available. Nevertheless our technique will still be advantageous for numerical calculations.

The matrices Δ touched upon here will be two-dimensional matrices, i.e., $M \times M$ matrices the elements of which are $N \times N$ matrices. To specify the elements of Δ (regarded as an $MN \times MN$ matrix) one needs four indices, or two vector indices $\mathbf{i} = (i, i_2)$, $\mathbf{j} = (j_1, j_2)$. The first component of the vector index represents the row (column) of blocks in which the element is located and the second the row (column) location inside the block.

If $F(z)$ is an analytic function of z over the entire eigenvalue spectrum of Δ, then the generalization of eq. (6) is as follows:

$$[F(\Delta)]_{\mathbf{kr}} = \sum_{\mathbf{j}} F(\Lambda_{\mathbf{j}})\, T_{\mathbf{kj}}\, T^{-1}_{\mathbf{jr}} \tag{141}$$

where Λ_j are the generalized eigenvalues of Δ (namely, M diagonal $N \times N$ -matrices) and T is the (generalized) matrix which brings Δ to diagonal form.

i) <u>Periodic Boundary Conditions</u>

In this subsection we shall consider sums arising from eigenvalues connected with asymmetric and symmetric two-dimensional circulant matrices.

The general <u>asymmetric</u> case leads to eigenvalues λ_{mn} of the form:

$$\lambda_{mn} = \sum_{j=0}^{M-1} \sum_{k=0}^{N-1} S_{jk}\, e^{i\frac{2\pi jm}{M}}\, e^{i\frac{2\pi kn}{N}}$$

$$m = 0, \ldots, m-1;\ n = 0, \ldots, n-1$$

Then, using the form of **T** given in eqs. (212), (216) of Appendix E

$$[F(\Delta)]_{pq} = \frac{1}{MN} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} F(\lambda_{mn}) \exp \left\{ 2\pi i \left[\frac{m(p_1 - q_1)}{M} + \frac{n(p_2 - q_2)}{N} \right] \right\}$$

$$p_1,\ q_1 = 0, \ldots, M - 1,\ p_2,\ q_2 = 0, \ldots, N - 1. \tag{143}$$

Eq. (143) shows that we are concerned here with sums of the type:

$$S_{MN} = \frac{1}{MN} \sum_{r=0}^{M-1} \sum_{\ell=0}^{N-1} F(\lambda_{r\ell})\, e^{-\frac{2\pi i rm}{M}}\, e^{-\frac{2\pi i \ell n}{N}} \tag{144}$$

where m,n are integers which can be restricted to the ranges $0 \leq m \leq M - 1$; $0 \leq n \leq N - 1$ because of periodicity. For $m = n = 0$, S_{MN} reduces to a simpler, trace-type sum. We define now the frequency generating function $\lambda(\theta, \varphi)$ by

$$\lambda(\theta, \varphi) = \sum_{j=0}^{M-1} \sum_{k=0}^{N-1} S_{jk}\, e^{i(j\theta + k\varphi)} \tag{145}$$

Clearly

$$\lambda_{r\ell} = \lambda \left(\frac{2\pi r}{M}, \frac{2\pi \ell}{N} \right) \tag{146}$$

The analytic function $F\{\lambda(\theta, \varphi)\}$ is assumed to have a double Fourier series expansion

$$F\{\lambda(\theta, \varphi)\} = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} A_{pq}\, e^{i(p\theta + q\varphi)} \tag{147}$$

where

$$A_{pq} = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} F\{\lambda(\theta, \varphi)\}\, e^{-i(p\theta+q\varphi)}\, d\theta\, d\varphi . \tag{148}$$

Again, only positive p, q are considered, since $\lambda(\theta, \varphi)$ and hence $F\{\lambda(\theta, \varphi)\}$ contain only positive powers of $e^{i\theta}$, $e^{i\varphi}$. In cases where $\lambda(\theta, \varphi)$ contains negative powers of $e^{i\theta}$ and $e^{i\varphi}$, the full expansion must be used.

Utilizing the expansion (147) we find

$$F(\lambda_{r\ell}) = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} A_{pq}\, e^{i\frac{2\pi rp}{M}} e^{i\frac{2\pi \ell q}{N}}$$

$$= \sum_{p=0}^{M-1} \sum_{q=0}^{N-1} A^*_{pq}\, e^{i\frac{2\pi rp}{M}} e^{i\frac{2\pi \ell q}{N}} \tag{149}$$

where

$$A^*_{pq} = \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} A_{p+jM,\, q+kN} . \tag{150}$$

Again, the analyticity of $F(z)$ insures the legitimacy of rearrangement of the series.

Insertion of (149) into (150) leads to

$$S_{MN} = A^*_{m,n} \tag{151}$$

The discussion preceding and following eq. (29) concerning the properties of the Fourier coefficients, is pertinent also here and need not be repeated.

The general symmetric case leads to eigenvalues $\lambda_{r\ell}$ of the form:

$$\lambda_{r\ell} = s_{00} + 2\sum_{k=1}^{N-1} s_{0k} \cos\frac{2\pi k\ell}{N'} + 2\eta\, s_{0N} \cos\frac{2\pi N\ell}{N'} + 2\sum_{j=1}^{M-1} s_{j0} \cos\frac{2\pi r j}{M'}$$

$$+ 4\sum_{j=1}^{M-1}\sum_{k=1}^{N-1} s_{jk} \cos\frac{2\pi j r}{M'} \cos\frac{2\pi\ell k}{N'} + 4\eta\sum_{j=1}^{M-1} s_{jN} \cos\frac{2\pi j r}{M'} \cos\frac{2\pi N\ell}{N'}$$

$$+ 2\epsilon\, s_{M0} \cos\frac{2\pi M r}{M'} + 4\epsilon\sum_{k=1}^{N-1} s_{Mk} \cos\frac{2\pi k\ell}{N^1} \cos\frac{2\pi M r}{M^1}$$

$$+ 4\epsilon\eta\, s_{MN} \cos\frac{2\pi M r}{M^1} \cos\frac{2\pi N\ell}{N^1} \tag{152}$$

where

$$\epsilon = \begin{cases} \frac{1}{2} & M' = 2M \\ 1 & M' = 2M+1 \end{cases} ; \quad \eta = \begin{cases} \frac{1}{2} & N' = 2N \\ 1 & N' = 2N+1 \end{cases} \tag{153}$$

We obtain the frequency distribution function $\lambda(\theta, \varphi)$ by substituting $\theta = 2\pi r/M'$; $\varphi = 2\pi\ell/N'$ in eq. (152). Then

$$F\{\lambda(\theta,\varphi\} = \frac{1}{4}A_{00} + \frac{1}{2}\sum_{p=1}^{\infty} A_{p0}\cos p\theta + \frac{1}{2}\sum_{q=1}^{\infty} A_{0q}\cos q\varphi$$

$$+ \sum_{p=1}^{\infty}\sum_{q=1}^{\infty} A_{pq}\cos p\theta\cos q\varphi \tag{154}$$

with

$$A_{pq} = \frac{1}{\pi^2}\int_0^{2\pi}\int_0^{2\pi} F\{\lambda(\theta,\varphi)\}\cos p\theta\cos d\theta d\varphi. \tag{155}$$

Then

$$F(\lambda_r\ell) = \sum_{p=0}^{M'-1}\sum_{q=0}^{N'-1} A^*_{pq}\cos\frac{2\pi p r}{M'}\cos\frac{2\pi q\ell}{N'} \tag{156}$$

where

$$\left.\begin{aligned}
A^*_{00} &= \frac{1}{4}A_{00} + \frac{1}{2}\sum_{k=1}^{\infty} A_{0,kN'} + \frac{1}{2}\sum_{j=1}^{\infty} A_{jM',0} + \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} A_{jM',kN'} \\
A^*_{0q} &= \frac{1}{2}\sum_{k=0}^{\infty} A_{0,q+kN'} + \sum_{j=1}^{\infty}\sum_{k=0}^{\infty} A_{jM',q+kN'} \\
q &> 0 \\
A^*_{p0} &= \frac{1}{2}\sum_{j=0}^{\infty} A_{p+jM',0} + \sum_{j=0}^{\infty}\sum_{k=1}^{\infty} A_{p+jM',kN'} \\
p &> 0 \\
A^*_{pq} &= \sum_{j=0}^{\infty}\sum_{k=0}^{\infty} A_{p+jM',q+kN'} \\
p,q &> 0
\end{aligned}\right\} \tag{157}$$

Then a sum of the type

$$S_{M'N'} = \frac{1}{M'N'} \sum_{r=0}^{M'-1} \sum_{\ell=0}^{N'-1} F(\lambda_{r\ell}) e^{-i\frac{2\pi rm}{M'}} e^{-i\frac{2\pi \ell n}{N'}} \tag{158}$$

in which m, n are as in eq. (144), can be rewritten with the aid of eq. (156):

$$S_{M'N'} = \frac{1}{4} A^*_{m,n} \tag{159}$$

If the exponentials in the sum (158) are replaced by the respective cosine terms, the modified sum is given by

$$S_{M'N'} = \frac{1}{4} \left\{ A^*_{M'-m,\ N'-n} + A^*_{M'-m,n} + A^*_{m,N'-n} + A^*_{m,n} \right\} . \tag{160}$$

For the trace sum with $m = n = 0$, we obtain:

$$S_{M'N'} = A^*_{00} . \tag{161}$$

We proceed now to calculations with specific functions $F(z)$.

1. The Inverse Δ^{-1}

In the symmetric case the integrals to be evaluated are

$$\begin{aligned} A_{pq} &= \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \frac{e^{-ip\theta} e^{-iq\varphi}\, d\theta\, d\varphi}{\sum_{j=0}^{M-1} \sum_{k=0}^{N-1} s_{jk}\, e^{ij\theta}\, e^{ik\varphi}} \\ &= \frac{1}{(2\pi i)^2} \int_{C'} \int_C \frac{d\zeta\, dz}{\zeta^{q+1}\, z^{p+1} \sum_{j=0}^{M-1} \sum_{k=0}^{N-1} s_{jk}\, z^j\, \zeta^k} \end{aligned} \tag{162}$$

where C' and C are unit circles in the ζ- and z-planes respectively. It is obvious that even though some formal results could be written down for the general case (e.g., a determinantal form for the contribution to A_{pq} from the poles at the origin), these would have no practical value. On the other hand if only a few of the s_{jk} do not vanish, certain exact and asymptotic results can be still derived. We shall not pursue this possibility here as illustrations will be given for the more interesting symmetric case.

In the symmetric case we treat only the case

$$\lambda(\theta, \varphi) = a + 2b \cos \theta + 2c \cos \varphi + 4d \cos \theta \cos \varphi \tag{163}$$

where the integrals to be evaluated are given by

$$A_{pq} = \frac{1}{\pi^2} \int_0^{2\pi} \int_0^{2\pi} \frac{\cos p\theta \cos q\varphi \, d\theta \, d\varphi}{a + 2b \cos \theta + 2c \cos \varphi + 4d \cos \theta \cos \varphi} \tag{164}$$

The following conditions are imposed on the coefficients:

$$|b| \geq |c| > 2|d| ; \quad b, c, d < 0 \tag{165}$$

It is clear that one integration can be immediately performed to yield an elementary function, and we shall do so in the sequel. Here we find it more convenient not to use contour integrals, the analysis being simpler in the real domain. Since for arbitrary p, q an exact result is not available, we give first the value of A_{00} where such a result exists. In Appendix B we have evaluated A_{00} for different ranges of the parameter a. Here we exhibit only one such result, eq. (22) there:

$$A_{00} = \frac{4}{\pi} \frac{1}{\sqrt{c^2 - 4d^2}} \frac{1}{\sqrt{(u-1)(v+1)}} K\left(\sqrt{\frac{2(u-v)}{(u-1)(v+1)}}\right) \tag{166}$$

where

$$u = \frac{a + 2|b|}{2(|c| - 2|d|)} \; ; \quad v = \frac{a - 2|b|}{2(|c| + 2|d|)} \tag{167}$$

and $K(k)$ is the complete elliptic integral of the first kind the modulus k of which is given by

$$k^2 = \frac{2(u-v)}{(u-1)(v+1)} \tag{168}$$

This generalizes results in the literature [11], including recent ones of Mathews and al. [18].

Appendix B also treats the asymptotic approximations of the general integral A_{pq}. For the case $d = 0$, exact results can be given for all A_{pq} by proceeding as follows:

$$A_{pq} = \frac{4}{\pi^2} \int_0^{\pi} \int_0^{\pi} \frac{\cos p\theta \cos q\varphi \, d\theta \, d\varphi}{a + 2b\cos\theta + 2c\cos\varphi} \tag{169}$$

Under the same restrictions as in eq. (165) with the additional condition $|a| \geq 2(|b| + |c| + 2|d|)$, the following identity can be used

$$\frac{1}{a + 2b\cos\theta + 2c\cos\varphi} = \int_0^{\infty} e^{-ax} e^{-2bx\cos\theta} e^{-2cx\cos\varphi} dx \tag{170}$$

Since

$$e^{-z\cos\psi} = J_0(iz) + 2\sum_{k=1}^{\infty} i^k J_k(iz)\cos k\psi \tag{171}$$

inserting (170) and (171) in eq. (169) we obtain:

$$\begin{aligned} A_{pq} = 4 \Big\{ & \delta_{po}\,\delta_{q0} \int_0^{\infty} e^{-ax} J_0(2bix)\, J_0(2cix)\, dx \\ & + 2(1-\delta_{q0})\,\delta_{p0}\, i^q \int_0^{\infty} e^{-ax} J_0(2bix)\, J_q(2cix)\, dx \\ & + 2(1-\delta_{p0})\,\delta_{q0}\, i^p \int_0^{\infty} e^{-ax} J_p(2bix)\, J_0(2cix)\, dx + 4(1-\delta_{po})(1+\delta_{q0})\, i^{p+q} \times \\ & \times \int_0^{\infty} e^{-ax} J_p(2bix)\, J_q(2cix)\, dx \Big\} \end{aligned} \tag{172}$$

According to Erdelyi [19] , the Laplace transforms in eq. (172) can be evaluated explicitly

$$\int_0^{\infty} e^{-ax} J_p(2bix)\, J_q(2cix)\, dx =$$

$$= \binom{p+q}{p} i^{p+q} \frac{b^p c^q}{(a+2|b|+2|c|)^{p+q+1}}\, \mathfrak{F}_2\left(p+q+1;\ p+1/2;\ q+1/2,\ 2p+1;\right.$$

$$\left. 2q+1;\ \frac{4|b|}{a+2|b|+2|c|},\ \frac{4|c|}{a+2|b|+2|c|}\right) \tag{173}$$

where $\mathfrak{F}_2$ is a hypergeometric function of two variables [15]. It can be shown that the expression for A_{00} reduces to a complete elliptic integral of the first kind, as expected from the case $d \neq 0$.

2. Exp $(t\Delta)$

For the asymmetric case the pertinent sums are of the form:

$$S_{MN} = \frac{1}{MN} \sum_{r=0}^{M-1} \sum_{\ell=0}^{N-1} \exp\left\{ t s_0 + t s_1 e^{i\frac{2\pi r}{M}} + t s_2 e^{i\frac{2\pi \ell}{N}} + t s_3 e^{i\frac{2\pi r}{M}} e^{i\frac{2\pi \ell}{N}} \right\} \times$$

$$\times\, e^{-\frac{2\pi i r m}{M}} e^{-\frac{2\pi i \ell n}{N}} \tag{174}$$

and no constraints need be placed on the s_j's.

The Fourier expansion is straightforward:

$$A_{pq} = \begin{cases} e^{t s_0}\, t^{p+q}\, s_1^p\, s_2^q \displaystyle\sum_{j=0}^{q} \frac{1}{j!\,(p-j)!\,(q-j)!} \left(\frac{s_3}{s_1 s_2}\right)^j & q \le p \\ e^{t s_0}\, t^{p+q}\, s_1^p\, s_2^q \displaystyle\sum_{j=0}^{p} \frac{1}{j!\,(p-j)!\,(q-j)!} \left(\frac{s_3}{s_1 s_2}\right)^j & q > p \end{cases} \tag{175}$$

These expressions simplify for $s_3 = 0$, to

$$A_{pq} = e^{t s_0} \frac{t^{p+q}\, s_1^p\, s_2^q}{p!\, q!} \tag{176}$$

and the summations involved in the evaluation of S_{MN} can be performed for p and q separately.

The symmetric case can be treated in terms of simple functions only for

$$\lambda(\theta, \varphi) = a + 2b \cos\theta + 2c \cos\varphi$$

Then

$$e^{t\lambda(\theta,\varphi)} = e^{ta}\, e^{2bt\cos\theta}\, e^{2ct\cos\varphi} \tag{178}$$

and we make use of the expansion (171), such that

$$A_{pq} = 4e^{ta}\, I_p(2bt)\, I_q(2ct); \quad p,q \ge 0 \tag{179}$$

As in the one-dimensional case, one can extend the above results to functions like $\frac{\sin}{\cos}(t\Delta)$, $\frac{\sinh}{\cosh}(t\Delta)$ and c^{Δ} (with c a constant), without difficulty.

4. The Frequency Distribution Function $\mathcal{G}(\omega^2)$

The sum to be evaluated here is

$$\mathcal{G}(\omega^2) = \frac{1}{MN} \sum_{r=0}^{M-1} \sum_{\ell=0}^{N-1} \delta(\omega^2 - \lambda_{r\ell}) \tag{180}$$

Hence we need the Fourier expansion of the generalized function $\delta\{\omega^2 - \lambda(\theta, \varphi)\}$. Since for the asymmetric case the eigenvalues $\lambda_{r\ell}$ can be complex, the appropriate eigenvalue distribution function $\mathcal{G}(\omega)$ would have to be defined over the complex plane. This is not done here and instead we treat only the real, symmetric case.

The frequency generating function $\lambda(\theta, \varphi)$ here is taken to be

$$\lambda(\theta, \varphi) = a + 2b\cos\theta + 2c\cos\varphi + 4d\cos\theta\cos\varphi \tag{181}$$

with the restrictions of eq. (165).

In Appendix C the Fourier expansion of the generalized function $\delta\{\omega^2 - \lambda(\theta, \varphi)\}$ is effected. Here we present only the first (dominant) term:

$\delta\{a - \omega^2 + 2b\cos\theta + 2c\cos\varphi + 4d\cos\theta\cos\varphi\} \approx$

$$\approx \frac{1}{4\pi^2}\sqrt{\frac{2}{c^2 - 4d^2}}\begin{cases} \dfrac{1}{\sqrt{u-v}}\, K\left(\sqrt{\dfrac{(1-v)(1+u)}{2(u-v)}}\right) \\ a - 2|b| - 2|c| - 4|d| < \omega^2 < a - 2|b| + 2|c| + 4|d| \\ \sqrt{\dfrac{2}{(1-v)(1+u)}}\, K\left(\sqrt{\dfrac{2(u-v)}{(1-v)(1+u)}}\right) \\ a - 2|b| + 2|c| + 4|d| < \omega^2 < a + 2|b| - 2|c| + 4|d| \\ \dfrac{1}{\sqrt{u-v}}\, K\left(\sqrt{\dfrac{(1-v)(1+u)}{2(u-v)}}\right) \\ a + 2|b| - 2|c| + 4|d| < \omega^2 < a + 2|b| + 2|c| - 4|d| \end{cases}$$

where $K(k)$ is the complete elliptic integral of the first kind with modulus $k\,(k < 1)$, and u, v are given by

$$u = \frac{a + 2|b| - \omega^2}{2(|c| - 2|d|)}\ ; \quad v = \frac{a - 2|b| - \omega^2}{2(|c| + 2|d|)} \tag{183}$$

The expression for $\mathcal{G}(\omega^2)$ is identical in the first term with that of $\delta\{\omega^2 - \lambda(\theta, \varphi)\}$, as can be seen from eq. (12). This result in eq. (182) is more general than that quoted by Montroll et al. [11] in two respects: 1. The addition of the mixing term $4d\cos\theta\cos\varphi$; 2. The constraints imposed on the parameters a, b, c and d are weaker than those ordinarily used. Moreover this evaluation exhibits the advantages of our method, since alternative integral representations for the δ-function lead, when mixing terms are included, to integrals which are not recognizable from existing tables.

ii. Rigid Boundary Conditions

As in the one-dimensional case, the formulas of this section differ from those of the previous one only because the sets $\{\theta_j\}$, $\{\varphi_k\}$ are modified. Again, it is clear that the changes will occur solely in the correction terms.

The sums treated here arise from eigenvalues connected with two-dimensional continuant matrices. The eigenvalues considered are of the type

$$\lambda_{r\ell} = a + 2b \cos \frac{\pi r}{M+1} + 2c \cos \frac{\pi \ell}{N+1} + 4d \cos \frac{\pi r}{M+1} \cos \frac{\pi \ell}{N+1} \tag{184}$$

and the matrix elements of $F(\Delta)$, on using the explicit form given in eq. (176) of Appendix E for the diagonalizing matrix T, will be

$$[F(\Delta)]_{pq} = \frac{4}{(M+1)(N+1)} \sum_{r=1}^{M} \sum_{\ell=1}^{N} F(\lambda_{r\ell}) \sin \frac{\pi r p_1}{M+1} \sin \frac{\pi r q_1}{M+1} \sin \frac{\pi \ell p_2}{N+1} \sin \frac{\pi \ell q_2}{N+1}$$

$$p_1, q_1 = 1, \ldots, M; \quad p_2, q_2 = 1, \ldots, N \tag{185}$$

Utilizing the relation

$$\sin x \sin y = \frac{1}{2} [\cos (x-y) - \cos (x+y)]$$

we see that our concern here is with a sum of the type

$$S_{MN} = \frac{1}{(M+1)(N+1)} \sum_{r=1}^{M} \sum_{\ell=1}^{N} F(\lambda_{r\ell}) \cos \frac{\pi r m}{M+1} \cos \frac{\pi \ell n}{N+1} \tag{186}$$

where, on account of periodicity the integers m, n can be restricted to the ranges $0 \le m \le 2M+1$; $0 \le n \le 2N+1$. For $m = n = 0$ S_{MN} reduces to a trace-type sum.

Now we assume for $F\{\lambda(\theta, \varphi)\}$ a Fourier expansion similar to that in eq. (154), with appropriate A_{pq}'s, and define quantities U_j, V_k

$$U_j = \frac{1}{M+1} \sum_{r=1}^{M} \cos \frac{\pi r j}{M+1} ; \quad V_k = \frac{1}{N+1} \sum_{\ell=1}^{N} \cos \frac{\pi k \ell}{N+1} \tag{187}$$

The sums appearing in (187) have been evaluated in terms of Kronecker δ's in eq. (128). Note also that $U_{-j} = U_j$ and $V_{-k} = V_k$. Then insertion of the Fourier expansion of $F(\lambda_{r\ell})$ and use of the U_j, V_k leads to the following form for S_{MN}

$$S_{MN} = \frac{1}{4} \sum_{p=0}^{\infty} \sum_{q=0} A_{pq}\, \epsilon_{pq}\, (U_{p-m} + U_{p+m})\, (V_{q-n} + V_{q+n}) \tag{188}$$

where

$$\epsilon_{pq} = \begin{cases} \frac{1}{4} & p = q = 0 \\ \frac{1}{2} & p = 0,\ q > 0; \quad p > 0,\ q = 0 \\ 1 & p > 0,\ q > 0 \end{cases} \tag{189}$$

If we further define

$$B_{r,s} = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} A_{pq}\, \epsilon_{pq}\, U_{p+r}\, V_{q+s} \tag{190}$$

then S_{MN} can be written as follows

$$S_{MN} = \frac{1}{4} \{B_{-m,-n} + B_{-m,n} + B_{m,-n} + B_{m,n}\} \tag{191}$$

Since the eigenvalue-generating function $\lambda(\theta,\varphi)$ considered here is identical with that of the symmetric case in the previous section, the Fourier coefficients for the various functions $F(z)$ coincide also. Hence there is no need to repeat the results, and no particular application will be made to the sums S_{MN}.

3.3 d-Dimensional Sums

This section is devoted to sums arising from problems in three or higher dimensions. The sums will be over analytic functions of eigenvalues of d-dimensional matrices. These matrices are straight-forward generalizations of the matrices dealt with previously. It must be borne in mind that if one disregards the d-dimensional partitioning of a generalized matrix, one is left with an ordinary matrix the elements of which can be specified by the usual two indices. On the otherhand if one has to keep track of the particular submatrices which contain the element in question, the two simple indices p,q are to be replaced by two d-dimensional vectors $\mathbf{p},\mathbf{q}$ the components of which take values from d appropriate ranges. Examples of these matrices, apart from the (lattice) dynamical matrices mentioned, are the matric representations of quantum-mechanical Hamiltonians, where the elements are specified by several quantum numbers. This shows also that the components p_j of the vector indices are sometimes taken from a set of N_j numbers not necessarily integers.

For the remainder of this section only the three-dimensional case will be considered. The elements of an analytic function of $\boldsymbol{\Delta}$ are given here by

$$[F(\boldsymbol{\Delta})]_{\mathbf{p},\mathbf{q}} = \sum_{\mathbf{k}} F(\Lambda_{\mathbf{k}})\, T_{\mathbf{pk}}\, T^{-1}_{\mathbf{kq}} \tag{192}$$

where Λ_k are generalized eigenvalues of $\boldsymbol{\Delta}$, $\mathbf{T}$ the (generalized) matrix which brings $\boldsymbol{\Delta}$ to diagonal form, and $\mathbf{p} = (p_1, p_2, p_3)$; $\mathbf{q} = (q_1, q_2, q_3)$, with p_j, q_j $\epsilon \{r_1^{(j)}, \ldots, r_{N_j}^{(j)}\}$. In the following the $r^{(j)}$ will be integers.

i. Periodic Boundary Conditions

Here we shall treat analytically only the simplest cases, since even for these closed form results are generally not available.

The general asymmetric case leads to eigenvalues of the form

$$\left.\begin{aligned} &\lambda_{pqr} = \sum_{j=0}^{N_1} \sum_{k=0}^{N_2} \sum_{\ell=0}^{N_3} s_{jk\ell}\, e^{i\frac{2\pi jp}{N_1}} e^{i\frac{2\pi kq}{N_2}} e^{i\frac{2\pi \ell r}{N_3}} \\ &p = 0, \ldots, N_1 - 1, \; q = 0, \ldots, N_2 - 1; \; r = 0, \ldots, N_3 - 1 \end{aligned}\right\} \tag{193}$$

Then using the form of $\mathbf{T}$ given in eq. ( ) of Appendix , we obtain

$$[F(\boldsymbol{\Delta})]_{uv} = \frac{1}{N_1 N_2 N_3} \sum_{p=0}^{N_1-1} \sum_{q=0}^{N_2-1} \sum_{r=0}^{N_3-1} F(\lambda_{pqr})\, e^{i\frac{2\pi p(u_1-v_1)}{N_1}} e^{i\frac{2\pi q(u_2-v_2)}{N_2}} \times e^{i\frac{2\pi r(u_3-v_3)}{N_3}} \tag{194}$$

Therefore we are concerned with sums of the type

$$S_{N_1N_2N_3} = \frac{1}{N_1 N_2 N_3} \sum_{p=0}^{N_1-1} \sum_{q=0}^{N_2-1} \sum_{r=0}^{N_3-1} F(\lambda_{pqr})\, e^{-\frac{2\pi i pn_1}{N_1}} e^{-\frac{2\pi i qn_2}{N_2}} e^{-\frac{2\pi i rn_3}{N_3}} \tag{195}$$

where n_1, n_2, n_3 are integers which can be restricted, because of periodicity, to the ranges:

$$0 \le n_1 \le N_1 - 1;\ 0 \le n_2 \le N_2 - 1;\ 0 \le n_3 \le N_3 - 1.$$

Proceeding as before, we define an eigenvalue generating function $\lambda(\theta, \varphi, \psi)$ and expand $F\{\lambda(\theta, \varphi, \psi)\}$ in a triple Fourier series. The final result is

$$S_{N_1 N_2 N_3} = A^*_{n_1 n_2 n_3} \tag{195}$$

Here

$$A^*_{p_1 p_2 p_3} = \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \sum_{\ell=0}^{\infty} A_{p_1+jN_1,\, p_2+kN_2,\, p_3+\ell N_3} \tag{197}$$

and

$$A_{jk\ell} = \frac{1}{(2\pi)^3} \iint_0^{2\pi}\!\int F\{\lambda(\theta, \varphi, \psi)\}\, e^{-i(j\theta+k\varphi+\ell\psi)}\, d\theta d\varphi d\psi \tag{198}$$

We have assumed $\lambda(\theta, \varphi, \psi)$ to contain only positive powers of $e^{i\theta}$, $e^{i\varphi}$, $e^{i\psi}$ and therefore the integers $j, k, \ell \ge 0$.

The general symmetric case leads to eigenvalues of the form:

$$\lambda_{pqr} = \sum_{j=0}^{N_1-1} \sum_{k=0}^{N_2-1} \sum_{\ell=0}^{N_3-1} s_{jk\ell} \cos\frac{2\pi pj}{N_1} \cos\frac{2\pi qk}{N_2} \cos\frac{2\pi r\ell}{N_3} \tag{199}$$

where the $s_{jk\ell}$'s satisfy certain identities, similar to those imposed in two dimensions. Then

$$F\{\lambda(\theta, \varphi, \psi)\} = \sum_{p_1=0}^{\infty} \sum_{p_2=0}^{\infty} \sum_{p_3=0}^{\infty} A_{p_1 p_2 p_3}\, \epsilon_{p_1 p_2 p_3} \cos p_1\theta \cos p_2\varphi \cos p_3\psi \tag{200}$$

where

$$\epsilon_{p_1p_2p_3} = \begin{cases} \frac{1}{8} & p_1 + p_2 + p_3 = 0 \\ \frac{1}{4} & p_1 + p_2 + p_3 = 1 \\ \frac{1}{2} & p_1 + p_2 + p_3 = 2 \\ 1 & p_1 + p_2 + p_3 \geq 3 \end{cases} \tag{201}$$

and

$$A_{p_1p_2p_3} = \frac{1}{\pi^3} \iint_0^{2\pi} \int F\{\lambda(\theta, \varphi, \psi)\} \cos p_1\theta \cos p_2\varphi \cos p_3\psi \, d\theta d\varphi d\psi \tag{202}$$

Hence a sum of the type

$$S_{N_1N_2N_3} = \frac{1}{N_1N_2N_3} \sum_{p=0}^{N_1-1} \sum_{q=0}^{N_2-1} \sum_{r=0}^{N_3-1} F(\lambda_{pqr}) \, e^{-2\pi i \left[\frac{pn_1}{N_1} + \frac{qn_2}{N_2} + \frac{rn_3}{N_3}\right]} \tag{203}$$

with n_1, n_2, n_3 as in eq. (195), can be rewritten as follows:

$$S_{N_1N_2N_3} = \frac{1}{8} A^*_{n_1n_2n_3} \tag{204}$$

and the A^*'s are given by

$$A^*_{pqr} = \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \sum_{\ell=0}^{\infty} \epsilon_{jk\ell} \, A_{p+jN_1,\, q+kN_2,\, r+\ell N_3} \tag{205}$$

When the exponentials in the sum (203) are replaced by the respective cosine terms the modified sum can be written as

$$S_{N_1N_1N_2} = \frac{1}{8} \sum_{\alpha,\beta,\gamma=-1}^{+1} A^*_{\alpha n_1+\frac{1-\alpha}{2}N_1,\ \beta_{n_2}+\frac{1-\beta}{2}N_2,\ \gamma n_3+\frac{1-\gamma}{2}N_3} \tag{206}$$

1. The Inverse Δ^{-1}

Here we shall treat only the symmetric case for the simplest frequency generating function $\lambda(\theta, \varphi, \psi)$:

$$\lambda(\theta, \varphi, \psi) = a + 2b \cos\theta + 2c \cos\varphi + 2d \cos\psi \tag{207}$$

The corresponding Fourier coefficients are

$$A_{pqr} = \frac{1}{\pi^3} \iiint_0^{2\pi} \frac{\cos k\theta \cos q\varphi \cos r\psi \, d\theta d\varphi d\psi}{a + 2b\cos\theta + 2c\cos\varphi + 2d\cos\psi} \tag{208}$$

The only exact results available are for A_{000}, and this only for particular relative values of a, b, c and d. For $a = -6b$ and $b = c = d < 0$, the integral has been evaluated by Watson [20], with the result

$$A_{000} \equiv \frac{3}{a\pi^3} \iiint_0^{2\pi} \frac{d\theta \, d\varphi \, d\psi}{3 - \cos\theta - \cos\varphi - \cos\psi} = \frac{96}{\pi^2 a} [18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6} \times$$

$$\times K^2 [(2-\sqrt{3})(\sqrt{3}-\sqrt{2})] \tag{209}$$

where $K(k)$ is the complete elliptic integral of the first kind.

Montroll [21] has generalized this result to the case $d, b = c < 0$ and $a = 2(2|b| + |d|)$, such that

$$A_{000} = \frac{1}{|b|\,\pi^3} \iiint_0^{2\pi} \frac{d\theta\, d\varphi\, d\psi}{(2 + \alpha^2) - \cos\theta - \cos\varphi - \alpha^2 \cos\psi}$$

$$= \frac{32}{\sqrt{|bd|}\,\pi^2} [\sqrt{\gamma + 1} - \sqrt{\gamma - 1}]\, K(k_1)\, K(k_2) \tag{210}$$

with

$$\alpha = \sqrt{\left|\frac{d}{b}\right|}; \qquad \gamma = \frac{4 + 3\alpha^2}{\alpha^2}$$

$$\left.\begin{aligned} k_1 &= \frac{1}{2} [\sqrt{\gamma - 1} - \sqrt{\gamma - 3}]\, [\sqrt{\gamma + 1} - \sqrt{\gamma - 1}] \\ k_2 &= \frac{1}{2} [\sqrt{\gamma - 1} + \sqrt{\gamma - 3}]\, [\sqrt{\gamma + 1} - \sqrt{\gamma - 1}] \end{aligned}\right\} \tag{211}$$

and $K(k)$ the first complete elliptic integral as before.

There exists a formal expression for A_{pqr} in terms of a hypergeometric function of three variables. The result arises as follows:

$$A_{pqr} = \frac{1}{\pi^3} \int_0^{\infty} dt \iiint_0^{2\pi} e^{-a\tau}\, e^{-\tau(2b\cos\theta + 2c\cos\varphi + 2d\cos\psi)}$$

$$\times \cos p\theta \cos q\varphi \cos r\psi\, d\theta\, d\varphi\, d\psi \tag{212}$$

where we assume $\Re e(a) > 0$. Since for integral n

$$\int_0^{2\pi} e^{-\beta\tau \cos x} \cos nx \, dx = 2\pi \, i^n \, J_n(\beta\tau i) \tag{213}$$

we obtain

$$A_{pqr} = 8 i^{p+q+r} \int_0^\infty e^{-a\tau} \, J_p(2b\tau i) \, J_q(2c\tau i) \, J_r(2d\tau i) \, dt \tag{214}$$

The integral in eq. (214) is a Laplace transform. Its value as given by [19] leads to

$$A_{pqr} = \frac{8(-1)^{p+q+r} \, b^p \, c^q \, d^r}{(a - 2b - 2c - 2d)^{p+q+r+1}} \, \frac{(p+q+r)!}{p! \, q! \, r!} \times \tag{215}$$

$$\times \, \mathfrak{F}_3 \left\{ p+q+r+1; \; p+\frac{1}{2}, \; q+\frac{1}{2}, \; r+\frac{1}{2}; \; 2p+1, \; 2q+1, \; 2r+1; \; -\frac{4b}{a-2b-2c-2d} \right.$$

$$\left. -\frac{4c}{a-2b-2c-2d}, \; -\frac{4d}{a-2b-2c-2d} \right\}$$

The function $\mathfrak{F}_3$, known as the Lauricella function, is a three-dimensional power series. Its properties have not been thoroughly investigated and its alternative representations, if any, are not known.

Tables for the general integral A_{pqr} are available for certain ranges of the parameters which appear in its denominator [22]. The same reference gives also asymptotic forms of A_{pqr} for large values of the indices.

Returning to A_{000} it can be shown that two integrations can be performed exactly in terms of complete elliptic integrals on using the results of Appendix B for the two-dimensional case, and this can be done even when $\lambda(\theta, \varphi, \psi)$ contains mixed cosine terms. But so far, attempts to carry out the third integration analytically have not been successful.

2. Exp $(t\Delta)$

For the asymmetric case we treat the sums

$$S_{N_1N_2N_3} = \frac{1}{N_1N_2N_3} \sum_{j=0}^{N_1-1} \sum_{k=0}^{N_2-1} \sum_{\ell=0}^{N_3-1} \exp\left\{ ts_0 + ts_1 e^{i\frac{2\pi j}{N_1}} + ts_2 e^{i\frac{2\pi k}{N_2}} + ts_3 e^{i\frac{2\pi \ell}{N_3}} \right\}$$

$$\times e^{-\frac{2\pi i n_1 j}{N_1}} e^{-\frac{2\pi i n_2 k}{N_2}} e^{-\frac{2\pi i n_3 \ell}{N_3}} \tag{216}$$

Since there is no mixing term, the Fourier coefficients can be immediately written down

$$A_{pqr} \equiv \frac{e^{ts_0}}{(2\pi)^3} \iiint_0^{2\pi} e^{-i(p\theta+q\varphi+r\psi)} \exp\{ts_1 e^{i\theta} + ts_2 e^{i\varphi} + ts_3 e^{i\psi}\}\, d\theta\, d\varphi\, d\psi$$

$$= \frac{e^{ts_0}\, t^{p+q+r}\, s_1^p s_2^q s_3^r}{p!\ q!\ r!} \tag{217}$$

The summations involved in the evaluation of the sum $S_{N_1N_2N_3}$ can be performed separately for p, q and r.

The symmetric case leads to the Fourier coefficients

$$A_{pqr} \equiv \frac{e^{ta}}{\pi^3} \iiint_0^{2\pi} \exp\{2bt\cos\theta + 2ct\cos\varphi + 2dt\cos\psi\}$$

$$\times \cos p\theta \cos q\varphi \cos r\psi\, d\theta\, d\varphi\, d\psi$$

$$= 8e^{ta}\, I_p(2bt)\, I_q(2ct)\, I_r(2dt) \tag{218}$$

where $I_\nu(z)$ is the modified Bessel function of the first kind.

3. Frequency Distribution Function

The remarks concerning the evaluation of the Fourier coefficients related to Δ^{-1} are pertinent also here. The triple integrals that are to be evaluated in order to find the Fourier expansion of the generalized function.

$$\delta(\omega^2 - a - 2b \cos\theta - 2c \cos\varphi - 2d \cos\psi)$$

present the same difficulties.

Therefore if $\mathcal{G}(\omega^2)$ is needed only for the conversion of finite triple sums into integrals, this approach will not be practical for numerical work because of the free parameter ω^2. On the other hand, our method is still useful.

CHAPTER IV

LATTICES WITH DEFECTS AND PERTURBATION THEORY

Defects and imperfections in crystal lattices have been the subject of numerous and relatively recent investigations [11]. The most widely used method for the treatment of such lattices is Montroll's method of Green's functions, developed and elaborated in collaboration with Potts, Maradudin and Weiss [23].

An outline of this method is presented below in connection with the evaluation of the frequencies of an arbitrary imperfect lattice. Later on the discussion will be specialized to the case of one isolated mass defect, so as to compare the results with those obtained from perturbation theory.

Let us assume that the dynamical matrix associated with an imperfect lattice is

$$\boldsymbol{\Delta} = \boldsymbol{\Delta}_0 - \boldsymbol{\Delta}' \tag{1}$$

where $\boldsymbol{\Delta}_0$ is the dynamical matrix connected with the perfect lattice, while $\boldsymbol{\Delta}'$ contains the deviations of the imperfect from the perfect lattice. The characteristic equations can be written as usual

$$(\boldsymbol{\Delta} - \lambda \mathbf{I})\, \mathbf{u} = 0 \quad \text{or} \quad (\boldsymbol{\Delta}_0 - \lambda \mathbf{I} - \boldsymbol{\Delta}')\, \mathbf{u} = 0 \tag{2}$$

in which $\mathbf{u}$ is an N-dimensional column vector.

Eq. (2) can be rewritten as follows:

$$\mathbf{u} = \mathbf{G}\boldsymbol{\Delta}'\, \mathbf{u} \tag{3}$$

$\mathbf{G}$ is the Green's matrix of $\boldsymbol{\Delta}_0$,

$$\mathbf{G} = (\boldsymbol{\Delta}_0 - \lambda\mathbf{I})^{-1} \tag{4}$$

defined for all λ not on the spectrum of $\boldsymbol{\Delta}_0$. Eq. (3) can be useful in solving for $\mathbf{u}$ by the method of successive approximations. More important is the fact that if only a few of the $\boldsymbol{\Delta}'$-elements are non-vanishing, then one can find the characteristic equation explicitly in terms of the Green's matrix elements from eq. (3). It is essential therefore to possess explicit expressions for the elements g_{rj} of $\mathbf{G}$. In eq. (22) of Appendix D these elements are given by

$$g_{rj} = \sum_{k=1}^{N} \frac{T_{rk}\, T^{-1}_{kj}}{\lambda_k^{(0)} - \lambda} \tag{5}$$

in which $\lambda_k^{(0)}$ and T_{pq} denote, respectively, the eigenvalues of $\boldsymbol{\Delta}_0$ and the elements of its diagonalizing matrix $\mathbf{T}$. For generalized matrices the scalar indices will be replaced by vectors of appropriate dimensionality.

For the case of one-dimensional systems with simple $\boldsymbol{\Delta}'$ perturbations, the characteristic equation can be written down directly without using Green's functions. For higher dimensional lattices, the method seems to be indispensable for finding the characteristic equation of the perturbed lattice, even though the exact forms of the Green's functions are not known, i.e., the sums in eq. (5) cannot be evaluated in closed form.

It is clear that once the characteristic equation is known, the mode of its solution is independent of the Green's function method. The same applies to the evaluation of the eigenvectors $\mathbf{u}$ of eq. (2).

In the rest of this chapter we apply second order perturbation theory to a monatomic linear chain with one isotopic impurity, symmetrically situated, and rigid boundary conditions.

We assume therefore

$$\Delta_0 = \begin{pmatrix} a & b & & & 0 \\ b & a & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & b \\ 0 & & & b & a \end{pmatrix}_{2n+1} ; \quad (\Delta')_{k\ell} = a' \, \delta_{k,n+1} \, \delta_{\ell,n+1} \tag{6}$$

with

$$\left.\begin{array}{ll} a = 2\alpha - M\omega^2 ; & b = -\alpha \\ a' = -\epsilon M \omega^2 ; & \epsilon = 1 - \dfrac{M'}{M} \end{array}\right\} \tag{7}$$

The eigenvalues of Δ_0 are

$$\lambda_k^{(0)} = a + 2b \cos \frac{\pi k}{2n+2} ; \quad k = 1, \ldots, 2n+1 \tag{8}$$

In the remainder of this chapter we shall use the notation $\theta = \pi/2n+1$. To apply perturbation theory we first bring Δ_0 to diagonal form by performing the similarity transformation $\mathbf{T}$ given in eq. (12) of Appendix E. Then the matrix to be treated by perturbation is

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{H}' \tag{9}$$

with

$$(\mathbf{H}_0)_{rk} = \lambda_k^{(0)} \, \delta_{rk} ; \quad \mathbf{H}'_{\ell j} = -\frac{a'}{n+1} \sin \frac{\pi \ell}{2} \sin \frac{\pi j}{2} \tag{10}$$

Since the eigenvalues $\lambda_k^{(0)}$ are simple we can use ordinary perturbation theory. Then to second order in a' the eigenvalues λ_k will be given by:

$$\lambda_k = a + 2b\cos k\theta - \frac{a'}{n+1}\left(\sin\frac{\pi k}{2}\right)^2$$

$$+ \left(\frac{a'}{n+1}\right)^2 \left(\sin\frac{\pi k}{2}\right)^2 \sum_{\substack{r=1 \\ r\neq k}}^{2n+1} \frac{\left(\sin\frac{\pi r}{2}\right)^2}{2b\,(\cos k\theta - \cos r\theta)} \qquad (11)$$

It is clear immediately from the form (10) of $\mathbf{H}'_{\ell j}$ and eq. (11) that for $k = 2j$; $j = 1, \ldots, n$, we obtain to all orders

$$\lambda_{2j} = \lambda_{2j}^{(0)} = a + 2b\cos\frac{\pi j}{n+1}\,; \qquad j = 1, \ldots, n \qquad (12)$$

Note that the eigenfrequencies in eq. (12) correspond also to a monatomic linear chain of n particles with rigid boundary conditions. The result that n frequencies are not perturbed by an isotopic mass defect situated at the center of symmetry can be arrived at also by purely matric methods.

Returning to eq. (11) and putting $k = 2j - 1$; $j = 1, \ldots, n+1$ we can write

$$\lambda_{2j-1} = a + 2b\cos(2j-1)\theta - \frac{a'}{n+1} + \frac{1}{2b}\left(\frac{a'}{n+1}\right)^2 \sum_{\substack{r=1 \\ r\neq j}}^{n+1} \frac{1}{\cos(2j-1)\theta - \cos(2r-1)\theta}$$

The restricted sum in eq. (13) can be rewritten as follows

$$\sum_{\substack{r=1 \\ r\neq j}}^{n+1} \frac{1}{\cos(2j-1)\theta - \cos(2r-1)\theta} = \sum_{\substack{r=1 \\ r\neq 2j-1}}^{2n+1} \frac{1}{\cos(2j-1)\theta - \cos r\theta} -$$

$$- \sum_{r=1}^{n} \frac{1}{\cos(2j-1)\theta - \cos\frac{\pi r}{n+1}} \tag{14}$$

The unrestricted sum in eq. (14) can be evaluated in closed form by using eq. (6) of Appendix D with

$$\left.\begin{aligned} F(\lambda) &= \frac{1}{U}\,[V^{n-1} - V^{-n-1}] \\ U &= \sqrt{\lambda^2 - 1}; \quad V = \lambda + U \end{aligned}\right\} \tag{15}$$

Then

$$F'(\lambda) = -\frac{\lambda}{U^2}\,F(\lambda) + \frac{n+1}{U^2}\,[V^{n+1} + V^{-n-1}] \tag{16}$$

Substituting $\cos(2j-1)\theta$ for λ in $F'(\lambda)/F(\lambda)$ we obtain the value of the unrestricted sum

$$\sum_{r=1}^{n} \frac{1}{\cos(2j-1)\theta - \cos\frac{\pi r}{n+1}} = \frac{\cos(2j-1)\theta}{\sin^2(2j-1)\theta} \tag{17}$$

To evaluate the restricted sum on the r.h.s. of eq. (14) we have to use formula (16) of Appendix D, this time with

$$F(\lambda) = \frac{1}{U}\,[V^{2n+2} - V^{-2n-2}] \tag{18}$$

where U and V are as defined in eq. (15). For this function we have

$$\begin{aligned} F'(\lambda) &= -\frac{\lambda}{U^2}\,F(\lambda) + \frac{2n+2}{U^2}\,[V^{2n+2} + V^{-2n-2}] \\ F''(\lambda) &= \left[\frac{(2n+2)^2 - 1}{U^2} + \frac{2\lambda^2}{U^4}\right] F(\lambda) - \frac{\lambda}{U^2}\,F'(\lambda) - \frac{4(n+1)\lambda}{U^4}\,[V^{2n+2} - V^{-2n-2}] \end{aligned} \tag{19}$$

Substituting $\cos(2j-1)\theta$ for λ in $F''(\lambda)/F'(\lambda)$ we finally obtain

$$\sum_{\substack{r=1 \\ r\neq 2j-1}}^{2n+1} \frac{1}{\cos(2j-1)\theta - \cos r\theta} = \frac{3}{2}\,\frac{\cos(2j-1)\theta}{\sin^2(2j-1)\theta} \tag{20}$$

Collecting results we can write for λ_k

$$\lambda_{2j-1} = a + 2b\cos(2j-1)\theta - \frac{a'}{n+1} + \frac{1}{4b}\left(\frac{a'}{n+1}\right)^2 \frac{\cos(2j-1)\theta}{\sin^2(2j-1)\theta}$$

$$j = 1, \ldots, n+1; \qquad \theta = \frac{\pi}{2n+2} \tag{21}$$

It can be shown that the contribution to λ_{2j-1} from third order vanishes identically and it is probably true that all odd order contributions vanish.

We proceed now to the evaluation of the eigenvectors to the same order of approximation. These are linear combinations of the eigenvectors $\mathbf{u}_r^{(0)}$ for the unperturbed lattice. In our case the components of $\mathbf{u}_r^{(0)}$ are

$$u^{(0)}_{\ell r} = \frac{1}{\sqrt{n+1}} \sin \frac{\pi r \ell}{2n+2} ; \qquad r, \ell = 1, \ldots, 2n+1 \tag{22}$$

Then if $\mathbf{u}_k$ is the eigenvector associated with λ_k of eq. (11) and $u_{\ell k}$ its components, we obtain on using eq. (22) and second order perturbation theory:

$$u_{\ell k} = \frac{1}{\sqrt{n+1}} \Bigg\{ \sin k\ell\theta - \frac{a'}{2b(n+1)} \sin\frac{\pi k}{2} \sum_{\substack{r=1 \\ r\neq k}}^{2n+1} \frac{\sin\frac{\pi r}{2} \sin r\ell\theta}{\cos k\theta - \cos r\theta}$$

$$+ \frac{1}{4b^2}\left(\frac{a'}{n+1}\right)^2 \sin\frac{\pi k}{2} \left[\sum_{\substack{p=1 \\ p\neq k}}^{2n+1} \frac{\sin\frac{\pi p}{2} \sin p\ell\theta}{\cos k\theta - \cos p\theta}\right] \left[\sum_{\substack{r=1 \\ r\neq k}}^{2n+1} \frac{\left(\sin\frac{\pi r}{2}\right)^2}{\cos k\theta - \cos r\theta}\right]$$

$$- \frac{1}{4b^2}\left(\frac{a'}{n+1}\right)^2 \left(\sin\frac{\pi k}{2}\right)^3 \sum_{\substack{r=1 \\ r\neq k}}^{2n+1} \frac{\sin\frac{\pi r}{2} \sin r\ell\theta}{(\cos k\theta - \cos r\theta)^2}$$

$$- \frac{1}{8b^2}\left(\frac{a'}{n+1}\right)^2 \left(\sin\frac{\pi k}{2}\right)^2 \sin k\ell\theta \sum_{\substack{r=1 \\ r\neq k}}^{2n+1} \frac{\left(\sin\frac{\pi r}{2}\right)^2}{(\cos k\theta - \cos r\theta)^2} \Bigg\} ; \quad \theta = \frac{\pi}{2n+2} ; \; \ell, k = 1, \ldots, 2n+1 \tag{23}$$

All of the sums in eq. (23) can be evaluated exactly when use is made of the results in Appendix D. We denote these sums by S_m, $m = 1, 2, \ldots, 5$ according to their order of appearance in eq. (23). It is also seen that S_1 and S_2 are identical.

From eq. (23) we immediately find that for $k = 2j$, $j = 1, \ldots, n$, $\mathbf{u}_{2j}$ coincides with $\mathbf{u}^{(0)}_{2j}$. Again this result can be shown to be exact by using matric methods.

We consider now the sums S_m for $k = 2j-1$, $j = 1, \ldots, n+1$. Then the sum S_3 is identical with the one exhibited on the l.h.s. of eq. (14), and we have

$$S_3 = \frac{1}{2} \frac{\cos(2j-1)\theta}{\sin^2(2j-1)\theta} \tag{24}$$

The sum S_5 can be written as follows:

$$S_5 = S_5' - S_5'' \tag{25}$$

where

$$S_5' = \sum_{\substack{r=1 \\ r \neq 2j-1}}^{2n+1} \frac{1}{(\cos(2j-1)\theta - \cos r\theta)^2} \; ; \quad S_5'' = \sum_{r=1}^{n} \frac{1}{\left(\cos(2j-1)\theta - \cos\frac{\pi r}{n+1}\right)^2} \tag{26}$$

The sum S_5' can be easily evaluated on using formula (20) of Appendix D with $F(\lambda)$ given in eq. (18) above:

$$S_5' = \frac{16(n+1)^2 \sin^2(2j-1)\theta - 17\cos^2(2j-1)\theta - 16}{12\sin^4(2j-1)\theta} \tag{27}$$

Similarly the sum S_5'' can be evaluated by using formula (7) of the same Appendix with $F(\lambda)$ as given in eq. (15). The result is

$$S_5'' = \frac{(n+1)^2 \sin^2(2j-1)\theta - 1}{\sin^4(2j-1)\theta} \tag{28}$$

Finally

$$S_5 = \frac{4(n+1)^2 \sin^2(2j-1)\theta - 17\cos^2(2j-1)\theta - 4}{12\sin^4\frac{\pi(2j-1)}{2n+2}} \tag{29}$$

The sum S_1 can be written as

$$S_1 = \frac{1}{2} [S_1' + S_1''] \tag{30}$$

where

$$\begin{matrix} S_1' \\ \\ S_1'' \end{matrix} = \left\{ \sum_{\substack{r=1 \\ r\neq 2j-1}}^{2n+1} \frac{\cos mr\theta}{\cos (2j-1)\theta - \cos r\theta} \quad \begin{matrix} m = n+1-\ell \\ \\ m = n+1+\ell \end{matrix} \right. \tag{31}$$

For $1 \leq m \leq 2n+2$ the sum in eq. (31) can be evaluated by using formula (15) of Appendix D, with

$$\left.\begin{aligned} f(\lambda) &= V^{2n+2-m} + V^{-2n-2+m} \\ F(\lambda) &= U\,[V^{-2n+2} - V^{-2n-2}] \end{aligned}\right\} \tag{32}$$

The result is

$$\sum_{\substack{r=1 \\ r\neq 2j-1}}^{2n+1} \frac{\cos mr\theta}{\cos (2j-1)\theta - \cos r\theta} = \frac{1}{2\sin^2 (2j-1)\theta} \Big\{1 - (-1)^m + [1+(-1)^m] \cos(2j-1)\theta$$

$$+ \cos (2j-1)m\theta \cos (2j-1)\theta - 2(2n+2-m) \sin(2j-1)m\theta \sin(2j-1)\theta\Big\} \tag{33}$$

If we assume $\ell \leq n+1$, then both values of m in eq. (31) satisfy the restriction $1 \leq m \leq 2n+2$ for which eq. (33) is valid and we can write for S_1:

$$S_1 = \frac{1}{2\sin^2(2j-1)\theta}\Big\{1-(-1)^{n+1-\ell}+[1+(-1)^{n+1-\ell}]\cos(2j-1)\theta$$

$$-2(n+1)\sin\frac{\pi(2j-1)}{2}\sin(2j-1)\theta\cos(2j-1)\ell\theta\Big\}\ ; \quad \ell \le n+1 \qquad (34)$$

For $\ell > n+1$, the sum S_1'' becomes

$$S_1'' = \sum_{\substack{r=1\\ r\neq 2j-1}}^{2n+1} \frac{(-1)^r \cos pr\theta}{\cos(2j-1)\theta - \cos r\theta} \qquad (35)$$

where

$$p = \ell - n - 1.$$

This sum can be readily evaluated by using formula (15) of Appendix D with

$$\left.\begin{aligned} f(\lambda) &= V^p + V^{-p} \\ F(\lambda) &= U\,[V^{2n+2} - V^{-2n-2}] \end{aligned}\right\} \qquad (36)$$

The result is

$$S_1'' = \frac{1}{2\sin^2(2j-1)\theta}\Big\{1-(-1)^p+[1+(-1)^p]\cos(2j-1)\theta$$

$$-2p\sin(2j-1)p\theta\sin(2j-1)\theta - \cos(2j-1)p\theta\cos(2j-1)\theta\Big\} \qquad (37)$$

Finally combining eq. (37) with the result in eq. (33) (for $m = \ell - n - 1$) we obtain

$$S_1 = \frac{1}{2\sin^2(2j-1)\theta} \left\{ 1 - (-1)^{\ell-n-1} + [1 + (-1)^{\ell-n-1}] \cos(2j-1)\theta \right.$$

$$\left. + 2(n+1) \sin\frac{\pi(2j-1)}{2} \sin(2j-1)\theta \cos(2j-1)\ell\theta \right\} \quad ; \; \ell > n+1 \tag{38}$$

The last sum to be evaluated is S_4, which again can be decomposed into two sums

$$S_4 = \frac{1}{2}[S_4' + S_4''] \tag{39}$$

where

$$\left.\begin{matrix} S_4' \\ \\ S_4'' \end{matrix}\right\} = \sum_{\substack{r=1 \\ r \neq 2j-1}}^{2n+1} \frac{\cos mr\theta}{(\cos(2j-1)\theta - \cos r\theta)^2} \qquad \begin{matrix} m = n+1-\ell \\ \\ m = n+1+\ell \end{matrix} \tag{40}$$

The sum in eq. (40) can be written down by using formula (19) of the Appendix with

$$\left.\begin{aligned} f(\lambda) &= V^{2n+2-m} + V^{-2n-2+m} \\ F(\lambda) &= U[V^{2n+2} - V^{-2n-2}] \end{aligned}\right\} \quad \text{for} \quad 1 \le m \le 2n+2 \tag{41}$$

and

$$\left.\begin{aligned} f(\lambda) &= V^{m} + V^{-m} \\ F(\lambda) &= U[V^{2n+2} - V^{-2n-2}] \end{aligned}\right\} \quad \text{for} \quad 2n+2 < m \le 4n+4$$

The results are:

$$\sum_{\substack{r=1\\ r\neq 2j-1}}^{2n+1} \frac{\cos mr\theta}{[\cos(2j-1)\theta - \cos r\theta]^2} = \frac{1}{2\sin^4(2j-1)\theta} \Big\{ 2[(-1)^m - 1]\cos(2j-1)\theta$$

$$- [1+(-1)^m][1+\cos^2(2j-1)\theta] + (2n+2-m)^2 \cos m(2j-1)\theta \sin^2(2j-1)\theta$$

$$+ 2(2n+2-m)\sin m(2j-1)\theta\cos(2j-1)\theta\sin(2j-1)\theta$$

$$- \frac{1}{2}\cos m(2j-1)\theta\cos^2(2j-1)\theta - \frac{\cos m(2j-1)\theta}{3\sin^2(2j-1)\theta}[4\sin^2(2j-1)\theta +$$

$$+ 15\cos^2(2j-1)\theta - 4(n+1)^2\sin^2(2j-1)\theta]\Big\}$$

$$;\ 1 \le m \le 2n+2 \tag{43}$$

and

$$\sum_{\substack{r=1\\ r\neq 2j-1}}^{2n+1} \frac{(-1)^r \cos pr\theta}{[\cos(2j-1)\theta - \cos r\theta]^2} = \frac{1}{2\sin^4(2j-1)\theta} \Big\{ 2[(-1)^p - 1]\cos(2j-1)\theta$$

$$- [(-1)^p + 1][1+\cos^2(2j-1)\theta] + 2p\cos(2j-1)\theta\sin(2j-1)\theta\sin p(2j-1)\theta$$

$$- p^2\cos p(2j-1)\theta\sin^2(2j-1)\theta + \frac{1}{2}\cos p(2j-1)\theta\cos^2(2j-1)\theta$$

$$+ \frac{\cos p(2j-1)\theta}{3\sin^2(2j-1)\theta}[4\sin^2(2j-1)\theta + 15\cos^2(2j-1)\theta$$

$$- 4(n+1)^2\sin^2(2j-1)\theta]\Big\} \tag{44}$$

where

$$1 \le p = m - 2n - 2 \le 2n \quad \text{and} \quad m > 2n+2.$$

On using these results with the appropriate values of m from eq. (40), and inserting in eq. (39), we obtain

$$S_4 = \frac{1}{2\sin^4(2j-1)\theta}\Big\{2\,[(-1)^{n+1-\ell}-1]\cos(2j-1)\theta - [(-1)^{n+1-\ell}+1]\,[1+\cos^2(2j-1)\theta]$$

$$+\, 2\ell(n+1)\sin\frac{\pi(2j-1)}{2}\sin^2(2j-1)\theta\sin\ell(2j-1)\theta$$

$$+\, 2(n+1)\sin\frac{\pi(2j-1)}{2}\sin(2j-1)\theta\cos(2j-1)\theta\sin\ell(2j-1)\theta\Big\};\ 1\le\ell\le n+1 \tag{45}$$

and

$$S_4 = \frac{1}{2\sin^4(2j-1)\theta}\Big\{2\,[(-1)^{\ell-n-1}-1]\cos(2j-1)\theta - [(-1)^{\ell-n-1}+1]\,[1+\cos^2(2j-1)\theta]$$

$$+\, 2(n+1)(2n+2-\ell)\sin\frac{\pi(2j-1)}{2}\sin^2(2j-1)\theta\sin\ell(2j-1)\theta$$

$$+\, 2(n+1)\sin\frac{\pi(2j-1)}{2}\sin(2j-1)\theta\cos(2j-1)\theta\cos\ell(2j-1)\theta\Big\};\ n+1<\ell\le 2n+1 \tag{46}$$

Returning to the perturbed eigenvalues of eq. (21), we remark that using the techniques developed here one can obtain

$$\sum_{k=1}^{2n+1}\lambda_k = (2n+1)a - a' \equiv \mathfrak{T}r\,(\Delta_0 - \Delta') \tag{47}$$

where λ_{2j} are as in eq. (12) and λ_{2j-1} as in eq. (21). This shows that in this order of approximation the sum of the approximate eigenvalues is equal to the sum of the exact eigenvalues of $\Delta_0 - \Delta'$.

The approximate perturbed frequencies of the linear lattice are obtained from the equations

$$\lambda_{2j-1} = 0; \quad j = 1, \ldots, n+1 \tag{48}$$

with λ_{2j-1} from eq. (21). All of these are quadratic equations in ω^2 except for the particular case $n = 2r$, $s = 1, 2, \ldots$, which leads for $2j - 1 = n+1$ to the particular frequency

$$\omega^2 = \frac{2\alpha}{M}\left\{1 + \frac{\epsilon}{n+1} + \left(\frac{\epsilon}{n+1}\right)^2\right\} \tag{49}$$

In all other cases we solve for ω^2 to second order in ϵ, choosing those solutions of the quadratic equations resulting in real ω's:

$$\omega^2_{2j-1} \doteq \frac{4\alpha}{M}\sin^2\frac{\pi(2j-1)}{4(n+1)}\left\{1 + \frac{\epsilon}{n+1} + \frac{1 + \frac{1}{2}\cos\frac{\pi(2j-1)}{2n+2}}{1 + \cos\frac{\pi(2j-1)}{2n+2}}\left(\frac{\epsilon}{n+1}\right)^2\right\} \tag{50}$$

Eq. (50) shows that the perturbed frequencies will be decreased or increased with regard to the unperturbed ones, according to whether $\epsilon < 0$ (a heavier impurity mass) or $\epsilon > 0$ (a lighter impurity mass). This is in agreement with general theorems of Rayleigh [24] concerning the effect of additional constraints on arbitrary vibrating systems.

It is of interest to note that if we put $4\alpha/M = \omega_L^2$ (ω_L is then the top of the frequency band) and take $\epsilon > 0$, one of the frequencies in eq. (50) will emerge above ω_L as n becomes large. This can be seen by considering ω^2_{2n+1} :

$$\omega^2_{2n+1} = \omega_L^2\cos^2\frac{\pi}{4(n+1)}\left\{1 + \frac{\epsilon}{n+1} + \frac{1 - \frac{1}{2}\cos\frac{\pi}{2n+2}}{1 - \cos\frac{\pi}{2n+2}}\left(\frac{\epsilon}{n+1}\right)^2\right\} \tag{51}$$

Proceeding to the limit $n \to \infty$ in eq. (51) we find

$$\omega_{LO}^2 \equiv \lim_{n \to \infty} \omega_{2n+1}^2 = \omega_L^2 \left\{ 1 + \left(\frac{2\epsilon}{\pi} \right)^2 \right\} \tag{52}$$

This is the frequency of the "localized" mode, and has been obtained here directly from perturbation theory, in contradiction to statements that this is impossible [11]. Montroll & al. have shown [8] that the exact localized mode frequency can be obtained by proceeding to the same limit from the original eigenvalue equation. Their result is

$$\omega_{LO}^2 = \frac{\omega_L^2}{2 - \epsilon^2} \tag{53}$$

The discrepancy between eqs. (52) and (53) to second order in ϵ is due to a difference in boundary conditions.

APPENDIX A

EQUATIONS OF MOTION FOR TWO- AND THREE-DIMENSIONAL RECTANGULAR LATTICES

1. Two-Dimensional Lattices

1.1 Free Boundaries

Let us denote by

$$\mathbf{u}_{\ell,m} = \begin{pmatrix} u_{\ell,m} \\ v_{\ell,m} \end{pmatrix} \tag{1}$$

the displacement of the particle located at the site $\ell \mathbf{a}_1 + m\,\mathbf{a}_2$. Then we can write, for particles not situated on the boundary, the equations

$$\begin{aligned} M\frac{d^2 \mathbf{u}_{\ell,m}}{dt^2} &= \begin{pmatrix} \alpha & 0 \\ 0 & \alpha' \end{pmatrix} \{\mathbf{u}_{\ell+1,m} - 2\,\mathbf{u}_{\ell,m} + \mathbf{u}_{\ell-1,m}\} \\ &+ \begin{pmatrix} \beta' & 0 \\ 0 & \beta \end{pmatrix} \{\mathbf{u}_{\ell,m+1} - 2\,\mathbf{u}_{\ell,m} + \mathbf{u}_{\ell,m-1}\} \\ &+ \begin{pmatrix} \gamma & \delta \\ \delta & \gamma' \end{pmatrix} \{\mathbf{u}_{\ell+1,m+1} - 2\,\mathbf{u}_{\ell,m} + \mathbf{u}_{\ell-1,m-1}\} \\ &+ \begin{pmatrix} \gamma & -\delta \\ -\delta & \gamma' \end{pmatrix} \{\mathbf{u}_{\ell-1,m+1} - 2\,\mathbf{u}_{\ell,m} + \mathbf{u}_{\ell+1,m-1}\} \end{aligned} \tag{2}$$

in which $\ell = 2, \ldots, N_1 - 1$; $m = 2, \ldots, N_2 - 1$, and where

$$\left.\begin{aligned}
&\alpha = \alpha_1; \quad \alpha' = \alpha_1'; \quad \beta = \alpha_2; \quad \beta' = \alpha_2' \\
&\gamma = \alpha_3' + \frac{a_1^2}{a_1^2 + a_2^2}(\alpha_3 - \alpha_3'); \quad \gamma' = \alpha_3' + \frac{a_2^2}{a_1^2 + a_2^2}(\alpha_3 - \alpha_3') \\
&\delta = \frac{a_1 a_2}{a_1^2 + a_2^2}(\alpha_3 - \alpha_3')
\end{aligned}\right\} \tag{3}$$

If we write

$$\mathbf{u}_{\ell,m} = \mathbf{U}_{\ell,m}\, e^{i\omega t} \tag{4}$$

the eqs. (2) can be put in the reduced form

$$\begin{aligned}
&\mathbf{A}\mathbf{U}_{\ell,m} + \mathbf{B}\,[\mathbf{U}_{\ell+1,m} + \mathbf{U}_{\ell-1,m}] + \mathbf{C}\,[\mathbf{U}_{\ell,m+1} + \mathbf{U}_{\ell,m-1}] \\
&\quad + \mathbf{D}\,[\mathbf{U}_{\ell+1,m+1} + \mathbf{U}_{\ell-1,m-1}] + \mathbf{E}\,[\mathbf{U}_{\ell-1,m+1} + \mathbf{U}_{\ell+1,m-1}] = 0
\end{aligned} \tag{5}$$

where

$$\begin{aligned}
&\mathbf{A} = \begin{pmatrix} 2(\alpha + \beta' + 2\gamma) - M\omega^2 & 0 \\ 0 & 2(\alpha' + \beta + 2\gamma') - M\omega^2 \end{pmatrix} \\
&\mathbf{B} = \begin{pmatrix} -\alpha & 0 \\ 0 & -\alpha' \end{pmatrix}; \quad \mathbf{C} = \begin{pmatrix} -\beta' & 0 \\ 0 & -\beta \end{pmatrix}; \quad \mathbf{D} = \begin{pmatrix} -\gamma & -\delta \\ -\delta & -\gamma' \end{pmatrix}; \quad \mathbf{E} = \begin{pmatrix} -\gamma & \delta \\ \delta & -\gamma' \end{pmatrix}
\end{aligned} \tag{6}$$

In writing down the eqs. (2) use was made of eqs. (60) and (61) for finding the appropriate force density tensors $\mathbf{A}, \mathbf{B}, \ldots, \mathbf{E}$.

One can write down the equations of motion for particles on the boundary in a similar fashion. These will differ from eqs. (2) since a smaller number of neighbors is involved. Here we shall only incorporate results in the dynamical matrix.

It is not difficult to find the dynamical matrix if one adopts the particle labeling shown in Fig. 3 of Chapter I. Using this one-dimensional labeling and the reduced equations of motion, one obtains the dynamical matrix exhibited in eq. (62) of Chapter I, with

$$\begin{aligned} \mathbf{A}_1 &= \mathbf{A}+\mathbf{B}+\mathbf{D}+\mathbf{E} & \mathbf{A}_3 &= \mathbf{A}+\mathbf{B}+\mathbf{C}+\mathbf{D}+2\mathbf{E} \\ \mathbf{A}_2 &= \mathbf{A}+\mathbf{C}+\mathbf{D}+\mathbf{E} & \mathbf{A}_4 &= \mathbf{A}+\mathbf{B}+\mathbf{C}+2\mathbf{D}+\mathbf{E} \end{aligned} \tag{7}$$

and $\mathbf{A}, \mathbf{B}, \ldots, \mathbf{E}$ as in eq. (6).

1.2 Rigid Boundaries

With the same notation as above, the equations of motion for interior particles are as in eq. (5). The equations for marginal particles are obtained by using eq. (2) and the observation that a rigid wall, by definition, cannot move; i.e., its displacement vector $\mathbf{u}$ is zero. The changes obtained when the appropriate $\mathbf{u}$'s are suppressed, have been incorporated in the dynamical matrix for a monatomic lattice as shown in eq. (78) of Chapter I.

1.3 Periodic Boundaries

Again for interior particles the reduced equations are those shown in eq. (5). The periodicity of the boundary conditions imply that there are no marginal particles. For instance, the particle labeled 1 in Fig. 3 of Chapter I has as immediate neighbors the eight particles labeled there 2, N_1+1, N_1+2, N_1, $2N_1$, $(N_2-1)N_1+1$, $(N_2-1)N_1+2$, and N_2N_1. The resulting dynamical matrix for a monatomic lattice is shown in eq. (93) of Chapter I.

2. Three-Dimensional Lattices

The unit vectors $\boldsymbol{\varepsilon}$, $\boldsymbol{\xi}$, $\boldsymbol{\eta}$ and the force constants associated with the 26 immediate neighbors of the model described in §1.3 are given below in three groups.

1. First Neighbors

$\varepsilon,\ \alpha$	$\xi,\ \alpha'$	$\eta,\ \alpha''$
$\{\mathbf{k},\ -\mathbf{k}\} \longleftrightarrow \alpha_1$	$\{\mathbf{i},\ -\mathbf{i}\} \longleftrightarrow \alpha'_1$	$\{\mathbf{j},\ \mathbf{j}\} \longleftrightarrow \alpha''_1$
$\{\mathbf{j},\ -\mathbf{j}\} \longleftrightarrow \alpha_2$	$\{\mathbf{k},\ -\mathbf{k}\} \longleftrightarrow \alpha'_2$	$\{\mathbf{i},\ \mathbf{i}\} \longleftrightarrow \alpha''_2$
$\{\mathbf{i},\ -\mathbf{i}\} \longleftrightarrow \alpha_3$	$\{\mathbf{j},\ -\mathbf{j}\} \longleftrightarrow \alpha'_3$	$\{\mathbf{k},\ \mathbf{k}\} \longleftrightarrow \alpha''_3$

2. Second Neighbors

ε	β	ξ	β'	η	β''
$\dfrac{a_2\mathbf{j} + a_3\mathbf{k}}{a_{23}}$	β_3	$\dfrac{-a_3\mathbf{j} + a_2\mathbf{k}}{a_{23}}$	β'_3	$\mathbf{i}$	β''_3
$\dfrac{-a_2\mathbf{j} + a_3\mathbf{k}}{a_{23}}$	β_3	$-\dfrac{a_3\mathbf{j} + a_2\mathbf{k}}{a_{23}}$	β'_3	$\mathbf{i}$	β''_3
$-\dfrac{a_2\mathbf{j} + a_3\mathbf{k}}{a_{23}}$	β_3	$\dfrac{a_3\mathbf{j} - a_2\mathbf{k}}{a_{23}}$	β'_3	$\mathbf{i}$	β''_3
$\dfrac{a_2\mathbf{j} - a_3\mathbf{k}}{a_{23}}$	β_3	$\dfrac{a_3\mathbf{j} + a_2\mathbf{k}}{a_{23}}$	β'_3	$\mathbf{i}$	β''_3
$\dfrac{a_1\mathbf{i} + a_3\mathbf{k}}{a_{13}}$	β_2	$\dfrac{-a_3\mathbf{i} + a_1\mathbf{k}}{a_{13}}$	β'_2	$-\mathbf{j}$	β''_2
$\dfrac{-a_1\mathbf{i} + a_3\mathbf{k}}{a_{13}}$	β_2	$-\dfrac{a_1\mathbf{i} + a_3\mathbf{k}}{a_{13}}$	β'_2	$-\mathbf{j}$	β''_2
$-\dfrac{a_1\mathbf{i} + a_3\mathbf{k}}{a_{13}}$	β_2	$\dfrac{a_3\mathbf{i} - a_1\mathbf{k}}{a_{13}}$	β'_2	$-\mathbf{j}$	β''_2
$\dfrac{a_1\mathbf{i} - a_3\mathbf{k}}{a_{13}}$	β_2	$\dfrac{a_3\mathbf{i} + a_1\mathbf{k}}{a_{13}}$	β'_2	$-\mathbf{j}$	β''_2
$\dfrac{a_1\mathbf{i} + a_2\mathbf{j}}{a_{12}}$	β_1	$\dfrac{-a_2\mathbf{i} + a_1\mathbf{j}}{a_{12}}$	β'_1	$\mathbf{k}$	β''_1

ϵ	β	ξ	β'	η	β''
$\frac{-a_1\mathbf{i}+a_2\mathbf{j}}{a_{12}}$	β_1	$-\frac{a_2\mathbf{i}+a_1\mathbf{j}}{a_{12}}$	β_1'	$\mathbf{k}$	β_1''
$-\frac{a_1\mathbf{i}+a_2\mathbf{j}}{a_{12}}$	β_1	$\frac{a_2\mathbf{i}-a_1\mathbf{j}}{a_{12}}$	β_1'	$\mathbf{k}$	β_1''
$\frac{a_1\mathbf{i}-a_2\mathbf{j}}{a_{12}}$	β_1	$\frac{a_2\mathbf{i}+a_1\mathbf{j}}{a_{12}}$	β_1'	$\mathbf{k}$	β_1''

Above we have used the definitions

$$a_{pq} \equiv \sqrt{a_p^2 + a_q^2}\,; \qquad p, q = 1,\ 2,\ 3 \tag{8}$$

3. Third Neighbors

The eight third-nearest neighbors are equivalent with respect to the central particle on which they act, and therefore only three force constants appear: γ, γ', γ'' associated with ϵ, ξ, η, respectively.

ϵ	ξ	η
$\frac{a_1\mathbf{i}+a_2\mathbf{j}+a_3\mathbf{k}}{a}$	$\frac{-a_2\mathbf{i}+a_1\mathbf{j}}{a_{12}}$	$\frac{-a_1a_3\mathbf{i}-a_2a_3\mathbf{j}+a_{12}^2\mathbf{k}}{a_{12}a}$
$\frac{a_1\mathbf{i}-a_2\mathbf{j}+a_3\mathbf{k}}{a}$	$\frac{a_2\mathbf{i}+a_1\mathbf{j}}{a_{12}}$	$\frac{-a_1a_3\mathbf{i}+a_2a_3\mathbf{j}+a_{12}^2\mathbf{k}}{a_{12}a}$
$\frac{a_1\mathbf{i}-a_2\mathbf{j}-a_3\mathbf{k}}{a}$	$\frac{a_2\mathbf{i}+a_1\mathbf{j}}{a_{12}}$	$\frac{a_1a_3\mathbf{i}-a_2a_3\mathbf{j}+a_{12}^2\mathbf{k}}{a_{12}a}$
$\frac{a_1\mathbf{i}+a_2\mathbf{j}-a_3\mathbf{k}}{a}$	$\frac{-a_2\mathbf{i}+a_1\mathbf{j}}{a_{12}}$	$\frac{a_1a_3\mathbf{i}+a_2a_3\mathbf{j}+a_{12}^2\mathbf{k}}{a_{12}a}$
$\frac{-a_1\mathbf{i}+a_2\mathbf{j}+a_3\mathbf{k}}{a}$	$-\frac{a_2\mathbf{i}+a_1\mathbf{j}}{a_{12}}$	$\frac{a_1a_3\mathbf{i}-a_2a_3\mathbf{j}+a_{12}^2\mathbf{k}}{a_{12}a}$

ϵ	ξ	η
$\dfrac{-a_1\,\mathbf{i} + a_2\,\mathbf{j} - a_3\,\mathbf{k}}{a}$	$-\dfrac{a_2\,\mathbf{i} + a_1\,\mathbf{j}}{a_{12}}$	$\dfrac{-a_1 a_3\,\mathbf{i} + a_2 a_3\,\mathbf{j} + a_{12}^2\,\mathbf{k}}{a_{12}\,a}$
$\dfrac{-a_1\,\mathbf{i} - a_2\,\mathbf{j} + a_3\,\mathbf{k}}{a}$	$\dfrac{a_2\,\mathbf{i} - a_1\,\mathbf{j}}{a_{12}}$	$\dfrac{a_1 a_3\,\mathbf{i} + a_2 a_3\,\mathbf{j} + a_{12}^2\,\mathbf{k}}{a_{12}\,a}$
$-\dfrac{a_1\,\mathbf{i} + a_2\,\mathbf{j} + a_3\,\mathbf{k}}{a}$	$\dfrac{a_2\,\mathbf{i} - a_1\,\mathbf{j}}{a_{12}}$	$\dfrac{-a_1 a_3\,\mathbf{i} - a_2 a_3\,\mathbf{j} + a_{12}^2\,\mathbf{k}}{a_{12}\,a}$

Here a_{12} is as in eq. (8) and

$$a \equiv \sqrt{a_1^2 + a_2^2 + a_3^2} \tag{9}$$

Just as in the two-dimensional case, the equations of motion for particles not on the boundaries are the same for all boundary conditions involved. To write these down, we denote by $\mathbf{u}_{\ell mn}$ the 3-dimensional displacement vector of the particle located at the equilibrium position $\ell\mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3$ and introduce the time-independent vectors $\mathbf{U}$,

$$\mathbf{u}_{\ell mn} = \mathbf{U}_{\ell mn}\, e^{i\omega t} \tag{10}$$

For a <u>monatomic</u> lattice the reduced equations of motion read

$$\begin{aligned}
&\mathbf{A}\mathbf{U}_{\ell mn} + \mathbf{B}_1(\mathbf{U}_{\ell-1\,mn} + \mathbf{U}_{\ell+1\,mn}) + \mathbf{B}_2(\mathbf{U}_{\ell\,m-1\,n} + \mathbf{U}_{\ell\,m+1\,n}) \\
&+ \mathbf{B}_3(\mathbf{U}_{\ell mn-1} + \mathbf{U}_{\ell mn+1}) + \mathbf{C}_1(\mathbf{U}_{\ell-1\,m-1\,n} + \mathbf{U}_{\ell+1\,m+1\,n}) + \mathbf{C}_2(\mathbf{U}_{\ell-1\,m+1\,n} + \mathbf{U}_{\ell+1\,m-1\,n}) \\
&+ \mathbf{C}_3(\mathbf{U}_{\ell-1\,m\,n-1} + \mathbf{U}_{\ell+1\,m\,n+1}) + \mathbf{C}_4(\mathbf{U}_{\ell-1\,m\,n+1} + \mathbf{U}_{\ell+1\,m\,n-1}) + \mathbf{C}_5(\mathbf{U}_{\ell\,m-1\,n-1} + \mathbf{U}_{\ell\,m+1\,n+1}) \\
&+ \mathbf{C}_6(\mathbf{U}_{\ell\,m-1\,n+1} + \mathbf{U}_{\ell\,m+1\,n-1}) + \mathbf{D}_1(\mathbf{U}_{\ell-1\,m-1\,n-1} + \mathbf{U}_{\ell+1\,m+1\,n+1}) + \mathbf{D}_2(\mathbf{U}_{\ell-1\,m+1\,n-1} + \mathbf{U}_{\ell+1\,m-1\,n+1}) \\
&+ \mathbf{D}_3(\mathbf{U}_{\ell-1\,m+1\,n+1} + \mathbf{U}_{\ell+1\,m-1\,n-1}) + \mathbf{D}_4(\mathbf{U}_{\ell-1\,m-1\,n+1} + \mathbf{U}_{\ell+1\,m+1\,n-1}) = 0
\end{aligned} \tag{11}$$

The 3×3 matrices $\mathbf{B}_1, \ldots, \mathbf{D}_4$ are the appropriate force density tensors preceded by a (-) sign and are given as follows

$$-\mathbf{B}_1 = \mathrm{diag}(\alpha_1\ \alpha_1'\ \alpha_1''); \quad -\mathbf{B}_2 = \mathrm{diag}(\alpha_2''\ \alpha_2\ \alpha_2'); \quad -\mathbf{B}_3 = \mathrm{diag}(\alpha_3'\ \alpha_3''\ \alpha_3) \tag{12}$$

$$\underset{r=1,2}{-\mathbf{C}_r} = \frac{\beta_1}{a_{12}^2}\begin{pmatrix} a_1^2 & (-1)^{r+1}a_1a_2 & 0 \\ (-1)^{r+1}a_1a_2 & a_2^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{\beta_1'}{a_{12}^2}\begin{pmatrix} a_2^2 & (-1)^r a_1a_2 & 0 \\ (-1)^r a_1a_2 & a_1^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} + $$

$$+ \beta_1''\ \mathrm{diag}(0\ 0\ 1) \tag{13}$$

$$\underset{r=3,4}{-\mathbf{C}_r} = \frac{\beta_2}{a_{13}^2}\begin{pmatrix} a_1^2 & 0 & (-1)^{r+1}a_1a_3 \\ 0 & 0 & 0 \\ (-1)^{r+1}a_1a_3 & 0 & a_3^2 \end{pmatrix} + \frac{\beta_2'}{a_{13}^2}\begin{pmatrix} a_3^2 & 0 & (-1)^r a_1a_3 \\ 0 & 0 & 0 \\ (-1)^r a_1a_3 & 0 & a_1^2 \end{pmatrix} + $$

$$+ \beta_2''\ \mathrm{diag}(0\ 1\ 0) \tag{14}$$

$$\underset{r=5,6}{-\mathbf{C}_r} = \frac{\beta_3}{a_{23}^2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & a_2^2 & (-1)^{r+1}a_2a_3 \\ 0 & (-1)^{r+1}a_2a_3 & a_3^2 \end{pmatrix} + \frac{\beta_3'}{a_{23}^2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & a_3^2 & (-1)^r a_2a_3 \\ 0 & (-1)^r a_2a_3 & a_2^2 \end{pmatrix} + $$

$$+ \beta_3''\ \mathrm{diag}(1\ 0\ 0) \tag{15}$$

$$\underset{r=1,2}{-\mathbf{D}_r} = \frac{\gamma}{a^2}\begin{pmatrix} a_1^2 & (-1)^{r+1}a_1a_2 & a_1a_3 \\ (-1)^{r+1}a_1a_2 & a_2^2 & (-1)^{r+1}a_2a_3 \\ a_1a_3 & (-1)^{r+1}a_2a_3 & a_3^2 \end{pmatrix} + \frac{\gamma'}{a_{12}^2}\begin{pmatrix} a_2^2 & (-1)^r a_1a_2 & 0 \\ (-1)^r a_1a_2 & a_1^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} + $$

$$+ \frac{\gamma''}{a^2a_{12}^2}\begin{pmatrix} a_1^2a_3^2 & (-1)^{r+1}a_1a_2a_3^2 & -a_1a_3a_{12}^2 \\ (-1)^{r+1}a_1a_2a_3^2 & a_2^2a_3^2 & (-1)^r a_2a_3a_{12}^2 \\ -a_1a_3a_{12}^2 & (-1)^r a_2a_3a_{12}^2 & a_{12}^4 \end{pmatrix} \tag{16}$$

$$-\underset{r=3,4}{\mathbf{D}_r} = \frac{\gamma}{a^2}\begin{pmatrix} a_1^2 & (-1)^r a_1 a_2 & -a_1 a_3 \\ (-1)^r a_1 a_2 & a_2^2 & (-1)^{r+1} a_2 a_3 \\ -a_1 a_3 & (-1)^{r+1} a_2 a_3 & a_3^2 \end{pmatrix} + \frac{\gamma'}{a_{12}^2}\begin{pmatrix} a_2^2 & (-1)^{r+1} a_1 a_2 & 0 \\ (-1)^{r+1} a_1 a_2 & a_1^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} +$$

$$+\frac{\gamma''}{a^2 a_{12}^2}\begin{pmatrix} a_1^2 a_3^2 & (-1)^r a_1 a_2 a_3^2 & a_1 a_3 a_{12}^2 \\ (-1)^r a_1 a_2 a_3^2 & & (-1)^r a_2 a_3 a_{12}^2 \\ a_1 a_3 a_{12}^2 & (-1)^r a_2 a_3 a_{12}^2 & a_{12}^4 \end{pmatrix} \qquad (17)$$

The matrix **A** in eq. (11) is given by

$$-\mathbf{A} = 2\sum_{r=1}^{3} \mathbf{B}_r + 2\sum_{r=1}^{6} \mathbf{C}_r + 2\sum_{r=1}^{4} \mathbf{D}_r + M\omega^2 \mathbf{I} \qquad (18)$$

The number of distinct force constants in this model is 21. For a cubic unit cell this number reduces to 9, since by symmetry $\alpha_1 = \alpha_2 = \alpha_3$; $\alpha_1' = \alpha_2' = \alpha_3'$; $\alpha_1'' = \alpha_2'' = \alpha_3''$; $\beta_1 = \beta_2 = \beta_3$; $\beta_1' = \beta_2' = \beta_3'$; and $\beta_1'' = \beta_2'' = \beta_3''$.

The dynamical matrices for the several boundary conditions are obtained without much effort by using the eqs. of motion (11) and by adopting, instead of (ℓ, m, n), the one-dimensional labeling of particles shown in Fig. 5 of Chapter I. The matrices are exhibited in the appropriate sections of the same chapter.

APPENDIX B

EVALUATION OF THE INTEGRAL

$$A_{pq} = \int_0^{\pi} \int_0^{\pi} \frac{\cos p\theta \cos q\varphi \, d\theta d\varphi}{a + 2b \cos \theta + 2c \cos \varphi + 4d \cos \theta \cos \varphi}$$

We consider first the case $p = q = 0$, when an exact result can be given. We proceed to integrate first over θ.

To perform this integration we define

$$A = a + 2c \cos \varphi; \quad B = b + 2d \cos \varphi . \tag{1}$$

Then

$$a + 2b \cos \theta + 2c \cos \varphi + 4d \cos \theta \cos \varphi \equiv A + 2B \cos \theta \tag{2}$$

and the first integral to be evaluated is

$$I = \int_0^{\pi} \frac{d\theta}{A + 2B \cos \theta} . \tag{3}$$

The value of I is given in [16] where different parameters are used. Our needs here require that we give all possible cases in a different form for the more general integral I_n:

$$I_n \equiv \int_0^{\pi} \frac{\cos n\theta}{A + 2B \cos \theta} \, d\theta =$$

$$
= \begin{cases} \dfrac{\pi}{\sqrt{A^2 - 4B^2}} \left(\dfrac{\sqrt{A^2 - 4B^2} - A \operatorname{sgn} A}{2B \operatorname{sgn} A} \right)^n \operatorname{sgn} A; & |A| > 2|B| \\[2ex] \dfrac{\pi}{2\sqrt{A^2 - 4B^2}} \left[\left(\dfrac{\sqrt{A^2 - 4B^2} - A}{2B} \right)^n - \left(- \dfrac{\sqrt{A^2 - 4B^2} + A}{2B} \right)^n \right]; & |A| \le 2|B| \\ \text{(In this case the integral exists only as a principal value)} & \end{cases} \tag{4}
$$

where

$$
\operatorname{sgn} A = \begin{cases} +1 & A > 0 \\ -1 & A < 0 . \end{cases} \tag{5}
$$

Then

$$
I = \begin{cases} \dfrac{\pi}{\sqrt{A^2 - 4B^2}} \operatorname{sgn} A & |A| > 2|B| \\ 0 & \text{otherwise} . \end{cases} \tag{6}
$$

We assume now that the following conditions are satisfied by b, c, and d:

$$
b,\ c,\ d < 0; \qquad |b| \ge |c| > 2|d| . \tag{7}
$$

Then it is clear that $B < 0$, and we have to consider the two possible cases for all φ: i) $A < 0$; ii) $A > 0$. The case $A = 0$ can be obtained as a limiting value from either i) or ii). If A vanishes for some φ's, the same treatment can be given for the subintervals where the cases i) and ii) are pertinent.

i) $A < 0$

Here the conditions $|A| > 2|B|$ and $0 \le \varphi \le \pi$ imply

$$
-(a + 2c \cos \varphi) > -2(b + 2d \cos \varphi) \tag{8}
$$

or using (7)

$$
\cos \varphi > \frac{a + 2|b|}{2(|c| - 2|d|)} . \tag{9}
$$

Let us define now

$$u \equiv \frac{a + 2|b|}{2(|c| - 2|d|)} . \tag{10}$$

The remaining integral will not vanish only if $u < 1$ since $-1 \leq \cos \varphi \leq 1$. This condition places a restriction on the possible values of the parameter a.

Then

$$A_{00} = -\pi \int_0^{\pi} \frac{d\varphi}{\sqrt{A^2 - 4B^2}} . \tag{11}$$

The substitution $x = \cos \varphi$ in eq. (11) yields

$$A_{00} = -\pi \int \frac{dx}{\sqrt{(1 - x^2)\,[(a - 2|c|\,x)^2 - 4(|b| + 2|d|\,x)^2]}} \tag{12}$$

where the limits of integration will be determined by considering the two possibilities: $u > -1$ or $u < -1$.

(1) $\underline{u < -1}$

$$A_{00} = \frac{-\pi}{2\sqrt{|c|^2 - 4|d|^2}} \int_{-1}^{+1} \frac{dx}{\sqrt{(1 - x^2)\,(v - x)\,(u - x)}} \tag{13}$$

and

$$v \equiv \frac{a - 2|b|}{2(|c| + 2|d|)} . \tag{14}$$

The integral in eq. (13) can be transformed into a complete elliptic integral of the first kind if the location of v with respect to the interval $[-1, 1]$ is given. For definiteness let us assume that $v < u$. Then a substitution prescribed by Erdelyi [15]

$$x = \frac{u - 1 - 2u \sin^2 \phi}{1 - u - 2 \sin^2 \phi} \tag{15}$$

leads to the result

$$A_{00} = - \frac{\pi}{\sqrt{|c|^2 - 4|d|^2}} \; \frac{1}{\sqrt{(1-u)(-1-v)}} \; K\left(\sqrt{\frac{2(u-v)}{(1-u)(-1-v)}}\right) \tag{16}$$

where K(k) is the complete elliptic integral of the first kind of modulus k.

(2) $\underline{u > -1}$

Again assuming $v < u$, we have the subcases $v < -1$ and $v > -1$. Then the integral A_{00} is given by

$$A_{00} = - \frac{\pi}{2\sqrt{|c|^2 - 4|d|^2}} \int_u^{+1} \frac{dx}{\sqrt{(1-x^2)(v-x)(u-x)}}$$

$$= - \frac{\pi}{\sqrt{|c|^2 - 4|d|^2}} \begin{cases} \dfrac{1}{\sqrt{2(u-v)}} \, K\left(\sqrt{\dfrac{(1-u)(-1-v)}{2(u-v)}}\right); & v < -1 \\[2ex] \dfrac{1}{\sqrt{(1-v)(1+u)}} \, K\left(\sqrt{\dfrac{(1-u)(1+v)}{(1-v)(1+u)}}\right); & v > -1 \end{cases} \tag{17}$$

ii) $\underline{A > 0}$

Here the conditions $|A| > 2|B|$ and $0 \leq \varphi \leq \pi$ imply

$$a + 2c \cos\varphi > -2(b + 2d\cos\varphi) \tag{18}$$

or using the inequalities (7) and definition (14) we get

$$\cos\varphi < v. \tag{19}$$

Hence if $v < -1$ the integral will vanish and two subcases have to be considered: (1) $-1 < v < 1$ and (2) $v > 1$.

(1) $\underline{-1 < v < 1}$

The substitution $x = \cos\varphi$ in eq. (11) yields in this case

$$A_{00} = \frac{\pi}{2\sqrt{|c|^2 - 4|d|^2}} \int_{-1}^{v} \frac{dx}{\sqrt{(1-x^2)(x-v)(x-u)}} \tag{20}$$

As before we assume $u > v$. The final result will again depend on whether $u > 1$ or $u < 1$. Performing the appropriate transformations we obtain

$$A_{00} = \frac{\pi}{\sqrt{|c|^2 - 4|d|^2}} \begin{cases} \dfrac{1}{\sqrt{(1-v)(1+u)}} K\left(\sqrt{\dfrac{(1+v)(1-u)}{(1-v)(1+u)}}\right); & u < 1 \\ \dfrac{1}{\sqrt{2(u-v)}} K\left(\sqrt{\dfrac{(1+v)(u-1)}{2(u-v)}}\right); & u > 1 \end{cases} \tag{21}$$

(2) $\underline{v > 1}$

A similar procedure produces the result

$$A_{00} = \frac{\pi}{2\sqrt{|c|^2 - 4|d|^2}} \int_{-1}^{+1} \frac{dx}{\sqrt{(1-x^2)(x-v)(x-u)}}$$

$$= \frac{\pi}{\sqrt{|c|^2 - 4|d|^2}} \frac{1}{\sqrt{(1+v)(u-1)}} K\left(\sqrt{\frac{2(u-v)}{(1+v)(u-1)}}\right). \tag{22}$$

We return now to the general integral A_{pq}, for which an asymptotic approximation is required when both p and q are large. We follow here Weiss et al. [41] who, in a different context, have evaluated a similar integral by making use of certain asymptotic results of Duffin [42]. The argument is based on the remark that the main contribution to A_{pq} comes from the neighborhood of the stationary point of the denominator, located here at $(\theta = 0,\ \varphi = 0)$. Expansion of the denominator around this point leads then to

$$A_{pq} \sim \int_0^{\pi}\int_0^{\pi} \frac{\cos p\theta \cos q\varphi \, d\theta \, d\varphi}{a + 2b + 2c + 4d - (c + 2d)\varphi^2 - (b + 2d - d\varphi^2)\theta^2}. \tag{23}$$

This can be written also as

$$A_{pq} \sim \int_0^{\pi}\int_0^{\pi} \frac{\cos q\varphi \cos p\theta \, d\theta \, d\varphi}{C + D\theta^2} \tag{24}$$

with

$$\left.\begin{aligned} C &\equiv a - 2(|b| + |c| + 2|d|) + (|c| + 2|d|)\,\varphi^2 \\ D &\equiv |b| + 2|d| - |d|\,\varphi^2 \end{aligned}\right\} . \tag{25}$$

The range of integration over θ can be taken as $(0, \infty)$ with an exponentially small error, since we assume p to be large:

$$A_{pq} \sim \int_0^{\pi} d\varphi \cos q\varphi \int_0^{\infty} \frac{\cos p\theta \, d\theta}{C + D\theta^2} . \tag{26}$$

We consider first the case $\operatorname{sgn} C = \operatorname{sgn} D$, for all φ's near $\varphi = 0$. This implies $a \geq 2|b| + 4|d|$ when eq. (7) is used. The inner integral is then an ordinary Fourier cosine transform and from Tables [19] we find:

$$A_{pq} \sim \int_0^{\pi} \frac{d\varphi \cos q\varphi}{D} \frac{\pi}{2} \sqrt{\frac{D}{C}} \exp\left\{ - p \sqrt{\frac{C}{D}} \right\}$$

$$= \frac{\pi}{2} \int_0^{\pi} \frac{\cos q\varphi}{\sqrt{CD}} \exp\left\{ - p \sqrt{\frac{C}{D}} \right\} d\varphi . \tag{27}$$

Since q is large we expand this result once more, this time in the neighborhood of $\varphi = 0$, and extend the integration over $(0,\infty)$:

$$A_{pq} \sim \frac{\pi}{2} \int_0^{\infty} \frac{\cos q\varphi}{R + S\varphi^2} \exp\left\{ - p\left[\rho + \sigma\varphi^2\right] \right\} d\varphi \tag{28}$$

in which

$$\left\{\begin{aligned} &\rho = \sqrt{\frac{a - 2(|b| + |c| + 2|d|)}{|b| + 2|d|}} ; \qquad \sigma = \frac{a|d| + |bc|}{2(|b| + 2|d|)^{3/2} \left[a - 2(|b| + |c| + 2|d|)\right]^{1/2}} \\ &R = \left[(a - 2(|b| + |c| + 2|d|))(|b| + 2|d|)\right]^{1/2}; \\ &S = \frac{(|c| + 2|d|)(|b| + 2|d|) - |d|\left[a - 2(|b| + |c| + 2|d|)\right]}{R} \end{aligned}\right. \tag{29}$$

We assume now $S > 0$. Then the integration in eq. (28) can be carried out [19]:

$$A_{pq} \sim \frac{\pi^2}{8\sqrt{RS}} e^{-p\rho} e^{\sqrt{p\sigma}\,R/S} \left[e^{-q\sqrt{R/S}} \operatorname{Erfc}\left(\sqrt{\frac{Rp\sigma}{S}} - \frac{q}{2\sqrt{p\sigma}}\right) + e^{q\sqrt{R/S}} \operatorname{Erfc}\left(\sqrt{\frac{Rp\sigma}{S}} + \frac{q}{2\sqrt{p\sigma}}\right)\right]. \tag{30}$$

For $q \to \infty$ the dominant term is the first one in the square brackets.

The case $S = 0$ leads again to a well defined result. Since originally we have considered values of φ only in the neighborhood of the origin, we disregard the singular case arising from $S < 0$.

We still have to consider the case $\operatorname{sgn} C \neq \operatorname{sgn} D$, for all φ near the origin. This will occur whenever $a - 2(|b| + |c| + 2|d|) < 0$. Then the inner integral in eq. (26) exists only as a principal value and we obtain

$$A_{pq} \sim -\frac{\pi}{2} \int_0^{\pi} \frac{\cos q\varphi}{\sqrt{-CD}} \sin p \sqrt{\frac{-C}{D}}\, d\varphi. \tag{31}$$

Expanding the functions $\sqrt{-C/D}$ and $\sqrt{-CD}$ around the origin $\varphi = 0$ and as before letting the upper limit of the integration go to infinity, A_{pq} can be written as

$$A_{pq} \sim -\frac{\pi}{2} \int_0^{\infty} \frac{\cos q\varphi}{R' - S'\varphi^2} \sin p[\rho' - \sigma'\varphi^2]\, d\varphi \tag{32}$$

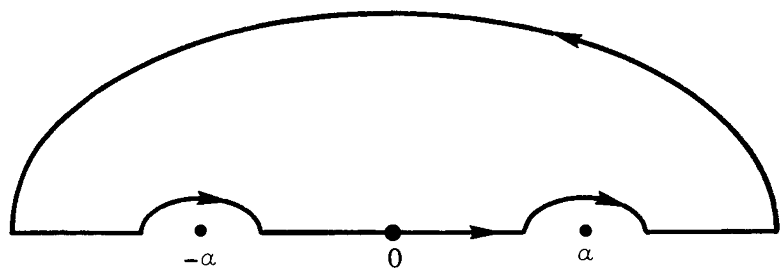
in which

$$\begin{cases} \rho' = \sqrt{\dfrac{2(|b| + |c| + 2|d|) - a}{|b| + 2|d|}}; \quad \sigma' = \dfrac{a|d| + |bc|}{2(|b| + 2|d|)^{3/2}\,[2(|b| + |c| + 2|d|) - a]^{1/2}} \\ R' = [(2(|b| + |c| + 2|d|) - a)(|b| + 2|d|)]^{1/2}; \\ S' = \dfrac{(|b| + 2|d|)(|c| + 2|d|) + (2(|b| + |c| + 2|d|) - a)|d|}{R'} \end{cases} \tag{33}$$

The integral in eq. (32) can be evaluated in the sense of a principal value by considering the integral of the function

$$\frac{e^{iqz} \sin p\,[\rho' - \sigma' z^2]}{z^2 - \alpha^2}$$

where $\alpha^2 = R'/S'$, along the contour shown in the figure.



The final result, obtained from residue theory, is

$$A_{pq} \sim -\frac{\pi^2}{4\sqrt{R'S'}} \sin q\sqrt{\frac{R'}{S'}} \sin p\left[\rho' - \sigma' \frac{R'}{S'}\right]. \tag{34}$$

APPENDIX C

FOURIER SERIES EXPANSION FOR

$\delta(a - \omega^2 + 2b \cos\theta + 2c \cos\varphi + 4d \cos\theta \cos\varphi)$

In the following we adapt the one-dimensional procedure of Lighthill [17] for expanding a generalized function in a Fourier series, to the two-dimensional case and apply this on the function of the title.

Setting

$$\delta(a - \omega^2 + 2b \cos\theta + 2c \cos\varphi + 4d \cos\theta \cos\varphi) = \sum_{m,n=-\infty}^{\infty} A_{mn}\, e^{im\theta}\, e^{in\varphi} \qquad (1)$$

the Fourier coefficients will be defined by

$$A_{mn} = \frac{1}{4\pi^2} \int_{-\infty}^{\infty} d\varphi\, e^{-in\varphi}\, V\left(\frac{\varphi}{2\pi}\right) \int_{-\infty}^{\infty} d\theta\, e^{-im\theta}\, U\left(\frac{\theta}{2\pi}\right) \times$$

$$\times\, \delta(a - \omega^2 + 2b \cos\theta + 2c \cos\varphi + 4d \cos\theta \cos\varphi) \qquad (2)$$

where the unitary functions U(x), V(y) have the following properties:

$$\sum_{m=-\infty}^{\infty} U(x + m\pi) = 1; \quad \sum_{n=-\infty}^{\infty} V(y + n\pi) = 1 \qquad (3)$$

for all x, y, and

$$\left.\begin{aligned} &U(x) = 0 \quad \text{for} \quad |x| \geq 1 \\ &U(x) + U(x-1) = 1 \quad \text{for} \quad 0 \leq x \leq 1 \\ &V(y) = 0 \quad \text{for} \quad |y| \geq 1 \\ &V(y) + V(y-1) = 1 \quad \text{for} \quad 0 \leq y \leq 1 \end{aligned}\right\} . \qquad (4)$$

Let us denote by $\theta_r^\pm$ the real roots of the equation

$$a - \omega^2 + 2c \cos \varphi + 2(b + 2d \cos \varphi) \cos \theta = 0 \tag{5}$$

considered as an equation in θ. Then

$$\theta_r^\pm = \begin{cases} \psi + 2r\pi \\ \\ -\psi + 2r\pi \end{cases} \qquad r = 0, \pm 1, \pm 2, \ldots \tag{6}$$

where ψ is taken as the principal branch of the function

$$\psi = \cos^{-1} \frac{\omega^2 - a - 2c \cos \varphi}{2(b + 2d \cos \varphi)} . \tag{7}$$

On the other hand the transformation properties of the δ-function lead to the representation

$$\delta(a - \omega^2 + 2b \cos \theta + 2c \cos \varphi + 4d \cos \theta \cos \varphi) =$$

$$= \sum_{r=-\infty}^{\infty} \frac{1}{2|b + 2d \cos \varphi|} \left[\frac{\delta(\theta - \theta_r^+)}{|\sin \theta_r^+|} + \frac{\delta(\theta - \theta_r^-)}{|\sin \theta_r^-|} \right] . \tag{8}$$

Inserting eq. (8) in eq. (2) and performing the integration over θ, we obtain:

$$A_{mn} = \frac{1}{4\pi^2} \int_{-\infty}^{\infty} d\varphi \, e^{-in\varphi} \, V\left(\frac{\varphi}{2\pi}\right) \frac{1}{2|b + 2d \cos \varphi|} \times$$

$$\times \sum_{r=-\infty}^{\infty} \left[U\left(\frac{\theta_r^+}{2\pi}\right) \frac{e^{-im\theta_r^+}}{|\sin \theta_r^+|} + U\left(\frac{\theta_r^-}{2\pi}\right) \frac{e^{-im\theta_r^-}}{|\sin \theta_r^-|} \right] . \tag{9}$$

Using now the form (6) of $\theta_r^\pm$ and taking account of the summation formula (3) for $U(x)$, the sum in (9) becomes simply

$$\frac{2 \cos m\psi}{|\sin \psi|} .$$

Therefore

$$A_{mn} = \frac{1}{4\pi^2} \int_{-\infty}^{\infty} d\varphi \, \frac{\cos m\psi}{|b + 2d \cos \varphi| \; |\sin \psi|} \, e^{-in\varphi} \, V\left(\frac{\varphi}{2\pi}\right). \tag{10}$$

The function of φ, the nth Fourier coefficient of which is to be evaluated in eq. (10), is now an ordinary function and its Fourier coefficients are defined in the usual way (Lighthill[17]). Hence

$$A_{mn} = \frac{1}{4\pi^2} \int_{-\pi}^{\pi} d\varphi \, \frac{\cos m\psi}{|b + 2d \cos \varphi| \; |\sin \psi|} \, e^{-in\varphi}$$

$$= \frac{1}{2\pi^2} \int_{0}^{\pi} \frac{\cos m\psi \cos n\varphi}{|b + 2d \cos \varphi| \; |\sin \psi|} \, d\varphi \, . \tag{11}$$

There exists a restriction on the integration over φ, since the assumption that the principal branch of (7) is to be taken, namely $0 \le \psi \le \pi$, leads to a condition on φ:

$$-1 \le \frac{\omega^2 - a - 2c \cos \varphi}{2(b + 2d \cos \varphi)} \le 1. \tag{12}$$

To find the limits of integration over φ, we must assume something about the parameters a, b, c, d (the range of values of ω^2 will follow automatically). We make the following choice

$$a > 2|b| + 2|c| + 4|d|; \quad |b| \ge |c| > 2|d|; \quad b,\ c,\ d < 0 \tag{13}$$

which represents the situation most frequently met in practice. Then solving for $\cos \varphi$ in eq. (12) and using eq. (13) we obtain

$$v \le \cos \varphi \le u \tag{14}$$

with

$$u \equiv \frac{a - \omega^2 + 2|b|}{2(|c - 2|d|)}; \quad v \equiv \frac{a - \omega^2 - 2|b|}{2(|c + 2|d|)} \, . \tag{15}$$

Since the largest possible range of $\cos\varphi$ is $-1 \le \cos\varphi \le 1$, we have to consider the positions of u, v relative to the interval $[-1, 1]$. A detailed analysis of the possible cases (under the assumptions (13)) furnishes the following results (a change of variable $\cos\varphi = x$ is implicit below):

$$A_{mn} = \begin{cases} \dfrac{1}{2\pi^2}\displaystyle\int_v^1 \dfrac{dx}{\sqrt{1-x^2}} f_{m,n}(x); & a-2|b|-2|c|-4|d| < \omega^2 < a-2|b|+2|c|+4|d| \\ & -1 < v < 1 < u \\ \dfrac{1}{2\pi^2}\displaystyle\int_{-1}^1 \dfrac{dx}{\sqrt{1-x^2}} f_{m,n}(x); & a-2|b|+2|c|+4|d| < \omega^2 < a+2|b|-2|c|+4|d| \\ & v < -1 < 1 < u \\ \dfrac{1}{2\pi^2}\displaystyle\int_{-1}^u \dfrac{dx}{\sqrt{1-x^2}} f_{m,n}(x); & a+2|b|-2|c|+4|d| < \omega^2 < a+2|b|+2|c|-4|d| \\ & v < -1 < u < 1 \end{cases} \tag{16}$$

in which

$$f_{mn}(x) = \frac{\cos n(\cos^{-1}x)\cos m\left(\cos^{-1}\dfrac{\omega^2 - a - 2cx}{2(b+2dx)}\right)}{|b+2dx|\left|\sin\left(\cos^{-1}\dfrac{\omega^2-a-2cx}{2(b+2dx)}\right)\right|}$$

$$= \frac{\cos n(\cos^{-1}x)\cos m\left(\cos^{-1}\dfrac{\omega^2 - a - 2cx}{2(b+2dx)}\right)}{\sqrt{|c|^2 - 4|d|^2}\sqrt{(x-v)(u-x)}}\ . \tag{17}$$

We note that a change in sign of m or n leaves A_{mn} invariant and hence the Fourier series for the δ-function will be a double cosine series. The theory of elliptic integrals [15] shows that with $f_{mn}(x)$ as in eq. (17) the integrals A_{mn} are in principle reducible to a linear combination of the three complete elliptic integrals, if a transformation to standard form is effected. For small values of m, n this can be done without much difficulty, but for large values it is more practical to find for A_{mn} asymptotic approximations.

We give below the explicit form of A_{00}. In the evaluation we use the appropriate transformations prescribed by Erdelyi [15].

$$A_{00} = \frac{1}{\pi^2 \sqrt{c^2 - 4d^2}} \begin{cases} \frac{1}{\sqrt{2(u-v)}} K\left(\sqrt{\frac{(1-v)(1+u)}{2(u-v)}}\right) \\ \frac{1}{\sqrt{1-v)(1+u)}} K\left(\sqrt{\frac{2(u-v)}{(1-v)(1+u)}}\right) \\ \frac{1}{\sqrt{2(u-v)}} K\left(\sqrt{\frac{(1-v)(1+u)}{2(u-v)}}\right) \end{cases} \tag{18}$$

The ranges of ω^2 for which (18) is valid are given in eq. (16).

We proceed now to find asymptotic expressions for A_{mn} and consider the three cases: (1) $n < m >> 1$; (2) $m < n >> 1$; (3) $m \approx n >> 1$.

Since A_{mn} has different forms in different ranges of ω^2, we discuss below only the first integral in eq. (16) which can be written as follows:*

$$I_{mn} = \frac{1}{2\pi^2 \sqrt{c^2 - 4d^2}} \int_0^{\cos^{-1} v} \frac{\cos n\varphi \cos m \left(\cos^{-1} \frac{a - \omega^2 - 2|c| \cos\varphi}{2(|b| + 2|d| \cos\varphi)}\right)}{\sqrt{(\cos\varphi - v)(u - \cos\varphi)}} d\varphi \tag{19}$$

where

$$-1 < v < 1 < u.$$

We see that I_{mn} has a branch point singularity at $\cos\varphi = v$ in the denominator and it is desirable therefore to use an approximation procedure which removes this singularity. Such a procedure is provided here by the stationary phase method.

Case 1: $n < m >> 1$

Here we consider the integral J_{mn},

$$J_{mn} = \frac{1}{\sqrt{c^2 - 4d^2}} \int_0^{\cos^{-1} v} g(\varphi)\, e^{imf(\varphi)}\, d\varphi \tag{20}$$

*The two other integrals in eq. (16) can be treated similarly.

in which

$$g(\varphi) = \frac{\cos n\varphi}{\sqrt{(\cos\varphi - v)(u - \cos\varphi)}} \; ; \qquad f(\varphi) = \cos^{-1} \frac{a - \omega^2 - 2|c| \cos\varphi}{2(|b| + 2|d| \cos\varphi)} \; . \tag{21}$$

Note that $I_{mn} = 1/2\, \pi^2\, \Re_e \{J_{mn}\}$. The function $f(\varphi)$ has a stationary point at $\varphi = 0$, and we obtain:

$$f(o) = \cos^{-1} \frac{a - \omega^2 - 2|c|}{2(|b| + 2|d|)}; \qquad f''(o) = - \frac{(a - \omega^2)\,|d| + |bc|}{\sqrt{c^2 - 4d^2}\,\sqrt{(1 - v)(u - 1)}\,(|b| + 2|d|)} \; . \tag{22}$$

It can also be easily verified that the function $g(\varphi)$ has the property

$$\lim_{\varphi \to 0} \frac{g(\varphi) - g(o)}{f'(\varphi)} = \lim_{\varphi \to 0} \frac{g'(\varphi)}{f''(\varphi)} < \infty \; . \tag{23}$$

Moreover, the function $(g(\varphi) - g(0))/f'(\varphi)$ has no singularity at $\cos\varphi = v$ and therefore is well-behaved throughout the interval of integration. Then all the conditions necessary for the application of the method are satisfied, and we find

$$J_{mn} = \sqrt{\frac{\pi}{m}} \; \frac{\sqrt{|b| + 2|d|}}{(c^2 - 4d^2)^{1/4}\,[(1 - v)(u - 1)]^{1/4}} \; \frac{1 - i}{2}\, e^{imf(o)} + O\left(\frac{1}{m}\right) \; . \tag{24}$$

The result in eq. (24) reflects the fact that sgn $f''(0) = -1$ and that the stationary point occurs at one end of the integration interval.

Finally

$$I_{mn} = \frac{\sqrt{|b| + 2|d|} \left\{ \cos m \left(\cos^{-1} \frac{a - \omega^2 - 2|c|}{2(|b| + 2|d|)} \right) + \sin m \left(\cos^{-1} \frac{a - \omega^2 - 2|c|}{2(|b| + 2|d|)} \right) \right\}}{4\sqrt{m\pi^3}\, \sqrt{(a - \omega^2)|d| + |bc|}\, (c^2 - 4d^2)^{1/4}\, [(1 - v)(u - 1)]^{1/4}}$$

$$+ O\left(\frac{1}{m}\right) \; . \tag{25}$$

For this order of approximation the result does not explicitly depend on n.

Case 2: $m < n \gg 1$

Here we first make a change of variable:

$$\cos\theta = \frac{a - \omega^2 - 2|c| \cos\varphi}{2(|b| + 2|d| \cos\varphi)} \,. \tag{26}$$

Then with this new variable, the integral I_{mn} becomes

$$I_{mn} = \frac{1}{\sqrt{b^2 - 4d^2}} \int_0^{\cos^{-1} v'} \frac{\cos m\theta \cos n \left(\cos^{-1} \dfrac{a - \omega^2 - 2|b| \cos\theta}{2(|c| + 2|d| \cos\theta)}\right)}{\sqrt{(\cos\theta - v')(u' - \cos\theta)}} \, d\theta \tag{27}$$

in which

$$v' \equiv \frac{a - \omega^2 - 2|c|}{2(|b| + 2|d|)}; \quad u' \equiv \frac{a - \omega^2 + 2|c|}{2(|b| - 2|d|)} \tag{28}$$

and

$$-1 < v' < 1 < u'.$$

The result follows immediately since now n has the role of m in the previous case also with respect to the form of the integrand. Then eq. (25) will be valid for this case too, when an appropriate identification of the parameters is carried out.

Case 3: $m \approx n \gg 1$

The author has been unable to find a meaningful asymptotic expression for this case by the stationary phase method. The method of steepest descent is not helpful either since here it becomes identical with the phase method.

APPENDIX D

PARTIAL FRACTION DECOMPOSITION AND SUMMATION OF FINITE SUMS

Let $F(\lambda)$ be a polynomial of degree N, and $f(\lambda)$ one of degree $M \leq N$. Assume that $F(\lambda)$ has j distinct roots λ_k with multiplicities p_k, such that

$$F(\lambda) = F_N \prod_{k=1}^{j} (\lambda - \lambda_k)^{p_k} . \qquad (1)$$

Then it is well-known that the following decomposition exists and is unique

$$\frac{f(\lambda)}{F(\lambda)} = \frac{f_M}{F_N} \delta_{M,N} + \sum_{k=1}^{j} \sum_{r=1}^{p_k} \frac{C_{rk}}{(\lambda - \lambda_k)^r} \qquad (2)$$

where C_{rk} are given by

$$C_{rk} = \frac{1}{(p_k - r)!} \frac{d^{p_k - r}}{d\lambda^{p_k - r}} \left\{ \frac{f(\lambda)(\lambda - \lambda_k)^{p_k}}{F(\lambda)} \right\} \Bigg|_{\lambda = \lambda_k} \qquad (3)$$

For simple roots, all $p_k = 1$ and the formula (2) becomes

$$\frac{f(\lambda)}{F(\lambda)} = \frac{f_M}{F_N} \delta_{M,N} + \sum_{k=1}^{N} \frac{C_k}{\lambda - \lambda_k} \qquad (4)$$

with

$$C_k = \frac{f(\lambda_k)}{F'(\lambda_k)} . \tag{5}$$

In the sequel we shall have use only for the simpler case (4) with the further restriction $M < N$. Several formulas are of particular interest:

$$\frac{F'(\lambda)}{F(\lambda)} = \sum_{k=1}^{N} \frac{1}{\lambda - \lambda_k} . \tag{6}$$

By repeated differentiation, eq. (6) yields

$$\frac{(-1)^{n-1}}{(n-1)!} \frac{d^{n-1}}{d\lambda^{n-1}} \left(\frac{F'(\lambda)}{F(\lambda)}\right) = \sum_{k=1}^{N} \frac{1}{(\lambda - \lambda_k)^n} \; ; \quad n \geq 1. \tag{7}$$

The result in eq. (7) can be extended by analytic continuation to all real n, the l.h.s. of eq. (7) being transformed then into an appropriate fractional derivative [43] of $\log F(\lambda)$.

These results suggest the possibility of their validity also for functions other than polynomials, e. g., functions possessing a discrete infinity of zeros which satisfy certain conditions of convergence. We shall not pursue this subject further here except for the following, well-known example:

Let $F(\lambda) = \sin \lambda$. Then formally

$$\sin \lambda = \prod_{n=-\infty}^{+\infty} (\lambda - \pi n) \tag{8}$$

and

$$\frac{F'(\lambda)}{F(\lambda)} \equiv \cot \lambda = \sum_{n=-\infty}^{+\infty} \frac{1}{\lambda - \pi n} . \tag{9}$$

A rearrangement is performed to produce convergence with the final result

$$\cot \lambda = \frac{1}{\lambda} + 2\lambda \sum_{n=1}^{\infty} \frac{1}{\lambda^2 - \pi^2 n^2} \tag{10}$$

otherwise obtained from complex function theory.

If the λ_k's are the characteristic roots of a matrix $\mathbf{\Delta}_N$, then eq. (7) gives a formula for evaluating the trace of $(\mathbf{\Delta}_N - \lambda \mathbf{I})^{-n}$, $F(\lambda)$ being the characteristic polynomial of $\mathbf{\Delta}_N$

$$F(\lambda) = |\mathbf{\Delta}_N - \lambda \mathbf{I}| . \tag{11}$$

The previous treatment can be extended in still another direction. Consider a sum of the type

$$S_r^{(1)} = \sum_{\substack{k=1 \\ k \neq r}}^{N} \frac{C_k}{\lambda_r - \lambda_k} . \tag{12}$$

To evaluate this sum we define a function $S^{(1)}(\lambda)$ which coincides with $S_r^{(1)}$ when $\lambda \to \lambda_r$:

$$S^{(1)}(\lambda) = \sum_{k=1}^{N} \frac{C_k}{\lambda - \lambda_k} - \frac{C_r}{\lambda - \lambda_r} = \frac{f(\lambda)}{F(\lambda)} - \frac{C_r}{\lambda - \lambda_r} . \tag{13}$$

The last result is obtained by substituting for the unrestricted sum from eq. (4), with $M < N$. $S^{(1)}(\lambda)$ can be rewritten as follows

$$S^{(1)}(\lambda) = \frac{f(\lambda) - C_r \dfrac{F(\lambda)}{\lambda - \lambda_r}}{F(\lambda)} . \tag{14}$$

It is to be noted now that $S^{(1)}(\lambda)$ becomes an indeterminate expression of the form 0/0, when $\lambda \to \lambda_r$. This is so because of the form (5) for the coefficients C_r. Using the L'Hôpital rule repeatedly we find

$$S_r^{(1)} = \frac{f'(\lambda_r)}{F'(\lambda_r)} - \frac{f(\lambda_r)F''(\lambda_r)}{2[F'(\lambda_r)]^2} . \tag{15}$$

A particularly simple relation is obtained for the case $f(\lambda) = F'(\lambda)$:

$$S_r^{(1)} \equiv \sum_{\substack{k=1 \\ k\neq r}}^{N} \frac{1}{\lambda_r - \lambda_k} = \frac{1}{2} \frac{F''(\lambda_r)}{F'(\lambda_r)} . \tag{16}$$

The evaluation of sums of higher powers

$$S_r^{(n)} \equiv \sum_{\substack{k=1 \\ k\neq r}}^{N} \frac{C_k}{(\lambda_r - \lambda_k)^n} \tag{17}$$

cannot be done simply by differentiating (15) or (16) with respect to λ_r, since $F'(\lambda_r)$, $F''(\lambda_r)$ depend on λ_r not only through their argument but also through their coefficients. It is much simpler therefore to use again the same procedure as above. We illustrate this for the sums (17) with $n = 2$, $S_r^{(2)}$.

We have to evaluate the expression

$$S_r^{(2)} \equiv \lim_{\lambda\to\lambda_r} \left\{ \sum_{k=1}^{N} \frac{C_k}{(\lambda - \lambda_k)^2} - \frac{C_r}{(\lambda - \lambda_r)^2} \right\}$$

$$= \lim_{\lambda\to\lambda_r} \left\{ -\frac{d}{d\lambda} \left(\frac{f(\lambda)}{F(\lambda)}\right) - \frac{C_r}{(\lambda - \lambda_r)^2} \right\}$$

$$= -\lim_{\lambda\to\lambda_r} \frac{f'(\lambda)F(\lambda) - f(\lambda)F'(\lambda) + C_r \left[\dfrac{F(\lambda)}{\lambda - \lambda_r}\right]^2}{[F(\lambda)]^2} \tag{18}$$

Again the limit process leads to the indeterminate form $0/0$ and we make use of the L'Hôpital rule several times to obtain:

$$S_r^{(2)} = -\frac{f''(\lambda_r)}{2F'(\lambda_r)} + \frac{f'(\lambda_r)F''(\lambda_r)}{2[F'(\lambda_r)]^2} - \frac{f(\lambda_r)[F''(\lambda_r)]^2}{4[F'(\lambda_r)]^3}$$

$$+ \frac{f(\lambda_r)F'''(\lambda_r)}{6[F'(\lambda_r)]^2} \quad . \tag{19}$$

For the case $f(\lambda) = F'(\lambda)$ we obtain the simpler expression

$$\sum_{\substack{k=1\\k\neq r}}^{N} \frac{1}{(\lambda_r - \lambda_k)^2} = \left[\frac{1}{2}\,\frac{F''(\lambda_r)}{F'(\lambda_r)}\right]^2 - \frac{1}{3}\,\frac{F'''(\lambda_r)}{F'(\lambda_r)} \quad .$$

For powers $n \geq 4$, the formulas become quite complicated. In Chapter IV the results in eqs. (16) and (20) are used to evaluate certain perturbation sums. Since one seldom considers perturbation approximations beyond the fourth order, the form of $S_r^{(n)}$ for arbitrary integral n is not needed.

The results in eqs. (16) and (20) can be extended to the functions discussed in the paragraph preceding eq. (8). Thus if again $F(\lambda) = \sin\lambda$ and in eq. (20) we take $\lambda_r = 0$, then

$$\sum_{k=-\infty}^{\infty} \frac{1}{\pi^2 k^2} = \frac{1}{3}$$

or

$$\sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6}$$

a well-known result, here following immediately from

$$F'(0) = 1; \; F''(0) = 0; \; \text{and} \; F'''(0) = -1.$$

In connection with applications below and in Chapter IV it is important to note that if <u>the polynomials $F(\lambda)$ and $f(\lambda)$ are known in closed form and if the roots λ_k are explicitly known also, then the formulas (4), (6), (7), (16) and (20), give closed form expressions for the corresponding finite sums.</u>

We proceed to apply some of these formulas to the exact evaluation of one-dimensional sums related to Green's functions of matrices appearing in the text.

The Green's matrix associated with a given matrix $\mathbf{\Delta}$ is by definition the matrix $\mathbf{G}$

$$\mathbf{G}(\lambda) \equiv (\mathbf{\Delta} - \lambda \mathbf{I})^{-1}. \tag{21}$$

If λ_k and $\mathbf{T}$ denote respectively the eigenvalues and diagonalizing matrix of $\mathbf{\Delta}$, then the elements $g_{rj}(\lambda)$ of $\mathbf{G}$ are given by

$$g_{rj}(\lambda) = \sum_{k=1}^{N} \frac{T_{rk}\, T^{-1}_{kj}}{\lambda_k - \lambda} \tag{22}$$

where we assume λ not to coincide with any of the eigenvalues of $\mathbf{\Delta}$.

It is readily seen that the sum in eq. (22) is of the type exhibited in eq. (4), with $M < N$ and $C_k \equiv - T_{rk} \; T^{-1}_{kj}$. If a polynomial $f_{rj}(\lambda)$ can be found such that

$$T_{rk}\, T^{-1}_{kj} = - \frac{f_{rj}(\lambda_k)}{F'(\lambda_k)} \tag{23}$$

where $F(\lambda)$ is the characteristic polynomial of $\mathbf{\Delta}$, then

$$g_{rj}(\lambda) = \frac{f_{rj}(\lambda)}{F(\lambda)} \; . \tag{24}$$

To illustrate the procedure we consider the Green's functions associated with a monatomic linear chain with fixed ends.

The dynamical matrix of this system is of the form shown in eq. (2) of Appendix E. Inserting in eq. (22) the λ_k and $T_{r\ell}$ there given, we find

$$g_{rj}(\lambda) = \frac{1}{N+1} \sum_{k=1}^{N} \left\{ \frac{\cos \frac{\pi(r-j)k}{N+1}}{a - \lambda + 2b\cos \frac{\pi k}{N+1}} + \frac{\cos \frac{\pi(r+j)k}{N+1}}{a - \lambda + 2b\cos \frac{\pi k}{N+1}} \right\} \tag{25}$$

$$r, j = 1, \ldots, N$$

Eq. (25) shows that we have to evaluate the sum

$$S(m, N) = \frac{1}{N+1} \sum_{k=1}^{N} \frac{\cos \frac{\pi m k}{N+1}}{\lambda - a - 2b\cos \frac{\pi k}{N+1}} . \tag{26}$$

Now eq. (7) of Appendix E gives for the characteristic polynomial of Δ

$$\mathcal{D}_N(\lambda) = (-1)^N b^{N+1} \frac{V^{N+1} - V^{-N-1}}{U} \tag{27}$$

with

$$U \equiv \sqrt{(\lambda - a)^2 - 4b^2} \; ; \; V \equiv \frac{\lambda - a + U}{2b} \tag{28}$$

It is not difficult to verify that if we take $F(\lambda)$ and $f(\lambda)$ in eq. (4) as follows

$$F(\lambda) = U^2 \mathcal{D}_N(\lambda) \; ; \; f(\lambda) = V^{N+1-m} + V^{-N-1+m} \tag{29}$$

where for the present $0 \le m \le N + 1$, then

$$C_k \equiv \frac{f(\lambda_k)}{F'(\lambda_k)} = \frac{1}{N+1} \cos \frac{\pi m k}{N+1} \quad ; k = 1, \ldots, N \tag{30}$$

and

$$C^{\pm} \equiv \frac{f(\lambda^{\pm})}{F'(\lambda^{\pm})} = \frac{(\pm 1)^m}{2(N+1)} \quad * \tag{31}$$

where

$$\lambda^{\pm} = a \pm 2b \, . \tag{32}$$

Finally we can write

$$S(m, N) = \frac{1}{U} \frac{V^{N+1-m} + V^{-N-1+m}}{V^{N+1} - V^{-N-1}} - \frac{1}{2(N+1)} \left[\frac{1}{\lambda - a - 2b} + \frac{(-1)^m}{\lambda - a + 2b} \right] \tag{33}$$

Since $m' = N + 1 - m$ satisfies $0 \le m' \le N + 1$, eq. (33) will be valid also for m', with the result:

$$S'(m, N) \equiv \frac{1}{N+1} \sum_{k=1}^{N} \frac{(-1)^k \cos \frac{\pi m k}{N+1}}{\lambda - a - 2b \cos \frac{\pi k}{N+1}} = \frac{1}{U} \frac{V^m + V^{-m}}{V^{N+1} - V^{-N-1}} -$$

$$- \frac{1}{2(N+1)} \left[\frac{1}{\lambda - a - 2b} + \frac{(-1)^{N+1-m}}{\lambda - a + 2b} \right] \tag{34}$$

*These coefficients are related to the polynomial U^2 in eq. (29).

The range of m in eq. (26) can be extended now to all integers by using eqs. (33) and (34).

For $m = 0$ we obtain from eq. (33)

$$\frac{1}{N+1} \sum_{k=1}^{N} \frac{1}{\lambda - a - 2b \cos \frac{\pi k}{N+1}} = - \frac{1}{N+1} \frac{\lambda - a}{U^2} + \frac{1}{U} \frac{V^{N+1} + V^{-N-1}}{V^{N+1} - V^{-N-1}} \tag{35}$$

It is easily seen now that

$$- g_{rj} = \begin{cases} S(r - j, N) + S(r + j, N) \\ \qquad r + j \leq N + 1 \\ \\ S(r - j, N) + S'(r + j - N - 1, N) \\ \qquad N + 1 < r + j \leq 2N \end{cases} \tag{36}$$

Other sums with closed form expressions can be obtained from (33) and (34) by addition, subtraction or proceeding to appropriate limits with the parameters involved. For instance, in the sum (33) the left hand side can be regarded as the Riemann sum associated with the integral

$$\frac{1}{\pi} \int_0^{\pi} \frac{\cos m\theta}{\lambda - a - 2b \cos \theta} \, d\theta$$

and letting $N \to \infty$ we obtain the value of this integral on the r.h.s. The value will depend on the position of V with respect to the unit circle.

We also remark that these results will be valid, if none of the denominators in the sums considered vanish, regardless of the nature of the parameters. If a, b were operators (e.g., matrices), the sole requirement for validity would be that these commute.

In principle the preceding treatment applies to finite sums in any number of dimensions. However, in practice, the application of these results is limited by the fact that the explicit forms of the appropriate polynomials are not known. In most cases one summation can be performed exactly but the rest have to be treated according to the methods of Chapter III.

APPENDIX E

MATRICES ASSOCIATED WITH PERIODIC SYSTEMS

Most of the material to be presented in this Appendix, while well-known, is rather scattered throughout the literature. Moreover the presentation there is frequently fragmentary, partial results being given as needed for specific applications. Also most of these results are obtained by determinantal methods which do not yield easily explicit expressions for the eigenvectors. For this reason the treatment to follow is done mainly by matrix methods, as these allow us to take into account more conveniently the various symmetries involved. The matrices to be subsequently listed are those met in the text together with some variants and generalizations which, to the author's knowledge, have not been published elsewhere. Each one of the matrices presented is accompanied, whenever possible, by its eigenvalues, eigenvectors and characteristic determinant.

The matrices will be classified according to the dimensionality of the problem from which they arise.

Part I. One Dimensional Matrices

1. Continuants

These matrices belong to particular subsets of the class of Jacobi matrices, the latter being defined by

$$J_N = \begin{pmatrix} a_1 & b_1 & & 0 \\ c_1 & \ddots & \ddots & b_{n-1} \\ & \ddots & \ddots & a_N \\ 0 & & & c_{N-1} \end{pmatrix} \tag{1}$$

(i) Simple Continuant

This matrix is defined by

$$\boldsymbol{\Delta}_N = \begin{pmatrix} a & b & & 0 \\ b & \ddots & \ddots & \\ & \ddots & \ddots & b \\ 0 & & b & a \end{pmatrix} \tag{2}$$

Its elements can be written in the form

$$(\boldsymbol{\Delta}_N)_{ij} = b\,\delta_{i-1,j} + a\,\delta_{ij} + b\,\delta_{i,j-1} \;;\; i,j = 1,\cdots, N \tag{3}$$

The characteristic polynomial is the determinant

$$\mathcal{D}_N(\lambda) \equiv |\boldsymbol{\Delta}_N - \lambda\,\mathbf{I}| \tag{4}$$

It can be easily verified that $\mathcal{D}_N(\lambda)$ satisfies the recurrence relation

$$\mathcal{D}_N = (a-\lambda)\,\mathcal{D}_{N-1} - b^2\,\mathcal{D}_{N-2} \tag{5}$$

The solution can be found by putting $\mathcal{D}_N = x^N$ and solving the quadratic equation in x that results. The solution is

$$\mathcal{D}_N(\lambda) = \frac{1}{\sqrt{(a-\lambda)^2 - 4b^2}}\left[\left(\frac{a-\lambda+\sqrt{(a-\lambda)^2-4b^2}}{2}\right)^{N+1} - \left(\frac{a-\lambda-\sqrt{(a-\lambda)^2-4b^2}}{2}\right)^{N+1}\right] \tag{6}$$

This can be written in a more symmetrical form as follows:

$$\mathcal{D}_N(\lambda) = (-1)^N\, b^{N+1}\, \frac{V^{N+1} - V^{-N-1}}{U} \tag{7}$$

where

$$U \equiv \sqrt{(\lambda-a)^2 - 4b^2} \;;\; V \equiv \frac{\lambda - a + U}{2b} \tag{8}$$

Various representations can be given to $\mathcal{D}_N(\lambda)$ when certain relations are imposed on a, λ and b. For instance, if one can write

$$a - \lambda = 2b \cos\varphi ; \quad 0 \leq \varphi \leq \pi$$

then

$$\mathcal{D}_N(\lambda) = (-1)^N b^N \frac{\sin(N+1)\varphi}{\sin\varphi} \tag{9}$$

The polynomial $\dfrac{\sin[(N+1)(\cos^{-1}x)]}{\sin(\cos^{-1}x)}$ is known as the Chebishev polynomial of the second kind.

The eigenvalues λ_k of $\mathbf{\Delta}_N$ can be immediately found from $\mathcal{D}_N(\lambda) = 0$ by using eq. (7):

$$\lambda_k = a + 2b\cos\frac{\pi k}{N+1} \; ; \; k = 1, \ldots, N \tag{10}$$

The eigenvectors $\mathbf{x}_k = (x_{1k} \cdots, x_{Nk})$ can be found by putting $x_{jk} = A_k \xi^j$ in the eigenvalue equation

$$(\mathbf{\Delta}_N - \lambda_k \mathbf{I}) \cdot \mathbf{x}_k = 0 \tag{11}$$

and solving the resulting quadratic equation in ξ.

The normalized eigenvectors thus obtained are the columns of the matrix $\mathbf{T}$ which brings $\mathbf{\Delta}_N$ to diagonal form:

$$T_{jk} = \sqrt{\frac{2}{N+1}} \sin\frac{\pi j k}{N+1} \tag{12}$$

$\mathbf{T}$ is a symmetric orthogonal matrix, $\mathbf{T}^{-1} = \mathbf{T}$, such that

$$\mathbf{T}^{-1} \mathbf{\Delta}_N \mathbf{T} = \mathbf{\Lambda}_N \tag{13}$$

with

$$(\mathbf{\Lambda}_N)_{jk} = \lambda_k \delta_{jk} \tag{14}$$

As $\mathbf{T}$ does not depend on the elements of $\mathbf{\Delta}_N$, the simple continuant matrices commute, since all of them can be brought to diagonal form by the same similarity transformation. In spite of this property, these matrices do not form a group with respect to multiplication since their powers are not simple continuants.

(ii) Asymmetric Simple Continuant

Let Δ_N be here given by

$$\Delta_N = \begin{pmatrix} a & b_1 & & 0 \\ c_1 & a & \ddots & \\ & \ddots & \ddots & b_{N-1} \\ 0 & & c_{N-1} & a \end{pmatrix} \tag{15}$$

where the b_i, c_i satisfy the relation

$$b_i c_i = b^2 \text{ for } i = 1, \cdots, N-1 \tag{16}$$

In particular for $b_i = \bar{c}_i$ (complex conjugate), Δ_N will be a hermitian matrix.

The eigenvectors of this matrix are the columns of the matrix **ST**, with S a diagonal matrix the elements of which are

$$S_{jj} = (c_1 c_2 \cdots c_{j-1} b_j b_{j+1} \cdots b_{N+1})^{1/2} \tag{17}$$

and **T** is the matrix given in eq. (12).

The eigenvalues are

$$\lambda_k = a + 2b \cos \frac{\pi k}{N+1} \; ; \; k = 1, \cdots, N \tag{18}$$

The characteristic polynomial (or determinant) is as in eq. (7).

(iii) Generalized Continuant

If one inquires what is the matrix with eigenvalues of the form

$$\lambda_k = a_0 + 2 \sum_{j=1}^{N} a_j \cos \frac{\pi k j}{N+1} + (-1)^j a_{N+1} \; ; \; k = 1, \cdots, N \tag{19}$$

and with the diagonalizing matrix $\mathbf{T}$ of eq. (12), one obtains the following interesting result:

$$\Delta_N = \begin{pmatrix} a_0 & a_1 & \cdots & a_{N-1} \\ & a_0 & \ddots & \vdots \\ & & \ddots & a_1 \\ \text{Symmetric} & & & a_0 \end{pmatrix} - \begin{pmatrix} a_2 & a_3 & \cdots & a_N & a_{N+1} \\ a_3 & & ⋰ & ⋰ & \\ \vdots & ⋰ & ⋰ & \text{Symmetric} & \\ a_N & ⋰ & & & \\ a_{N+1} & & & & \end{pmatrix} \tag{20}$$

This matrix can be decomposed as follows:

$$\Delta_N = \sum_{j=0}^{N+1} a_j \, \Delta^{(j)} \tag{21}$$

where

$$\Delta^{(0)} = I_N \; ; \; \Delta^{(1)} = \begin{pmatrix} 0 & 1 & & 0 \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ 0 & & 1 & 0 \end{pmatrix} ; \; \Delta^{(N+1)} = \begin{pmatrix} 0 & & 1 \\ & ⋰ & \\ 1 & & 0 \end{pmatrix}$$

$$\Delta^{(j)} = \begin{array}{r} j-2 \left\{ \begin{array}{c} \\ \\ \end{array} \right. \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{pmatrix} \overbrace{0 \cdots 0}^{j-2} & -1 & 0 & 1 & \cdots & 1 & & & \\ \vdots \;⋰ & ⋰ & & & & & & 0 & \\ 0 & & & & & & & & 0 \\ -1 & & & 0 & & & & & -1 \\ 0 & & & & & & & ⋰ & \\ 1 & \ddots & & & & & 0 & & \\ & & \ddots & & & ⋰ & \vdots & & \\ 0 & & & 1 & 0 & -1 & \underbrace{0 \cdots 0}_{j-2} & & \end{pmatrix} \begin{array}{l} \\ \\ \\ \\ \\ \left. \begin{array}{c} \\ \\ \end{array} \right\} j-2 \\ \\ \end{array} ; \; j = 2, \cdots, N \tag{22}$$

Not all of these matrices are independent, in fact

$$\Delta^{(N+1-j)} = -\Delta^{(N+1)}\,\Delta^{(j)} \quad \begin{cases} j = 0, \cdots, \frac{N}{2}; \; N \text{ even} \\ \\ j = 0, \cdots, \frac{N-1}{2}; \; N \text{ odd} \end{cases} \tag{23}$$

The number of independent matrices is $(N/2)+2$ for N even and $(N+1)/2+2$ for N odd.

An important particular case is obtained when we put $a_j = 0$ for $j = 3, \ldots, N+1$:

$$\Delta_N = \begin{pmatrix} a_0 - a_2 & a_1 & a_2 & & 0 \\ a_1 & a_0 & \ddots & \ddots & a_2 \\ a_2 & \ddots & \ddots & \ddots & a_1 \\ & \ddots & \ddots & a_0 & a_0 - a_2 \\ 0 & & a_2 & a_1 & \end{pmatrix} \tag{24}$$

with eigenvalues

$$\lambda_k = a_0 + 2\,a_1 \cos\frac{\pi k}{N+1} + 2\,a_2 \cos\frac{2\pi k}{N+1} \tag{25}$$

$$k = 1, \cdots, N$$

The determinant of $\Delta_N - \lambda\,\mathbf{I}$ with Δ_N given in eq. (24) can be easily evaluated by writing

$$|\Delta_N - \lambda\,\mathbf{I}| = \prod_{k=1}^{N} (\lambda_k - \lambda)$$

Using the identity

$$\cos\frac{2\pi k}{N+1} = 2\cos^2\frac{\pi k}{N+1} - 1$$

and the form (25) of λ_k, we can write

$$\lambda_k - \lambda = \left(a_1 + 2 b_1 \cos \frac{\pi k}{N+1}\right) \left(a_2 + 2 b_2 \cos \frac{\pi k}{N+1}\right)$$

where

$$a_1 = \frac{b - \sqrt{b^2 - 4c(a - 2c - \lambda)}}{2\sqrt{c}} \; ; \; a_2 = \frac{b + \sqrt{b^2 - 4c(a - 2c - \lambda)}}{2\sqrt{c}}$$

$$b_1 = \sqrt{c} \, ; \; b_2 = \sqrt{c}$$

Then the characteristic determinant is

$$|\mathbf{\Delta}_N - \lambda \mathbf{I}| = \mathcal{D}_N^{(1)}(\lambda) \, \mathcal{D}_N^{(2)}(\lambda)$$

in which the $\mathcal{D}_N^{(i)}(\lambda)$ are given by eqs. (6) or (7) with $a - \lambda$ replaced by a_i and b by b_i.

(iv) Alternating Continuant

Let $\mathbf{\Delta}_N$ have the form

$$\mathbf{\Delta}_N = \begin{pmatrix} u & & b & & & \\ & v & & \ddots & & \\ b & & u & & \ddots & \\ & \ddots & & v & & b \\ & & \ddots & & \ddots & \\ & & & b & & \end{pmatrix} \qquad (26)$$

where the last term on the main diagonal is v for N even and u for N odd. Accordingly, we treat these two cases separately.

(1) $\underline{N = 2n}$

One can write the following decomposition for Δ_{2n}:

$$\Delta_{2n} = \begin{pmatrix} \frac{u+v}{2} & b & & & 0 \\ b & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & b \\ 0 & & & b & \frac{u+v}{2} \end{pmatrix} + \frac{u-v}{2} \begin{pmatrix} 1 & & & & 0 \\ & -1 & & & \\ & & \ddots & & \\ & & & 1 & \\ 0 & & & & -1 \end{pmatrix} \qquad (27)$$

We apply the similarity transformation $\mathbf{T}$ of eq. (12) on Δ_{2n} , with the result

$$\mathbf{T}^{-1} \Delta_{2n} \mathbf{T} = \Lambda'_{2n} + \frac{u-v}{2} \mathbf{R}_{2n} \qquad (28)$$

where

$$(\Lambda'_{2n})_{k\ell} = \left(\frac{u+v}{2} + 2b \cos \frac{\pi k}{2n+1} \right) \delta_{k\ell} \qquad (29)$$

and

$$\mathbf{R}_{2n} = \begin{pmatrix} 0 & & 1 \\ & 1 & \\ 1 & & 0 \end{pmatrix} \qquad (30)$$

The matrix given by eq. (28) belongs to the class of matrices $\{\mathbf{Z}\}$ defined by

$$\mathbf{Z}_{2n} = \begin{pmatrix} x_1 & & & 0 \\ & x_2 & & \\ & & \ddots & \\ 0 & & & x_{2n} \end{pmatrix} + \begin{pmatrix} 0 & & & y_1 \\ & & y_2 & \\ & \iddots & & \\ y_{2n} & & & 0 \end{pmatrix} \qquad (31)$$

It is not difficult to prove that a similarity transformation $\mathbf{P}$ brings $\mathbf{Z}$ to the form:

$$\mathbf{P}^{-1} \mathbf{Z} \mathbf{P} = \begin{pmatrix} \mathbf{Z}^{(1)} & & & \\ & \mathbf{Z}^{(2)} & & 0 \\ & & \ddots & \\ 0 & & & \mathbf{Z}^{(n)} \end{pmatrix} \qquad (32)$$

where $\mathbf{P}$ is the permutation matrix

$$P_{kj} = \begin{cases} \delta_{j,2k-1}; & k = 1, \ldots, n \\ \delta_{j,2(2n-k+1)}; & k = n+1, \ldots, 2n \end{cases} \qquad (33)$$

and

$$\mathbf{Z}^{(k)} = \begin{pmatrix} x_k & y_k \\ y_{2n-k+1} & x_{2n-k+1} \end{pmatrix}; \qquad k = 1, \ldots, n \tag{34}$$

The eigenvalues of $\mathbf{Z}_{2n}$ are then

$$\lambda_k^{\pm}(\mathbf{Z}) = \frac{x_k + x_{2n-k+1}}{2} \pm \sqrt{\left(\frac{x_k - x_{2n-k+1}}{2}\right)^2 + y_k\, y_{2n-k+1}} \tag{35}$$

$$k = 1, \ldots, n$$

Using the above results we find for the eigenvalues of $\mathbf{\Delta}_{2n}$

$$\lambda_k^{\pm}(\mathbf{\Delta}) = \frac{u + v}{2} \pm \sqrt{\left(\frac{u - v}{2}\right)^2 + \left(2b \cos \frac{\pi k}{2n + 1}\right)^2} \tag{36}$$

$$k = 1, \ldots, n$$

and these appear in the order $\lambda_1^+, \lambda_1^-, \lambda_2^+, \lambda_2^-, \ldots, \lambda_n^-$. The eigenvectors of $\mathbf{\Delta}_{2n}$ are the columns of the matrix **TPS**, with **T** given by eq. (12), **P** by eq. (33), and S is the matrix

$$\mathbf{S} = \begin{pmatrix} \mathbf{S}^{(1)} & & & \\ & \mathbf{S}^{(2)} & & \\ & & \ddots & \\ & & & \mathbf{S}^{(n)} \end{pmatrix} \tag{37}$$

in which $\mathbf{S}^{(k)}$ is a 2×2-matrix diagonalizing the matrix $\mathbf{\Delta}^{(k)}$,

$$\mathbf{\Delta}^{(k)} = \begin{pmatrix} \dfrac{u + v}{2} + 2b \cos \dfrac{\pi k}{2n + 1} & \dfrac{u - v}{2} \\ \dfrac{u - v}{2} & \dfrac{u + v}{2} + 2b \cos \dfrac{\pi(2n + 1 - k)}{2n + 1} \end{pmatrix} \tag{38}$$

The characteristic polynomial of $\mathbf{\Delta}_{2n}$ can be shown to have the form $\mathcal{D}_{2n}(\lambda)$ if $a - \lambda$ is replaced by $\sqrt{(u-\lambda)(v-\lambda)}$ in eqs. (6) or (7).

(2) $\underline{N = 2n + 1}$

Making a decomposition similar to eq. (27) and following the same procedure as above we find that the eigenvectors of Δ_{2n+1} are the columns of the matrix **TPS**, where **T** is given by eq. (12), **P** is defined as

$$P_{kj} = \begin{cases} \delta_{j,2k-1}; & k = 1, \ldots, n+1 \\ \delta_{j,2(2n+2-k)}; & k = n+2, \ldots, 2n+1 \end{cases} \tag{39}$$

S is the matrix

$$\mathbf{S} = \begin{pmatrix} S^{(1)} & & & 0 & \\ & S^{(2)} & & & \\ & & \ddots & & \\ 0 & & & S^{(n)} & \\ & & & & 1 \end{pmatrix} \tag{40}$$

where $S^{(k)}$ is the 2×2 matrix diagonalizing the matrix $\Delta^{(k)}$,

$$\Delta^{(k)} = \begin{pmatrix} \frac{u+v}{2} + 2b\cos\frac{\pi k}{2n+2} & \frac{u-v}{2} \\ \frac{u-v}{2} & \frac{u+v}{2} + 2b\cos\frac{\pi(2n+2-k)}{2n+2} \end{pmatrix} \tag{41}$$

The eigenvalues are

$$\lambda_k^{\pm} = \frac{u+v}{2} \pm \sqrt{\left(\frac{u-v}{2}\right)^2 + \left(2b\cos\frac{\pi k}{2n+2}\right)^2}$$

$$k = 1, \ldots, n \tag{42}$$

$$\lambda_{2n+1} = u$$

and their order is $\lambda_1^+, \lambda_1^-, \ldots, \lambda_n^+, \lambda_n^-, \lambda_{2n+1}$.

The characteristic polynomial of Δ_{2n+1} can be found by using the recurrence relation

$$|\Delta_{2n+1} - \lambda \mathbf{I}| + b^2 |\Delta_{2n-1} - \lambda \mathbf{I}| = (u - \lambda)\, \mathcal{D}_{2n}(\lambda) \tag{43}$$

where $\mathscr{D}_{2n}(\lambda)$ is the characteristic polynomial of $\mathbf{\Delta}_{2n}$ described in the previous subsection. The solution is

$$|\mathbf{\Delta}_{2n+1} - \lambda \mathbf{I}| = (-1)^n (u - \lambda)\, b^{2n} \sum_{k=0}^{n} (-1)^k \frac{\mathscr{D}_{2k}(\lambda)}{b^{2k}} \tag{44}$$

Performing the summation in eq. (44) by utilizing eq. (7), we obtain

$$|\mathbf{\Delta}_{2n+1} - \lambda \mathbf{I}| = \sqrt{\frac{u-\lambda}{v-\lambda}}\; \mathscr{D}_{2n+1}(\lambda) \tag{45}$$

where $\mathscr{D}_{2n+1}(\lambda)$ is given again by eq. (7), with $a - \lambda$ replaced by $\sqrt{(u-\lambda)(v-\lambda)}$.

(v) <u>Alternating Continuant Generalized</u>

Let $\mathbf{\Delta}_{2n+1}$ be the matrix

$$\mathbf{\Delta}_{2n+1} = \begin{pmatrix} u & b & & & & \\ b & v & c & & 0 & \\ & c & u & \ddots & & \\ & & \ddots & \ddots & b & \\ & 0 & & b & v & c \\ & & & & c & u \end{pmatrix} \tag{46}$$

To find the eigenvalues and eigenvectors of this matrix we make use of a decomposition of the eigenvalue equations, first employed by Born [25], which is of some independent interest. Let the equations mentioned be

$$(\mathbf{\Delta}_{2n+1} - \lambda \mathbf{I}) \cdot \mathbf{x} = 0 \tag{47}$$

where $\mathbf{x}$ is a $2n+1$-dimensional column vector.

We rewrite the eq's (47) as follows:

$$(u - \lambda)\, \mathbf{I}_n \cdot \mathbf{x}^0 = - \begin{pmatrix} b & & & 0 \\ c & \ddots & & \\ & \ddots & \ddots & \\ 0 & & c & b \end{pmatrix} \cdot \mathbf{x}^e \tag{48}$$

$$(v - \lambda)\,\mathbf{I}_n \cdot \mathbf{x}^e = - \begin{pmatrix} b & c & & 0 \\ & \ddots & \ddots & \\ & & \ddots & c \\ 0 & & & b \end{pmatrix} \cdot \mathbf{x}^0 - c x_{2n+1} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} \tag{49}$$

$$(u - \lambda)\, x_{2n+1} = - c x_{2n} \tag{50}$$

The n-dimensional column vectors $\mathbf{x}^0$, $\mathbf{x}^e$ are defined by

$$\mathbf{x}^0 = \begin{pmatrix} x_1 \\ x_3 \\ \vdots \\ x_{2n-1} \end{pmatrix}; \quad \mathbf{x}^e = \begin{pmatrix} x_2 \\ x_4 \\ \vdots \\ x_{2n} \end{pmatrix} \tag{51}$$

Inserting the value of $\mathbf{x}^0$ from eq. (48) into eq. (49), we obtain

$$\begin{pmatrix} b^2 + c^2 - (u - \lambda)(v - \lambda) & bc & & & 0 \\ bc & b^2 + c^2 - (u - \lambda)(v - \lambda) & bc & & \\ & bc & \ddots & \ddots & \\ & & \ddots & b^2 + c^2 - (u - \lambda)(v - \lambda) & bc \\ 0 & & & bc & b^2 - (u - \lambda)(v - \lambda) \end{pmatrix} \cdot \mathbf{x}^e - c(u - \lambda)\, x_{2n+1} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} \tag{52}$$

Using eq. (50), we finally obtain:

$$\begin{pmatrix} \alpha & \beta & & 0 \\ \beta & \alpha & \ddots & \\ & \ddots & \ddots & \beta \\ 0 & & \beta & \alpha \end{pmatrix} \cdot \mathbf{x}^e = 0 \tag{53}$$

with

$$\alpha = b^2 + c^2 - (u - \lambda)(v - \lambda); \qquad \beta = bc \tag{54}$$

The matrix appearing in eq. (53) is a simple continuant and therefore equating to zero its known eigenvalues we get n quadratic equations for λ:

$$b^2 + c^2 - (u - \lambda)(v - \lambda) + 2bc \cos \frac{\pi k}{n+1} = 0; \quad k = 1, \ldots, n \tag{55}$$

We have found in this manner 2n eigenvalues of $\mathbf{\Delta}_{2n+1}$;

$$\lambda_k^{\pm} = \frac{u+v}{2} \pm \sqrt{\left(\frac{u-v}{2}\right)^2 + (b-c)^2 + \left(2\sqrt{bc}\cos\frac{\pi k}{2n+2}\right)} \tag{56}$$

$$k = 1, \ldots, n$$

For $b = c$ these eigenvalues reduce indeed to those given in eq. (42). Also we have found for the components of $\mathbf{x}_k^e$:

$$x_{jk}^e = \sin\frac{\pi jk}{n+1}; \qquad j, k = 1, \ldots, n \tag{57}$$

and

$$\mathbf{x}_k^{0\,\pm} = \frac{1}{\lambda_k^{\pm} - u}\begin{pmatrix} b & & & 0 \\ c & \ddots & & \\ & \ddots & \ddots & \\ 0 & & \ddots & b \\ & & & c \end{pmatrix} \cdot \mathbf{x}_k^e; \qquad k = 1, \ldots, n \tag{58}$$

The remaining eigenvalue is easily seen to be equal to u,

$$\lambda_{2n+1} = u \tag{59}$$

with the eigenvector

$$\mathbf{x}_{2n+1} = \begin{cases} x_{2k,\,2n+1} = 0; & k = 1, \ldots, n \\ x_{2k+1,\,2n+1} = \left(-\frac{b}{c}\right)^k; & k = 0, \ldots, n \end{cases} \tag{60}$$

Note that the eigenvectors we found have not been normalized, but the normalization (if needed) presents no difficulties. From the mode of solution it is seen that the characteristic polynomial of $\mathbf{\Delta}_{2n+1}$ is given by:

$$|\mathbf{\Delta}_{2n+1} - \lambda\mathbf{I}| = (u-\lambda)\,\mathcal{D}_n(\lambda) \tag{61}$$

in which $\mathcal{D}_n(\lambda)$ is as in eq. (6), with $a - \lambda$ replaced by $b^2 + c^2 - (u-\lambda)(v-\lambda)$.

For the matrix of even order Δ_{2n} ,

$$\Delta_{2n} = \begin{pmatrix} u & b & & & & 0 \\ b & v & c & & & \\ & c & \ddots & \ddots & & \\ & & \ddots & \ddots & c & \\ & & & c & u & b \\ 0 & & & & b & v \end{pmatrix} \tag{62}$$

no analytic results are available, since the eigenvalues cannot be explicitly found for $b \neq c$.

(vi) Variants of the Continuant

(1)

$$\Delta_N = \begin{pmatrix} a+b & b & & & 0 \\ b & a & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & a & b \\ 0 & & & b & a+b \end{pmatrix} \tag{63}$$

Using methods similar to those employed previously for the simple continuent, we obtain the eigenvalues

$$\lambda_k = a + 2b \cos \frac{\pi k}{N}; \quad k = 0, \ldots, N-1 \tag{64}$$

and the normalized eigenvectors as columns of the orthogonal matrix $\mathbf{T}$

$$\left.\begin{array}{ll} T_{jk} = \sqrt{\dfrac{2}{N}} \cos \left(j - \dfrac{1}{2}\right) \dfrac{\pi k}{N} & \\ k \neq 0 & j = 1, \ldots, N \\ T_{j0} = \dfrac{1}{\sqrt{N}} & \end{array}\right\} \tag{65}$$

Note that all matrices $\mathbf{\Delta}_N$ of this type commute as they are brought to diagonal form by the same similarity transformation.

The characteristic polynomial is

$$|\mathbf{\Delta}_N - \lambda \mathbf{I}| = (a - \lambda + 2b)\, \mathcal{D}_{N-1}(\lambda) \tag{66}$$

where $\mathcal{D}_{N-1}(\lambda)$ is given by eq. (6).

(2)

$$\mathbf{\Delta}_N = \begin{pmatrix} a-b & b & & & \\ b & a & \ddots & & 0 \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & b \\ 0 & & \ddots & & a \\ & & & b & a-b \end{pmatrix} \tag{67}$$

The eigenvalues are

$$\lambda_j = a + 2b \cos \frac{\pi j}{N}; \qquad j = 1, \ldots, N \tag{68}$$

and the diagonalizing orthogonal matrix $\mathbf{T}$ is

$$\left.\begin{aligned} T_{kj} &= \sqrt{\frac{2}{N}} \sin \frac{\pi(k - 1/2)\, j}{N} \\ j &\neq N \qquad\qquad\qquad\qquad k = 1, \ldots, N \\ T_{kN} &= \frac{(-1)^k}{\sqrt{N}} \end{aligned}\right\} \tag{69}$$

The characteristic polynomial is given by

$$|\mathbf{\Delta}_N - \lambda \mathbf{I}| = (a - \lambda - 2b)\, \mathcal{D}_{N-1}(\lambda) \tag{70}$$

in which $\mathcal{D}_{N-1}(\lambda)$ is again as in eq. (6).

(3)

$$\boldsymbol{\Delta}_n = \begin{pmatrix} a+b & b & & 0 \\ b & a & \ddots & \\ & \ddots & \ddots & b \\ 0 & & b & a-b \end{pmatrix} \tag{71}$$

The eigenvalues are

$$\lambda_j = a + 2b \cos \frac{\pi (j - 1/2)}{N} ; \qquad j = 1, \ldots, N \tag{72}$$

The eigenvectors are columns of the orthogonal matrix $\mathbf{T}$

$$T_{kj} = \sqrt{\frac{2}{N}} \cos \frac{\pi (k - 1/2)(j - 1/2)}{N} \tag{73}$$

$$k, j = 1, \ldots, N$$

The characteristic polynomial is

$$|\boldsymbol{\Delta}_N - \lambda \mathbf{I}| = \mathcal{D}_N(\lambda) - b^2 \mathcal{D}_{N-2} \tag{74}$$

(4)

$$\boldsymbol{\Delta}_N^{\pm} = \begin{pmatrix} a \pm b & b & & 0 \\ b & a & \ddots & \\ & \ddots & \ddots & b \\ 0 & & b & a \end{pmatrix} \tag{75}$$

Eigenvalues

$$\left.\begin{aligned} \lambda_k^+ &= a + 2b\cos\frac{\pi(2k-1)}{2N+1} \\ & \qquad\qquad\qquad\qquad k = 1, \ldots, N \\ \lambda_k^- &= a + 2b\cos\frac{2\pi k}{2N+1} \end{aligned}\right\} \tag{76}$$

The diagonalizing matrices $\mathbf{T}^+$, $\mathbf{T}^-$ are orthogonal

$$\left.\begin{aligned} T_{kj}^+ &= \frac{2}{\sqrt{2N+1}}\cos\frac{\pi(2k-1)(2j-1)}{2(2N+1)} \\ & \qquad\qquad\qquad\qquad k, j = 1, \ldots, N \\ T_{kj}^- &= \frac{2}{\sqrt{2N+1}}\sin\frac{\pi(2k-1)\,j}{2N+1} \end{aligned}\right\} \tag{77}$$

and

$$|\boldsymbol{\Delta}_N^{\pm} - \lambda\mathbf{I}| = (a - \lambda \pm b)\,\mathcal{D}_{N-1}(\lambda) - b^2\,\mathcal{D}_{N-2}(\lambda) \tag{78}$$

(5)

$$\boldsymbol{\Delta}_{2n} = \begin{pmatrix} a+c & b & & & & \\ b & a & c & & 0 & \\ & c & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & 0 & & c & a & b \\ & & & & b & a+c \end{pmatrix} \tag{79'}$$

The elements on the first upper and lower diagonals are alternatingly b and c. This matrix is associated with a monatomic linear chain with free ends and alternating spacing constants.

We give below the derivation of the eigenvectors and eigenvalues since it illustrates a frequently used device in problems with similar symmetries.

The eigenvector equation

$$(\mathbf{\Delta}_{2n} - \lambda\mathbf{I}) \cdot \mathbf{x} = 0 \tag{80'}$$

when written in full, leads to two prototype equations

$$\left.\begin{aligned} bx_{2j-1} + (a - \lambda)\, x_{2j} + cx_{2j+1} &= 0 \\ cx_{2j} + (a - \lambda)\, x_{2j+1} + bx_{2j+2} &= 0 \end{aligned}\right\} \tag{81'}$$

$$j = 1, \ldots, n - 1$$

and two boundary conditions

$$\left.\begin{aligned} (a - \lambda + c)\, x_1 + bx_2 &= 0 \\ bx_{2n-1} + (a - \lambda + c)\, x_{2n} &= 0 \end{aligned}\right\} \tag{82'}$$

We put

$$x_{2j-1} = Ay^{2j-1}; \quad x_{2j} = By^{2j} \tag{83'}$$

and insert in eq's (81') to obtain

$$\left.\begin{aligned} (b + cy^2)\, A + (a - \lambda)\, yB &= 0 \\ (a - \lambda)\, yA + (c + by^2)\, B &= 0 \end{aligned}\right\} \tag{84'}$$

A non-trivial solution for A, B requires y to satisfy the equation

$$(b + cy^2)\,(c + by^2) - (a - \lambda)\, y^2 = 0 \tag{85'}$$

or

$$y_{\pm}^2 = \frac{1}{2bc} \left\{ (a - \lambda)^2 - b^2 - c^2 \pm \sqrt{\left[(a - \lambda)^2 - b^2 - c^2\right]^2 - 4b^2c^2} \right\} \tag{86'}$$

Let us put now

$$(a - \lambda)^2 - b^2 - c^2 = 2bc \cos 2\theta \tag{87'}$$

Then

$$y_{\pm} = e^{\pm i\theta} \tag{88'}$$

Inserting this in eq. (84') we find

$$\left.\begin{aligned} B_1 &= -\frac{be^{-i\theta} + ce^{i\theta}}{a - \lambda} A_1 \\ B_2 &= -\frac{be^{i\theta} + ce^{-i\theta}}{a - \lambda} A_2 \end{aligned}\right\} \tag{89'}$$

Introducing now

$$\left.\begin{aligned} x_{2j-1} &= A_1 e^{i(2j-1)\theta} + A_2 e^{-i(2j-1)\theta} \\ x_{2j} &= B_1 e^{i2j\theta} + B_2 e^{-i2j\theta} \end{aligned}\right\} \tag{90'}$$

into eq. (82') and making use of eq's (87') and (89'), we finally obtain a system of two equations for A_1, A_2. The requirement of a non-trivial solution for these yields an equation for θ:

$$\sin 2n\theta \; [b^2 - (a - \lambda + c)^2] = 0 \tag{91'}$$

Then, by inspection of the original matrix, we find that the only admissible roots of $\sin 2n\theta = 0$ are

$$\theta_k = \frac{\pi k}{2n}; \quad k = 1, \ldots, n-1 \tag{92'}$$

with the remaining two roots furnished by $b^2 - (a - \lambda + c)^2 = 0$.

The eigenvalues can be finally given as

$$\left.\begin{aligned} \lambda_k^{\pm} &= a \pm \sqrt{b^2 + 2bc\cos\frac{\pi k}{n} + c^2}; \quad k = 1, \ldots, n-1 \\ \lambda_n^{\pm} &= a + c \pm b \end{aligned}\right\} \tag{93'}$$

For each λ there exists one linear relation between A_1 and A_2. Eliminating one of them and introducing its expression in eq's (90'), we obtain the components of the respective eigenvector. The matrix $\mathbf{T}_{2n}$ which brings $\mathbf{\Delta}$ to diagonal form should have the normalized eigenvectors for its columns.

(6)

$$\mathbf{\Delta}_N = \begin{pmatrix} a & \sqrt{2}\,b & & & 0 \\ \sqrt{2}\,b & a & b & & \\ & b & \ddots & \ddots & \\ & & \ddots & \ddots & b \\ 0 & & & b & a \end{pmatrix}$$

The eigenvalues are

$$\lambda_j = a + 2b\cos\frac{\pi(j - 1/2)}{N}; \quad j = 1, \ldots, N \tag{80}$$

The eigenvectors are columns of the matrix **ST**, where

$$T_{kj} = \cos\frac{\pi(k-1)(j-1/2)}{N}; \quad k, j = 1, \ldots, N \tag{81}$$

and the matrix **S** is given by

$$S_{ij} = \begin{cases} \sqrt{2}\ \delta_{i1} \\ \\ \delta_{ij}\ ; \quad j = 2, \ldots, N \end{cases} \tag{82}$$

Note that while the rows of **T** are pairwise orthogonal, this not so for the columns (eigenvectors), and hence **T** is not an orthogonal matrix.

The characteristic polynomial is

$$|\mathbf{\Delta}_N - \lambda \mathbf{I}| = \mathcal{D}_N(\lambda) - b^2\, \mathcal{D}_N(\lambda) \tag{83}$$

where again $\mathcal{D}_N(\lambda)$ is of the form (6). It is of interest to note that if one puts $a - \lambda \equiv \mathbf{x}$, then it can be shown that $|\mathbf{\Delta}_N - \lambda \mathbf{I}|$ is proportional to the Chebishev polynomial of the first kind, defined by

$$\mathfrak{T}_N(x) = \cos N\,(\cos^{-1} x) \tag{84}$$

(7)

$$\mathbf{\Delta}_{2n} = \begin{pmatrix} u+b & b & & & & \\ b & v & \ddots & & 0 & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & u & b & \\ 0 & & & \ddots & & \\ & & & b & v+b \end{pmatrix} \tag{85}$$

This matrix is associated with a diatomic linear chain with free ends. We give below the derivation of its eigenvalues and eigenvectors since again this exhibits an approach useful for problems of this sort.

The equations to be solved are

$$(\mathbf{\Delta}_{2n} - \lambda \mathbf{I}) \cdot \mathbf{x} = 0 \tag{86}$$

where $\mathbf{x}$ is a $2n$-dimensional vector. We divide now each equation in (86) by b and define:

$$\xi \equiv \frac{u - \lambda}{b}; \qquad \eta \equiv \frac{v - \lambda}{b} \tag{87}$$

We make also the substitution

$$\mathbf{x} = \mathbf{S} \cdot \mathbf{y} \tag{88}$$

where the diagonal matrix S is given, in an obvious notation, by

$$\mathbf{S} = \mathrm{diag}\left(\sqrt{\eta},\ \sqrt{\xi},\ \ldots,\ \sqrt{\eta},\ \sqrt{\xi}\right) \tag{89}$$

By inspection it is clear that neither u nor v are eigenvalues and hence ξ, $\eta \neq 0$. We multiply now the matrix $\Delta_{2n} - \lambda \mathbf{I}$ on the left by the diagonal matrix S' defined by

$$S' = \mathrm{diag}\left(\frac{1}{\sqrt{\xi}}, \frac{1}{\sqrt{\eta}},\ \ldots, \frac{1}{\sqrt{\xi}}, \frac{1}{\sqrt{\eta}}\right) \tag{90}$$

This operation does not change the eigenvalues because the null space of $(\Delta_{2n} - \lambda \mathbf{I})\, S$ is identical with that of $S'\,(\Delta_{2n} - \lambda\mathbf{I})\, S$ (the null space of S' contains only the 0-vector). After all these transformations, eq. (86) becomes:

$$\begin{pmatrix} a+\alpha & 1 & & & & \\ 1 & a & 1 & & & \\ & 1 & \ddots & \ddots & & \\ & & \ddots & a & 1 & \\ & & & 1 & a+\frac{1}{\alpha} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ \vdots \\ y_{2n} \end{pmatrix} = 0 \tag{91}$$

in which

$$a \equiv \sqrt{\xi\eta}; \qquad \alpha \equiv \sqrt{\frac{\eta}{\xi}} \tag{92}$$

Eqs. (91) can be solved by putting

$$y_r = y^r; \quad a = -2\cos\theta \tag{93}$$

in the rth equation of (91). We find then

$$y_r = Ae^{ir\theta} + Be^{-ir\theta} \tag{94}$$

where the constants A, B will be determined from the first and last eq's in (91). The process of elimination finally yields the eigenvalues equation

$$(\alpha e^{-i\theta} - 1)(\alpha e^{i\theta} - 1)(e^{i2n\theta} - e^{-i2n\theta}) = 0 \tag{95}$$

By referring to the original matrix it can be shown that the only admissible solutions of

$$e^{i2n\theta} - e^{-i2n\theta} = 0 \tag{96}$$

are

$$\theta_k = \frac{k\pi}{2n}; \quad k = 1, \ldots, n-1 \tag{97}$$

The two remaining values of θ are solutions of the equation

$$\alpha^2 - 2\alpha\cos\theta + 1 = 0 \tag{98}$$

Eq. (97) yields the eigenvalues

$$\lambda_k^{\pm} = \frac{u+v}{2} \pm \sqrt{\left(\frac{u-v}{2}\right) \pm \left(2b\cos\frac{\pi k}{2n}\right)^2}; \quad k = 1, \ldots, n-1 \tag{99}$$

Eq. (98) when expressed in terms of ξ, η becomes

$$\xi\eta + \xi + \eta = 0 \tag{100}$$

with the solutions (the so-called surface modes)

$$\lambda_0^{\pm} = \frac{u+v}{2} + b \pm \sqrt{\left(\frac{u-v}{2}\right)^2 + b^2} \tag{101}$$

The eigenvectors corresponding to the eigenvalues (99) are $S_k^{\pm} \cdot y_{\pm}^{(k)}$ where

$$y_{\pm}^{(k)} = \alpha_k^{\pm} \begin{pmatrix} 0 \\ \sin\frac{\pi k}{2n} \\ \vdots \\ \sin\frac{\pi k(r-1)}{2n} \\ \vdots \\ \sin\frac{\pi k(2n-1)}{2n} \end{pmatrix} - \begin{pmatrix} \sin\frac{\pi k}{2n} \\ \vdots \\ \sin\frac{\pi k r}{2n} \\ \vdots \\ \sin\frac{\theta k(2n-1)}{2n} \\ 0 \end{pmatrix} \tag{102}$$

and $S_k^{\pm}$ is the matrix S of eq. (89) with λ replaced by $\lambda_k^{\pm}$, while those corresponding to the eigenvalues $\lambda_0^{\pm}$ are $S_0^{\pm} \cdot y_{\pm}^{(0)}$ where

$$y_{\pm}^{(0)} = \begin{pmatrix} \alpha_0^{\pm} \\ \vdots \\ (\alpha_0^{\pm})^r \\ \vdots \\ (\alpha_0^{\pm})^{2n} \end{pmatrix} \tag{103}$$

and

$$\alpha_k^{\pm} = \sqrt{\frac{v-\lambda_k^{\pm}}{u-\lambda_k^{\pm}}}; \qquad k = 0, 1, \ldots, n-1 \tag{104}$$

The eigenvectors presented above are not normalized. The characteristic polynomial is

$$|\Delta_{2n} - \lambda I| = \mathcal{D}_{2n}(\lambda) - b\left(\sqrt{\frac{u-\lambda}{v-\lambda}} + \sqrt{\frac{v-\lambda}{u-\lambda}}\right)\mathcal{D}_{2n-1}(\lambda) + b^2\,\mathcal{D}_{2n-2}(\lambda) \tag{105}$$

where all the polynomials $\mathbb{D}_j$ in eq. (105) have the form shown in eq. (6), with $a - \lambda$ replaced by $\sqrt{(u - \lambda)(v - \lambda)}$.

We note that such analytic results do not exist for the matrix of odd order

$$\Delta_{2n+1} = \begin{pmatrix} u+b & b & & & 0 \\ b & v & \ddots & & \\ & \ddots & u & \ddots & \\ & & \ddots & v & b \\ 0 & & & b & u+b \end{pmatrix} \tag{106}$$

though its characteristic determinant can be written down without difficulty.

2. Associated Jacobi Matrices

i) Let Δ_N denote the matrix

$$\Delta_N = \begin{pmatrix} a_1 & 0 & b_1 & & & 0 \\ 0 & a_2 & 0 & \ddots & & \\ c_1 & 0 & \ddots & \ddots & \ddots & b_{N-2} \\ & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & & c_{N-2} & & 0 & a_N \end{pmatrix} \tag{107}$$

We exhibit below a similarity transformation which reduces Δ_N to a diagonal block matrix composed of simple Jacobi matrices. We treat separately the cases $N = 2n$, and $N = 2n + 1$.

(1) $\underline{N = 2n}$

We define a permutation π_{2n}

$$\pi_{2n} \equiv \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \; . \; . \; . \; 2n \\ \\ 1 & n+1 & 2 & n+2 & 3 \; . \; . \; . \; 2n \end{pmatrix} \tag{108}$$

When we apply this permutation on the columns of the unit matrix $\mathbf{I}_{2n}$, we obtain a permutation matrix $\mathbf{P}_{2n}$ with the property

$$\mathbf{P}_{2n}^{-1} \boldsymbol{\Delta}_{2n} \mathbf{P}_{2n} = \left(\begin{array}{cccccc|cccccc}
a_1 & b_1 & & & 0 & & & & & & & \\
c_1 & a_3 & b_3 & & & & & & & & & \\
 & c_3 & \ddots & \ddots & & & & & & 0 & & \\
 & & \ddots & \ddots & b_{2n-3} & & & & & & & \\
 & 0 & & c_{2n-3} & a_{2n-1} & & & & & & & \\
\hline
 & & & & & & a_2 & b_2 & & & & \\
 & & & & & & c_2 & a_4 & b_4 & & 0 & \\
 & & 0 & & & & & c_4 & \ddots & \ddots & & \\
 & & & & & & & 0 & \ddots & \ddots & b_{2n-2} & \\
 & & & & & & & & & c_{2n-2} & a_{2n} &
\end{array}\right) \tag{109}$$

Note that $\mathbf{P}_{2n}$ is orthogonal so that $\mathbf{P}_{2n}^{-1} = \tilde{\mathbf{P}}_{2n}$, where $\tilde{\mathbf{P}}_{2n}$ denotes the transpose of $\mathbf{P}_{2n}$. The elements of $\mathbf{P}_{2n}$ are given by

$$(\mathbf{P}_{2n})_{ij} = \begin{cases} \delta_{i,2j-1} & j = 1, \; . \; . \; . \; , n \\ \\ \delta_{i,2(j-m)} & j = n+1, \; . \; . \; . \; , 2n \end{cases} \tag{110}$$

(2) $\underline{N = 2n + 1}$

On applying the permutation

$$\pi_{2n+1} = \begin{pmatrix} 1 & 2 & 3 & 4 & \cdots & 2n & 2n+1 \\ \\ 1 & n+2 & 2 & n+3 & \cdots & 2n+1 & n+1 \end{pmatrix} \tag{111}$$

on the columns of the unit matrix $\mathbf{I}_{2n+1}$ we obtain the permutation matrix which brings $\mathbf{\Delta}_{2n+1}$ to block-diagonal form:

$$(\mathbf{P}_{2n+1})_{ij} = \begin{cases} \delta_{i,2j-1} & j = 1, \ldots, n+1 \\ \\ \delta_{i,2(j-n-1)}; & j = n+2, \ldots, 2n+1 \end{cases} \tag{112}$$

and

$$\mathbf{P}^{-1}_{2n+1}\,\mathbf{\Delta}_{2n+1}\,\mathbf{P}_{2n+1} = \left(\begin{array}{c|c} \begin{matrix} a_1 & b_1 & & 0 \\ c_1 & a_3 & \ddots & \\ & \ddots & \ddots & b_{2n-1} \\ 0 & & c_{2n-1} & a_{2n+1} \end{matrix} & 0 \\ \hline 0 & \begin{matrix} a_2 & b_2 & & 0 \\ c_2 & a_4 & \ddots & \\ & \ddots & \ddots & b_{2n-2} \\ 0 & & c_{2n-2} & a_{2n} \end{matrix} \end{array}\right) \tag{113}$$

These reductions enable us to obtain eigenvalues and eigenvectors for $\mathbf{\Delta}_N$ in eq. (107) if the resulting block matrices belong to any one of the classes of matrices previously described.

(ii) If Δ_N denotes the matrix

$$\Delta_N = \begin{pmatrix} a_1 & \overbrace{0 \;\cdots\; 0}^{p-1} & & b_1 & & \\ \left.\begin{matrix} 0 \\ \vdots \\ 0 \end{matrix}\right\}{\scriptstyle p-1} & a_2 & & & \ddots & \\ & & \ddots & & & b_{N-p} \\ & & & \ddots & & 0 \\ c_1 & & & & \ddots & \vdots \\ & c_2 & & & & \vdots \\ & & \ddots & & \ddots & 0 \\ 0 & & c_{N-p} & 0 \cdots 0 & & a_N \end{pmatrix}$$

it is still possible to effect a similar reduction. This is done by assuming $N = \ell p + r$ (i.e., $N = r \bmod(p)$), where $0 \le r \le p-1$. The appropriate permutation here is $\pi_{\ell p + r}$ defined by

$$\left.\begin{aligned} & pk \to (p-1)\ell + r + k; \quad k = 1, \ldots, \ell \\ & pk + n \to (p-1-n)\ell + k + 1; \quad \begin{cases} n = 1, \ldots, r \Rightarrow k = 0, \ldots, \ell \\ n = r+1, \ldots, p-1 \Rightarrow k = 0, \ldots, \ell-1 \end{cases} \end{aligned}\right\} \tag{115}$$

The permutation matrix **P**, obtained by applying $\pi_{\ell p + r}$ on the columns of the unit matrix, reduces the matrix Δ_N to a block-diagonal form in which the first r blocks are $(\ell + 1) \times (\ell + 1)$ Jacobi matrices and the remaining $p - r$ are $\ell \times \ell$-matrices of similar type.

3. Circulant Matrices

i) Simple Asymmetric

Let Δ_N be the matrix

$$\Delta_N = \begin{pmatrix} s_0 & s_1 & s_2 & \cdots & s_{N-1} \\ s_{N-1} & s_0 & s_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & s_2 \\ s_2 & & \ddots & \ddots & s_1 \\ s_1 & s_2 & \cdots & s_{N-1} & s_0 \end{pmatrix} \tag{116}$$

The rows of this matrix are cyclic permutations of the first row and hence the notation

$$\Delta_N = (s_0\ s_1\ s_2\ \cdots\ s_{N-1})_{cyc} \tag{117}$$

is self-explanatory. The elements of Δ_N can be written also as

$$(\Delta_N)_{kr} = \begin{cases} s_{r-k} & r \geq k \\ s_{N-(k-r)} & k > r \end{cases} \qquad k, r = 0, \ldots, N-1 \tag{118}$$

The eigenvalues and eigenvectors can be found in several ways but the most elegant procedure is based on the observation that Δ_N can be written as a linear combination of powers of a single matrix,

$$\Delta_N = \sum_{j=0}^{N-1} s_j\, Q^j \tag{119}$$

in which $\mathbf{Q}$ is of the form

$$\mathbf{Q} = \begin{pmatrix} 0 & 1 & & \\ 0 & & 1 & 0 \\ \vdots & & & \ddots \\ 0 & & 0 & 1 \\ 1 & 0 & \cdots & 0 \end{pmatrix} \tag{120}$$

$\mathbf{Q}$ is a permutation matrix arising from the application of the cyclic permutation π_c

$$\pi_c = \begin{pmatrix} 1 & 2 & 3 & \cdots & N-1 & N \\ 2 & 3 & 4 & \cdots & N & 1 \end{pmatrix} \tag{121}$$

on the columns of the unit matrix. The powers of π_c form a (commutative) subgroup of the permutation group, and this property is shared also by the matrix representation $\mathbf{Q}$. Since $(\pi_c)^N = \mathfrak{I}$ (the identity permutation) we obtain

$$\mathbf{Q}^N = \mathbf{I} \tag{122}$$

This shows immediately that the eigenvalues of $\mathbf{Q}$ are $e^{i2\pi k/N}$, $k = 0, 1, \ldots,$ $N - 1$. A simple calculation then yields also the eigenvectors. Returning to $\mathbf{\Delta}_N$ we can write for the eigenvalues

$$\lambda_k = \sum_{j=0}^{N-1} s_j \, e^{i2\pi kj/N}; \quad k = 0, \ldots, N-1 \tag{123}$$

The normalized eigenvectors are the columns of the unitary matrix $\mathbf{U}$ which brings $\mathbf{\Delta}_N$ to diagonal form

$$\mathbf{U}_{r\ell} = \frac{1}{\sqrt{N}} e^{i \frac{2\pi r \ell}{N}}; \quad r, \ell = 0, \ldots, N-1 \tag{124}$$

It is clear, from eq. (119) or the form of $\mathbf{U}$, that any two circulant matrices commute.

The characteristic determinant cannot be written down in closed form for the general case. We give below its form for two particular cases:

(1) $\underline{s_j = 0;\ j = 3, \ldots, N-1}$

$$|\mathbf{\Delta}_N - \lambda \mathbf{I}| = (s_0 - \lambda)^N - \left[\left(-\frac{s_1}{2} + \sqrt{\left(\frac{s_1}{2}\right)^2 - (s_0 - \lambda) s_2}\right)^N + \left(-\frac{s_1}{2} - \sqrt{\left(\frac{s_1}{2}\right)^2 - (s_0 - \lambda) s_2}\right)^N\right] + s_2^N \tag{125}$$

(2) $\underline{s_j = 0;\ j = 2, \ldots, N-2}$

$$|\mathbf{\Delta}_N - \lambda \mathbf{I}| = (-1)^{N-1} \left\{ s_1^N - \left[\left(-\frac{s_0 - \lambda}{2} + \sqrt{\left(\frac{s_0 - \lambda}{2}\right)^2 - s_1 s_{N-1}}\right)^N + \left(-\frac{s_0 - \lambda}{2} - \sqrt{\left(\frac{s_0 - \lambda}{2}\right)^2 - s_1 s_{N-1}}\right)^N\right] + s_{N-1}^N \right\} \tag{126}$$

Various generalizations of the asymmetric circulant are possible [26]. We mention here one of the simplest: instead of applying the permutation π_c of eq. (121) on the columns of the unit matrix, one applies it on the columns of an arbitrary diagonal matrix $\mathbf{A} = \mathrm{diag}\,(a_1\ a_2 \cdots a_N)$. The resulting generalized circulant $\mathbf{\Delta}'_N$ is of the form:

$$\mathbf{\Delta}'_N = \sum_{j=0}^{N-1} s_j\ (\mathbf{Q}')^j \tag{127}$$

where

$$\mathbf{Q}' = \begin{pmatrix} 0 & a_2 & & & 0 \\ \vdots & & a_3 & & \\ \vdots & & 0 & \ddots & \\ 0 & & & & a_N \\ a_1 & 0 & \cdots & \cdots & 0 \end{pmatrix} \tag{128}$$

The eigenvalues of $\mathbf{\Delta}'_N$ are then

$$\lambda'_k = \sum_{j=0}^{N-1} s_j \left(\sqrt[N]{a_1\ a_2 \cdots a_N}\right)^j e^{i\frac{2\pi k j}{N}}\ ;\ k = 0, \ldots, N-1 \tag{129}$$

and its jth eivenvector is given by the column

$$
\begin{pmatrix}
1 \\
\dfrac{a_1 a_3 \cdots a_N}{x_j^{N-1}} \\
\vdots \\
\dfrac{a_1 a_{k+2} \cdots a_N}{x_j^{N-k}} \\
\vdots \\
\dfrac{a_1}{x_j}
\end{pmatrix}
\tag{130}
$$

in which

$$
x_j = \sqrt[N]{a_1 \cdots a_N}\; e^{i\frac{2\pi j}{N}}; \quad j = 0, \ldots, N-1 \tag{131}
$$

(ii) Alternating Asymmetric

We consider the matrix

$$
\Delta_{2n} = \begin{pmatrix}
u & s_1 & \cdots & \cdots & s_{2n-1} \\
s_{2n-1} & v & s_1 & \cdots & s_{2n-2} \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
\vdots & & \ddots & \ddots & s_1 \\
s_1 & \cdots & \cdots & s_{2n-1} & v
\end{pmatrix}
\tag{132}
$$

Δ_{2n} can be put in the form

$$
\Delta_{2n} = \left(\frac{u+v}{2},\ s_1 \ldots s_{2n-1}\right)_{cyc.} + \frac{u-v}{2}\,\mathbf{J} \tag{133}
$$

where $\mathbf{J}$ is the same as the second matrix on the l.h.s. of eq. (27). The first matrix in eq. (133) is a simple circulant and we apply on Δ_{2n} the similarity transformation $\mathbf{U}$ of eq. (124). Then

$$\Delta'_{2n} \equiv \mathbf{U}^{-1}\, \Delta_{2n}\, \mathbf{U} = \mathbf{M} + \frac{u-v}{2}\, \mathbf{J}' \tag{134}$$

where

$$\left.\begin{aligned} M_{rj} &= \mu_j\, \delta_{rj} \\ & \qquad\qquad\qquad j = 0, \ldots, 2n-1 \\ \mu_j &= \frac{u+v}{2} + \sum_{\ell=0}^{2n-1} s_\ell\, e^{i\frac{2\pi j \ell}{N}} \end{aligned}\right\} \tag{135}$$

and

$$\mathbf{J}' = \left(\begin{array}{c|c} 0 & \mathbf{I}_n \\ \hline \mathbf{I}_n & 0 \end{array}\right) \tag{136}$$

We further apply on Δ'_{2n} a similarity transformation $\mathbf{P}$,

$$P_{kj} = \begin{cases} \delta_{j,\,2k} & ;\ k = 0, \ldots, n-1 \\ \delta_{j,\,2k-2n+1} & ;\ k = n, \ldots, 2n-1 \end{cases} \tag{137}$$

such that

$$\mathbf{P}^{-1}\, \Delta'_{2n}\, \mathbf{P} = \mathrm{diag}\,(\mathbf{A}_0, \mathbf{A}_1, \ldots, \mathbf{A}_{n-1}) \tag{138}$$

where

$$\mathbf{A}_r = \begin{pmatrix} \mu_r & \dfrac{u - v}{2} \\ \\ \dfrac{u - v}{2} & \mu_{r+n} \end{pmatrix} \tag{139}$$

It is of some interest to note that the permutation $\mathbf{P}$ of eq. (137) is a special case of the permutations (115) which reduce displaced Jacobi matrices. The effect of $\mathbf{P}$ on a matrix Λ of the type

$$\Lambda_{2n} = \begin{pmatrix} \Lambda^a & \Lambda^b \\ \\ \Lambda^c & \Lambda^d \end{pmatrix}$$

where the Λ's are $n \times n$ diagonal matrices, is as follows:

$$\mathbf{P}^{-1} \Lambda_{2n} \mathbf{P} = \mathrm{diag}(\Lambda_1, \Lambda_2, \ldots, \Lambda_n)$$

where

$$\Lambda_r = \begin{pmatrix} \lambda_r^a & \lambda_r^b \\ \\ \lambda_r^c & \lambda_r^d \end{pmatrix}$$

The eigenvalues and eigenvectors of $\mathbf{A}_r$ can be easily found. We summarize: the eigenvalues of $\mathbf{\Delta}_{2n}$ are

$$\lambda_r^{\pm} = \frac{\mu_r + \mu_{r+n}}{2} \pm \sqrt{\left(\frac{\mu_r - \mu_{r+n}}{2}\right)^2 + \left(\frac{u - v}{2}\right)^2} \; ; \qquad r = 0, \ldots, n - 1 \tag{140}$$

the order of appearance being $\lambda_0^+ \lambda_0^- \ldots \lambda_{n-1}^+ \lambda_{n-1}^-$. The eigenvectors are the columns of the matrix $\mathbf{UPS}$, with $\mathbf{U}$ and $\mathbf{P}$ as described above, while S is given by

$$S = \mathrm{diag}(S_0, S_1, \ldots, S_{n-1}) \tag{141}$$

in which S_r is the 2×2-matrix diagonalizing the matrix $\mathbf{A}_r$ of eq. (139).

Analytic results, such as given above, have not yet been found for alternating circulants of odd order.

(iii) Doubly Alternating Asymmetric

Let $\mathbf{\Delta}_{2n}$ be the matrix

$$\mathbf{\Delta}_{2n} = \begin{pmatrix} s_0 & s_1 & \cdots & & & & s_{2n-1} \\ \sigma_{2n-1} & \sigma_0 & \sigma_1 & \cdots & & & \sigma_{2n-2} \\ s_{2n-2} & s_{2n-1} & s_0 & s_1 & \cdots & & s_{2n-3} \\ \sigma_{2n-3} & \cdots & \sigma_0 \sigma_1 & \cdots & & & \sigma_{2n-4} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ s_2 & s_3 & \cdots & & s_{2n-1} & s_0 & s_1 \\ \sigma_1 & \sigma_2 & \cdots & & & \sigma_{2n-1} & \sigma_0 \end{pmatrix}$$

In the sequel we shall employ the notation

$$\mathbf{\Delta}_{2n} = \begin{pmatrix} s_0 & s_1 & \cdots & s_{2n-1} \\ \\ \sigma_{2n-1} & \sigma_0 & \sigma_1 \cdots & \sigma_{2n-2} \end{pmatrix}_{\mathrm{cyc.}}$$

Let us define now the permutation matrix **P**

$$P_{kj} = \begin{cases} \delta_{k,2j} & ;\ j = 0, \ldots, n-1 \\ \\ \delta_{k,2(j-n)+1} & ;\ j = n, \ldots, 2n-1 \end{cases} \tag{143}$$

Then

$$\mathbf{P}^{-1} \Delta_{2n} \mathbf{P} = \begin{pmatrix} \mathbf{A}_n & \mathbf{B}_n \\ \\ \mathbf{C}_n & \mathbf{D}_n \end{pmatrix} \tag{144}$$

where $\mathbf{A}_n$, $\mathbf{B}_n$, $\mathbf{C}_n$ and $\mathbf{D}_n$ are simple circulant matrices given by

$$\left.\begin{aligned} \mathbf{A}_n &= (s_0\ s_2\ s_4\ \ldots\ s_{2n-2})_{cyc.} \\ \mathbf{B}_n &= (s_1\ s_3\ s_5\ \ldots\ s_{2n-1})_{cyc.} \\ \mathbf{C}_n &= (\sigma_1\ \sigma_3\ \sigma_5\ \ldots\ \sigma_{2n-1})_{cyc.} \\ \mathbf{D}_n &= (\sigma_0\ \sigma_2\ \sigma_4\ \ldots\ \sigma_{2n-2})_{cyc.} \end{aligned}\right\} \tag{145}$$

We apply now a similarity transformation **U** on eq. (144),

$$\mathbf{U} = \begin{pmatrix} \mathbf{U}_n & 0 \\ \\ 0 & \mathbf{U}_n \end{pmatrix} \tag{146}$$

in which $\mathbf{U}_n$ is the unitary matrix of eq. (124). The resulting matrix is

$$U^{-1} P^{-1} \Delta_{2N} P U = \begin{pmatrix} \Lambda^A & \Lambda^B \\ \Lambda^C & \Lambda^D \end{pmatrix} \tag{147}$$

where Λ^A is the diagonal form of A, Λ^B that of B, etc. A further permutation Q, of the form exhibited in eq. (137), brings the matrix in eq. (147) to the form

$$Q^{-1} U^{-1} P^{-1} \Delta_{2N} P U Q = \mathrm{diag}(A_0, A_1, \ldots, A_{n-1}) \tag{148}$$

where

$$A_k = \begin{pmatrix} \lambda_k^A & \lambda_k^B \\ \lambda_k^C & \lambda_k^D \end{pmatrix} \tag{149}$$

Finally the eigenvalues of Δ_{2n} are given by:

$$\lambda_k^{\pm} = \frac{\lambda_k^A + \lambda_k^D}{2} \pm \sqrt{\left(\frac{\lambda_k^A - \lambda_k^D}{2}\right)^2 + \lambda_k^B \lambda_k^C} \tag{150}$$

The eigenvectors are the columns of the matrix $PUQS$, where

$$S = \mathrm{diag}(S_0, S_1, \ldots, S_{n-1}) \tag{151}$$

and the S_k are 2×2-matrices diagonalizing the A_k of eq. (149).

(iv) Simple Symmetric

(1) $N = 2n$

$$\Delta_{2n} = (s_0\ s_1 \ldots s_n\ s_{n-1} \ldots s_1)_{cyc.} \tag{152}$$

This is a special case of the simple asymmetric matrix (116), its eigenvalues are

$$\lambda_k = s_0 + 2 \sum_{j=1}^{n-1} s_j \cos \frac{\pi k j}{n} + (-1)^k s_n \tag{153}$$

$$k = 0, \ldots, 2n - 1$$

while the eigenvectors remain the same.

(2) <u>$N = 2n + 1$</u>

$$\Delta_{2n+1} = (s_0 \; s_1 \; \cdots \; s_n \; s_{n-1} \; \cdots \; s_1)_{cyc.} \tag{154}$$

$$\lambda_k = s_0 + 2 \sum_{j=1}^{n} s_j \cos \frac{2\pi k j}{2n+1} \quad ; \; k = 0, \ldots, 2n \tag{155}$$

Again the eigenvectors are the same as those for (166).

For the simple case $s_j = 0, \; j = 2, \ldots, n$ there is no need to distinguish between the parities of N, the eigenvalues of

$$\Delta_N = (s_0 \; s_1 \; 0 \; \cdots \; 0 \; s_1)_{cyc.} \tag{156}$$

being given by

$$\lambda_k = s_0 + 2s_1 \cos \frac{2\pi k}{N} \quad ; \; k = 0, \ldots, N - 1 \tag{157}$$

The same is true for the slightly more general case

$$\Delta_N = (s_0 \; s_1 \; s_2 \; 0 \; . \; . \; . \; 0 \; s_2 \; s_1)_{cyc.} \tag{158}$$

for which

$$\lambda_k = s_0 + 2s_1 \cos \frac{2\pi k}{N} + 2s_2 \cos \frac{4\pi k}{N}$$

$$k = 0, \; . \; . \; . \; , \; N - 1 . \qquad 159)$$

The characteristic polynomials for (156) and (158) can be easily obtained b using eqs. (125) and (126).

(v) Doubly Alternating Symmetric

Let

$$\Delta_{2n} = \begin{pmatrix} s_0 & s_1 & \cdots & s_n & s_{n-1} & \cdots & s_1 \\ \\ \sigma_1 & \sigma_0 & \sigma_1 & \cdots & \sigma_n & \sigma_{n-1} & \cdots & \sigma_2 \end{pmatrix}_{cyc.} \tag{160}$$

be a special case of eq. (142). The eigenvalues and eigenvectors are easily obtained from those of (142). Below we exhibit only one particular case of (142) which appears more frequently:

$$\Delta_{2n} = \begin{pmatrix} s_0 & s_1 & 0 & \ldots & 0 & s_2 \\ \\ s_1 & \sigma_0 & s_2 & 0 & \ldots & 0 \end{pmatrix}_{cyc.} \tag{161}$$

The eigenvalues are

$$\lambda_k^{\pm} = \frac{s_0 + \sigma_0}{2} \pm \sqrt{\left(\frac{s_0 - \sigma_0}{2}\right)^2 + s_1^2 + 2 s_1 s_2 \cos \frac{2\pi k}{n} + s_2^2}$$

$$k = 0, \ldots, n-1 \tag{162}$$

The characteristic polynomial of $\mathbf{\Delta}_{2n}$ in (161) is given by

$$|\mathbf{\Delta}_{2n} - \lambda \mathbf{I}| = \mathbb{D}_n(\lambda) - s_1^2 s_2^2 \mathbb{D}_{n-2}(\lambda) - 2(s_1 s_2)^n \tag{163}$$

where $\mathbb{D}_n(\lambda)$, $\mathbb{D}_{n-2}(\lambda)$ are as in eq. (6), with $a - \lambda$ replaced by $(u - \lambda)(v - \lambda) - (s_1^2 - s_2^2)$, and b replaced by $-s_1 s_2$.

(vi) Skew-Circulant

Let

$$\mathbf{\Delta}_N = \begin{pmatrix} s_0 & s_1 & \cdots & & s_{N-1} \\ -s_{N-1} & s_0 & s_1 & \cdots & s_{N-2} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ & & & & s_1 \\ -s_1 & \cdots & & -s_{N-1} & s_0 \end{pmatrix} \tag{164}$$

Making use of methods similar to the ones described above we find the eigenvalues

$$\lambda_k = \sum_{j=0}^{N-1} s_j \, e^{\frac{i\pi(2k+1)j}{N}} \; ; \; k = 0, \ldots, N-1$$

The eigenvectors are the columns of the unitary matrix $\mathbf{U}$ which brings Δ_N to diagonal form

$$U_{kj} = \frac{1}{\sqrt{N}} \; e^{i\frac{\pi(2j+1)k}{N}} \; ; \; k, \; j = 0, \ldots, N-1 \; . \tag{166}$$

Here also some generalizations are possible but we shall not be further concerned with these, except for the following case of an alternating skew circulant

$$\Delta_{2n} = \begin{pmatrix} u & s_1 & \cdots & & s_{2n-1} \\ -s_{2n-1} & v & \ddots & & \vdots \\ \vdots & \ddots & \ddots & u & s_1 \\ & & & & v \\ -s_1 & \cdots & & -s_{2n-1} & \end{pmatrix} \tag{167}$$

The eigenvalues are

$$\lambda_k^{\pm} = \frac{\mu_k + \mu_{k+n}}{2} \pm \sqrt{\left(\frac{\mu_k - \mu_{k+n}}{2}\right)^2 + \left(\frac{u - v}{2}\right)^2} \tag{168}$$

$$k = 0, \ldots, n-1$$

in which

$$\mu_k = \frac{u + v}{2} + \sum_{j=1}^{2n-1} s_j \; e^{i\frac{\pi(2k+1)j}{2n}} \tag{169}$$

The eigenvectors are columns of the matrix $\mathbf{UPS}$, with $\mathbf{U}$ given by eq. (166), $\mathbf{P}$ by eq. (137) and $\mathbf{S}$ by

$$S = \mathrm{diag}(S_0, S_1, \ldots, S_{n-1}) \tag{170}$$

where S_k is a 2×2-matrix diagonalizing the matrix $\mathbf{A}_k$

$$\mathbf{A}_k = \begin{pmatrix} \mu_k & \frac{u-v}{2} \\ \frac{u-v}{2} & \mu_{k+n} \end{pmatrix} \tag{171}$$

We conclude this discussion of one dimensional matrices with the remark that no restrictions, as to relative values, were imposed on any of the parameters involved. Hence, all the results presented are universally valid. We shall see below that this is true also for higher dimensions.

Part II. Two Dimensional Matrices

Introduction

It is remarked in the text that whatever the dimensionality of the problem from which a matrix originates, the matrix is always an ordinary one, i.e., its elements are complex or real numbers and only two indices are needed to specify all of them. On the other hand it happens in many cases that the matrices considered may be handled more conveniently if some partition into blocks can be effected. This is particularly so when a large number of elements vanish. In this fashion the concept of a generalized matrix arises. Several problems confront us once a partition is obtained: for instance, the individual blocks may not commute and just as important, properties of the original matrix may not carry over to the partitioned matrix, e.g., symmetry in the ordinary elements does not necessarily imply symmetry in the matric elements.

We exhibit below results which parallel those in Part I. It is clear that whenever a one-dimensional matrix can be brought to diagonal form by a similarity transformation which is independent of the matrix elements, the corresponding result for a generalized matrix can be obtained automatically, regardless of the commutativity of the appropriate block matrices. For other cases though, commutativity is essential.

1. Continuant Matrices

i) Simple Continuant

Let Δ be the $N_1N_2 \times N_1N_2$ -matrix

$$\Delta = \begin{pmatrix} F & G & & & 0 \\ G & F & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & G \\ 0 & & & G & F \end{pmatrix}_{N_2} \qquad (172)$$

in which **F**, **G** are $N_1 \times N_1$-matrices. A reduction of $\boldsymbol{\Delta}$ to block-diagonal form can be effected immediately by using the similarity transformation $\mathbf{T}_{N_2} \otimes \mathbf{I}_{N_2}$, with $\mathbf{T}_{N_2}$ given by eq. (12), $\mathbf{I}_{N_1}$ the unit matrix and the Kronecker (or direct) product $\otimes$ being defined as follows

$$\left(\mathbf{T}_{N_2} \otimes \mathbf{I}_{N_1}\right)_{kj} = \left(\mathbf{T}_{N_2}\right)_{kj} \mathbf{I}_{N_1}; \quad k,\ j = 1, \cdots, N_2 \tag{173}$$

The reduced matrix $\boldsymbol{\Delta}'$ will have therefore the form:

$$\Delta'_{r\ell} \equiv \left[\left(\mathbf{T}_{N_2} \otimes \mathbf{I}_{N_1}\right)^{-1} \boldsymbol{\Delta}\left(\mathbf{T}_{N_2} \otimes \mathbf{I}_{N_1}\right)\right]_{r\ell} = \left\{\mathbf{F} + 2\mathbf{G} \cos \frac{\pi r}{N_2 + 1}\right\} \delta_{r\ell} \tag{174}$$

Note that this reduction is independent of the commutativity of **F** with **G**. The matrices defined in eq. (174) may be termed the generalized eigenvalues of $\boldsymbol{\Delta}$. It is clear that the actual eigenvalues of $\boldsymbol{\Delta}$ will be those of the N_2 $N_1 \times N_1$-matrices of eq. (174). Using the matrices of Part I, a whole body of results can be obtained for all those cases where **F** and **G** can be simultaneously diagonalized. Here we discuss only the case of **F** and **G** being simple continuant:

$$\mathbf{F} = \begin{pmatrix} A & B & & & 0 \\ B & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & B \\ 0 & & & B & A \end{pmatrix}; \quad \mathbf{G} = \begin{pmatrix} C & D & & & 0 \\ D & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & D \\ 0 & & & D & C \end{pmatrix} \tag{175}$$

Then the transformation $\mathbf{I}_{N_2} \otimes \mathbf{T}_{N_1}$, with $\mathbf{T}_{N_1}$ as in eq. (12), brings $\boldsymbol{\Delta}'$ to diagonal form. The eigenvalues of $\boldsymbol{\Delta}$ are

$$\lambda_{kj} = A + 2B \cos \frac{\pi k}{N_1 + 1} + 2C \cos \frac{\pi j}{N_2 + 1} + 4D \cos \frac{\pi k}{N_1 + 1} \cos \frac{\pi j}{N_2 + 1}$$
$$k = 1, \ldots, N_1; \quad j = 1, \ldots, N_2 \tag{175}$$

The eigenvectors are the columns of the matrix $(\mathbf{T}_{N_2} \otimes \mathbf{I}_{N_1})(\mathbf{I}_{N_2} \otimes \mathbf{T}_{N_1}) = \mathbf{T}_{N_2} \otimes \mathbf{T}_{N_1}$. The elements of this matrix (in vector index notation) are:

$$\left(\mathbf{T}_{N_2} \otimes \mathbf{T}_{N_1}\right)_{\mathbf{pq}} = \frac{2}{\sqrt{(N_1+1)(N_2+1)}} \sin\frac{\pi p_1 q_1}{N_1+1} \sin\frac{\pi p_2 q_2}{N_2+1} \tag{176}$$

where $\mathbf{p} = (p_1, p_2)$; $\mathbf{q} = (q_1, q_2)$ and $p_1, q_1 = 1, \cdots, N_1$; p_2, $q_2 = 1, \cdots, N_2$.

The results above are still valid when A, B, C, D become arbitrary matrices.

(ii) Alternating Continuant

Let Δ be the matrix

$$\Delta = \begin{pmatrix} \mathbf{F}_1 & \mathbf{G} & & & \\ \mathbf{G} & \mathbf{F}_2 & \ddots & & \\ & \ddots & \mathbf{F}_1 & \ddots & \\ & & \ddots & \ddots & \mathbf{G} \\ & & & \mathbf{G} & \mathbf{F} \end{pmatrix}_{N_2} \tag{177}$$

The matrices $\mathbf{F}_1, \mathbf{F}_2, \mathbf{G}$ are $N_1 \times N_1$-matrices, and when N_2 is odd the last $\mathbf{F}$ matrix in (177) is $\mathbf{F}_1$ while for even N_2 it is $\mathbf{F}_2$. We have to treat these two cases separately.

(1) $N_2 = 2n_2$

We follow the procedure of the one-dimensional case and apply the similarity transformations $\mathbf{T}_2 \mathbf{P}_2 = (\mathbf{T}_{2n_2} \otimes \mathbf{I}_{N_1})(\mathbf{P}_{2n_2} \otimes \mathbf{I}_{N_1})$, where $\mathbf{T}_{2n_2}$ is given by eq. (12) and $\mathbf{P}_{2n_2}$ by eq. (33). The result is

$$\mathbf{P}_2^{-1} \mathbf{T}_2^{-1} \Delta \mathbf{T}_2 \mathbf{P}_2 = \mathrm{diag}(\mathbf{H}_1, \mathbf{H}_2, \cdots, \mathbf{H}_{n_2}) \tag{178}$$

where

$$\mathbf{H}_k = \begin{pmatrix} \dfrac{\mathbf{F}_1 + \mathbf{F}_2}{2} + 2\mathbf{G}\cos\dfrac{\pi k}{2n_2+1} & \dfrac{\mathbf{F}_1 - \mathbf{F}_2}{2} \\ \dfrac{\mathbf{F}_1 - \mathbf{F}_2}{2} & \dfrac{\mathbf{F}_1 + \mathbf{F}_2}{2} + 2\mathbf{G}\cos\dfrac{\pi(2n_2+1-k)}{2n_2+1} \end{pmatrix} \tag{179}$$

If the three matrices F_1, F_2 and G commute, then the same similarity transformation S_{N_1} (whenever this exists) will bring them to diagonal form, and we write

$$S^{-1} P_2^{-1} T_2^{-1} \Delta T_2 P_2 S = \text{diag}\,(\Delta_1, \Delta_2, \cdots, \Delta_{n_2}) \tag{180}$$

where

$$S = I_{2n_2} \otimes S_{N_1} \tag{181}$$

and

$$\Delta_k = \begin{pmatrix} \dfrac{\Lambda^{F_1} + \Lambda^{F_2}}{2} + 2\Lambda^G \cos\dfrac{\pi k}{2n_2+1} & \dfrac{\Lambda^{F_1} - \Lambda^{F_2}}{2} \\ \dfrac{\Lambda^{F_1} - \Lambda^{F_2}}{2} & \dfrac{\Lambda^{F_1} + \Lambda^{F_2}}{2} - 2\Lambda^G \cos\dfrac{\pi k}{2n_2+1} \end{pmatrix} \tag{182}$$

The $N_1 \times N_1$ matrices $\Lambda^{F_1}, \Lambda^{F_2}, \Lambda^G$ are the diagonal forms of F_1, F_2 and G respectively. Each Δ_k can now be brought to a block-diagonal form, the blocks being 2×2 matrices Δ_{kj},

$$\Delta_{kj} = \begin{pmatrix} \dfrac{\lambda_j^{F_1} + \lambda_j^{F_2}}{2} + 2{}_j^G \cos\dfrac{\pi k}{2n_2+1} & \dfrac{\lambda_j^{F_1} - \lambda_j^{F_2}}{2} \\ \dfrac{\lambda_j^{F_1} - \lambda_j^{F_2}}{2} & \dfrac{\lambda_j^{F_1} + \lambda_j^{F_2}}{2} - 2\lambda_j^G \cos\dfrac{\pi k}{2n_2+1} \end{pmatrix} \tag{183}$$

$j = 1, \cdots, N_1$

The similarity transformation Q_{2N_1} needed, is as defined in eq. (137) (there it is denoted by P). It is a simple matter now to write down the eigenvalues of Δ_{kj} and its eigenvectors. Returning to the original matrix Δ, we see that its eigenvectors are the columns of the matrix $T_2 P_2 S Q R$ where T_2, P_2, S have been already defined above, and

$$\mathbf{Q} = \mathbf{I}_{n_2} \otimes \mathbf{Q}_{2N_1} \tag{184}$$

$$\mathbf{R} = \operatorname{diag}\,(\mathbf{R}_{11}, \mathbf{R}_{12}, \cdots, \mathbf{R}_{n_2 N_1}) \tag{185}$$

The $\mathbf{R}_{kj}$ in eq. (185) are the 2×2-matrices which bring $\boldsymbol{\Delta}_{kj}$ to diagonal form.

In certain applications (e.g., a diatomic lattice) we encounter the case where $\mathbf{F}_1, \mathbf{F}_2$ and $\mathbf{G}$ do not commute. If these matrices are entirely arbitrary no further reduction of $\boldsymbol{\Delta}$ is possible. Below we treat one particular case which admits of a complete reduction even though commutativity does not exist:

$$\mathbf{F}_1 = \begin{pmatrix} A_1 & B & & 0 \\ B & A_2 & \ddots & \\ & \ddots & \ddots & B \\ 0 & & B & A \end{pmatrix}; \qquad \mathbf{F}_2 = \begin{pmatrix} A_2 & B & & 0 \\ B & A_1 & \ddots & \\ & \ddots & \ddots & B \\ 0 & & B & A \end{pmatrix} \tag{186}$$

$$\mathbf{G} = \begin{pmatrix} C & D & & 0 \\ D & \ddots & \ddots & \\ & \ddots & \ddots & D \\ 0 & & D & C \end{pmatrix} \tag{187}$$

The last A's in F_1, F_2 will be A_2, A_1 respectively for N_1 even, and A_1, A_2 for N_1 odd. It is easily seen then that the matrix H_k of eq. (179) can be written in the form

$$\mathbf{H}_k = \begin{pmatrix} \mathbf{H}_k^+ & \mathbf{J} \\ \mathbf{J} & \mathbf{H}_k^- \end{pmatrix} \tag{188}$$

where $\mathbf{H}_k^{\pm}$ are continuant matrices with elements

$$(\mathbf{H}_k^{\pm})_{rj} = \left(B \pm 2D \cos \frac{\pi k}{2n_2+1}\right)(\delta_{r,j+1} + \delta_{r,j-1}) +$$

$$+ \left(\frac{A_1 + A_2}{2} \pm 2\,C \cos \frac{\pi k}{2n_2+1}\right) \delta_{rj} \tag{189}$$

and

$$\mathbf{J} = \mathrm{diag}\left(\frac{A_1 - A_2}{2}, -\frac{A_1 - A_2}{2}, \cdots, \frac{A_1 - A_2}{2}, -\frac{A_1 - A_2}{2}\right) \tag{190}$$

Since the $\mathbf{H}_k^{\pm}$'s are continuant, the transformation $\mathbf{T}_{N_1}$ of eq. (12) will bring them simultaneously to diagonal form. Also we have already shown how the $\mathbf{J}$ matrix transforms under $\mathbf{T}$ in eq. (30). Hence on applying the transformation $\mathbf{T}_1 = \mathbf{I}_{2n_2} \otimes \mathbf{T}_{N_1}$ on the matrix of eq. (178), we obtain

$$\mathbf{T}_1^{-1}\, \mathbf{P}_2^{-1}\, \mathbf{T}_2^{-1}\, \Delta\, \mathbf{T}_2\, \mathbf{P}_2\, \mathbf{T}_1 = \mathrm{diag}\,(\mathbf{H}'_1, \mathbf{H}'_2, \cdots, \mathbf{H}'_{n_2}) \tag{191}$$

where

$$\mathbf{H}'_k = \begin{pmatrix} \mathbf{M}_k^{+} & 0 \\ & \\ 0 & \mathbf{M}_k^{-} \end{pmatrix} + \frac{A_1 - A_2}{2}\begin{pmatrix} 0 & & 1 \\ & & 1 \\ & 1 \,\cdot^{\cdot^{\cdot}} & \\ 1 & & 0 \end{pmatrix} \tag{192}$$

The diagonal matrices $\mathbf{M}_k^{\pm}$ contain the eigenvalues of $\mathbf{H}_k^{\pm}$. We employ now the permutation matrix $\mathbf{P}_1 = \mathbf{I}_{n_2} \otimes \mathbf{P}_{2N_1}$, with $\mathbf{P}_{2N_1}$ defined in eq. (33), to bring $\mathbf{H}'_k$ to a block-diagonal matrix, the blocks being the 2×2-matrices Δ'_{kj}

$$\Delta'_{kj} = \begin{pmatrix} \mu_{kj}^{+} & \dfrac{A_1 - A_2}{2} \\ & \\ \dfrac{A_1 - A_2}{2} & \mu_{kj}^{-} \end{pmatrix}; \; k = 1, \cdots, n_2;\; j = 1, \cdots, N_1 \tag{193}$$

with

$$\mu_{kj}^{\pm} = \frac{A_1 + A_2}{2} \pm 2\,C \cos\frac{\pi k}{2n_2 + 1} + 2\left(B \pm 2\,D \cos\frac{\pi k}{2n_2 + 1}\right)\cos\frac{\pi j}{N_1 + 1} \tag{194}$$

Finally the eigenvalues of the original matrix Δ are given by

$$\lambda_{kj}^{\pm} = \frac{\mu_{kj}^{+} + \mu_{kj}^{-}}{2} \pm \sqrt{\left(\frac{\mu_{kj}^{+} - \mu_{kj}^{-}}{2}\right)^2 + \left(\frac{A_1 - A_2}{2}\right)^2} \tag{195}$$

$$k = 1, \cdots, n_2\;;\; j = 1, \cdots, N_1$$

The eigenvectors are the columns of the matrix $T_2\, P_2\, T_1\, P_1\, S$, where T_2, P_2, T_1, P_1 have already been defined and S is the matrix

$$S = \operatorname{diag}\,(S_{11}, S_{12}, \cdots, S_{n_2 N_1}) \tag{196}$$

the S_{kj} being the 2×2-matrices diagonalizing Δ'_{kj} of eq. (193).

(2) $\underline{N_2 = 2n_2 + 1}$

It is readily shown, in a manner identical to the case of N_2 even, that the eigenvalues of Δ for <u>non-commuting</u> F_1, F_2, G are

$$\lambda^{\pm}_{kj} = \frac{\mu^{+}_{kj} + \mu^{-}_{kj}}{2} \pm \sqrt{\left(\frac{\mu^{+}_{kj} - \mu^{-}_{kj}}{2}\right)^2 + \left(\frac{A_1 - A_2}{2}\right)^2} \tag{197}$$

$$k = 1, \cdots, n_2 \;;\; j = 1, \cdots, N_1$$

where

$$\mu^{\pm}_{kj} = \frac{A_1 + A_2}{2} \pm 2\,C \cos \frac{\pi k}{2\,(n_2 + 1)} + 2\left(B \pm 2\,D \cos \frac{\pi k}{2\,(n_2 + 1)}\right) \cos \frac{\pi j}{N_1 + 1} \tag{198}$$

The other N_1 eigenvalues are those of the matrix F_1, which for N_1 even are given by eq. (36) and for N_1 odd by eq. (42), when u, v are replaced by A_1, A_2 respectively.

Trivial changes in the transformation matrices of the even N_2-case will quickly yield the eigenvectors for the present case.

Similarly, for <u>commuting</u> F_1, F_2 and G, the eigenvalues of Δ will be the roots of the matrices

$$\Delta_{kj} = \begin{pmatrix} \dfrac{\lambda^{F_1}_j + \lambda^{F_2}_j}{2} + 2\,\lambda^G_j \cos \dfrac{\pi k}{2\,(n_2 + 1)} & \dfrac{\lambda^{F_1}_j - \lambda^{F_2}_j}{2} \\[2ex] \dfrac{\lambda^{F_1}_j - \lambda^{F_2}_j}{2} & \dfrac{\lambda^{F_1}_j + \lambda^{F_2}_j}{2} - 2\,\lambda^G_j \cos \dfrac{\pi k}{2\,(n_2 + 1)} \end{pmatrix} \tag{199}$$

$$k = 1, \cdots, n_2 \;;\; j = 1, \cdots, N_1$$

To these roots one has to add the eigenvalues of $\mathbf{F}_1$ in order to obtain the complete spectrum of Δ.

We conclude this section with the following remark: the reductions performed in the non-commuting case will be still valid to a certain extent if the numbers A, B, C and D are replaced by matrices. Thus if these are arbitrary matrices eq. (193) remains valid, further reduction being dependent on the nature of A, B, C, D. We shall make use of this result in our treatment of higher dimensional matrices. Here we mention one case arising in a two-dimensional lattice problem: A, B, C and D are 2×2-diagonal matrices. Then eqs. (195), (197) are valid if these matrices are replaced by their respective diagonal elements.

(iii) Variants of the Continuant

(1) Let Δ be the matrix

$$\Delta = \begin{pmatrix} \mathbf{F}+\mathbf{G} & \mathbf{G} & & & \\ \mathbf{G} & \mathbf{F} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \mathbf{F} & \mathbf{G} \\ & & & \mathbf{G} & \mathbf{F}+\mathbf{G} \end{pmatrix}_{N_2} \tag{200}$$

and $\mathbf{F}, \mathbf{G}$ are $N_1 \times N_1$-matrices.

We define now a similarity transformation $\mathbf{T}_2 = \mathbf{T}_{N_2} \otimes \mathbf{I}_{N_1}$, where $\mathbf{T}_{N_2}$ is the orthogonal transformation of eq. (65). Then

$$\mathbf{T}_2^{-1}\, \Delta\, \mathbf{T}_2 = \operatorname{diag}(\mathbf{H}_0, \mathbf{H}_1, \cdots, \mathbf{H}_{N_2-1}) \tag{201}$$

with

$$\mathbf{H}_k = \mathbf{F} + 2\,\mathbf{G} \cos\frac{\pi k}{N_2}\,;\ k = 0, \cdots, N_2 - 1 \tag{202}$$

This reduction is valid for arbitrary $\mathbf{F}, \mathbf{G}$. Further reduction will depend on the nature of $\mathbf{F}, \mathbf{G}$. If in particular $\mathbf{F}$ and $\mathbf{G}$ commute, then the same similarity transformation S_{N_1} will bring them to diagonal form and the eigenvalues of Δ will be

$$\lambda_{kj} = \lambda_j^F + 2\lambda_j^G \cos\frac{\pi k}{N_2}; \qquad \begin{matrix} k = 0, \cdots, N_2 - 1 \\ j = 1, \cdots, N_1 \end{matrix} \tag{203}$$

where λ_j^F and λ_j^G are the eigenvalues of $\mathbf{F}$ and $\mathbf{G}$ respectively.

We make use of eq. (203) for the special case

$$\mathbf{F} = \begin{pmatrix} A+B & B & & & 0 \\ B & A & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & A & B \\ 0 & & & B & A+B \end{pmatrix}_{N_1} ; \quad \mathbf{G} = \begin{pmatrix} C & & & 0 \\ & C & & \\ & & \ddots & \\ 0 & & & C \end{pmatrix}_{N_1} \tag{204}$$

Then we can identify S_{N_1} with $\mathbf{T}_{N_1}$ from eq. (65), and the eigenvalues of Δ will be given by:

$$\lambda_{kj} = A + 2B\cos\frac{\pi j}{N_1} + 2C\cos\frac{\pi k}{N_2}; \qquad \begin{matrix} k = 0, \cdots, N_2 - 1 \\ j = 0, \cdots, N_1 - 1 \end{matrix} \tag{205}$$

The eigenvectors are the columns of the matrix

$$\mathbf{T} \equiv (\mathbf{T}_{N_2} \otimes \mathbf{I}_{N_1})(\mathbf{I}_{N_2} \otimes \mathbf{T}_{N_1}) = \mathbf{T}_{N_2} \otimes \mathbf{T}_{N_1}$$

Note that the result in eq. (205) remains valid even when A, B and C become arbitrary matrices.

(2) Here we consider the alternating matrix

$$\mathbf{\Delta} = \begin{pmatrix} \mathbf{F}_1 + \mathbf{G} & \mathbf{G} & & & 0 \\ \mathbf{G} & \mathbf{F}_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \mathbf{F}_1 & \mathbf{G} \\ 0 & & & \mathbf{G} & \mathbf{F}_2 + \mathbf{G} \end{pmatrix}_{2n_2} \tag{206}$$

Again F_1, F_2 and G are $N_1 \times N_1$-matrices. If we employ the results for the one-dimensional case (85), we can show – provided the matrices F_1, F_2, G commute and G possesses an inverse – that the eigenvalues of Δ are the roots of the equations

$$(F_1 - \lambda I)(F_2 - \lambda I) - 4 G^2 \cos^2 \frac{\pi k}{N_2} = 0 \tag{207}$$

$$k = 1, \cdots, n_2 - 1$$

and

$$(F_1 - \lambda I)(F_2 - \lambda I) + G[F_1 - \lambda I + F_2 - \lambda I] = 0 \tag{208}$$

The eigenvectors will follow just as in the one-dimensional case. Since by assumption F_1, F_2 and G commute, the eigenvalues of Δ will be the roots of the equation

$$\left.\begin{aligned} &(\lambda_j^{F_1} - \lambda)(\lambda_j^{F_2} - \lambda) - 4(\lambda_j^{G})^2 \cos^2 \frac{\pi k}{n_2} = 0 \\ &\qquad\qquad\qquad\qquad k = 1, \cdots, n_2 - 1 \\ &\qquad\qquad\qquad\qquad j = 1, \cdots, N_1 \\ &(\lambda_j^{F_1} - \lambda)(\lambda_j^{F_2} - \lambda) + \lambda_j^{G}\left[\lambda_j^{F_1} - \lambda + \lambda_j^{F_2} - \lambda\right] = 0 \end{aligned}\right\} \tag{209}$$

The more interesting case of <u>non-commuting</u> F_1, F_2 where

$$F_1 = \begin{pmatrix} A_1 + B & B & & & \\ B & A_2 & \ddots & & 0 \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & B \\ & & & B & A_2 + B \end{pmatrix} ; \quad F_2 = \begin{pmatrix} A_2 + B & B & & & \\ B & A_1 & \ddots & & 0 \\ & \ddots & A_2 & \ddots & \\ & 0 & \ddots & \ddots & B \\ & & & B & A_1 + B \end{pmatrix}$$

$$G = \begin{pmatrix} C & & & \\ & C & & 0 \\ & & \ddots & \\ & 0 & & C \end{pmatrix} \tag{210}$$

has up to the present resisted all efforts toward its diagonalization.

2. Circulant Matrices

(i) Simple Asymmetric

Here we consider the matrix

$$\Delta = (A_0\ A_1\ \cdots\ ,A_{N_2-1})_{cyc.} \tag{211}$$

in which the A_k are $N_1 \times N_1$ -matrices.

The similarity transformation $U_2 = U_{N_2} \otimes I_{N_1}$, with U_{N_2} given by eq. (124), reduces Δ to the form

$$U_2^{-1}\,\Delta\,U_2 = \mathrm{diag}\,(\Delta_0, \Delta_1, \cdots, \Delta_{N_2-1}) \tag{212}$$

where

$$\Delta_r = \sum_{j=0}^{N_2-1} A_j\, e^{i\,\frac{2\pi r j}{N_2}}\ ;\ r = 0, \cdots, N_2 - 1 \tag{213}$$

Further reductions will depend on the nature of A_j. If for instance all A_j commute then the transformation $S \equiv I_{N_2} \otimes S_{N_1}$ – where S_{N_1} brings the A_j simultaneously to diagonal form – will completely diagonalize Δ:

$$S^{-1}\,U_2^{-1}\,\Delta\,U_2\,S = \mathrm{diag}\,(\lambda_{00}\ \lambda_{01}\ \cdots\ \lambda_{N_2-1,N_1}) \tag{214}$$

in which

$$\lambda_{rk} = \sum_{j=0}^{N_2-1} \lambda_k^{A_j}\, e^{i\,\frac{2\pi r j}{N_2}}\ ;\ \left.\begin{array}{l} k = 1, \cdots, N_1 \\ r = 0, \cdots, N_2 - 1 \end{array}\right\} \tag{215}$$

The eigenvectors are the columns of the matrix $U_{N_2} \otimes S_{N_1}$.

The special case in which the matrices A_{N_2} are circulant is of particular interest: the matrix S_{N_1} is then the U_{N_1} of eq. (124) and the eigenvalues are

$$\lambda_{rk} = \sum_{j=0}^{N_2-1} \sum_{\ell=0}^{N_1-1} A_{j\ell}\, e^{i\,\frac{2\pi k \ell}{N_1}}\, e^{i\,\frac{2\pi r j}{N_2}} \tag{216}$$

The result in eq. (216) remains valid when the $A_{j\ell}$ become arbitrary matrices since the diagonalizing transformation does not depend on the matric elements of Δ.

(ii) Doubly Alternating Asymmetric

The matrix to be considered here is

$$\Delta = \begin{pmatrix} A_0\ A_1 & \cdots\ A_{2n_2-1} \\ \\ B_{2n_2-1}\ B_0\ B_1 & \cdots\ B_{2n_2-2} \end{pmatrix}_{cyc.} \tag{217}$$

We have already used this notation in eq. (142). Here the A's and B's are $N_1 \times N_1$-matrices. We define the similarity transformation $P_2 \equiv P_{2n_2} \otimes I_{N_1}$ with P_{2n_2} given by eq. (143). Then

$$P_2^{-1}\,\Delta\,P_2 = \begin{pmatrix} \Delta^{(1)} & \Delta^{(2)} \\ \\ \Delta^{(3)} & \Delta^{(4)} \end{pmatrix} \tag{218}$$

where $\Delta^{(r)}$ are the generalized simple circulants

$$\left.\begin{aligned} \Delta^{(1)} &= (A_0\ A_2\ \cdots\ A_{2n_2-2})_{cyc.} \\ \Delta^{(2)} &= (A_1\ A_3\ \cdots\ A_{2n_2-1})_{cyc.} \\ \Delta^{(3)} &= (B_1\ B_3\ \cdots\ B_{2n_2-1})_{cyc.} \\ \Delta^{(4)} &= (B_0\ B_2\ \cdots\ B_{2n_2-2})_{cyc.} \end{aligned}\right\} \tag{219}$$

We apply now on eq. (218) the similarity transformation $U_2' \equiv I_2 \otimes U_2$ where U_2 is as in eq. (212). The result will be

$$U_2'^{-1}\,P_2^{-1}\,\Delta\,P_2\,U_2' = \begin{pmatrix} K^{(1)} & K^{(2)} \\ \\ K^{(3)} & K^{(4)} \end{pmatrix} \tag{220}$$

where $\mathbf{K}^{(r)}$ is the block-diagonal form of $\mathbf{\Delta}^{(r)}$, r = 1, 2, 3, 4. A further permutation $\mathbf{P}_1 = \mathbf{Q}_{2n_2} \otimes \mathbf{I}_{N_1}$, with $\mathbf{Q}_{2n_2}$ as in eq. (137), brings the matrix in eq. (220) to the form

$$\mathbf{P}_1^{-1}\,\mathbf{U}_2'^{-1}\,\mathbf{P}_2^{-1}\,\mathbf{\Delta}\,\mathbf{P}_2\,\mathbf{U}_2'\,\mathbf{P}_1 = \mathrm{diag}\,(\mathbf{H}_0, \mathbf{H}_1, \ldots, \mathbf{H}_{n_2-1}) \tag{221}$$

The matrices $\mathbf{H}_k$ are given by

$$\mathbf{H}_k = \begin{pmatrix} \mathbf{K}_k^{(1)} & \mathbf{K}_k^{(2)} \\ \mathbf{K}_k^{(3)} & \mathbf{K}_k^{(4)} \end{pmatrix} \tag{222}$$

and $\mathbf{K}_k^{(r)}$, r = 1, $\cdots$, 4; k = 0, $\cdots$, $n_2 - 1$ is the k th block of $\mathbf{K}^{(r)}$, similar in form to $\mathbf{\Delta}_k$ of eq. (213).

To reduce the $\mathbf{H}_k$ we need at this point to know the commutation properties of the $\mathbf{A}$'s and $\mathbf{B}$'s. Assume first that all these matrices commute: then, if $\mathbf{U}_{N_1}$ denotes their common diagonalizing matrix, we obtain the matrix $\mathbf{H}_k'$

$$\mathbf{H}_k' \equiv (\mathbf{I}_2 \otimes \mathbf{U}_{N_1})^{-1}\,\mathbf{H}_k\,(\mathbf{I}_2 \otimes \mathbf{U}_{N_1}) = \begin{pmatrix} \Lambda_k^{(1)} & \Lambda_k^{(2)} \\ \Lambda_k^{(3)} & \Lambda_k^{(4)} \end{pmatrix} \tag{223}$$

where $\Lambda_k^{(r)}$ is the diagonal form of $\mathbf{K}_k^{(r)}$. Now, the permutation $\mathbf{P}_{2N_1}$ defined in eq. (137), when applied on $\mathbf{H}_k'$ leads to the matrix

$$\mathbf{P}_{2N_1}^{-1}\,\mathbf{H}_k'\,\mathbf{P}_{2N_1} = \mathrm{diag}\,(\mathbf{J}_{k_1}, \mathbf{J}_{k_2}, \cdots, \mathbf{J}_{kN_1}) \tag{224}$$

where

$$\mathbf{J}_{kr} = \begin{pmatrix} \lambda_{kr}^{(1)} & \lambda_{kr}^{(2)} \\ \lambda_{kr}^{(3)} & \lambda_{kr}^{(4)} \end{pmatrix} \quad \left.\begin{matrix} k = 0, \ldots, n_2 - 1 \\ \\ r = 1, \ldots, N_1 \end{matrix}\right\} \tag{225}$$

Finally the eigenvalues of the original matrix Δ are

$$\lambda_{kr}^{\pm} = \frac{\lambda_{kr}^{(1)} + \lambda_{kr}^{(4)}}{2} \pm \sqrt{\left(\frac{\lambda_{kr}^{(1)} - \lambda_{kr}^{(4)}}{2}\right)^2 + \lambda_{kr}^{(2)} \lambda_{kr}^{(3)}} \tag{226}$$

$$k = 0, \ldots, n_2 - 1; \; r = 1, \ldots, N_1$$

The eigenvectors are the columns of the product of the various transformations employed.

We return now to the original matrix Δ and assume that <u>not all</u> of the A's and B's commute. For simplicity we shall assume that $A_1, A_2, \cdots, A_{2n_2-1}$ coincide with $B_1, B_2, \cdots, B_{2n_2-1}$ and all are simple circulant matrices, while A_0 and B_0 are alternating circulant of the following type:

$$A_0 = \begin{pmatrix} \alpha & A_{01} & A_{02} & \cdots & A_{0N_1-1} \\ A_{0N_1-1} & \beta & A_{01} & A_{02} & \cdots & A_{0N_1-2} \end{pmatrix}_{cyc.}$$

$$B_0 = \begin{pmatrix} \beta & A_{01} & A_{02} & \cdots & A_{0N_1-1} \\ A_{0N_1-1} & \alpha & A_{01} & A_{02} & \cdots & A_{0N_1 2} \end{pmatrix}_{cyc.} \tag{227}$$

Let us denote by Δ_0 the generalized simple circulant

$$\Delta_0 = \left(\frac{A_0 + B_0}{2}, A_1, A_2, \ldots, A_{2n_2-1}\right)_{cyc.} \tag{228}$$

Then the matrix Δ can be written also as

$$\Delta = \Delta_0 + \frac{A_0 - B_0}{2} \mathrm{diag}\,(I_{N_1}, -I_{N_1}, \ldots, I_{N_1}, -I_{N_1})_{2n_2}. \tag{229}$$

Then the transformation U_2 of eq. (212), with $N_2 = 2n_2$, reduces Δ_0 to block-diagonal form, and on applying it on Δ it yields

$$U_2^{-1} \Delta U_2 = \mathrm{diag}(\Delta^{(0)}, \Delta^{(1)}, \ldots, \Delta^{(2n_2-1)}) + J \tag{230}$$

in which

$$\Delta^{(k)} = \frac{A_0 + B_0}{2} + \sum_{j=1}^{2n_2 - 1} A_j \, e^{i\frac{\pi k j}{n_2}} \tag{231}$$

$$J = \left(\begin{array}{c|c} 0 & \begin{matrix} \frac{A_0 - B_0}{2} & & 0 \\ & \ddots & \\ 0 & & \frac{A_0 - B_0}{2} \end{matrix} \\ \hline \begin{matrix} \frac{A_0 - B_0}{2} & & 0 \\ & \ddots & \\ 0 & & \frac{A_0 - B_0}{2} \end{matrix} & 0 \end{array}\right) \begin{array}{l} \}\, n_2 \\ \\ \}\, n_2 \end{array} \tag{232}$$

$$\qquad\quad \underbrace{\qquad\qquad}_{n_2} \qquad\qquad \underbrace{\qquad}_{n_2}$$

A further reduction of the matrix in eq. (230) is provided by the permutation $P_2 = P_{2n_2} \otimes I_{N_1}$, with P_{2n_2} given by eq. (137),

$$P_2^{-1} \, U^{-1} \, \Delta \, U_2 \, P_2 = \mathrm{diag}(H_0, H_1, \ldots, H_{n_2 - 1}) \tag{233}$$

where

$$H_k = \begin{pmatrix} \Delta^{(k)} & \frac{A_0 - B_0}{2} \\ \frac{A_0 - B_0}{2} & \Delta^{(k+n_2)} \end{pmatrix} \tag{234}$$

$$k = 0, \ldots, n_2 - 1$$

At this point we must assume $N_1 = 2n_1$ since no analytic solution is known for the odd case. Hence, if this is so, we can write:

$$\frac{A_0 - B_0}{2} = \frac{\alpha - \beta}{2} \, \mathrm{diag}\,(1, -1, \ldots, 1, -1)_{2n_1} \tag{235}$$

On the other hand the $\Delta^{(k)}$'s are simple circulant and can be brought simultaneously to diagonal form by the transformation U_{2n_1} defined in eq. (124). If we apply on H_k the transformation $I_2 \otimes U_{2n_1}$ we obtain

$$(\mathbf{I}_2 \otimes \mathbf{U}_{2n_1})^{-1} \mathbf{H}_k(\mathbf{I}_2 \otimes \mathbf{U}_{2n_1}) = \mathrm{diag}(\Lambda_0^{(k)}, \Lambda_1^{(k)}, \Lambda_0^{(k+n_2)}, \Lambda_1^{(k+n_2)}) + \frac{\alpha - \beta}{2} \begin{pmatrix} 0 & & & \mathbf{I}_{n_1} \\ & & \mathbf{I}_{n_1} & \\ & \mathbf{I}_{n_1} & & \\ \mathbf{I}_{n_1} & & & 0 \end{pmatrix} \tag{236}$$

in which $\Lambda_0^{(r)}$ contains the first n_1 eigenvalues of $\Delta^{(r)}$ and $\Lambda_1^{(r)}$ the n_1 succeeding ones.

The similarity permutation $\mathbf{I}_{n_1} \otimes \mathbf{P}_4$, with

$$\mathbf{P}_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{237}$$

brings the matrix of eq. (236) to the form

$$(\mathbf{I}_{n_1} \otimes \mathbf{P}_4)^{-1} (\mathbf{I}_2 \otimes \mathbf{U}_{2n_1})^{-1} \mathbf{H}_k (\mathbf{I}_2 \otimes \mathbf{U}_{2n_1})(\mathbf{I}_{n_1} \otimes \mathbf{P}_4) = \mathrm{diag}(\mathbf{H}_k^{(0)}, \mathbf{H}_k^{(1)}) \tag{238}$$

where

$$\mathbf{H}_k^{(0)} = \begin{pmatrix} \Lambda_0^{(k)} & \frac{\alpha-\beta}{2} \mathbf{I}_{n_1} \\ \frac{\alpha-\beta}{2} \mathbf{I}_{n_1} & \Lambda_1^{(k+n_2)} \end{pmatrix} \; ; \; \mathbf{H}_k^{(1)} = \begin{pmatrix} \Lambda_1^{(k)} & \frac{\alpha-\beta}{2} \mathbf{I}_{n_1} \\ \frac{\alpha-\beta}{2} \mathbf{I}_{n_1} & \Lambda_0^{(k+n_2)} \end{pmatrix} \tag{239}$$

We apply now the permutation $\mathbf{P}_{2n_1}$, defined in eq. (137), on $\mathbf{H}_k^{(0)}$ and $\mathbf{H}_k^{(1)}$ to obtain

$$\left.\begin{aligned} \mathbf{P}_{2n_1}^{-1} \mathbf{H}_k^{(0)} \mathbf{P}_{2n_1} &= \mathrm{diag}(\mathbf{K}_{k0}^{(0)}, \mathbf{K}_{k1}^{(0)}, \ldots, \mathbf{K}_{kn_1-1}^{(0)}) \\ \mathbf{P}_{2n_1}^{-1} \mathbf{H}_k^{(1)} \mathbf{P}_{2n_1} &= \mathrm{diag}(\mathbf{K}_{k0}^{(1)}, \mathbf{K}_{k1}^{(1)}, \ldots, \mathbf{K}_{kn_1-1}^{(1)}) \end{aligned}\right\} \tag{240}$$

where

$$\mathbf{K}^{(0)}_{kj} = \begin{pmatrix} \lambda^{(k)}_j & \frac{\alpha-\beta}{2} \\ \\ \frac{\alpha-\beta}{2} & \lambda^{(k+n_2)}_{j+n_1} \end{pmatrix} ; \quad \mathbf{K}^{(1)}_{kj} = \begin{pmatrix} \lambda^{(k)}_{j+n_1} & \frac{\alpha-\beta}{2} \\ \\ \frac{\alpha-\beta}{2} & \lambda^{(k+n_2)}_{j} \end{pmatrix} \tag{241}$$

In eq. (241) $\lambda^{(r)}_{\ell}$ is by definition the ℓth eigenvalue of the matrix $\Delta^{(r)}$ of eq. (231). Again the entire reduction up to this point remains valid if the $\lambda^{(r)}_{\ell}$'s become matrices. It is an easy matter now to write down the eigenvalues of Δ, after solving the quadratic equations arising from $\mathbf{K}^{(0)}_j$ and $\mathbf{K}^{(1)}_j$. The eigenvectors will be the columns of the matrix $\mathbf{U}_2\,\mathbf{P}_2\,\mathbf{U}_1\,\mathbf{Q}\,\mathbf{P}_1\,\mathbf{S}$, where $\mathbf{U}_2$ is defined in eq. (230), $\mathbf{P}_2$ in eq. (233), $\mathbf{U}_1 \equiv (\mathbf{I}_{2n_2} \otimes \mathbf{U}_{2n})$ and $\mathbf{U}_{2n_1}$ as in eq. (124), $\mathbf{Q} \equiv (\mathbf{I}_{n_1n_2} \otimes \mathbf{P}_4)$, $\mathbf{P}_1 \equiv (\mathbf{I}_{2n_2} \otimes \mathbf{P}_{2n_1})$ and $\mathbf{P}_{2n_1}$ as in eq. (137), and finally $\mathbf{S} \equiv \operatorname{diag}(\mathbf{S}^{(0)}_{00}, \mathbf{S}^{(0)}_{01}, \cdots, \mathbf{S}^{(1)}_{n_2-1,\,n_1-1})$, in which $\mathbf{S}^{(r)}_{kj}$ is a 2×2-matrix diagonalizing $\mathbf{K}^{(4)}_{kj}$, $r = 0, 1$.

(iii) Symmetric Circulants

As in the one-dimensional case, the results for the symmetric circulants follow automatically from those for the asymmetric ones and therefore will not be treated further here.

Part III. Three Dimensional Matrices

The results to be obtained in the following depend largely on those of Parts I and II. Since we have shown in Part II how partial diagonalizations can be effected in several cases involving arbitrary matrix elements, here we shall proceed dirsctly to the matrices of interest.

1. Continuants

(i) Simple Continuant

Let Δ be the $N_1N_2N_3$ matrix

$$\Delta = \begin{pmatrix} S & T & & & 0 \\ T & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & T \\ 0 & & & T & S \end{pmatrix}_{N_2} \tag{242}$$

with

$$S = \begin{pmatrix} F & G & & & 0 \\ & \ddots & \ddots & & \\ G & & \ddots & \ddots & \\ & \ddots & & \ddots & G \\ 0 & & G & & F \end{pmatrix}_{N_3}, \quad T = \begin{pmatrix} H & K & & & 0 \\ & \ddots & \ddots & & \\ K & & \ddots & \ddots & \\ & \ddots & & \ddots & K \\ 0 & & K & & H \end{pmatrix}_{N_3} \tag{243}$$

(See page 230 for Equation 243a)

All of the matrices above are generalized or ordinary simple continuant matrices, and we can write down the eigenvalues and eigenvectors immediately:

$$\left.\begin{aligned} \lambda_{jkr} &= A + 2B_1 \cos j\theta + 2B_2 \cos k\varphi + 2B_3 \cos r\psi \\ &\quad + 4C_1 \cos j\theta \cos k\varphi + 4C_3 \cos j\theta \cos r\psi + 4C_5 \cos k\varphi \cos r\psi \\ &\quad + 8D_1 \cos j\theta \cos k\varphi \cos r\psi \\ \theta &= \frac{\pi}{N_1 + 1}; \quad \varphi = \frac{\pi}{N_2 + 1}; \quad \psi = \frac{\pi}{N_3 + 1} \\ j &= 1, \ldots, N_1; \quad k = 1, \ldots, N_2; \quad r = 1, \ldots, N_3 \end{aligned}\right\} \tag{244}$$

This result remains valid if A, B_i, C_i and D_1 become arbitrary matrices.

$$\mathbf{F} = \begin{pmatrix} A & B_1 & & 0 \\ B_1 & \ddots & \ddots & \\ & \ddots & \ddots & B_1 \\ 0 & & B_1 & A \end{pmatrix}_{N_1} ; \quad \mathbf{G} = \begin{pmatrix} B_3 & C_3 & & 0 \\ C_3 & \ddots & \ddots & \\ & \ddots & \ddots & C_3 \\ 0 & & C_3 & B_3 \end{pmatrix}_{N_1} ; \quad \mathbf{H} = \begin{pmatrix} B_2 & C_1 & & 0 \\ C_1 & \ddots & \ddots & \\ & \ddots & \ddots & C_1 \\ 0 & & C_1 & B_2 \end{pmatrix}_{N_1} ; \quad \mathbf{K} = \begin{pmatrix} C_5 & D_1 & & 0 \\ D_1 & \ddots & \ddots & \\ & \ddots & \ddots & D_1 \\ 0 & & D_1 & C_5 \end{pmatrix}_{N_1} \qquad (243$$

The eigenvectors of Δ are the columns of the matrix $T_{N_2} \otimes T_{N_3} \otimes T_{N_1}$, where T_{N_i} are given by eq. (12).

(ii) Alternating Continuant

The matrix to be considered here is of the form

$$\Delta = \begin{pmatrix} S_1 & T & & & 0 \\ T & S_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & T \\ 0 & & & T & S_* \end{pmatrix}_{N_2} \tag{245}$$

where

$$S_* = \begin{cases} S_1; & N_2 = 2n_2 + 1 \\ S_2; & N_2 = 2n_2 \end{cases} \tag{246}$$

Also

$$S_1 = \begin{pmatrix} F_1 & G & & & 0 \\ G & F_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & G \\ 0 & & & G & F' \end{pmatrix}_{N_3} ; \quad S_2 = \begin{pmatrix} F_2 & G & & & 0 \\ G & F_1 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & G \\ 0 & & & G & F'' \end{pmatrix}_{N_3} \tag{247}$$

$$F' = \begin{cases} F_1; & N_3 = 2n_3 + 1 \\ F_2; & N_3 = 2n_3 \end{cases} ; \quad F'' = \begin{cases} F_2; & N_3 = 2n_3 + 1 \\ F_1; & N_3 = 2n_3 \end{cases} \tag{248}$$

and

$$F_1 = \begin{pmatrix} A_1 & B_1 & & & 0 \\ B_1 & A_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & B_1 \\ 0 & & & B_1 & A' \end{pmatrix}; \quad F_2 = \begin{pmatrix} A_2 & B_1 & & & 0 \\ B_1 & A_1 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & B_1 \\ 0 & & & B_1 & A'' \end{pmatrix} \tag{249}$$

$$A' = \begin{cases} A_1; & N_1 = 2n_1 + 1 \\ A_2; & N_1 = 2n_1 \end{cases}; \quad A'' = \begin{cases} A_2; & N_1 = 2n_1 + 1 \\ A_1; & N_1 = 2n_1 \end{cases} \tag{250}$$

The matrices $\mathbf{T}$ and $\mathbf{G}$ are as in eq. (243).

For simplicity we shall choose $N_2 = 2n_2$, $N_3 = 2n_3$ and $N_1 = 2n_1$. All other possible choices lead to soluble cases and the procedure to be followed is similar to the one used below.

First note that (S_1, S_2) and (F_1, F_2) are pairs of non-commuting matrices. We proceed as in the two-dimensional case, and apply successively the transformations $T_2 P_2$,

$$\mathbf{P}_2^{-1} \mathbf{T}_2^{-1} \Delta \mathbf{T}_2 \mathbf{P}_2 = \mathrm{diag}\,(\Omega_1, \Omega_2, \ldots, \Omega_{n_2}) \tag{251}$$

where

$$\mathbf{T}_2 = (\mathbf{T}_{2n_2} \otimes \mathbf{I}_{N_3}) \otimes \mathbf{I}_{N_1}; \quad \mathbf{P}_2 = (\mathbf{P}_{2n_2} \otimes \mathbf{I}_{N_3}) \otimes \mathbf{I}_{N_1} \tag{252}$$

with $\mathbf{T}_{2n_2}$, $\mathbf{P}_{2n_2}$ as in eq. (178),

$$\Omega_k = \begin{pmatrix} \Lambda_k & \frac{S_1 - S_2}{2} \\ \frac{S_1 - S_2}{2} & \Lambda_{2n_2 - k + 1} \end{pmatrix} \tag{253}$$

and

$$\Lambda_k = \frac{S_1 + S_2}{2} + 2T \cos k\varphi; \quad \varphi = \frac{\pi}{2n_2 + 1} \tag{254}$$

Recalling the definitions of the various matrices in eq. (254), it is easily seen that the Λ_ℓ's are generalized continuants the matrix elements of which are

$$(\Lambda_k)_{pq} = \left(\frac{F_1 + F_2}{2} + 2H \cos k\varphi\right) \delta_{pq} + (G + 2K \cos k\varphi)\ (\delta_{p,q+1} + \delta_{p,q-1}) \quad (255)$$

and

$$\frac{S_1 - S_2}{2} = \mathrm{diag}\left(\frac{F_1 - F_2}{2}, -\frac{F_1 - F_2}{2}, \ldots, \frac{F_1 - F_2}{2}, -\frac{F_1 - F_2}{2}\right)_{2n_3} \quad (256)$$

We apply now successively the transformations $T_3 = (I_{2n_2} \otimes T_{2n_3}) \otimes I_{2n_1}$ and $P_3 = (I_{2n_2} \otimes P_{2n_3}) \otimes I_{2n_1}$ —with T_{2n_3} as in eq. (12) and P_{2n_3} as in eq. (33)—on eq. (251) to obtain

$$(T_2 P_2 T_3 P_3)^{-1} \Delta T_2 P_2 T_3 P_3 = \mathrm{diag}\ (\Omega_{11}, \Omega_{12}, \ldots, \Omega_{n_2 \cdot 2n_3}) \quad (257)$$

in which

$$\Omega_{kr} = \begin{pmatrix} \Lambda_{kr} & \dfrac{F_1 - F_2}{2} \\ \dfrac{F_1 - F_2}{2} & \Lambda_{2n_2-k+1,\, 2n_3-r+1} \end{pmatrix} \quad (258)$$

and

$$\left.\begin{aligned} \Lambda_{\ell m} &= \frac{F_1 + F_2}{2} + 2H \cos \ell\varphi + 2\ [G + 2K \cos \ell\varphi]\ \cos m\psi \\ \ell &= 1, \ldots, 2n_2; \quad m = 1, \ldots, 2n_3; \quad \psi = \frac{\pi}{2n_3 + 1} \end{aligned}\right\} \quad (259)$$

Again we observe that the $\Lambda_{\ell m}$ of eq. (258) are continuants with the elements

$$\begin{aligned} (\Lambda_{\ell m})_{pq} &= \left\{\frac{A_1 + A_2}{2} + 2B_2 \cos \ell\varphi + 2\ [B_3 + 2C_5 \cos \ell\varphi]\ \cos m\psi\right\} \delta_{pq} + \\ &+ \{B_1 + 2C_1 \cos \ell\varphi + 2\,[C_3 + 2D_1 \cos \ell\varphi]\ \cos m\psi\}\ (\delta_{p,q+1} + \delta_{p,q-1}) \\ &p, q = 1, \ldots, 2n_1 \end{aligned} \quad (260)$$

and

$$\frac{F_1 - F_2}{2} = \mathrm{diag}\left(\frac{A_1 - A_2}{2}, -\frac{A_1 - A_2}{2}, \ldots, -\frac{A_1 - A_2}{2}\right)_{2n_1} \tag{261}$$

If we apply on eq. (257) the successive transformations $T_1 = (I_{2n_2} \otimes I_{2n_3}) \otimes T_{2n_1}$, $P_1 = (I_{2n_2} \otimes I_{2n_3}) \otimes P_{2n_1}$, with T_{2n_1} and P_{2n_1} as in eq.'s (12) and (33) respectively, we get

$$(T_2 P_2 T_3 P_3 T_1 P_1)^{-1} \Delta T_2 P_2 T_3 P_3 T_1 P_1 = \mathrm{diag}(\Omega_{111}, \Omega_{112}, \ldots, \Omega_{n_2, 2n_3, 2n_1}) \tag{262}$$

where

$$\Omega_{krj} = \begin{pmatrix} \Lambda_{krj} & \dfrac{A_1 - A_2}{2} \\ \dfrac{A_1 - A_2}{2} & \Lambda_{2n_2-k+1,\, 2n_3-r+1,\, 2n_1-j+1} \end{pmatrix} \tag{263}$$

and

$$\Lambda_{\ell mn} = \frac{A_1 + A_2}{2} + 2B_1 \cos n\theta + 2B_2 \cos \ell\varphi + 2B_3 \cos m\psi$$

$$+ 4C_1 \cos n\theta \cos \ell\varphi + 4C_3 \cos n\theta \cos m\psi + 4C_5 \cos \ell\varphi \cos m\psi$$

$$+ 8D_1 \cos n\theta \cos \ell\varphi \cos m\psi$$

$$\ell = 1, \ldots, 2n_2, \; m = 1, \ldots 2n_3; \; n = 1, \ldots, 2n_1; \; \theta = \frac{\pi}{2n_1 + 1} \tag{264}$$

It is easy now to find the eigenvalues of Ω_{krj}, provided that all capital letters in eq. (263) and (264) denote either scalars or diagonal matrices. Thus

$$\lambda^{\pm}_{jkr} = \frac{\mu^{+}_{jkr} + \mu^{-}_{jkr}}{2} \pm \sqrt{\left(\frac{\mu^{+}_{jkr} - \mu^{-}_{jkr}}{2}\right)^2 + \left(\frac{A_1 - A_2}{2}\right)^2} \tag{265}$$

$$j = 1, \ldots, 2n_1; \quad k = 1, \ldots, n_2; \quad r = 1, \ldots, 2n_3$$

in which μ^{+}_{jkr} is identical with Λ_{krj} of eq. (264) and μ^{-}_{jkr} has the same form as μ^{+}_{jkr} but each cosine enters with a (−) sign.

(iii) <u>A Simple Variant</u>

Let

$$\Delta = \begin{pmatrix} S+T & T & & & 0 \\ T & S & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & S & T \\ 0 & & & T & S+T \end{pmatrix} \tag{266}$$

where

$$S = \begin{pmatrix} F+G & G & & & 0 \\ G & F & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & F & G \\ 0 & & & G & F+G \end{pmatrix}_{N_3} ; \quad T = \begin{pmatrix} H+K & K & & & 0 \\ K & H & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & H & K \\ 0 & & & K & H+K \end{pmatrix}_{N_3}$$

$$F = \begin{pmatrix} A+B_1 & B_1 & & & 0 \\ B_1 & A & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & A & B_1 \\ 0 & & & B_1 & A+B_1 \end{pmatrix}_{N_1} ; \quad G = \begin{pmatrix} B_3+C_3 & C_3 & & & 0 \\ C_3 & B_3 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & B_3 & C_3 \\ 0 & & & C_3 & B_3+C_3 \end{pmatrix}_{N_1} ; \quad H = \begin{pmatrix} B_2+C_1 & C_1 & & & 0 \\ C_1 & B_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & B_2 & C_1 \\ 0 & & & C_1 & B_2+C_1 \end{pmatrix}_{N_1} \tag{267}$$

$$K = \begin{pmatrix} C_5+D_1 & D_1 & & & 0 \\ D_1 & C_5 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & C_5 & D_1 \\ 0 & & & D_1 & C_5+D_1 \end{pmatrix}_{N_1}$$

Just as for the case (i) above the eigenvalues can be written down immediately:

$$\left.\begin{aligned}
\lambda_{jkr} &= A + 2B_1 \cos j\theta + 2B_2 \cos k\varphi + 2B_3 \cos r\psi \\
&\quad + 4C_1 \cos j\theta \cos k\varphi + 4C_3 \cos j\theta \cos r\psi + 4C_5 \cos k\varphi \cos r\psi \\
&\quad + 8D_1 \cos j\theta \cos k\varphi \cos r\psi \\
\theta &= \frac{\pi}{N_1};\quad \varphi = \frac{\pi}{N_2};\quad \psi = \frac{\pi}{N_3};\quad j = 0, \ldots, N_1 - 1;\ k = 0, \ldots, N_2 - 1;\ r = 0, \ldots, N_3 - 1
\end{aligned}\right\} \tag{268}$$

The eigenvectors are the columns of the matrix $T_{N_2} \otimes T_{N_3} \otimes T_{N_1}$, with T_{N_i} given by eq. (65).

2. Circulants

(i) Simple Asymmetric

It is clear from the previous treatment that general results can be written down for arbitrary three-dimensional circulants, the elements and sub-elements of which are also arbitrary circulants. For the sake of simplicity we restrict the following discussion to the simpler and more frequently met matrix

$$\Delta = \begin{pmatrix} S & T & & & \tilde{T} \\ \tilde{T} & \ddots & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & T \\ T & & & \tilde{T} & S \end{pmatrix}_{N_2} \tag{269}$$

in which

$$
\left.
\begin{aligned}
&S = \begin{pmatrix} F & G & & & \tilde{G} \\ \tilde{G} & \ddots & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & G \\ G & & & \tilde{G} & F \end{pmatrix}_{N_3} ; \quad T = \begin{pmatrix} H & K & & & L \\ L & \ddots & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & K \\ K & & & L & H \end{pmatrix}_{N_3} \\
&F = \begin{pmatrix} A & B_1 & & & B_1 \\ B_1 & \ddots & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & B_1 \\ B_1 & & & B_1 & A \end{pmatrix}_{N_1} ; \quad G = \begin{pmatrix} B_3 & C_3 & & & C_4 \\ C_4 & \ddots & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & C_3 \\ C_3 & & & C_4 & B_3 \end{pmatrix}_{N_1} \\
&H = \begin{pmatrix} B_2 & C_1 & & & C_2 \\ C_2 & \ddots & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & C_1 \\ C_1 & & & C_2 & B_2 \end{pmatrix}_{N_1} ; \quad K = \begin{pmatrix} C_5 & D_1 & & & D_3 \\ D_3 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & D_1 \\ D_1 & & & D_3 & C_5 \end{pmatrix}_{N_1} ; \quad L = \begin{pmatrix} C_6 & D_4 & & & D_2 \\ D_2 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & D_4 \\ D_4 & & & D_2 & C_6 \end{pmatrix}_{N_1}
\end{aligned}
\right\} \qquad (270)
$$

We assume Δ to have ordinary symmetry* (in the elements A, B,C, D) and therefore the transposed block matrices in eq. (269) and eq. (270) are transposed as ordinary matrices also. This means, for instance, that

$$
\tilde{T} = \begin{pmatrix} \tilde{H} & \tilde{L} & & & \tilde{K} \\ \tilde{K} & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \tilde{L} \\ \tilde{L} & & & \tilde{K} & \tilde{H} \end{pmatrix} \qquad (271)
$$

*The asymmetry in the title of this section refers to the form of Δ as a block matrix.

with similar expressions for $\tilde{\mathbf{H}}$, $\tilde{\mathbf{K}}$ and $\tilde{\mathbf{L}}$ if these in turn are generalized matrices.

The eigenvalues of $\boldsymbol{\Delta}$ are

$$
\begin{aligned}
\boldsymbol{\lambda}_{jkr} = {} & \mathbf{A} + 2\mathbf{B}_1 \cos j\theta + \mathbf{B}_2 e^{ik\varphi} + \tilde{\mathbf{B}}_2 e^{-ik\varphi} + \mathbf{B}_3 e^{-ir\psi} + \tilde{\mathbf{B}}_3 e^{-ir\psi} + \mathbf{C}_1 e^{i(j\theta+k\varphi)} \\
& + \tilde{\mathbf{C}}_1 e^{-i(j\theta+k\varphi)} + \mathbf{C}_2 e^{i(k\varphi-j\theta)} + \tilde{\mathbf{C}}_2 e^{-i(k\varphi-j\theta)} + \mathbf{C}_3 e^{i(j\theta+r\psi)} + \tilde{\mathbf{C}}_3 e^{-i(j\theta+r\psi)} \\
& + \mathbf{C}_4 e^{-i(j\theta-r\psi)} + \tilde{\mathbf{C}}_4 e^{i(j\theta-r\psi)} + \mathbf{C}_5 e^{i(k\varphi+r\psi)} + \tilde{\mathbf{C}}_5 e^{-i(k\varphi+r\psi)} + \\
& + \mathbf{C}_6 e^{i(k\varphi-r\psi)} + \tilde{\mathbf{C}}_6 e^{-i(k\varphi-r\psi)} + \mathbf{D}_1 e^{i(j\theta+k\varphi+r\psi)} + \tilde{\mathbf{D}}_1 e^{-i(j\theta+k\varphi+r\psi)} + \\
& + \mathbf{D}_2 e^{-i(j\theta-k\varphi+r\psi)} + \tilde{\mathbf{D}}_2 e^{i(j\theta-k\varphi+r\psi)} + \mathbf{D}_3 e^{i(-j\theta+k\varphi+r\psi)} + \tilde{\mathbf{D}}_3 e^{i(j\theta-k\varphi-r\psi)} + \\
& + \mathbf{D}_4 e^{i(j\theta+k\varphi-r\psi)} + \tilde{\mathbf{D}}_4 e^{-i(j\theta+k\varphi-r\psi)}
\end{aligned}
\tag{272}
$$

where

$$
\left.
\begin{aligned}
& \theta = \frac{2\pi}{\mathbf{N}_1}; \quad \varphi = \frac{2\pi}{\mathbf{N}_2}; \quad \psi = \frac{2\pi}{\mathbf{N}_3} \\
& j = 0, \ldots, \mathbf{N}_1 - 1; \quad k = 0, \ldots, \mathbf{N}_2 - 1; \quad r = 0, \ldots, \mathbf{N}_3 - 1
\end{aligned}
\right\}
\tag{273}
$$

The eigenvalues λ_{jkr} in eq. (272) were written under the assumption that $\mathbf{A}, \mathbf{B}_1, \ldots, \mathbf{D}_4$ were matrices. If we assume these to be either diagonal or symmetric, we obtain the simplified expression

$$
\begin{aligned}
\boldsymbol{\lambda}_{jkr} = {} & \mathbf{A} + 2\mathbf{B}_1 \cos j\theta + 2\mathbf{B}_2 \cos k\varphi + 2\mathbf{B}_3 \cos r\psi + \\
& + 2\mathbf{C}_1 \cos(j\theta + k\varphi) + 2\mathbf{C}_2 \cos(j\theta - k\varphi) + 2\mathbf{C}_3 \cos(j\theta + r\psi) + \\
& + 2\mathbf{C}_4 \cos(j\theta - r\psi) + 2\mathbf{C}_5 \cos(k\varphi + r\psi) + 2\mathbf{C}_6 \cos(k\varphi - r\psi) + \\
& + 2\mathbf{D}_1 \cos(j\theta + k\varphi + r\psi) + 2\mathbf{D}_2 \cos(j\theta - k\varphi + r\psi) + 2\mathbf{D}_3 \cos(j\theta - k\varphi - r\psi) \\
& + 2\mathbf{D}_4 \cos(j\theta + k\varphi - r\psi)
\end{aligned}
\tag{274}
$$

with θ, φ, ψ and j, k, r as in eq. (273).

The eigenvectors will be the columns of the matrix $U_{N_2} \otimes U_{N_3} \otimes U_{N_1}$, with U's as in eq. (124).

ii) Alternating Asymmetric

The matrix considered here is of the form

$$\Delta = \begin{pmatrix} S_1 & T & & & \tilde{T} \\ \tilde{T} & S_2 & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & T \\ T & & & \tilde{T} & S_2 \end{pmatrix}_{N_2} \qquad N_2 = 2n_2 \tag{275}$$

with S_1 , S_2 regularly alternating along the main diagonal of Δ and

$$S_1 = \begin{pmatrix} F_1 & G & & & \tilde{G} \\ \tilde{G} & F_2 & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & G \\ G & & & \tilde{G} & F_2 \end{pmatrix}_{N_3} ; \quad S_2 = \begin{pmatrix} F_2 & G & & & \tilde{G} \\ G & F_1 & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & G \\ G & & & \tilde{G} & F_1 \end{pmatrix}_{N_3} ; \quad N_3 = 2n_3 \tag{276}$$

$$F_1 = \begin{pmatrix} A_1 & B_1 & & & B_1 \\ B_1 & A_2 & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & B_1 \\ B_1 & & & B_1 & A_2 \end{pmatrix}_{N_1} ; \quad F_2 = \begin{pmatrix} A_2 & B_1 & & & B_1 \\ B_1 & A_1 & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & B_1 \\ B_1 & & & B_1 & A_1 \end{pmatrix}_{N_1} ; \quad N_1 = 2n_1 \tag{277}$$

F_1 and F_1 alternate regularly along the main diagonals of S_1, S_2 and so do A_1 and A_2 in F_1 , F_2. The matrices T and G are as defined in eq. (270).

We remark that the matrices S_1 , F_1 do not commute with S_2, F_2, respectively. To diagonalize Δ we put it in the form

$$\Delta = \Delta_0 + \mathrm{diag}\left(\frac{S_1 - S_2}{2}, -\frac{S_1 - S_2}{2}, \ldots, -\frac{S_1 - S_2}{2}\right)$$

in which $\pm 1/2\ (S_1 - S_2)$ alternate regularly and

$$\Delta_0 = \left(\frac{S_1 + S_2}{2},\ T,\ 0 \ldots 0\ \tilde{T}\right)_{\text{cyc.}} \tag{279}$$

The transformation U_2 which reduces Δ_0 to block-diagonal form is given by

$$U_2 = (U_{N_2} \otimes I_{N_3}) \otimes I_{N_1} \tag{280}$$

with U_{N_2} as in eq. (124). Then we can write

$$U_2^{-1}\, \Delta\, U_2 = \operatorname{diag}\,(\Delta^{(0)},\ \Delta^{(1)},\ \ldots,\ \Delta^{(2n_2-1)}) + J \tag{281}$$

where

$$\begin{aligned} \Delta^{(k)} &= \frac{1}{2}\,(S_1 + S_2) + T\, e^{ik\varphi} + \tilde{T}\, e^{-ik\varphi} \\ k &= 0,\ \ldots,\ 2n_2 - 1; \qquad \varphi = \pi/n_2 \end{aligned} \tag{282}$$

and

$$J = \begin{pmatrix} 0 & J_1 \\ J_1 & 0 \end{pmatrix} \tag{283}$$

with

$$J_1 = I_{n_2} \otimes \frac{1}{2}\,(S_1 - S_2) \tag{284}$$

A further reduction is provided by the permutation

$$P_2 = (P_{N_2} \otimes I_{N_3}) \otimes I_{N_1} \tag{285}$$

with P_{N_2} given in eq. (137) (for $n = n_2$). The result of this permutation is

$$(U_2\, P_2)^{-1}\, \Delta\, U_2\, P_2 = \operatorname{diag}\,(H_0,\ H_1,\ \ldots,\ H_{n_2-1}) \tag{286}$$

in which

$$\mathbf{H}_k = \begin{pmatrix} \Delta^{(k)} & \frac{1}{2}(\mathbf{S}_1 - \mathbf{S}_2) \\ \frac{1}{2}(\mathbf{S}_1 - \mathbf{S}_2) & \Delta^{(k+n_2)} \end{pmatrix}; \quad k = 0, \ldots, n_2 - 1 \tag{287}$$

Now, the matrix $1/2\ (\mathbf{S}_1 - \mathbf{S}_2)$ is of the form

$$\frac{1}{2}(\mathbf{S}_1 - \mathbf{S}_2) = \mathrm{diag}\left(\frac{\mathbf{F}_1 - \mathbf{F}_2}{2}, -\frac{\mathbf{F}_1 - \mathbf{F}_2}{2}, \ldots, -\frac{\mathbf{F}_1 - \mathbf{F}_2}{2}\right) \tag{288}$$

where $\pm 1/2\ (\mathbf{F}_1 - \mathbf{F}_2)$ alternate regularly, while the $\Delta^{(\ell)}$ are all generalized simple circulants. Therefore is we apply on $\mathbf{H}_k$ the transformation $\mathbf{V}_1$,

$$\mathbf{V}_1 = (\mathbf{I}_2 \otimes \mathbf{U}_{N_3}) \otimes \mathbf{I}_{N_1} \tag{289}$$

with $\mathbf{U}_{N_3}$ as in eq. (124), we obtain

$$\mathbf{V}_1^{-1}\,\mathbf{H}_k\,\mathbf{V}_1 = \mathrm{diag}\left(\Lambda_0^{(k)}, \Lambda_1^{(k)}, \Lambda_0^{(k+n_2)}, \Lambda_1^{(k+n_2)}\right) + \mathbf{J}' \tag{290}$$

in which $\Lambda_0^{(\ell)}$ contains the first n_3 (generalized) eigenvalues of $\Delta^{(\ell)}$ and $\Lambda_1^{(\ell)}$ the n_3 succeeding ones. The matrix $\mathbf{J}'$ is given by

$$\mathbf{J}' = \begin{pmatrix} & 0 & & \mathbf{J}_1' \\ & & \mathbf{J}_1' & \\ & \mathbf{J}_1' & & 0 \\ \mathbf{J}_1' & & & \end{pmatrix} \tag{291}$$

with

$$\mathbf{J}_1' = \mathbf{I}_{n_3} \otimes \frac{1}{2}(\mathbf{F}_1 - \mathbf{F}_2) \tag{292}$$

The similarity transformation $\mathbf{V}_2 = \mathbf{I}_{n_3} \otimes \mathbf{P}_4$, with $\mathbf{P}_4$ as defined in eq. (237), brings the matrix in eq. (290) to the form

$$(\mathbf{V}_1\,\mathbf{V}_2)^{-1}\,\mathbf{H}_k\,\mathbf{V}_1\mathbf{V}_2 = \mathrm{diag}\ (\mathbf{H}_k^{(0)}, \mathbf{H}_k^{(1)}) \tag{293}$$

where

$$\mathbf{H}_k^{(0)} = \begin{pmatrix} \Lambda_0^{(k)} & \mathbf{J}_1' \\ \mathbf{J}_1' & \Lambda^{(k+n_2)} \end{pmatrix}; \quad \mathbf{H}_k^{(1)} = \begin{pmatrix} \Lambda_1^{(k)} & \mathbf{J}_1' \\ \mathbf{J}_1' & \Lambda_0^{(k+n_2)} \end{pmatrix} \tag{294}$$

We apply now the permutation

$$\mathbf{P}_3 = \mathbf{P}_{2n_3} \otimes \mathbf{I}_{N_1} \tag{295}$$

with $\mathbf{P}_{2n_3}$ as in eq. (137), on $\mathbf{H}_k^{(0)}$ and $\mathbf{H}_k^{(1)}$:

$$\left.\begin{aligned} \mathbf{P}_3^{-1}\,\mathbf{H}_k^{(0)}\,\mathbf{P}_3 &= \mathrm{diag}\,(\mathbf{K}_{k0}^{(0)}, \mathbf{K}_{k1}^{(0)}, \ldots, \mathbf{K}_{kn_3-1}^{(0)}) \\ \mathbf{P}_3^{-1}\,\mathbf{H}_k^{(1)}\,\mathbf{P}_3 &= \mathrm{diag}\,(\mathbf{K}_{k0}^{(1)}, \mathbf{K}_{k1}^{(1)}, \ldots, \mathbf{K}_{kn_3-1}^{(1)} \end{aligned}\right\} \tag{296}$$

in which

$$\mathbf{K}_{kr}^{(0)} = \begin{pmatrix} \Lambda_{kr} & \frac{1}{2}(\mathbf{F}_1 - \mathbf{F}_2) \\ \frac{1}{2}(\mathbf{F}_1 - \mathbf{F}_2) & \Lambda_{k+n_2,\,r+n_3} \end{pmatrix}; \quad \mathbf{K}_{kr}^{(1)} = \begin{pmatrix} \Lambda_{k,\,r+n_3} & \frac{1}{2}(\mathbf{F}_1 - \mathbf{F}_2) \\ \frac{1}{2}(\mathbf{F}_1 - \mathbf{F}_2) & \Lambda_{k+n_2,\,r} \end{pmatrix} \tag{297}$$

$$k = 0, \ldots, n_2 - 1; \quad r = 0, \ldots, n_3 - 1$$

and where

$$\begin{aligned} \Lambda_{pq} = \frac{1}{2}(\mathbf{F}_1 + \mathbf{F}_2) &+ \mathbf{H}\,e^{ip\varphi} + \widetilde{\mathbf{H}}\,e^{-ip\varphi} + \mathbf{G}\,e^{iq\psi} \\ &+ \widetilde{\mathbf{G}}\,e^{-iq\psi} + \mathbf{K}\,e^{i(p\varphi+q\psi)} + \widetilde{\mathbf{K}}\,e^{-i(p\varphi+q\psi)} \\ &+ \mathbf{L}\,e^{i(p\varphi-q\psi)} + \widetilde{\mathbf{L}}\,e^{-i(p\varphi-q\psi)} \end{aligned} \tag{298}$$

with

$$\varphi = \pi/n_2; \quad \psi = \pi/n_3; \quad p = 0, \ldots, 2n_2 - 1; \quad q = 0, \ldots, 2n_3 - 1$$

The matrices Λ_{pq} are again circulant, while

$$\frac{1}{2}(\mathbf{F}_1 - \mathbf{F}_2) = \mathrm{diag}\left(\frac{\mathbf{A}_1 - \mathbf{A}_2}{2}, -\frac{\mathbf{A}_1 - \mathbf{A}_2}{2}, \ldots, -\frac{\mathbf{A}_1 - \mathbf{A}_2}{2}\right) \tag{299}$$

in which $\pm 1/2\ (\mathbf{A}_1 - \mathbf{A}_2)$ alternate regularly. Then if we apply on $\mathbf{K}^{(0)}_{kr}$ and $\mathbf{K}^{(1)}_{kr}$ the transformation

$$\mathbf{U}_3 = \mathbf{I}_2 \otimes \mathbf{U}_{2n_1} \tag{300}$$

we obtain

$$\mathbf{U}_3^{-1}\, \mathbf{K}^{(0)}_{kr}\, \mathbf{U}_3 = \mathrm{diag}\,(\Lambda^{(0)}_{kr}\ \Lambda^{(1)}_{kr}\ \Lambda^{(0)}_{k+n_2,\,r+n_3}\ \Lambda^{(1)}_{k+n_2,\,r+n_3}) + \mathbf{W} \tag{301}$$

where $\Lambda^{(0)}_{pq}$ contains the n_1 first eigenvalues of Λ_{pq}, and $\Lambda^{(1)}_{pq}$ the n_1 succeeding ones. Also

$$\mathbf{W} = \begin{pmatrix} & 0 & & \mathbf{W}_1 \\ & & \mathbf{W}_1 & \\ & \mathbf{W}_1 & & 0 \\ \mathbf{W}_1 & & & \end{pmatrix} ; \quad \mathbf{W}_1 = \mathbf{I}_{n_1} \otimes \frac{1}{2}(\mathbf{A}_1 - \mathbf{A}_2) \tag{302}$$

The similarity permutation $\mathbf{V}_3 = \mathbf{I}_{n_1} \otimes \mathbf{P}_4$, with $\mathbf{P}_4$ as in eq. (237), brings the matrix of eq. (301) to the form

$$(\mathbf{U}_3\, \mathbf{V}_3)^{-1}\, \mathbf{K}^{(0)}_{kr}\, \mathbf{U}_3\, \mathbf{V}_3 = \mathrm{diag}\,(\mathbf{X}^{(0)}_{kr},\ \mathbf{Y}^{(0)}_{kr}) \tag{303}$$

in which

$$\mathbf{X}^{(0)}_{kr} = \begin{pmatrix} \Lambda^{(0)}_{kr} & \mathbf{W}_1 \\ \mathbf{W}_1 & \Lambda^{(1)}_{k+n_2,\,r+n_3} \end{pmatrix} ; \quad \mathbf{Y}^{(0)}_{kr} = \begin{pmatrix} \Lambda^{(1)}_{kr} & \mathbf{W}_1 \\ \mathbf{W}_1 & \Lambda_{k+n_2,\,r+n_3} \end{pmatrix} \tag{304}$$

Applying the permutation $\mathbf{P}_{2n_1}$ defined in eq. (137), we finally obtain

$$\left.\begin{aligned} \mathbf{P}^{-1}_{2n_1}\, \mathbf{X}^{(0)}_{kr}\, \mathbf{P}_{2n_1} &= \mathrm{diag}\,(\Omega^{(x,0)}_{0kr},\ \Omega^{(x,0)}_{1kr},\ \ldots,\ \Omega^{(x,0)}_{n_1-1\,kr}) \\ \mathbf{P}^{-1}_{2n_1}\, \mathbf{Y}^{(0)}_{kr}\, \mathbf{P}_{2n_1} &= \mathrm{diag}\,(\Omega^{(y,0)}_{0kr},\ \Omega^{(y,0)}_{1kr},\ \ldots,\ \Omega^{(y,0)}_{n_1-1\,kr}) \end{aligned}\right\} \tag{305}$$

in which

$$\Omega^{(x,0)}_{jkr} = \begin{pmatrix} \Lambda_{jkr} & \frac{1}{2}(A_1 - A_2) \\ \frac{1}{2}(A_1 - A_2) & \Lambda_{j+n_1\, k+n_2\, r+n_3} \end{pmatrix} ; \quad \Lambda^{(y,0)}_{jkr} = \begin{pmatrix} \Lambda_{j+n_1\, kr} & \frac{1}{2}(A_1 - A_2) \\ \frac{1}{2}(A_1 - A_2) & \Lambda_{jk+n_2\, r+n_3} \end{pmatrix}$$

$$j = 0, \ldots, n_1 - 1; \quad k = 0, \ldots, n_2 - 1; \quad r = 0, \ldots, n_3 - 1 \tag{306}$$

and the expressions $\Lambda_{\ell mn}$ coincide with the ones given in eq. (272), if **A** there is replaced by $1/2\ (A_1 + A_2)$.

The same procedure gives for $K^{(1)}_{kr}$ the matrices

$$\Omega^{(x,1)}_{jkr} = \begin{pmatrix} \Lambda_{jkr+n_3} & \frac{1}{2}(A_1 - A_2) \\ \frac{1}{2}(A_1 - A_2) & \Lambda_{j+n_1\, k+n_2\, r} \end{pmatrix} ; \quad \Omega^{(y,1)}_{jkr} = \begin{pmatrix} \Lambda_{j+n_1\, k\, r+n_3} & \frac{1}{2}(A_1 - A_2) \\ \frac{1}{2}(A_1 - A_2) & \Lambda_{jk+n_2\, r} \end{pmatrix} \tag{307}$$

This is the reduction required. It is simple now to find the eigenvalues if the matrices $A_1, \ldots, D_4$ are diagonal or can be simultaneously diagonalized.

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