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Symmetries of the second-difference matrix and the finite Fourier transform

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The finite Fourier transformation is well known to diagonalize the second-difference matrix and has been thus applied extensively to describe finite crystal lattices and electric networks. In setting out to find all transformations having this property, we obtain a multiparameter class of them. While permutations and unitary scaling of the eigenvectors constitute the trivial freedom of choice common to all diagonalization processes, the second-difference matrix has a larger symmetry group among whose elements we find the dihedral 'manifest' symmetry transformations of the lattice. The latter are nevertheless sufficient for the unique specification of eigenvectors in various symmetry-adapted bases for the constrained lattice. The free symmetry parameters are shown to lead to a complete set of conserved quantities for the physical lattice motion.

I. INTRODUCTION

The Fourier integral transform owes its success to the well-known property of turning differential equations with constant coefficients into algebraic ones, amenable to an easier solution. Similarly, the finite Fourier transform has found use in the uncoupling of lattice and network equations as it diagonalizes the second-difference matrix. This is briefly reviewed in section II. In this article we find constructively the eigenvalues and eigenvectors of this matrix. In section III we thus find the largest class of transformations which have this property; the usual finite Fourier transform is only one –perhaps the simplest– unitary member of this class. In section IV we examine the freedom in the class, relating it to the symmetry group and eigenvalue degeneracies; this group contains the "manifest"

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discrete dihedral symmetries of an N-point lattice. As shown in section V, symmetry adaptation, i.e. the requirement that some dihedral operation constitute a definite symmetry, resolves the transformation ambiguity up to the trivial freedom of permutation and unitary scaling. Finally, in section VI we show that the symmetry group leads us to the independent conservation laws for the physical N-point lattice motion defined as sesquilinear invariants in phase space.

II. THE LATTICE EQUATIONS OF MOTION AND THE FOURIER TRANSFORM

Consider a closed linear lattice consisting of N equal masses M_n which can be numbered in some convenient fashion modulo N and which are pairwise connected by springs, k_{nm} being the Hooke constant of the spring connecting masses number n and m. If f_n is the displacement from equilibrium of mass n, its equation of motion will be [1, 2]

$$\begin{aligned} -M_n \ddot{f}_n &= k_{nn} f_n + \sum_{n \neq m} k_{nm}(f_n - f_m) \\ &= \sum_m [-k_{nm} + \delta_{n,m}(k_{nn} + \sum_r k_{nr})] f_m \\ &= \sum_m \kappa_{nm} f_m \quad , \qquad n = 1, 2, \ldots, N \quad . \end{aligned} \tag{1}$$

Here we are allowing each mass to be connected to its equilibrium position through a spring k_{nn}; the last member defines the elements of a symmetric interaction matrix $\mathbf{K} = \| \kappa_{nm} \|$. Sums over dummy indices extend from 1 to N.

The *simple* lattice case assumes that all springs connecting qth neighbours are equal, i.e. that κ_{nm} is a function of $q = |n - m|$ only. The interaction matrix $\mathbf{K}$ contains then at most $[N/2]$ different elements ($[r]$ is the largest integer which does not exceed r) and is constant along the main and parallel diagonals. The set of equations (1) can be written then as a vector equation

$$\mathbf{M}\ddot{\mathbf{f}} = -\mathbf{K}\mathbf{f} = \left(\sum_{q=0}^{[N/2]} k_q \Delta^q \right) \mathbf{f} \quad , \qquad k_q \geqslant 0 \quad , \tag{2}$$

where $\mathbf{M} = M\mathbf{1}$ for the case when all masses are equal and

$$\Delta = \begin{pmatrix} -2 & 1 & 0 & . & . & . & . & . & 0 & 1 \\ 1 & -2 & 1 & . & . & . & . & . & 0 & 0 \\ 0 & 1 & -2 & & & & & & & . \\ . & . & . & . & & & & & & . \\ . & . & . & & . & & & & & . \\ . & . & & & & & . & & & . \\ . & . & & & & & & . & & . \\ 0 & 0 & & & & & & & -2 & 1 \\ 1 & 0 & & & & & 0 & & 1 & -2 \end{pmatrix} \qquad (3a)$$

is the second-difference matrix. As

$$(\Delta^p)_{mn} = (-1)^{m+n-p} \binom{2p}{p+m-n}$$

$$= (\Delta^p)_{m,N-n} = (\Delta^p)_{N-m,n} \quad , \qquad (3b)$$

the k_p's in (2) can be put easily in terms of the pth neighbour interaction Hooke constants $\kappa_{n,n\pm p}$.

The task of finding the normal modes and frequencies of the simple lattice (2) is thus equivalent to the diagonalization of (3). This can be achived through the unitary *Fourier transform* matrix defined as

$$\mathbf{F} = \| F_{mn} \| = \| N^{½} \exp(-2imn/N) \| \quad . \qquad (4)$$

Indeed, one has

$$\mathbf{F}^{-1} \Delta \mathbf{F} = \Lambda \quad , \qquad \Lambda = \| -4\delta_{m,n} \sin^2 (\pi n/N) \| \quad , \qquad (5)$$

as can be easily verified through the summation formula

$$x^a + x^{a+1} + \ldots + x^{a+b} = \begin{cases} (1-x)^{-1} x^a (1-x^{b+1}) \ , & x \neq 1 \\ b+1 \ , & x = 1 \ , \end{cases} \qquad (6)$$

upon letting $a = 1$, $b = N-1$, $x = \exp(-2\pi i[n-m]/N)$, and performing some algebra. The Fourier matrix **F** has the properties of being: a) unitary, b) symmetric, c) expressed as (4) it is a *periodic* matrix (i.e. $F_{m,n} = F_{m',n'}$ for $m \equiv m'$ mod N and $n \equiv n'$ mod N), d) $F_{m,n} = F^*_{m,N-n} = F^*_{N-m,n}$. Once we have found a transform matrix with the property (5), the lattice equations of motion (2) uncouple into N second-order differential equations for the components of $\tilde{\mathbf{f}} = \mathbf{F}^{-1}\mathbf{f}$:

$$-\kappa_n \tilde{f}_n = M\ddot{\tilde{f}}_n\ , \qquad \kappa_n = -\sum_{q=0}^{[N/2]} k_q \lambda_n^q\ , \qquad n = 1, 2, \ldots, N\ , \quad (7a)$$

which represent N independent *pseudo*-oscillators, in the sense of being mathematical entities which obey the oscillator equations of motion with Hooke constants of κ_n. The solutions to (7a) are

$$\tilde{f}_n(t) = \tilde{f}_n(0)\cos(\omega_n t) + \dot{\tilde{f}}_n(0)\sin(\omega_n t)/\omega_n\ , \quad \omega_n = (\kappa_n/M)^{1/2}\ ,$$

$$n = 1, 2, \ldots, N\ , \qquad (7b)$$

which formally include the case $n = N$ ($\omega_N = 0$) which represents the free drift motion of the whole lattice as $\tilde{f}_N(t) = \tilde{f}_N(0) + \dot{\tilde{f}}_N(0)t$. The original solutions to (2) are then found as the components of $\mathbf{f} = \mathbf{F}\tilde{\mathbf{f}}$.

These are all well known facts. What we intend to do here is to find the eigenvalues and eigenvectors of Δ, i.e. the matrices Φ and Λ such that

$$\Delta\Phi = \Phi\Lambda\ , \qquad \Lambda = \|\delta_{mn}\lambda_n\|\ . \qquad (8)$$

In the process we shall be able to parametrize the freedom of this class of matrices and point out the particularities of the Fourier matrix.

III. DIAGONALIZATION OF THE SECOND-DIFFERENCE MATRIX

The elements of any matrix $\Phi = \|\varphi_{mn}\|$ that is to diagonalize Δ are constrained, due to (8), through the relations

$$-(2+\lambda_n)\varphi_{1,n} + \varphi_{2,n} + \varphi_{N,n} = 0 \qquad (9a)$$

$$\varphi_{m-1,n} - (2+\lambda_n)\,\varphi_{m,n} + \varphi_{m+1,n} = 0\ ,$$

$$m = 2, 3, \ldots, N-1 \qquad (9b)$$

$$\varphi_{1,n} + \varphi_{N-1,n} - (2+\lambda_n)\,\varphi_{N,n} = 0 \,,$$

$$n = 1, 2, \ldots, N \,. \tag{9c}$$

The first two recursion relations [3] show that any $\varphi_{m+1,n}$ can be put in terms of $\varphi_{1,n}$ and $\varphi_{N,n}$, with coefficients which can be only *polynomials* in $2+\lambda_n$. More precisely, we have

$$\varphi_{m+1,n} = U_m(x_n)\varphi_{1,n} + V_{m-1}(x_n)\varphi_{N,n} \,, \tag{10a}$$

$$x_n = 1 + \lambda_n/2 \,, \tag{10b}$$

where $U_q(x)$ and $V_q(x)$ are polynomials of degree q in x, as we can easily see replacing (10a) in (9b):

$$\begin{aligned} \varphi_{m+1,n} &= 2x_n\varphi_{m,n} - \varphi_{m-1,n} \\ &= [2x_n U_{m-1}(x_n) - U_{m-2}(x_n)]\varphi_{1,n} \\ &\quad + [2x_n V_{m-2}(x_n) - V_{m-3}(x_n)]\varphi_{N,n} \,. \end{aligned} \tag{11}$$

Comparison with (10) gives the recursion relation for $U_m(x)$:

$$U_m(x) = 2xU_{m-1}(x) - U_{m-2}(x) \,,$$

$$m = 2, 3, \ldots, N-1 \,. \tag{12}$$

and an identical one for $V_m(x)$. The base of the recursion is found considering $\varphi_{1n} = 1 \cdot \varphi_{1n} + 0 \cdot \varphi_{Nn}$ which implies $U_0(x) = 1$ and formally $V_{-1}(x) = 0$; equation (9a) yields $U_1(x) = 2x$ and $V_0(x) = -1$, while the next step sets $V_1(x) = -2x$. It follows that $V_m(x) = -U_m(x)$. The fact that Δ is a tridiagonal matrix, constant along the main and parallel diagonals, has constrained $U_m(x)$ to satisfy a *three*-term recursion relation with coefficients independent of m. This result can be compared with the Christoffel-Darboux formulae and base values for orthogonal polynomials. Indeed, Eq. (12) is found to characterize precisely the Chebyshev polynomials of the second kind [4]:

$$U_m(x) = \sin([m+1]\arccos x)/\sin(\arccos x) \quad . \tag{13}$$

Since the three-term recursion (9a)-(9b) closes in (9c), there are two conditions we have to impose for their proper matching. These will yield the values of x_n in Eqs. (10)-(13). Equations (10) for $m = N-1$ read —collecting terms—

$$U_{N-1}(x_n)\,\varphi_{1,n} - [U_{N-2}(x_n) + 1]\,\varphi_{N,n} = 0 \ , \tag{14a}$$

while the equality of the two expressions for $\varphi_{N-1,n}$, one obtained from (10) for $m = N-2$ and the other from (9c), lead to

$$[U_{N-2}(x_n) + 1]\,\varphi_{1,n} - [U_{N-3}(x_n) + 2x_n]\,\varphi_{N,n} = 0 \ . \tag{14b}$$

The values x_n for which (14) are a consistent system of homogeneous equations will yield the eigenvalues of Δ. If all coefficients in (14) are zero for a particular eigenvalue, this will be doubly degenerate as $\varphi_{1,n}$ and $\varphi_{N,n}$ are independent. If (14a) and (14b) have non-zero coefficients but are proportional, the eigenvalue will be simple. In both cases, the determinant of the system (14) must vanish:

$$[U_{N-2}(x_n) + 1]^2 - U_{N-1}(x_n)[U_{N-3}(x_n) + 2x_n] = 0 \ . \tag{15a}$$

Replacement of (13) into (15a) and some algebra involving trigonometric identities leads to

$$\sin\theta_n[1 - \cos(N\theta_n)] = 0 \ , \quad \cos\theta_n = x_n = 1 + \lambda_n/2 \ . \tag{15b}$$

The roots of (15b) lie at $\theta_n = 2\pi k/N$ for k integer. In the x_n-variable, these are

$$x_n = \cos(2\pi k/N) \ , \qquad k = 0, 1, 2, \ldots, [N/2] \ . \tag{16}$$

As the distinct roots are less than N, some of these must be degenerate and this can be analyzed as follows: the zeros of $U_m(x)$ lie at $\cos(k\pi/[m+1])$ while $U_m(\pm 1) = (\pm 1)^m(m+1)$. Examination of the system (14) shows that, for N odd, $k = 1, 2, \ldots, (N-1)/2$, the coefficients are zero. The same happens for N even at $k = 1, 2, \ldots, N/2 - 1$ and, as remarked following Eqs. (14), these eigenvalues must be doubly degenerate. This leaves one missing eigenvalue for N odd: this is $k = 0$, i.e. $x_n = 1$ for which $\varphi_{1,n} = \varphi_{N,n}$. When N is even, the two missing eigenvalues are accounted for by $k = 0$, as before; in addition, $k = N/2$, i.e. $x_n = -1$ for which $\varphi_{1,n} = -\varphi_{N,n}$.

The numbering of the eigenvalues presents us with the first freedom of choice. It is of a trivial kind since it is common to all diagonalization procedures: if Φ diagonalizes Δ then $\Phi\mathbf{P}$, $\mathbf{P}$ being a permutation matrix (see below), will also diagonalize Δ. Permutation matrices have one non-zero unit element in each row and in each column: $P_{mn} = \delta_{m,p(n)}$ where $p(n)$ is a one-to-one function of the set of points $(1, 2, ..., N)$ onto itself. The identity permutation is $p(n) = n$ while the matrix inverse to $\mathbf{P}$ is $\mathbf{P}^T$, as $(\mathbf{P}^{-1})_{mn} = \delta_{p(m),n} = P_{nm}$. Permutation matrices are real and unitary. Acting on a diagonal matrix Λ, $\mathbf{P}^{-1}\Lambda\mathbf{P}$ only replaces λ_n by $\lambda_{p(n)}$. It is thus a simple matter to order the eigenvalues λ_n stemming from (10b)-(16) according to k as

$$\lambda_n = 2\,[\cos(2\pi n/N) - 1] = -4\sin^2(\pi n/N)\ , \qquad n = 1, 2, ..., N\ , \tag{17a}$$

the two-fold degenerate eigenvalue pairs being $\lambda_n = \lambda_{N-n}$. The non-degenerate ones are $\lambda_N = 0$ and, when N is even, $\lambda_{N/2} = -4$. According to the ordering implied by (17a), the degenerate eigenvector components are given by (10)-(13)-(16) through

$$\varphi_{m,n} = \varphi_{N,n}\,\{\cos(2\pi mn/N) + [\gamma_n - \cos(2\pi n/N)] \times \sin(2\pi mn/N)/\sin(2\pi n/N)\}\ , \tag{17b}$$

$$\gamma_n = \varphi_{1,n}/\varphi_{N,n}\ , \qquad N/2 \neq n = 1, 2, ..., N-1\ . \tag{17c}$$

The eigenvectors corresponding to the non-degenerate eigenvalues are, as stated before,

$$\varphi_{m,N} = \varphi_{N,N} \text{ and, when } N \text{ even, } \varphi_{m,N/2} = (-1)^m\varphi_{N,N/2}\ . \tag{17d}$$

IV. DIHEDRAL SYMMETRY AND EIGENVALUE DEGENERACY

The simple lattice equations of motion are invariant under a set of "manifest" transformations involving a renumeration of the constitutent masses. These can be analyzed through noting that the matrix Δ in Eq. (3)

is invariant under certain similarity transformations involving permutations of rows and columns. We can easily determine those permutations **P** for which $\mathbf{P}^{-1}\Delta\mathbf{P} = \Delta$. The *m-n* element of the left hand side of this equation reads

$$(\mathbf{P}^{-1}\Delta\mathbf{P})_{mn} = \sum_{r,s} P^{-1}_{mr}\Delta_{rs}P_{sn}$$

$$= \sum_{r,s} \delta_{p(m),r}[-2\delta_{r,s} + \delta_{r,s-1} + \delta_{r,s+1}]\,\delta_{s,p(n)}$$

$$= -2\delta_{m,n} + \delta_{m,p^{-1}(p(n)-1)} + \delta_{m,p^{-1}(p(n)+1)}\,, \qquad (18a)$$

where all rows and columns are considered, as usual, modulo N. Equation (18a) will equal Δ_{mn} if and only if

$$\text{either } p(n \pm 1) = p(n) \pm 1 \text{ or } p(n \pm 1) = p(n) \mp 1\,. \qquad (18b)$$

The first case defines rotations, while the second requires reflections, as detailed below. The set of all permutations leaving Δ invariant define the dihedral group of matrices $\mathcal{D}_N$. If Φ diagonalizes Δ and **D** is an element of $\mathcal{D}_N$ then clearly $\mathbf{D}\Phi$ will also diagonalize Δ. This involves dihedral transformations between the *rows* of Φ. The trivial permutations seen in the last section involved permutations of the *columns* of this matrix.

The conditions (18b) imply that two neighbouring masses in a circular lattice remain adjacent after the transformation. This can be achieved under rotations of the circle or inversions through a diameter. Consider first the rotation matrix $\mathbf{R} = \| \delta_{m,n+1} \|$ which, when acting from the left on Φ will shift the rows of Φ downwards by one unit, the Nth row of Φ being the first of $\mathbf{R}\Phi$. All other cyclic permutations of the rows can be produced by powers of this matrix:

$$\mathbf{R}^k = \| \delta_{m,N+k} \| = \begin{pmatrix} \mathbf{0} & \mathbf{1}_k \\ \mathbf{1}_{N-k} & \mathbf{0} \end{pmatrix}, \qquad \mathbf{R}^N = \mathbf{1}_N\,, \qquad (19a)$$

where $\mathbf{1}_q$ is the $q \times q$ unit matrix and the **0**'s are appropiate rectangular null matrices. Next, *inversions* can be characterized by the rows which are left in place. If N is odd, one row must always be invariant. Thus, we define the matrices

$$\mathbf{I}_k = \| \delta_{m,\, N+2k-n} \| = \begin{pmatrix} \mathbf{A}_{N-2k-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_{2k+1} \end{pmatrix}$$

$$= \mathbf{R}^k \, \mathbf{I}_0 \, \mathbf{R}^{-k} \, , \qquad (19b)$$

where $\mathbf{A}_q$ is the $q \times q$ antidiagonal unit matrix. When N is even, then, in addition to the kth row, its antipodal, the $(N/2 + k)$th row is also invariant. When N is even, we have, moreover, one more class of inversions: those where no row is left invariant. This is accomplished through the matrices

$$\mathbf{K}_k = \| \delta_{m,\, N+2k+1-n} \| = \begin{pmatrix} \mathbf{A}_{N-2k} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_{2k} \end{pmatrix}$$

$$= \mathbf{R}^k \mathbf{K}_0 \mathbf{R}^{-k} \, . \qquad (19c)$$

Through simple counting we can verify that in every case $\mathcal{D}_N$ has $2N$ elements, meaning that for every matrix Φ diagonalizing Δ, that many distinct matrices $\mathbf{D}\Phi$ can be produced. In terms of the physical lattice, the $\mathbf{R}^k$ rotate the system through k times the inter-mass angle, the $\mathbf{I}_k$ reflect the system across a diameter passing through mass k, while $\mathbf{K}_k$ performs the same across a diameter through the midpoints of the springs joining masses k and $k + 1$, and masses $N/2 + k$ and $N/2 + k + 1$.

Although the symmetries above are all the *manifest* symmetries of the lattice, they are far from being all the symmetries. To see this, consider the diagonal matrix Λ, which is equivalent —through the Fourier transformation— to Δ. Clearly, if $\varphi_{\cdot n}$ and $\varphi_{\cdot N-n}$ are two linearly independent eigenvectors corresponding to the same eigenvalue $\lambda_n = \lambda_{N-n}$, two independent linear combinations of these will also qualify to define an eigenbasis for Δ. If we denote by $\mathbf{T}_n$ and $N \times N$ non-singular matrix which has the elements of the unit matrix except for the intersections of the nth and $(N-n)$th rows and columns, then $\mathbf{T}_n^{-1} \Lambda \, \mathbf{T}_n = \Lambda$. Consequently, if Φ diagonalizes Δ, so will $\Phi \, \mathbf{T}_n$.

Now, each $\mathbf{T}_n$ may have four complex parameters and $\mathbf{T}_n \mathbf{T}_{n'} = \mathbf{T}_{n'} \mathbf{T}_n$ for $n \neq n'$. For N odd there are thus four complex free parameters for each of the $(N-1)/2$ degenerate eigenvalue pairs, while for N even, we have $N/2 - 1$ degenerate pairs. In addition, non-degenerate eigenvalues can have their corresponding eigenvectors multiplied by any complex number. To this end one can define $\mathbf{T}_N$ as a diagonal matrix with 1's except for the N-N element, and similarly for $\mathbf{T}_{N/2}$, when N is even. The total number of complex free parameters is thus $2N - 1$ for N odd and $2N - 2$ for N even. This total equals the number of free parameters in the Fourier matrix (17b)-(17d). In fact, through products with $\mathbf{T}_n$'s we can produce, out of a given Φ, any other Δ-diagonalizing matrix.

One may wonder if, for every matrix D in $\mathcal{D}_N$, we have a corresponding product $\Pi_n \mathbf{T}_n = \mathbf{T}$ such that $\mathbf{D}\Phi = \Phi\mathbf{T}$. Indeed, one can easily find its corresponding $\mathbf{T} = \Phi^{-1}\mathbf{D}\Phi$. What is perhaps surprising is that in the analysis of the structure of $\Phi\mathbf{T}\Phi^{-1}$ one finds that the dihedral group $\mathcal{D}_N$ of manifest symmetries of the lattice is embedded as a discrete subgroup in the continuous group of all $\Pi_n \mathbf{T}_n$, which qualifies then as the hidden symmetry group of the system. We shall not go into this here, although the Lie-theoretical results of this observation are interesting in their own right.

A well known property of the eigenvectors of Hermitean matrices is that those corresponding to different eigenvalues are orthogonal with respect to the natural sesquilinear inner product $(\mathbf{u}, \mathbf{v}) = \Sigma_n u_n^* v_n$. Those which correspond to the same eigenvalue, in our case $\lambda_n = \lambda_{N-n}$, need not be. In fact, from (17b) and the summation formula (7), we find

$$(\varphi_{\cdot n}, \varphi_{\cdot N-n}) = \varphi^*_{N,n}\varphi_{N,N-n}(N/2)[\gamma_n^*\gamma_{N-n} - (\gamma_n^* + \gamma_{N-n})$$

$$\times \cos(2\pi n/N) + 1]/\sin^2(2\pi n/N) ,$$

$$N/2 \neq n = 1, 2, \ldots, N-1 . \qquad (20a)$$

In order that the two independent eigenvectors be orthogonal, it is necessary that γ_n and γ_{N-n} be related by

$$\gamma_{N-n} = [\gamma_n^* \cos(2\pi n/N) - 1]/[\gamma_n^* - \cos(2\pi n/N)] . \qquad (20b)$$

Finally, each eigenvector will be normalized when $(\varphi_{\cdot n}, \varphi_{\cdot n}) = 1$. This implies, through a procedure parallel to that followed in (19), that $\varphi_{N,n}$ and γ_n be related by

$$|\varphi_{N,n}| = \{(N/2)[1 + |\gamma_n|^2 - 2\,\mathrm{Re}\,(\gamma)\cos(2\pi n/N)]\}^{-1/2}\sin(2\pi n/N)$$

$$N/2 \neq n = 1, 2, \ldots, N-1 , \qquad (21a)$$

while for the two non-degenerate eigenvalues, one has

$$|\varphi_{N,\,N}| = N^{-1/2} \text{ and, when } N \text{ even, } |\varphi_{N,\,N/2}| = N^{-1/2} \ . \tag{21b}$$

The commonly defined Fourier transform **F** in (5) is a unitary matrix which can be seen to stem from the choice.

$$\gamma_n^{\mathrm{F}} = \exp(-2\pi i n/N) \ , \quad n = 1, 2, ..., (N-1)/2 \ , \tag{22}$$

and $\varphi_{Nn}^{\mathrm{F}} = N^{-1/2}$, $n = 1, 2, ..., N$. It is clear that from **F** we can obtain any other Δ-diagonalizing matrix Φ through right multiplication by matrices $\mathbf{T}_n$ as $\Phi = \mathbf{F}\Pi_n \mathbf{T}_n$.

V. DEGENERACY RESOLUTION THROUGH DIHEDRAL SYMMETRY

As we have seen, the Δ matrix does not lead to a unique specification of its eigenvectors due to the degeneracy in its eigenvalues. We now search for other matrices commuting with Δ which may provide the missing labels. Although any matrix $\mathbf{F}(\Pi_n \mathbf{T}_n)\mathbf{F}^{-1}$ will commute with Δ since $\Pi_n \mathbf{T}_n$ commutes with Λ, we are generally interested in those matrices which can be given a clear geometric meaning, such as the subset $\mathcal{D}_N$. These will provide the eigenvectors with definite symmetry under lattice rotations and inversions. For the former, a unique classification will be obtained, coinciding with the usual Fourier basis. For the latter, the various bases can serve to describe lattices with constraints: if N is even, lattices with two fixed masses —endpoints— or two fixed spring midpoints; if N is odd, lattices with one fixed mass and one fixed spring midpoint. As all the matrices (19) are unitary, their eigenvalues will be of modulus one and their nondegenerate eigenspaces, orthogonal. The inversion matrices (19b) and (19c) are, moreover, Hermitean. Their spectrum can therefore consist only of the points +1 and −1. The Δ-degenerate spaces will separate into odd- and even-symmetry eigenvectors.

Consider first the matrix Φ as defined through (8) and diagonalizing one of the rotation operators:

$$\mathbf{R}^k \Phi = \Phi \hat{\mathbf{R}}^k \ \Leftrightarrow \ \varphi_{m-k,\,n} = \rho_n \varphi_{m,\,n} \ , \ \hat{\mathbf{R}}^k = \| \delta_{mn} \rho_n^{(k)} \| \ , \tag{23a}$$

Using (17) in (23a) yields, in terms of the free parameters $\varphi_{N,n}$ and γ_n, the relation

$$\varphi_{N,n}\{\rho_n^{(k)}\gamma_n \sin(2\pi mn/N) - \rho_n^{(k)}\sin(2\pi[m-1]n/N)$$

$$-\gamma_n \sin(2\pi[m-k]n/N) + \sin(2\pi[m-k-1]n/N)\} = 0 \ ,$$

$$m, n = 1, 2, ..., N \ . \qquad (23b)$$

These equations for $m = 0$ and $m = 1$ yield the eigenvalues of $\mathbf{R}^k$ as

$$\rho_n^{(k)} = \exp(2\pi ikn/N) = \rho_{N-n}^{(k)*} \ , \qquad n = 1, 2, ..., N \ . \qquad (24a)$$

The corresponding eigenvectors are defined by

$$\gamma_n = \exp(-2\pi ikn/N) = \gamma_{N-n}^* \ , \qquad n = 1, 2, ..., N \ , \qquad (24b)$$

leaving the $\varphi_{N,n}$ free. We see that Δ-degeneracy is indeed lifted since the two orthogonal vectors with the same eigenvalue under Δ have complex conjugate —hence distinct— eigenvalues under $\mathbf{R}^k$. Only when $k = 0$ or $k = N/2$ when N even, does the degeneracy remain unresolved. The reason for this is due to the fact that $\mathbf{R}^0$ and $\mathbf{R}^{N/2}$ commute with all the elements in $\mathcal{D}_N$ (they are the center of the group). They can be thus diagonalized together with any other element of $\mathcal{D}_N$. If we ask that the matrix Φ be unitary, condition (21a) will impose $|\varphi_{N,n}| = N^{-1/2}$, $N/2 \neq n \neq N$, leaving only the N phases of the $\varphi_{N,n}$ free. It is interesting to note that the Fourier transform matrix can be defined up to column phases as that transformation which diagonalizes $\mathbf{R}^k$ for any k that is not a non-trivial divisor of N. If this condition is satisfied, there will be no degenerate eigenvalues, and the form (17)-(24) gives the proper eigenvectors.

The matrix Φ can also be defined through (8) and either of the relations

$$\mathbf{I}_k\Phi = \Phi\hat{\mathbf{I}}_k \Leftrightarrow \varphi_{2k-m,n} = \iota_n^{(k)}\varphi_{m,n} \ , \quad \hat{\mathbf{I}}_k = \|\delta_{m,n}\,\iota_n^{(k)}\| \qquad (25a)$$

$$\mathbf{K}_{k'}\Phi = \Phi\hat{\mathbf{K}}_{k'} \Leftrightarrow \varphi_{2k'+1-m,n} = \kappa_n^{(k')}\varphi_{m,n} \ , \quad \hat{\mathbf{K}}_{k'} = \|\delta_{mn}\,\kappa_n^{(k')}\| \qquad (25b)$$

for some k or k'. The two nondegenerate eigenvectors (17d) correspond to the eigenvalue $+1$ under $\mathbf{I}_k$ and under $\mathbf{K}_{k'}$ to $+1$ and $(-1)^n$, respectively. Equations (25) lead through (17) to the relation

$$\varphi_{N,n}\{\mu_n^{(k)}\gamma_n \sin(2\pi mn/N) - \mu_n^{(k)} \sin(2\pi[m-1]n/N)$$

$$-\gamma_n \sin(2\pi[\xi^{(k)} - m]n/N) + \sin(2\pi[\xi^{(k)} - 1 - m]n/N)\} = 0 \ ,$$

$$m, n = 1, 2, \ldots, N \ , \qquad (26)$$

where $\mu_n^{(k)}$ is $2n$ and $\xi^{(k)}$ is $2k$ for $\mathbf{I}_k$, while for $\mathbf{K}_k$ they are $\kappa_n^{(k)}$ and $2k+1$, respectively.

In what follows immediately below we exclude $\mathbf{I}_0$ from our considerations. Equations (26) for $m = 0$ and $m = 1$ lead to the determination of $\mu_n^{(k)} = \pm 1$ for $N \neq n \neq N/2$. This shows that the eigenvalues of these operators will indeed resolve the Δ-degeneracy. Correspondingly, one has

$$\gamma_n^{(+1)} = \cos(2\pi[\xi^{(k)}/2 - 1]n/N)/\cos(\pi\xi^{(k)}n/N) \ , \qquad (27a)$$

$$\gamma_n^{(-1)} = \sin(2\pi[\xi^{(k)}/2 - 1]n/N)/\sin(\pi\xi^{(k)}n/N) \ ,$$

$$N \neq n \neq N/2 \ , \qquad (27b)$$

leaving the $\varphi_{N,n}$ free. The unitary condition (21a) furthermore imposes the restrictions:

$$|\varphi_{N,n}^{(+1)}| = (N/2)^{-1/2} \, |\cos(\pi\xi^{(k)}n/N)| \ , \qquad (28a)$$

$$|\varphi_{N,n}^{(-1)}| = (N/2)^{-1/2} \, |\sin(\pi\xi^{(k)}n/N)| \ , \qquad N/2 \neq n \neq N \ , \qquad (28b)$$

leaving again only phases free. The case for $\mathbf{I}_0$ is somewhat special. If the eigenvalue is $+1$, we obtain from the preceding formulae $\varphi_n^{(+1)} = \cos(2\pi n/N)$ and $|\varphi_{Nn}^{(+1)}| = (N/2)^{-1/2}$. If the eigenvalue is -1, since the operator leaves the Nth component in place, we obtain $\varphi_{N,n}^{(-1)} = 0$, and the ratio $\varphi_n^{(-1)}$ is meaningless. As long as we consider the product $\varphi_{N,n}^{(-1)}\varphi_n^{(-1)}$ to be finite, we can make sense out of (26) and obtain $\varphi_{mn}^{(-1)} = C_n \sin(2\pi\, mn/N)$ with $|C_n| = (N/2)^{-1/2}$, again leaving the phase freedom.

We conclude that any of the dihedral matrices (excepting $\mathbf{R}^0 = \mathbf{1}$ and $\mathbf{R}^{N/2}$) suffices to resolve the degeneracy in the Δ eigenvector problem. The requirement of unitarity further leaves only the unavoidable phase ambiguity in each of the vectors.

VI. SYMMETRY AND CONSERVATION LAWS FOR THE SIMPLE LATTICE

In this section we shall see how the symmetry group of the lattice can be used in order to find constants of motion for the system. The lattice equations of motion, Eq. (2), can be written as a first-order differential equation in a 2N-dimensional configuration-velocity space whose elements and transformation matrices we shall denote with a caret. Thus we write

$$\begin{pmatrix} 0 & 1 \\ -\mathbf{M}^{-1}\mathbf{K} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{f} \\ \dot{\mathbf{f}} \end{pmatrix} = \frac{d}{dt} \begin{pmatrix} \mathbf{f} \\ \dot{\mathbf{f}} \end{pmatrix} , \qquad \text{i.e. } \hat{\mathbf{H}}\hat{\mathbf{f}} = \frac{d}{dt}\hat{\mathbf{f}} . \tag{29}$$

The first component of this equation defines $\dot{\mathbf{f}}$ as $d\mathbf{f}/dt$, while the second one reproduces (2) with this definition.

The solution of the equation of motion (29) can be written in terms of the initial conditions (at time $t = 0$) as [2]

$$\begin{pmatrix} \mathbf{f}(t) \\ \dot{\mathbf{f}}(t) \end{pmatrix} = \exp \left[t \begin{pmatrix} 0 & 1 \\ -\mathbf{M}^{-1}\mathbf{K} & 0 \end{pmatrix} \right] \begin{pmatrix} \mathbf{f}(0) \\ \dot{\mathbf{f}}(0) \end{pmatrix} ,$$

$$\text{i.e. } \hat{\mathbf{f}}(t) = \exp(t\mathbf{H})\, \hat{\mathbf{f}}(0) . \tag{30}$$

This leads to the definition of the time-evolution operator of the system.

We are interested here in constructing sesquilinear forms in this 2N-dimensional space of the form

$$E(\mathbf{f}) = (\mathbf{f}^\dagger\ \dot{\mathbf{f}}^\dagger) \begin{pmatrix} \mathbf{E}_a & \mathbf{E}_b \\ \mathbf{E}_c & \mathbf{E}_d \end{pmatrix} \begin{pmatrix} \mathbf{f} \\ \dot{\mathbf{f}} \end{pmatrix} ,$$

$$\text{i.e.} \quad E(\mathbf{f}) = \hat{\mathbf{f}}^\dagger \hat{\mathbf{E}}\, \hat{\mathbf{f}} , \tag{31}$$

which are to be *conserved*, i.e., are to be independent of time as $\hat{\mathbf{f}}$ is allowed to evolve according to (30). Equation (30), when substituted in (31), yields the relation

$$\exp(t\hat{\mathbf{H}}^\dagger)\hat{\mathbf{E}} = \hat{\mathbf{E}}\, \exp(-t\hat{\mathbf{H}}) . \tag{32a}$$

This relation holds true if and only if the derivative of this expression with respect to t at $t = 0$ holds, i.e.,

$$\hat{H}^{\dagger}\hat{E} = -\hat{E}\hat{H} . \tag{32b}$$

Written out in $N \times N$ matrix form, this result embodies four matrix equations:

$$\mathbf{K}^{\dagger}\mathbf{M}^{\dagger-1}\mathbf{E}_c + \mathbf{E}_b\mathbf{M}^{-1}\mathbf{K} = \mathbf{0} , \qquad \mathbf{M}^{-1}\mathbf{K}\mathbf{E}_d - \mathbf{E}_a = \mathbf{0} ,$$

$$\mathbf{E}_a - \mathbf{E}_d\mathbf{M}^{-1}\mathbf{K} = \mathbf{0} , \qquad \mathbf{E}_b + \mathbf{E}_c = \mathbf{0} . \tag{33}$$

In the case of the simple lattice, i.e., when $\mathbf{M} = M\mathbf{1}$ and $\mathbf{K}$ is symmetric and built as a sum of powers of Δ (barring accidental symmetries as, for instance, when all qth-neighbour springs are equal and independent of q), Eqs. (33) are equivalent to the system

$$\Delta\mathbf{E}_d = \mathbf{E}_d\Delta , \qquad \mathbf{E}_a = M^{-1}\mathbf{K}\mathbf{E}_d , \tag{34a}$$

$$\Delta\mathbf{E}_b = \mathbf{E}_b\Delta , \qquad \mathbf{E}_c = -\mathbf{E}_b . \tag{34b}$$

In this system the submatrices $\mathbf{E}_d$ and $\mathbf{E}_b$ should commute with Δ, while the other two are determined once the first pair is given.

The set of $2N \times 2N$ matrices $\hat{\mathbf{E}}$ with the property (32) forms a complex vector space since any linear combination of such matrices will again have property (32). We are thus interested in finding a basis for this space. In section IV we saw that the "manifest" symmetry dihedral matrices (19) commute with Δ. Moreover, it was seen that the full symmetry group was provided by the matrices $\mathbf{T}_n$ which commute with Λ, so it follows that $\Phi\,\mathbf{T}_n\Phi^{-1}$ will commute with Δ. The arbitrariness in the choice of Φ has no effect on this result.

The matrices $\mathbf{T}_n$ can be written as

$$\mathbf{T}_n = \mathbf{1} + \sum_{\mu=1}^{4} a_n^{\mu}\,\tau_{\mu}^{(n)} , \qquad n = 1, 2, \ldots, [(N-1)/2] , \tag{35a}$$

where $\mathbf{1}$ is the $N \times N$ unit matrix. The $\tau_{\mu}^{(n)}$ are matrices whose non-zero elements are

$$\tau_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \tau_2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\tau_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \tau_4 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{35b}$$

placed in the intersections of the nth and $(N-n)$th rows and columns. For the special cases $\nu = N$ and, when N even, $\nu = N/2$, we can write $\mathbf{T}_\nu$ in terms of matrices $\tau^{(\nu)}$ with a single 1 in the N-N or $N/2$-$N/2$ position:

$$\mathbf{T}_\nu = \mathbf{1} + a_\nu \tau^{(\nu)}, \qquad \tau^{(\nu)} = \| \delta_{n,\nu} \delta_{m,\nu} \| , \tag{35c}$$

Since $\mathbf{1}$ obviously commutes with Δ and can be expressed as a sum of τ's, a basis for the matrices which commute with Δ is given thus by $\Phi \tau_\mu^{(n)} \Phi^{-1}$ for $n = 1, 2, ..., N$ (excluding double-counting and, when $n = N$ or $N/2$ we simply disregard the index μ and use (35c) for its definition). Counting the number of degenerate eigenvalue pairs with a four-dimensional matrix basis (35a) and the non-degenerate ones with a one-dimensional basis (35c), and doubling this number for the two equations in (34), we conclude that the space of conserved sesquilinear forms (31) is $(4N-2)$-dimensional for N odd and $(4N-4)$-dimensional for N even. Note that when the coefficients a_n in (35) are real, the matrices are Hermitean.

We shall now proceed to determine the physical meaning of each of the basis vectors of this space as we let first $\mathbf{E}_d$ run over all $\Phi\tau_\mu^{(n)} \Phi^{-1}$ and $\mathbf{E}_b = \mathbf{0}$, and second consider $\mathbf{E}_d = \mathbf{0}$ and $\mathbf{E}_b$ to be the $\Phi\tau_\mu^{(n)} \Phi^{-1}$. We recall that the vector $\tilde{\mathbf{f}} = \Phi^{-1}\mathbf{f}$ is the Fourier transform vector of $\mathbf{f}$. If Φ coincides with the usual Fourier transform matrix (5) or if Φ is a unitary matrix, then $\tilde{\mathbf{f}}^\dagger = \mathbf{f}^\dagger\Phi$; if not, then $\mathbf{f}^\dagger \Phi = \tilde{\mathbf{f}}^\dagger \mathbf{S}$, with $\mathbf{S} = \Phi^\dagger\Phi$ being a matrix which effects linear combinations in the degenerate eigenvalue planes. For the sake of conciseness we shall assume below that Φ is unitary. A simple substitution will yield the other cases.

Using the first set of conditions described above, we obtain the constans of motion

$$E_\mu^{(n)}(\mathbf{f}) = \dot{\tilde{\mathbf{f}}}^\dagger \tau_\mu^{(n)} \dot{\tilde{\mathbf{f}}} + M^{-1} \tilde{\mathbf{f}}^\dagger \tilde{\mathbf{K}} \tau_\mu^{(n)} \tilde{\mathbf{f}} ,$$

$$n = 1, 2, ..., [N/2] , \quad \text{or } n = N . \tag{36a}$$

For the second case, after multiplying $\mathbf{E}_b$ by i and changing letters for notational convinience, we obtain

$$F_\mu^{(n)}(\mathbf{f}) = i(\tilde{\mathbf{f}}^\dagger \tau_\mu^{(n)} \dot{\tilde{\mathbf{f}}} - \dot{\tilde{\mathbf{f}}}^\dagger \tau_\mu^{(n)} \tilde{\mathbf{f}}) ,$$

$$n = 1, 2, ..., [N/2] , \text{ or } n = N . \qquad (36b)$$

The first observation is that the constants of motion $E_1^{(n)}$ and $F_1^{(n)}$ involve only the nth componets of $\tilde{\mathbf{f}}$, while $E_2^{(n)}$ and $F_2^{(n)}$ only the $(N-n)$th component. The other two will involve both the nth and $(N-n)$th components. The E's have the general form of energies, involving quadratic expressions in the velocity plus cuadratic expressions in the elongation, in fact, one has that

$$ME_1^{(n)}(\mathbf{f}) = M|\dot{\tilde{f}}_n|^2 + \kappa_n |\tilde{f}_n|^2 = ME_2^{(N-n)} ,$$

$$n = 1, 2, ..., N . \qquad (37)$$

Thus, the E's are the energies associated to each of the Fourier partial waves, generalized in the sense of holding also for partial waves defined through any of the Δ-diagonalizing unitary matrices Φ. These are N real, positive quantities where we recall that $\lambda_n \leqslant 0$. Next, for $\mu = 3$ and 4, one finds

$$E_3^{(n)}(\mathbf{f}) = 2\,\mathrm{Re}(\dot{\tilde{f}}_n^* \dot{\tilde{f}}_{N-n} + M^{-1} \kappa_n \tilde{f}_n^* \tilde{f}_{N-n}) , \qquad (38a)$$

$$E_4^{(n)}(\mathbf{f}) = 2\,\mathrm{Im}(\dot{\tilde{f}}_n^* \dot{\tilde{f}}_{N-n} + M^{-1} \kappa_n \tilde{f}_n^* \tilde{f}_{N-n}) ,$$

$$n = 1, 2, ..., [(N-1)/2] , \qquad (38b)$$

which are $2[(N-1)/2]$ real quantities.

We now continue in the same manner with the F's in (36b). These will have the form of angular momenta, as suggested below. The conserved quantities are

$$F_1^{(n)}(\mathbf{f}) = 2\,\mathrm{Im}(\dot{\tilde{f}}_n^* \tilde{f}_n) = F_2^{(N-n)}(\mathbf{f})$$

$$n = 1, 2, ..., N \qquad (39)$$

and

$$F_3^{(n)}(\mathbf{f}) = 2\,\mathrm{Im}(\dot{\tilde{f}}_n^{\,*}\tilde{f}_{N-n} + \dot{\tilde{f}}_{N-n}^{\,*}\tilde{f}_n)\;, \tag{40a}$$

$$F_4^{(n)}\,\mathbf{f} = -2\,\mathrm{Re}(\dot{\tilde{f}}_n^{\,*}\tilde{f}_{N-n} - \dot{\tilde{f}}_{N-n}^{\,*}\tilde{f}_n)\;,\; n = 1, 2, ..., [(N-1)/2]\;, \tag{40b}$$

The total number of constants of motion equals the number of real plus imaginary parts of the free parameters of Φ seen in Sect. IV, namely $2(2N-1)$ for N odd and $2(2N-2)$ for N even.

We shall now reduce this large set of constants of motion by considering the actual physical lattice where the elongations and velocities are real quantities and where we will have no more than the $2N$ constants of motion afforded by the $2N$ initial conditions. To this end, consider first the usual Fourier transform (5) and the Fourier partial waves associated to it. Since $F^*_{mn} = F_{m,N-n} = F_{N-m,n}$, it follows that when $\mathbf{f}$ is a real vector, then $\tilde{f}^*_m = \tilde{f}_{N-m}$, and similarly for the velocities. With this restriction, it is easy to see that the number of independent constants reduces: in (37), one has $E_1^{(n)} = E_4^{(n)-n)}$, while in (38), one has $E_3^{(n)} = E_3^{(N-n)}$ and $E_4^{(n)} = -E_4^{(N-n)}$. Finally, in (39), one has the relation

$$F_1^{(n)}(\mathbf{f}) = -i(\dot{\tilde{f}}_{N-n}\tilde{f}_n - \dot{\tilde{f}}_n\tilde{f}_{N-n}) = -F_1^{(N-n)}(\mathbf{f})\,,\,. \tag{41}$$

This result assigns to this constant of motion the meaning of an angular momentum in the uncoupled Fourier pseudo-oscillator planes corresponding to the degenerate eigenvalues. Lastly, in (40), one has that $F_3^{(n)}$ and $F_4^{(n)}$ are identically zero.

We note the identity $4(E_1^{(n)})^2 = (E_3^{(n)})^2 + (E_4^{(n)})^2$, valid for $n = N$ and, when N even, for $n = N/2$ as well. If none of the interaction matrix eigenvalues κ_n is zero, we see through simple counting, thus, that we are provided with $2N-1$ real constants of the motion when N is odd, and $2N-2$ constants when N is even. If for one or more $\bar{n}$ the interaction operator eigenvalue $\kappa_{\bar{n}}$ is zero, (as in the case of the simple wave equation, where $\mathbf{K} = -k\Delta$ and $\kappa_N = 0$), then $4(E_1^{(\bar{n})})^2 + (E_3^{(\bar{n})})^2 + (E_4^{(\bar{n})})^2$, and we loose that number of constants of the motion. This is due to the fact that if we replace $\tilde{f}_{\bar{n}}$ by $\tilde{f}_{\bar{n}} + c\dot{\tilde{f}}_{\bar{n}}$, for any real c, none of the sesquilinear constants of the motion is altered. This corresponds to adding to $\mathbf{f}$ a vector with components $cF_{n\bar{n}}(\mathbf{F}^\dagger\,\dot{\mathbf{f}})_{\bar{n}}$, $n = 1, 2, ..., N$. For the wave equation case, this is any real constant vector.

Finally, if any non-usual Fourier basis $\tilde{\mathbf{f}}$ is used, but related to the Fourier transform basis through $\tilde{\mathbf{f}} = (\Pi_n T_n)\bar{\mathbf{f}}$, it will effect at most linear combinations in the degenerate eigenvalue planes. It is easy to see then from (36) that the new $E_\mu^{(n)}$'s will be linear combinations of the old $E_\mu^{(n)}$'s in (37)-(38), the coefficients being sesquilinear functions of the transforming matrices $\mathbf{T}_n$. The same holds for the $F_\mu^{(n)}$'s. In any case, though, we remain with $2N$ independent constants of motion.

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RESUMEN

La transformación de Fourier finita, como es bien sabido, diagonaliza a la matrix de segunda diferencia y por ello ha sido usada extensamente para describir mallas cristalinas y redes eléctricas. Al proponernos encontrar todas las matrices con esta propiedad, obtenemos un conjunto multiparamétrico de ellas. Las permutaciones y los cambios de norma de los vectores propios constituyen los grados de libertad triviales, comunes a todos los procesos de diagonalización. Sin embargo, la matriz de segunda diferencia posee un grupo de simetrías más amplio. Entre los elementos de este grupo continuo encontramos las simetrías manifiestas de transformaciones dihedrales de la malla. Estos últimos son, sin embargo, suficientes para la elección única de una base de vectores propios ortonormales adaptados de acuerdo a varias simetrías para las redes constreñidas. Los parámetros de las simetrías no-triviales llevan a un conjunto completo de cantidades conservadas bajo el movimiento de una malla física.