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Travelling waves, symmetries and invariant quadratic forms in discrete systems

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We consider discrete, finite systems which abide Klein-Gordon, damped wave, or Helmholtz difference-differential equations. The evolution operator of these systems is diagonal in the travelling-wave basis. There, the symmetry properties are most evident. We construct the complete set of sesquilinear and bilinear time-invariant forms associated to a factor ring of the phase-space symmetry group of the system. The associated constants of the motion have the structure of energies and angular momenta. Their homogeneity under geometric (dihedral) transformations and time inversions is examined, as well as their positivity properties. Lastly, in letting the elements of the system approach a continuum, and imposing Poincaré or Euclidean invariance, we obtain the positive inner products for the Klein-Gordon positive-energy solution space and for the oscillatory Helmholtz solution space.

I. INTRODUCTION

I.1 Lattices

Consider a system with N elements whose configuration and motion at a given time t are determined completely by a set of observables $\mathbf{f}_n(t)$, $n = 1, 2, ..., N$, the subindex referring to the nth element of the system, and the components of this vector encompassing all the information needed to specify the state of the element. In the first five sections we shall treat as a concrete model a system composed of point masses M_n, $n = 1, 2, ..., N$ and springs joining these masses with Hooke's constants $k_{nn'} = k_{n'n}$ for the spring joining masses number n and n', inmersed in a viscous medium with damping constant C_n for the nth mass, with one space degree of freedom, specified by its elongation, $f_n(t)$, *for the* nth mass at time t. Such a mechanical model will be referred to as a discrete N-element *lattice* [1].

I.2 Equation of motion

It is well known that the equation of motion for each element of the lattice can be set up considering the forces acting on it: the sum of the forces on the nth mass due to its connecting springs is $-\Sigma_{n'} k_{nn'}[f_n(t) - f_{n'}(t)]$, a spring tying M_n to its equilibrium position will yield a force of $-k_{nn} f_n(t)$ and the viscous force $-Cn\dot{f}_n(t)$. The mass M_n will respond with an acceleration $\ddot{f}_n(t)$, leading to the equations of motion

$$M_n \ddot{f}_n(t) + C_n \dot{f}_n(t) + \sum_{n'=1}^{N} k_{nn'}[f_n(t) - f_{n'}(t)] + k_{nn} f_n(t) = 0 \ . \qquad (1.1)$$

This is a coupled set of equations. The purpose of harmonic analysis is to solve (1.1) through uncoupling the equations of the set such that only ordinary differential equations are left to solve. Fourier analysis is useful to this purpose since it uncouples the particular case of a *homogeneous* lattice, i.e., a lattice which consists of equal masses M, damping constants C, and a set of springs whose Hooke's constants depend only on the 'distance' between the masses as $k_{n,n'} = k_{|n-n'|}$.

It is convenient to think of such a lattice arranging the masses around a circle, numbered by successive values of n, with k_p being the Hooke's constant of the springs between pth neighbours. Slight care is needed for the upper value of p: when N is odd, it is $P(N) = (N-1)/2$ while when N is even, it is $P(N) = N/2$. In the last case the Hooke's constant between the antipodal pair should be divided by two, to give $k_{N/2}$, as two pth neighbours are assumed in writing (1.1).

We can then write (1.1) as the N-dimensional vector equation

$$M\ddot{\mathbf{f}}(t) + C\dot{\mathbf{f}}(t) + \mathbf{K}\mathbf{f}(t) = 0 \ , \quad \mathbf{f}(t) = \|f_n(t)\| \ , \qquad (1.2)$$

where $\mathbf{K}$ will be referred to as the *interaction* matrix; its elements can be found through elementary manipulation of the sum in (1.1), as $\mathbf{K} = \|K_{nn'}\|$,

$$K_{nn'} = -k_{|n-n'|} + \delta_{n,n'}\Big(k_0 + \sum_{n''=1}^{N} k_{|n-n''|}\Big) \ . \qquad (1.3)$$

It is a *symmetric, circulating* matrix. When only first neighbour interactions are present ($k_0 = 0, k_1 \neq 0, k_p = 0, p = 2, 3, \ldots, P(N)$) then K is $-k_1$ times the second-difference matrix ($\mathbf{K} = -k_1\Delta$):

$$\Delta = \|\Delta_{nn'}\| \ , \quad \Delta_{nn'} = -2\delta_{n,n'} + \delta_{n,n'+1} + \delta_{n,n'-1} \qquad (1.4)$$

with n and n' counted modulo N. Farther-neighbour interaction matrices -up to qth neighbours, say- are expressible as a linear combination of $\Delta^p, p = 0, 1, \ldots, q$.

I.3 The Fourier transform

The N-dimensional Fourier transform is a change of coordinates in N-space brought about by the Fourier matrix

$$\mathbf{F} = \|F_{nm}\| \ , \quad F_{nm} = N^{-1/2} \exp(-2\pi imn/N) \ . \qquad (1.5)$$

It is one within a class of matrices [2] which diagonalize Δ:

$$\mathbf{F}^{-1}\Delta\mathbf{F} = \|\delta_{m,m'}\lambda_m\| \ , \quad \lambda_m = -4\sin^2(\pi m/N) \ . \qquad (1.6)$$

It is unitary: $\mathbf{F}^{-1} = \mathbf{F}^{\dagger}$ and a fourth root of the unit matrix: $\mathbf{F}^4 = 1$. The general homogeneous lattice interaction matrix K is also diagonalized, then, as

$$\mathbf{F}^{-1}\mathbf{K}\mathbf{F} = \|\delta_{m\,m'}\mu_m\| \qquad (1.7a)$$

$$\mu_m = k_0 + 4\sum_{p=1}^{P(N)} k_p \sin^2(\pi pm/N) = \mu_{N-m} \ . \qquad (1.7b)$$

The set of N equations (1.2) then uncouples into N separate ordinary differential equations of second order whose solution is well known, and which will be briefly reviewed in section II.

I.4 Phase space

The main point we wish to make in section III is that the description of the homogeneous lattice and its solutions takes the simplest conceptual form when we use the $2N$-dimensional phase space of the lattice. We know

from elementary mechanics that for vibrating lattices, the complete specification of the state of motion requires both the positions $f_n(t)$ and the velocities $\dot{f}_n(t)$ of the masses, or equivalently, the momenta $M\dot{f}_n(t)$. In these terms, the N-component equation of motion (1.2) should be written as the $2N$-component equation

$$\mathsf{H}\mathsf{f}(t) = \partial_t \mathsf{f}(t) \ , \tag{1.8a}$$

$$\mathsf{H} = \begin{pmatrix} \mathsf{O} & M^{-1}\mathsf{1} \\ -\mathsf{K} & -CM^{-1}\mathsf{1} \end{pmatrix} ,$$

$$\mathsf{f}(t) \begin{pmatrix} \|f_n(t)\| \\ \|f_{N+n}(t)\| \end{pmatrix} = \begin{pmatrix} \|f_n(t)\| \\ M\|\dot{f}_n(t)\| \end{pmatrix} \tag{1.8b}$$

Hencefort, the *boldface sans serif* type will be reserved for vectors and matrices in the $2N$-dimensional phase-space of the system.

Equation (1.8a) is an evolution equation with a *generator* H and a first-order time derivative. Replacing second- with first-order differential operators is the basic step here. It leads to simple formal solutions

$$\mathsf{f}(t) = \exp(t\mathsf{H})\mathsf{f}(0) = \mathsf{G}(t)\mathsf{f}(0) \ , \tag{1.9}$$

where $\mathsf{G}(t)$ is the Green's or *evolution* operator of the system, and has the general form of a one-parameter Lie group element. The travelling-wave basis is the basis where the operators in (1.8) and (1.9) are completely diagonal.

I.5 Particular cases

We shall systematically stress some particular systems:

A) The (discrete) Klein-Gordon equation: Eqs. (1.2)-(1.3) with $M = c^{-2} = 1, C = 0, k_0 = \kappa^2, k_1 = 1$ and $k_p = 0$ for $p = 2, 3, ..., P(N)$.

B) The (discrete) wave equation, with $M = c^{-2} = 1, k_0 = 0, k_1 = 1$, and $k_p = 0$, $p = 2, 3, ..., P(N)$. We shall distinguish between the damped ($C > 0$) and undamped ($C = 0$) cases.

C) The (discrete) Helmholtz equation: $M = 1, C = 0, k_0 = \kappa^2, k_1 = -1$ and $k_p = 0$ for $p = 2, 3, ..., P(N)$.

I.6 Symmetry

Section IV is devoted to find the symmetry group of the general system encompassing A)-C). There is a 'manifest' geometric dihedral symmetry group $\mathcal{D}_N$ for the homogeneous lattice, of course. In the travelling-wave basis, however, a larger symmetry group, containing a finite $\mathcal{D}_N \otimes \mathcal{D}_N$ subgroup is seen to describe the system under transformations in phase space.

I.7 Quadratic invariants

In section V we relate a subring of the $\mathcal{D}_N \otimes \mathcal{D}_N$ group ring with the set of quadratic forms. This relation has been established, to the best of our knowledge, for systems which are symmetric under continuous groups of transformations, where for each of the linearly independent Lie generators we have one invariant quadratic form. These are here equivalently described through a factor subring of the symmetry group ring, and lead to the specification of the complete set of sesquilinear and bilinear time-invariant forms and constants of the motion. This is, moreover, not coincident with the total number of constants of the motion *linear* in the initial conditions, but a set of equivalence classes of the latter. We then restrict our quadratic set to the subset invariant under the geometric $\mathcal{D}_N$ symmetry group of the lattice, and find two types of invariants: energy-type and angular momentum-type.

I.8 The continuum limit

In section VI we let $N \to \infty$ and arrive at the description of homogeneous non-compact media subject to the Klein-Gordon and Helmholtz partial differential equations. There we can further demand Poincaré or Euclidean invariance for the quadratic forms obtaining the unique inner products (and subspaces where these are positive definite) which ensure the unitarity of all phase space transformations in these groups.

Basically, our aim is to extend the study of groups of canonical transformations from quantum mechanics [3] to certain discrete, finite systems, and also to certain continuous systems whose governing equations contain second-order time derivatives [4, 5]. By and large, it seems that matrix-operator realizations of Lie algebras, Lie groups as well as the Hilbert spaces one can define for them, have been slighted in the literature. In this article we try to give a more complete account of the inner products one can construct, as well as a better insight of the workings of group theory on discrete systems.

II. FUNDAMENTAL SOLUTIONS AND NORMAL MODES

In this section we give a résumé of the Fourier solution method for the second-order equation of motion (1.2). This will serve to extablish a framework and introduce notation.

II.1 Uncoupling

Applying $\mathbf{F}^{-1}$ to the left of (1.2) and defining the new vector $\tilde{\mathbf{f}}(t) = \mathbf{F}^{-1}\mathbf{f}(t)$ we find the components of the latter to satisfy the uncoupled set of equations

$$M\ddot{\tilde{f}}_m(t) + C\dot{\tilde{f}}_m(t) + \mu_m \tilde{f}_m(t) = 0 \ , \quad m = 1, 2, \ldots, N \ . \tag{2.1}$$

II.2 Oscillating solutions

The solutions of equations (2.1) are in general damped oscillatory functions. In terms of the initial values $\tilde{f}_m(0)$ and $\dot{\tilde{f}}_m(0)$ they can be expressed as

$$\tilde{f}_m(t) = [\dot{\tilde{G}}_m(t) + 2\Gamma\tilde{G}_m(t)]\tilde{f}_m(0) + \tilde{G}_m(t)\dot{\tilde{f}}_m(0) \ , \tag{2.2a}$$

where $\tilde{G}_m(t)$ are the set of Green's functions for damped one-dimensional oscillators

$$\tilde{G}_m(t) = e^{-\Gamma t}(\omega_m^e)^{-1}\sin(\omega_m^e t) = (2i\omega_m^e)^{-1}(e^{i\omega_m^+ t} - e^{i\omega_m^- t}) \ , \tag{2.2b}$$

with damping constant and effective frequency of oscillation given by

$$\Gamma = C/2M \ , \quad \omega_m^e = [\mu_m/M - \Gamma^2]^{1/2} = \omega_{N-m}^e \ . \tag{2.2c}$$

In the last expression of (2.2b), the partial-wave Green's function is displayed as a linear combination of two complex-frequency parts with

$$\omega_m^\pm = \pm\omega_m^e + i\Gamma \ . \tag{2.2d}$$

The general character of the possible solutions for the homogeneous latti-
ces depends on the possible values of μ_m in (1.7b). If some of the Hooke's

constants are negative –i.e., the oscillators are repulsive– then it may occur that some of the μ_m's are negative. For those values of m for which $\mu_m > \Gamma^2 M$, the effective frequency ω_m^e is real and the solutions (2.2a) have an in general damped oscillatory behaviour. As both $\tilde{G}_m(t)$ and its time derivative $\dot{\tilde{G}}_m(t)$ are even functions of ω_m^e, it is sufficient to consider the positive value of the square root in (2.2c).

II.3 Exponential solutions

If there exist values of m for which $\mu_m < \Gamma^2 M$, the effective frequency ω_m^e will be purely imaginary. The Green's function (2.2b) then takes the form

$$\tilde{G}_m(t) = e^{-\Gamma t}(w_m^e)^{-1}\sinh(w_m^e t) = (2w_m^e)^{-1}(e^{i\omega_m^+ t} - e^{i\omega_m^- t}) \ , \tag{2.3a}$$

$$i\omega_m^e = w_m^e = [\Gamma^2 - \mu_m/M]^{-1/2} = w_{N-m}^e \ , \tag{2.3b}$$

$$i\omega_m^\pm = -\Gamma \pm w_m^e \ , \tag{2.3c}$$

where again it is sufficient to consider the positive values of the square root for the values of w_m^e. The associated solutions will be called *exponential.*

II.4 Critical solutions

Finally, *critical* solutions may exist for some m_c when $\mu_{m_c} = \Gamma^2 M$, so $\omega_{m_c}^e = 0$. The solutions of (2.1) will then have the form (2.2a) with

$$\tilde{G}_{m_0}(t) = te^{-\Gamma t} \ . \tag{2.4}$$

This form could have been obtained from (2.2b) or (2.3a) letting $\omega_m^e \to 0$. The solutions (2.2a) are then linear combinations of $t\,e^{-\Gamma t}$ and $e^{-\Gamma t}$. In the case of the undamped wave equation, the $m = 0$ solution is allways critical.

II.5 Green's operator

Once we have found the solutions $\tilde{f}_m(t)$, $m = 1, 2, \ldots, N$, as determined

through the initial conditions $\tilde{f}_m(0)$ and $\dot{\tilde{f}}_m(0)$, we may revert to the 'physical' elongation basis $f_n(t)$, $n = 1, 2, ..., N$ and write them as the components of

$$\mathrm{f}(t) = \mathrm{F}\tilde{\mathrm{f}}(t) = [\dot{G}(t) + 2\Gamma \mathrm{G}(t)]\mathrm{f}(0) + \mathrm{G}(t)\ \dot{\mathrm{f}}(0)\ , \tag{2.5a}$$

where *Green's operator* is given by the matrix

$$\mathrm{G}(t) = \mathrm{F}\tilde{\mathrm{G}}(t)\mathrm{F}^{-1}\ ,\quad \tilde{\mathrm{G}}(t) = \|\delta_{m,m'}\tilde{G}_m(t)\|\ , \tag{2.5b}$$

which is symmetric and circulating.

II.6 Fundamental solutions

Two sets of initial conditions are important here: those giving rise to *fundamental solutions* and those giving rise to *normal modes*. The first ones are obtained through taking the $2N$ components of $\mathrm{f}(0)$ and $\dot{\mathrm{f}}(0)$ to be nonzero one at a time. These represent the motion of a lattice which starts from rest with one mass out of equilibrium, and one which starts from equilibrium with one mass moving in the positive direction with unit velocity. The $2N$ fundamental solutions obtained in this way are the N columns of $\dot{\mathrm{G}}(t) + 2\Gamma\ \mathrm{G}(t)$ and the N columns of $\mathrm{G}(t)$, respectively. The most general set of initial conditions can be written as a linear combination of these, as stated by (2.5).

II.7 Normal modes

The set of normal modes is obtained by taking the $2N$ components of $\tilde{\mathrm{f}}(0)$ and $\dot{\tilde{\mathrm{f}}}(0)$ to be nonzero one at a time. As the components of $\tilde{\mathrm{f}}(t)$ follow uncoupled motions, only one $\tilde{f}_{\bar{m}}(t)$ will be nonzero, that of $\tilde{f}_{\bar{m}}(0)$ and/or $\dot{\tilde{f}}_{\bar{m}}(0)$. When we revert to the 'physical' elongations $f(t) = F\tilde{\mathrm{f}}(t)$, they will appear as the $\bar{m}$th column of F multiplied by the common factor $\tilde{f}_{\bar{m}}(t)$, i.e., $f_n^{(\bar{m})}(t) = F_{n\bar{m}}\tilde{f}_{\bar{m}}(t)$ for $n = 1, 2, ..., N$, with no sum on $\bar{m}$. The solutions are then *separable* functions of the mass position n and of time t. Normal modes are thus time-modulated standing waves in the lattice, which beats with (complex) frequencies $\omega_m^{\pm}$. The phase of the motion is linearly related to $\arctan[\tilde{f}_{\bar{m}}(0)/\dot{\tilde{f}}_{\bar{m}}(0)]$.

The descriptions of the lattice motion in terms of the coupled elongations $f_n(t)$ or the uncoupled normal mode coordinates $\tilde{f}_m(t)$ are related through the Fourier transform. We would like now to present a third set

of coordinates which we deem more convenient in the description of the motion of a lattice: the travelling-wave basis. Mathematically it results from the search for the simplest description of the solutions to the $2N$-component first-order equation (1.8a), rather than the N-component second-order equations (1.2) or (2.1). It will be shown to lead quickly to a description of the invariant quadratic forms for a lattice.

III. TRAVELLING WAVES

The evolution form (1.8) for the lattice equations of motion makes use of a $2N$-dimensional matrix H, whose diagonalization we now address. Indeed, in the last section we used the $N \times N$ Fourier matrix F to diagonalize the interaction matrix K. In $2N$-dimensional terms, this is a reduction to block-diagonal form:

$$\mathrm{F}^{-1}\mathrm{H}\mathrm{F} = \begin{pmatrix} \mathrm{F}^{-1} & 0 \\ 0 & \mathrm{F}^{-1} \end{pmatrix}\begin{pmatrix} 0 & M^{-1}1 \\ -\mathrm{K} & -CM^{-1}1 \end{pmatrix}\begin{pmatrix} \mathrm{F} & 0 \\ 0 & \mathrm{F} \end{pmatrix} =$$

$$= \begin{pmatrix} 0 & M^{-1}1 \\ -\|\delta_{mm'}\mu_m\| & -CM^{-1}1 \end{pmatrix} = \tilde{\mathrm{H}}\ . \tag{3.1}$$

III.1 Complete diagonalization

When none of the μ_m is zero, the complete diagonalization of H can be achieved through a further similarity transformation which acts on the submatrix of $\tilde{\mathrm{H}}$ constituted by its mth and $(N + m)$th rows and columns as

$$(\mathrm{V}^{(m)})^{-1}\begin{pmatrix} 0 & M^{-1} \\ -\mu_m & CM^{-1} \end{pmatrix}\mathrm{V}^{(m)} = \begin{pmatrix} i\omega_m^{+} & 0 \\ 0 & i\omega_m^{-} \end{pmatrix}\ , \tag{3.2a}$$

$$\mathrm{V}^{(m)} = M^{-1/2}(\omega_m^{e})^{-1}\begin{pmatrix} 1 & 1 \\ iM\omega_m^{+} & iM\omega_m^{-} \end{pmatrix}\ . \tag{3.2b}$$

The eigenvalues $i\omega_m^{\dagger}$ are given in (2.2d), and we have chosen $\det \mathbf{V}^{(m)} = -2i/\omega_m^e$.

III.2 Null eigenvalues

In order to simplify the discussion, we shall normally assume that there are no critical solutions, i.e., $\omega_m^e \neq 0$; to avoid them, we can always introduce a small change in, say, k_0. All basis-independent results can be regained by letting this k_0 regain its former value. Those arguments which are specific to travelling waves, however, do not. For the latter we may define $\mathbf{V}^{(m_c)} = 1$ whenever $\omega_{m_c}^e = 0$. Special comments will be inserted to cover these cases.

III.3 The travelling-wave basis

Composing (3.1) and (3.2) we obtain

$$\mathbf{X}^{-1}\mathbf{H}\mathbf{X} = \bar{\mathbf{H}} = i\begin{pmatrix} \|\delta_{m,m'}\omega_m^{+}\| & 0 \\ 0 & \|\delta_{m,m'}\omega_m^{-}\| \end{pmatrix}, \tag{3.3a}$$

$$\mathbf{X} = M^{-1/2}\begin{pmatrix} \|F_{nm}/\omega_m^e\| & \|F_{nm}/\omega_m^e\| \\ iM\|F_{nm}\,\omega_m^{+}/\omega_m^e\| & iM\|F_{nm}\,\omega_m^{-}/\omega_m^e\| \end{pmatrix}, \tag{3.3b}$$

$$\mathbf{X}^{-1} = \frac{1}{2}iM^{-1/2}\begin{pmatrix} iM\|\omega_m^{-}F_{mn}^{*}\| & -\|F_{mn}^{*}\| \\ -iM\|\omega_m^{+}F_{mn}^{*}\| & \|F_{mn}^{*}\| \end{pmatrix}. \tag{3.3c}$$

The $2N$-dimensional vector

$$\bar{\mathbf{f}}(t) = \mathbf{X}^{-1}\mathbf{f}(t) = \begin{pmatrix} \|\bar{f}_{m,\rightarrow}(t)\| \\ \|\bar{f}_{m,\leftarrow}(t)\| \end{pmatrix}, \tag{3.4}$$

will be then subject to a particularly simple evolution equation: Eq. (1.8a) with the diagonal matrix $\bar{\mathbf{H}}$ in place of $\mathbf{H}$. Its solution, in terms of the $t = 0$ conditions, is

$$\bar{\mathbf{f}}(t) = \bar{\mathbf{G}}(t)\bar{\mathbf{f}}(0), \quad \bar{\mathbf{G}}(t) = \begin{pmatrix} \|\delta_{m,m'}e^{i\omega_m^{+}t}\| & 0 \\ 0 & \|\delta_{m,m'}e^{i\omega_m^{-}t}\| \end{pmatrix}. \tag{3.5}$$

Application of $\mathbf{X}$ to this equation then yields the description of the elongations and velocities of each of the lattice masses as the components of $\mathbf{f}(t)$, in terms of the $2N$ linear combination coefficients $\bar{\mathbf{f}}(0)$ times the elements of each of the rows of $\mathbf{X}\bar{\mathbf{G}}(t)$. Again, one preferred set of initial conditions is important: that obtained through taking the $\bar{f}_{m,\rightarrow}(0)$, $\bar{f}_{m,\leftarrow}(0)$, $m = 1, \ldots, N$ to be nonzero one at a time. Then, the corresponding set of $2N$ solutions, which will be recognized below as the set of *travelling waves* in the system, are given by the $2N$ columns of $\mathbf{X}\bar{\mathbf{G}}(t)$.

It should be noted that the $N \times N$ submatrices in $\mathbf{X}$ and $\bar{\mathbf{G}}(t)$ are invariant under the simultaneous permutation of the mth and $(N-m)$th rows and columns, [i.e., $F_{m,n} = F_{N-m,N-n}$, $\omega_m^{\pm} = \omega_{N-m}^{\pm}$ by (1.5), (1.7b) and (2.2c)]. The origin of this property is due to the invariance of a homogeneous lattice under inversions mapping the position n onto the position $N-n$. This particular inversion keeps the mass at N at its place; if N is even, also the $N/2$ mass is invariant. In conforming with the Brillouin convention, we shall henceforth consider the N values of the indices to lie, whenever convenient, in the range of integers, for N odd, between $-P(N)$ and $P(N)$, for N even, between $-P(N)+1$ and $P(N)$. Although we count modulo N, we shall sometimes speak of 'low' and 'high' partial waves, meaning those near $m = 0$ and $m = N/2$ respectively.

We define the $(m, \rightleftarrows)$-travelling waves as the lattice solutions given by

$$\mathbf{w}^{m,\rightarrow}(t) = \|w_n^{m,\rightarrow}(t)\| = (\mathbf{X}\bar{\mathbf{G}}(t))_{\cdot,m} = \mathbf{w}^{m,\rightarrow}(0)e^{i\omega_m^{+}t}, \tag{3.6a}$$

$$\mathbf{w}^{m,\leftarrow}(t) = \|w_n^{m,\leftarrow}(t)\| = (\mathbf{X}\bar{\mathbf{G}}(t))_{\cdot,N+m} = \mathbf{w}^{m,\leftarrow}(0)e^{i\omega_m^{-}t}, \tag{3.6b}$$

$$w_n^{m,\rightleftarrows}(t) = (MN)^{-1/2}(\omega_m^e)^{-1}\exp i(\omega_m^{\pm}t - 2\pi mn/N)$$

$$= (MN)^{-1/2}(\omega_m^e)^{-1}\exp(-2\pi im[n - v_m^{\rightleftarrows}t]/N), \tag{3.6c}$$

$$v_m^{\rightleftarrows} = N\omega_m^{\pm}/2\pi m = N(i\Gamma \pm \omega_m^e)/2\pi m. \tag{3.6d}$$

III.4 Velocity

The set of $2N$ independent solutions (3.6) represent *waveforms* of the

lattice, [i.e., they are proportional to complex exponentials in the mass position n], labelled by m and $\rightleftarrows$ which *travel*, as they are functions of $n - v_m^{\rightleftarrows} t$. The in general complex *velocity* $v_m^{\rightleftarrows}$ is given in (3.6d) in units of interparticle separation per unit time.

It might appear that counting modulo N we may change the range of velocities in (3.6d), since $v_m^{\rightleftarrows} \neq v_{N+m}^{\rightleftarrows}$. That this is not the case should be obvious from the invariance of the second member of (3.6c) under $m \to N + m$ *for integer values of* n, i.e., for the actual mass positions. There is a concommitant apparent paradox: higher values of $|m|$ seem to entail a greater average movement of the masses although the travelling waves have a smaller velocity. The fact which sets intuition straight is that the wave number (the number of wavelenghts around the lattice) also incrases with (in fact, is) $|m|$ [7].

Since it is the heart of the matter, we should restate that the travelling wave solutions $w_n^{m\rightleftarrows}(t)$ as we have defined them here, are functions of $n - v_m^{\rightleftarrows} t$ due to the fact that (a) they are constructed as the eigenvectors of H, and hence G(t) is a completely diagonal matrix with linear exponential dependence on t, and (b) the lattice being homogeneous, the diagonalizing matrix X contains the factor F which has a linear exponential dependence on the row index n. Exponents sum and the proportionality between the linear dependences is the velocity of the wave. This can be a real quantity, but in general it will be complex, meaning that damped oscillating or exponential behaviour are at work.

At this point we should particularize our discussion to the three cases listed in subsection I.5, so that the nuances of (3.6) be properly clarified.

III.5 The Klein-Gordon case

First, for the case of the discrete Klein-Gordon equation [$M = 1$, $C = 0$, $k_0 = \kappa^2$, $k_1 = 1$; $k_p = 0$, $p = 2, \ldots, P(N)$], as $\mu_0 = \kappa^2 \leqslant \mu_n \leqslant \kappa^2 + 4 = \mu_{N/2}$, undamped oscillating solutions exist with frequencies in the range $\omega_0^e = \kappa \leqslant \omega_m^e \leqslant (\kappa^2 + 4)^{1/2} = \omega_{N/2}^e$, monotonically increasing in $(0, N/2)$ and decreasing in $(-N/2, 0)$. Here $v_m^{\rightleftarrows} = \pm N\omega_m^e/2\pi m$ is a real propagation velocity for waves moving in the direction of, or against, increasing mass position n. As $v_m^{\rightleftarrows}$ is a function of m, dispersion of signals will in general occur. The only consistent degeneracy in the velocity is between $+|m|$ and $-|m|$ waves [c.f., Eqs. (1.7b) and (2.2c) for $m \neq 0$ and $m \neq N/2$]. We have $v_m^{\rightleftarrows} = v_{-m}^{\rightleftarrows} = -v_{-m}^{\rightleftarrows}$. These pairs of waves travelling in the same direction, however, differ through their initial conditions as $w^{m,\rightleftarrows}(0) = [w^{-m',\rightleftarrows}(0)]^*$; through linear combinations, hence, two independent waves can always

be constructed. Linear combination of travelling waves, however, does not yield a travelling wave. The $m = 0$ 'travelling' waves $w^{0,\rightleftarrows}$ merit special consideration. They are realized in a lattice, subject to the discrete Klein-Gordon equation, with initial conditions given by all masses being equally displaced from equilibrium: $w_n^{0,\rightleftarrows}(0) = (MN)^{-1/2}(\omega_0^e)^{-1}$ with mass velocities given by $\pm i\omega_0^e$ times this elongation, i.e., $w^{0,\rightarrow}(0)$ has the masses moving 'up' and $w^{0,\leftarrow}$ moving 'down'. The ensuing motion will be oscillatory, but as a travelling wave, the $m = 0$ waves have no definite sense or velocity of motion in the basic Brillouin range. [If we shift this range to $m = 1, 2, \ldots, N$, however, and view $w^{N,\rightleftarrows}(0)$ as initial conditions of wave number N rather than 0, their propagation velocity will be $\pm\omega_0^e/2\pi$ from (3.6d).] Out of linear combinations of $w^{0,\rightarrow}(t)$ and $w^{0,\leftarrow}(t)$ we can build solutions whose position or velocity at $t = 0$ are zero, i.e., we may revert to the normal mode solution basis described in Sect. II. Finally, the $m = N/2$ travelling waves (for N even) exhibit the smallest velocity in the basic Brillouin range (ω_0^e/π) and –as the $m = 0$ waves– do not have degenerate companions.

The most general solution for the homogeneous lattice (and for the general case contemplated in Sect. I) can be written as a linear combination of (3.6a, b) as

$$\mathrm{f}(t) = \sum_{\sigma=\rightleftarrows} \sum_{m} c_{m,\sigma} \mathrm{w}^{m,\sigma}(t) \ , \tag{3.7a}$$

where the linear combination coefficients are given in terms of the initial conditions as

$$c_{m,\rightleftarrows} = \left\{ \begin{array}{l} \overline{\mathrm{f}}_{m,\rightarrow}(0) = [\mathrm{X}^{-1}\mathrm{f}(0)]_m \\ \\ \overline{\mathrm{f}}_{m,\leftarrow}(0) = [\mathrm{X}^{-1}\mathrm{f}(0)]_{N+m} \end{array} \right\}$$

$$= \mp\frac{1}{2}M^{1/2} \sum_{n=1}^{N} F_{mn}^{*}(\omega_m^{\mp} f_n(0) + i\dot{f}_n(0)) \ . \tag{3.7b}$$

III.6 The wave equation and critical solutions

Lattices abiding the undamped wave equation can be described through the simple expedient of letting $\kappa^2 \to 0^+$ in the Klein-Gordon set of solu-

tions. The only point to note is that the $m = 0$ solutions now become critical as $\mu_0 = 0$ and $\omega_0^e = 0$. Although the travelling-wave form (3.6) becomes infinite, its presence in any solution (3.7a) remains well defined. In fact, *any* critical solution m_c, for damped or undamped lattices can be considered through letting $\omega_{m_c}^e \to 0$ in the expansion (3.7) and using (3.6a,b). The corresponding m_c summand is, when written out,

$$c_{m_c,\rightarrow} w_n^{m_c\rightarrow}(t) + c_{m_c,\leftarrow} w_n^{m_c,\leftarrow}(t)$$

$$= F_{m_c,n} e^{-\Gamma t}\{(\omega_{m_c}^e)^{-1} \sin(\omega_{m_c}^e t) \sum_{n'} F_{m_c,n'}^* [\Gamma f_{n'}(0) + \dot{f}_{n'}(0)]$$

$$+ \cos(\omega_{m_c}^e t) \sum_{n'} F_{m_c,n'}^* f_{n'}(0)\}$$

$$\xrightarrow[\omega_{m_c}^e \to 0]{} F_{m_c,n} e^{-\Gamma t} \sum_{n'} F_{m_c,n'}^* [(\Gamma t + 1) f_{n'}(0) + t\dot{f}_{n'}(0)]$$

$$= F_{m_c,n} e^{-\Gamma t}[(\Gamma t + 1)\bar{f}_{m_c}(0) + t\dot{\bar{f}}_{m_c}(0)] \ . \tag{3.8a}$$

This is a basis-independent statement for the m_c-mode subspace, as it sums over the two travelling-wave components. According to our convention in Subsect. III.2, defining $V^{(m_c)} = 1$ sets through (3.4) the critical travelling wave components as $\bar{f}_{m_c,\rightarrow}(t) = \bar{f}_{m_c}(t)$ and $\bar{f}_{m_c,\leftarrow}(t) = M\dot{\bar{f}}_{m_c}(t)$. Correspondingly using $\bar{f}_{m_c}(0) = c_{m_c,\rightarrow}$ and $\dot{\bar{f}}_{m_c}(0) = M^{-1} c_{m_c,\rightarrow}$ in (3.8) we may define the 'critical travelling waves' themselves as

$$w_n^{m_c,\rightarrow}(t) = F_{m_c,n}(\Gamma t + 1)e^{-\Gamma t} \tag{3.8b}$$

and, so as to supplement (3.6) for the critical cases,

$$w_n^{m_c,\leftarrow}(t) = F_{m_c,n}\, t e^{-\Gamma t}/M \ . \tag{3.8c}$$

[Applying the denomination 'travelling waves' to (3.8b,c) is a misnomer, though, as they are *not* functions of $n - vt$].

III.7 The damped wave equation

Next, the solutions which describe lattices abiding the damped ($C >$

0) wave equation should be analyzed. The discussion in Sect. II and specially equation (2.2d) point to the fact that through a redefinition of functions $g(t) = e^{\Gamma t} f(t)$, the vector equation (1.2) for $f(t)$ becomes a similar vector equation for $g(t)$ with the replacements $C \mapsto 0$, $K \mapsto K - M\Gamma^2$ 1. This is equivalent, hence, to an undamped wave equation lattice *with a repulsive spring* of Hooke's constant $k_0 = -M\Gamma^2$ pushing each particle away from its equilibrium position, and can be thought of as a Klein-Gordon lattice with a negative value of κ^2. We thus proceed to analyze the latter system, as it will also expedite our presentation of the Helmholtz equation, below.

III.8 Klein-Gordon equation with negative κ^2

When the Klein-Gordon equation contains a negative constant $\kappa^2 = -\lambda$, $\lambda = M\Gamma^2 > 0$, then there will be a non-empty range of m's such that $\mu_m < 0$. At least $\mu_0 < 0$, and at most (if $\lambda > 4$) all μ_m's will be negative. Negative μ_m's lead to purely imaginary (negative) values of the corresponding ω_m^e's [c.f., Eq. (2.3b) with $\Gamma = 0$]. In this region, the 'travelling wave' basis (3.6) separates $w^{m,\rightarrow}(t)$, the growing-exponential solution $\sim \exp(i\omega_m^+ t) = \exp(w_m^e t)$, from $w^{m,\leftarrow}(t)$, the decreasing-exponential solution $\sim \exp(i\omega_m^- t) = \exp(-w_m^e t)$.

The lower- $|m|$ solutions are always of this kind because they represent states of the lattice where the attractive interparticle springs, being on the average little deformed, are overwhelmed by the repulsion each particle experiences from its equilibrium position. This is always true for the $m = 0$ solution, as there the interparticle springs are not acting at all. At the other extreme, the $m = P(N)$ solution represents a lattice configuration where neighbouring masses have opposite elongations so that the attractive springs have the best chance of overwhelming the repulsive ones. Finally, two critical solutions may exist if for some m_c, $\mu_{m_c} = 0$. These have been described in (3.8) and need not be repeated here.

III.9 The damped wave equation, revisited

Returning briefly to the damped wave equation through the inverse function redefinition $f(t) = e^{-\Gamma t} g(t)$ and $g(t)$ having been described above, we see that the oscillation frequencies $\omega_m^{\pm}$ are obtained through a shift by $i\Gamma$, of $\pm\, \omega_m^e$. It should be noted carefully that the damped-oscillatory solutions have an m-independent damping Γ, while for the overdamped solutions, the damping depends on m, and for $w^{m,\rightarrow}(t)$

is in the range $[0, \Gamma)$ while for $w^{m,\leftarrow}(t)$ it is in $(\Gamma, 2\Gamma)$. In the sequel we shall exclude damping from the equations under consideration.

III.10 The Helmholtz equation

We turn last to the Helmholtz equation: $[M = 1, C = 0, k_0 = \kappa^2, k_1 = -1; k_p = 0, p = 2, 3, \ldots P(N)]$, noting that the attractive and repulsive springs are exchanged with respect to the case examined in III.8. The highest eigenvalue of the interaction operator is $\mu_0 = \kappa^2 > 0$ and the lowest is $\mu_{N/2} = \kappa^2 - 4$. If $\kappa^2 < 4$, all μ_m are positive, all frequencies ω_m^e are real and all solutions are oscillating. If $\kappa^2 > 4$, the highest-$|m|$ frequencies will be imaginary leading to exponentially increasing and decreasing solutions $w^{m,\rightleftharpoons}(t)$. In the last cases, the repulsive interparticle springs overwhelm the oscillators which bind the masses to their equilibrium positions. Small-curvature lattice solutions, on the other hand, are stable.

As in former cases, critical solutions may exist, and if so, are of the form (3.8). We should note, finally, that the discrete Laplace equation for a lattice is obtained in the limit $\kappa^2 \to 0^+$.

In every case, we see that the travelling-wave basis, whose general form was written in (3.6), has a well-defined mathematical meaning (as an eigenbasis for H), providing a convenient division of the solutions into oscillatory, critical and exponentially decreasing and increasing solutions. It should be noted that each of these sets generates a time-invariant vector subspace of the $2N$-dimensional space of motions of the lattice.

IV. SYMMETRIES OF THE HOMOGENEOUS LATTICE

A homogeneous lattice can be alternatively defined as a system whose description is invariant under a subgroup of the group of permutations of its constituent elements, this subset being the *dihedral* group which we introduce below.

IV.1 The dihedral group

We denote a given permutation P of the N elements of a system (numbered by $n = 1, 2, \ldots, N$), through

$$P^{\pi}\{n\} = \{\pi(n)\}\,, \tag{4.1}$$

where $\pi(n)$ is the new position, under permutation, of the old mass number n. Thus π is specified by the values it takes for $n = 1, 2, \ldots, N$. The set (4.1) of permutations forms a group.

The *dihedral* subgroup $\mathcal{D}_N$ can be pictured as acting on a set of N equally spaced masses on a circle and is composed by the following elements:

a) Rotations by $2\pi k/N$, $k = 0, 1, \ldots, N-1$ (which can be counted modulo N):

$$R^k\{n\} = \{n + k\}\,, \quad \text{i.e., } \pi(n) = n + k \quad (\text{modulo } N). \tag{4.2a}$$

In particular $R^N = R^0 = 1$ is the identity transformation.

b) Inversions through a diameter, leaving the kth mass invariant

$$I_k\{n\} = \{N + 2k - n\}\,, \quad \text{i.e., } \pi(n) = N + 2k - n \quad (\text{modulo } N). \tag{4.2b}$$

When N is odd, we let k range through $N \equiv 0, 1, 2, \ldots, N-1$. When N is even, I_k leaves invariant both mass k and its antipodal, mass $k + N/2$, so $I_k = I_{k+N/2}$ and it is sufficient to let k range through $0, 1, 2, \ldots, N/2 - 1$. When N is even, we can also have inversions through the midpoints of pairs of masses

$$J_k\{n\} = \{N + 2k + 1 - n\}\,,$$

$$\text{i. e., } \pi(n) = N + 2k + 1 - n \quad (\text{modulo } N)\,, \tag{4.2c}$$

with k ranging through $0, 1, 2, \ldots, N/2 - 1$. In every case, there are $2N$ elements in (4.2), defining $\mathcal{D}_N$. Inversion and multiplication of two elements in $\mathcal{D}_N$ is easily carried out through inversion and sequential application of (4.2). Such operations, as can be easily verified, yield another element in $\mathcal{D}_N$. This set, hence, forms a group. We shall denote by D the general element of $\mathcal{D}_N$.

IV.2 $N \times N$ representations of $\mathcal{D}_N$

The dihedral transformations (4.2) leave the neighbour relation in the lattice invariant, since they rotate and reflect 'rigidly' the representing circle. They are also *all* the permutations with this property. It is perhaps intuitively obvious by now that the dihedral transformations should leave the dynamics of the homogeneous lattice invariant, since they transform

a lattice —masses and springs; i.e., neighbour relations— into another lattice indistinguishable dynamically from the first. To make this notion precise, we *represent* the dihedral group elements (4.2) through $N \times N$ matrices which act on the lattice configuration N-vector f through permuting its rows:

$$P^{\pi} \leftrightarrow \mathrm{P}^{\pi} = ||P^{\pi}_{n,n'}|| \ , \quad P^{\pi}_{n,n'} = \delta_{n,\pi(n')} \ . \tag{4.3}$$

The rotations R^k in (4.2a) are thus represented by a matrix R^k with nonzero entries 1, placed on a subdiagonal which is k places to the lower left of the main diagonal, counted modulo N, i.e., it is a circulating matrix where the lower-left subdiagonal continues as an upper-right subdiagonal $N - k$ places up from the main one:

$$\mathrm{R}^k = ||\delta_{n,n'+k}|| \ . \tag{4.4a}$$

Clearly, $\mathrm{R}^N = \mathrm{R}^0 = 1$ and $\mathrm{R}^{-1} = (\mathrm{R}^1)^{-1}$. The inversions I_k in (4.2b) are represented by sub-antidiagonal matrices I_k whose nonzero entries are 1's at $n + n' = 2k$ and $2k + N$, i.e., strung from the $(2k - 1, 1)$ to the $(1, N - 2k - 1)$ positions which, since the matrices are anticirculating, continue from the $(N, 2k)$ to the $(2k, N)$ positions, counted modulo N:

$$\mathrm{I}_k = ||\delta_{n+n',2k}|| \ . \tag{4.4b}$$

Lastly, for N even, the J_k in (4.2c) are represented by other anticirculating sub-antidiagonal matrices J_k with 1's at $n + n' = 2k + 1$ and $2k + N + 1$, i.e., on sub-antidiagonals from the $(N - k, 1)$ to the $(1, N - k)$ and the $(N, N - k - 1)$ to the $(N - k - 1, N)$ positions:

$$\mathrm{J}_k = ||\delta_{n+n',2k+1}|| \ . \tag{4.4c}$$

The inversion and multiplication of two of these matrices yields the matrix which represents the inverse and product of the corresponding group elements in $\mathcal{D}_N$. Note that all matrices P^{π} are real, unitary matrices, i.e., $\mathrm{P}^{\dagger}\mathrm{P} = 1 = \mathrm{P}\mathrm{P}^{\dagger}$, where the dagger ($\dagger$) indicates adjunction, that is, transposition and conjugation. We shall write D for the general $N \times N$ matrix representing the dihedral group element $D \in \mathcal{D}_N$. Finally, we shall

economize space by not distinguishing explicitely the group elements from their matrix representatives, and refer to them as $\mathrm{D} \in \mathcal{D}_N$.

IV.3 Mapping solutions into solutions

If we write C for any linear combination of the D-matrices, we can state clearly the invariance of the homogeneous lattice dynamics as follows. If the configuration N-vector $\mathrm{f}(t)$ is a solution to the equation of motion of a homogeneous lattice equation (1.2), then $\mathrm{C}\,\mathrm{f}(t)$ is also a solution to the same equation.

The proof of this statement reduces to showing that C commutes with the interaction matrix K, i.e., $\mathrm{C}\,\mathrm{K} = \mathrm{K}\mathrm{C}$. The similarity action of a permutation matrix P on any matrix M as $\mathrm{M} \mapsto \mathrm{P}\mathrm{M}\mathrm{P}^{-1}$, is to subject the row and column entries of M to the same permutation which P effects on the rows of the column vector f. Rotations R^k perform $M_{n,n'} \rightarrow M_{n+k,n'+k}$ and hence translate (modulo N) the entries by k units along the direction of the main diagonal. This leaves invariant all circulating matrices, in particular, the circulating matrix K in (1.3). The I_k invert the rows and columns of M accross the (k, k) entry, while the J_k do the same accross the midpoint between the (k, k) and $(k + 1, k + 1)$ entries. In particular, if M is a circulating matrix, the I_k's and J_k's have the net effect of transposing M. Recalling that K is a symmetric circulating matrix, we have $\mathrm{D}\mathrm{K} = \mathrm{K}\mathrm{D}$ for $\mathrm{D} \in \mathcal{D}_N$. Performing linear combination of the dihedral matrices D into C's completes the proof.

The converse of the statement is also true, namely, that if some $N \times N$ matrix C commutes with a symmetric circulating matrix K, the C must be a linear combination of the $2N$ matrices D of the dihedral group $\mathcal{D}_N$. The proof proceeds through noting that the circulation and symmetry properties are equivalent to commutation with the rotation and inversion representative matrices.

IV.4 The dihedral group ring and its representation

It should be pointed out that under the additional vector-space operation of linear combination, the set of dihedral matrices (4.4) are *not* linearly independent: When N is odd,

$$\sum_{k=0}^{N-1} \mathrm{I}_k = \sum_{k=0}^{N-1} \mathrm{R}^k$$

is a matrix filled with 1's, while when N is even,

a lattice —masses and springs; i.e., neighbour relations— into another lattice indistinguishable dynamically from the first. To make this notion precise, we *represent* the dihedral group elements (4.2) through $N \times N$ matrices which act on the lattice configuration N-vector f through permuting its rows:

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The rotations R^k in (4.2a) are thus represented by a matrix R^k with nonzero entries 1, placed on a subdiagonal which is k places to the lower left of the main diagonal, counted modulo N, i.e., it is a circulating matrix where the lower-left subdiagonal continues as an upper-right subdiagonal $N - k$ places up from the main one:

$$\mathrm{R}^k = ||\delta_{n,n'+k}|| \ . \tag{4.4a}$$

Clearly, $\mathrm{R}^N = \mathrm{R}^0 = 1$ and $\mathrm{R}^{-1} = (\mathrm{R}^1)^{-1}$. The inversions I_k in (4.2b) are represented by sub-antidiagonal matrices I_k whose nonzero entries are 1's at $n + n' = 2k$ and $2k + N$, i.e., strung from the $(2k - 1, 1)$ to the $(1, N - 2k - 1)$ positions which, since the matrices are anticirculating, continue from the $(N, 2k)$ to the $(2k, N)$ positions, counted modulo N:

$$\mathrm{I}_k = ||\delta_{n+n',2k}|| \ . \tag{4.4b}$$

Lastly, for N even, the J_k in (4.2c) are represented by other anticirculating sub-antidiagonal matrices J_k with 1's at $n + n' = 2k + 1$ and $2k + N + 1$, i.e., on sub-antidiagonals from the $(N - k, 1)$ to the $(1, N - k)$ and the $(N, N - k - 1)$ to the $(N - k - 1, N)$ positions:

$$\mathrm{J}_k = ||\delta_{n+n',2k+1}|| \ . \tag{4.4c}$$

The inversion and multiplication of two of these matrices yields the matrix which represents the inverse and product of the corresponding group elements in $\mathcal{D}_N$. Note that all matrices P^{π} are real, unitary matrices, i.e., $\mathrm{P}^{\dagger}\,\mathrm{P} = 1 = \mathrm{P}\,\mathrm{P}^{\dagger}$, where the dagger ($\dagger$) indicates adjunction, that is, transposition and conjugation. We shall write D for the general $N \times N$ matrix representing the dihedral group element $D \in \mathcal{D}_N$. Finally, we shall

economize space by not distinguishing explicitely the group elements from their matrix representatives, and refer to them as $\mathrm{D} \in \mathcal{D}_N$.

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The proof of this statement reduces to showing that C commutes with the interaction matrix K, i.e., $\mathrm{C\,K} = \mathrm{KC}$. The similarity action of a permutation matrix P on any matrix M as $\mathrm{M} \mapsto \mathrm{PMP}^{-1}$, is to subject the row and column entries of M to the same permutation which P effects on the rows of the column vector f. Rotations R^k perform $M_{n,n'} \to M_{n+k,n'+k}$ and hence translate (modulo N) the entries by k units along the direction of the main diagonal. This leaves invariant all circulating matrices, in particular, the circulating matrix K in (1.3). The I_k invert the rows and columns of M accross the (k, k) entry, while the J_k do the same accross the midpoint between the (k, k) and $(k + 1, k + 1)$ entries. In particular, if M is a circulating matrix, the I_k's and J_k's have the net effect of transposing M. Recalling that K is a symmetric circulating matrix, we have $\mathrm{DK} = \mathrm{KD}$ for $\mathrm{D} \in \mathcal{D}_N$. Performing linear combination of the dihedral matrices D into C's completes the proof.

The converse of the statement is also true, namely, that if some $N \times N$ matrix C commutes with a symmetric circulating matrix K, the C must be a linear combination of the $2N$ matrices D of the dihedral group $\mathcal{D}_N$. The proof proceeds through noting that the circulation and symmetry properties are equivalent to commutation with the rotation and inversion representative matrices.

IV.4 The dihedral group ring and its representation

It should be pointed out that under the additional vector-space operation of linear combination, the set of dihedral matrices (4.4) are *not* linearly independent: When N is odd,

$$\sum_{k=0}^{N-1} \mathrm{I}_k = \sum_{k=0}^{N-1} \mathrm{R}^k$$

is a matrix filled with 1's, while when N is even,

$$\sum_{k=0}^{N/2-1} (I_k - J_k) = \sum_{k=0}^{N-1} (-1)^k R^k$$

is filled with 1's and (-1)'s in alternate checker-board positions. These matrices are both circulating and anticirculating and commute with all linear combinations C of D's representing $\mathcal{D}_N$. The described linear vector space of circulating ($\Sigma_k c_k R^k$) plus anticirculating ($\Sigma_k a_k I^k$ or $\Sigma_k a_k I_k + \Sigma_k b_k J_k$ for N odd or even) matrices has thus dimension $2N-1$ for N odd and $2N-2$ for N even. We shall call this vector space $\mathcal{C}_N$.

The elements of $\mathcal{C}_N$ are subject to closed operations of multiplication and linear combination, and contain the unit matrix. We see thus that $\mathcal{C}_N$ has the structure of a *ring with identity*. This object can also be defined, equivalently, as the factor ring of the dihedral group ring by a central subring. The latter has one element, $\Sigma_k R^k - \Sigma_k I_k$ when N is odd; when N is even, it has two elements, $\Sigma_k R^k - \Sigma_k(I_k + J_k)$ and $\Sigma_k(-1)^k R^k - \Sigma_k(I_k - J_k)$.

Had we directed our paper to the search for the most general $\mathcal{C}_N$ -invariant interaction, we would have arrived at the homogeneous lattice interaction.

IV.5 The full group of symmetries of the interaction operator

We saw above that C f(t) is a C-transformed solution of the lattice obtained from f(t). It is obtained through applying the *same* element C of $\mathcal{C}_N$ on the elongation components $f_n(t) = \mathsf{f}_n(t)$ and on the momentum components $Mf_n(t) = \mathsf{f}_{N+n}(t)$. This is due –as we remarked briefly before– to the property

$$\mathsf{C}_d \mathsf{G}(t) = \mathsf{G}(t)\mathsf{C}_d, \quad \mathsf{C}_d = \begin{pmatrix} \mathsf{C} & 0 \\ 0 & \mathsf{C} \end{pmatrix}, \quad \mathsf{C} \in \mathcal{C}_N . \tag{4.5}$$

Under the (temporary) assumption that the positions and momenta undergo the same transformation, we now describe the action of this dihedral group $\mathcal{D}_N$ on the travelling wave basis (3.6)-(3.7). The representation of the elements D of $\mathcal{D}_N$ in this basis is obtained applying to (4.4) the similarity transformation X in (3.3b)

$$\bar{\mathsf{D}}_d = \mathsf{X}^{-1}\mathsf{D}_d\mathsf{X} = \begin{pmatrix} \tilde{\mathsf{D}} & 0 \\ 0 & \tilde{\mathsf{D}} \end{pmatrix}, \quad \tilde{\mathsf{D}} = \mathsf{F}^{-1}\mathsf{D}\mathsf{F}, \quad \mathsf{D} \in \mathcal{D}_N . \tag{4.6}$$

The Fourier transform of the dihedral representation matrices (4.4) are the unitary matrices [8]

$$\tilde{R}^k = \|\delta_{m,m'} \exp(2\pi ikm/N)\| = \tilde{R}^{N-k\dagger} = \tilde{R}^{kT}, \tag{4.7a}$$

$$\tilde{I}_k = \|\delta_{m+m',0} \exp(4\pi ikm/N)\| = \tilde{I}_k^{\dagger} = \tilde{I}_{N-k}^{T} . \tag{4.7b}$$

$$\tilde{J}_k = \|\delta_{m+m',0} \exp(2\pi i[2k+1]m/N)\| = \tilde{J}_k^{\dagger} = \tilde{I}_{N-k-1}^{T} , \tag{4.7c}$$

where M^T is the transpose of M. Eqs. (4.7) provide a representation of $\mathcal{D}_N$ unitarily equivalent to the representation afforded by (4.4). In the basis (4.7) it is evident why (4.6) commutes with the diagonal $\bar{G}(t)$ in (3.5). The rotations $\tilde{R}^k$ in (4.7a) are diagonal, while the inversions $\tilde{I}_k$ and $\tilde{J}_k$ in (4.7b) and (4.7c) mix degenerate eigenvalues. In the travelling-wave basis, moreover, we see two limitations of our geometric-symmetry approach: two $N \times N$ blocks of $\bar{D}_d$ in (4.6) represent the *same* element of the discrete $\mathcal{D}_N$ group. In searching in this basis for *all* $2N \times 2N$ matrices commuting with the diagonal $\bar{G}(t)$, the upper and lower block of (4.6) may be clearly taken as independent, and moreover, each eigenvalue space may be subject to an arbitrary linear combination $GL(2, R)$ if the eigenvalue is doubly degenerate: $\mu_m = \mu_{N-m}$, or $GL(1, R)$ if it is single as μ_0 or, when N even, $\mu_{N/2}$. Furthermore, if *accidental* degeneracies occur (as in the case of pth-neighbour interaction lattices, i.e., $\mu_{m_1} = \mu_{m_2}$, $m_1 \neq m_2 \neq N - m_1$), then the four- (or more-) dimensional solution space associated to that frequency may be subject to arbitrary $GL(4, R)$ (or larger) linear transformations. Lastly, if some eigenvalue becomes zero as $\mu_{m_c} = 0$, the corresponding solutions become critical and the structure of the commuting group of matrices changes abruptly. Instead of $GL(2, R)$ we have S_2, the three-parameter solvable group of upper-triangular matrices. Since we have not insisted on the critical cases, where the travelling wave transformation X becomes singular [Eqs. (3.3)], we shall gloss over the exact description of this group contraction phenomenon. Further, we shall also avoid detailing the accidental degeneracy cases, which do not occur in the ordinary (first-neighbour interaction) Klein-Gordon or Helmholtz cases.

IV.6 Lie algebras vs rings

We have thus the "complete" symmetry group found in Ref. 2, where

the corresponding Lie algebra is also analyzed. The point we want to make here is that the said algebra representations and its applications in the next section are equivalently described through a ring structure associated to the $\mathcal{C}_N$ ring, which represents phase-space transformation in the lattice equation of motion. To this end we define

$$\overrightarrow{\mathsf{C}} = \begin{pmatrix} \tilde{\mathsf{C}} & 0 \\ 0 & 0 \end{pmatrix}, \quad \overleftarrow{\mathsf{C}} = \begin{pmatrix} 0 & 0 \\ 0 & \tilde{\mathsf{C}}' \end{pmatrix}, \quad \tilde{\mathsf{C}} = \mathsf{F}^{-1}\mathsf{C}\mathsf{F} \;;\; \mathsf{C}, \mathsf{C}' \in \mathcal{C}_N \;. \tag{4.8}$$

When the $\tilde{\mathsf{C}}$, $\tilde{\mathsf{C}}'$ are the $\mathcal{D}_N$ group representation matrices D in (4.7), the corresponding $\overrightarrow{\mathsf{D}}$ provide a $2N \times 2N$ representation of the *direct product* group $\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow}$, the first and second factors acting on right- and left-travelling waves. A larger symmetry group of the homogeneous lattice equation (1.2) is thus $\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow}$ which contains the 'geometric' dihedral $\mathcal{D}_N$ as its diagonal subgroup $(\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow})_d$ and is contained in the full symmetry group of subsection IV.5. Thence the subindex 'd' in (4.6). Henceforth, we shall denote by $\overline{\mathsf{D}}$ the $2N \times 2N$ matrix with two independent $\mathcal{D}_N$-blocks.

The elongation-and-momentum basis representation of (4.8) can be found through $\mathsf{C} = \mathsf{X}\overline{\mathsf{C}}\mathsf{X}^{-1}$. This matrix will in general mix the elongation and momentum components of $\mathsf{f}(t)$, as canonical transformations do. We shall not write out the $4N$ elements D of $\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow}$ in this representation, since they do not reduce beyond the block form of X and their explicit expression is not needed in the following results. This underlines the fact that the description of the symmetries of the homogeneous lattice is more transparent in the travelling wave basis than in the fundamental solution or normal mode bases.

Under linear combination, the $4N$ matrices (4.8) obtained letting $\tilde{\mathsf{D}}$ and $\tilde{\mathsf{D}}'$ range independently over (4.7) generate a linear vector space and ring $\mathcal{C}_N^{\rightarrow} \oplus \mathcal{C}_N^{\leftarrow}$ of dimension $2(2N-1)$ for N odd, and $2(2N-2)$ for N even. This space will be identified in the next section with the space of invariant quadratic forms, related to constants of the motion. In preparation for this we introduce a more convenient basis for $\mathcal{C}_N^{\rightarrow} \oplus \mathcal{C}_N^{\leftarrow}$: Matrices with a single nonzero element.

IV.7 A basis for the ring $\mathcal{C}_N^{\rightarrow} \oplus \mathcal{C}_N^{\leftarrow}$

Out of the rotations (4.7a) we define the $N \times N$ matrices

$$\tilde{\mathsf{E}}_\ell = \|\delta_{m,m'}\delta_{m\ell}\| = N^{-1/2}\sum_{k=0}^{N-1} F_{\ell k}\tilde{\mathsf{R}}^k \;, \quad \ell = 0, 1, \ldots, N-1 \;, \tag{4.9a}$$

counting indices modulo N. Out of the inversions (4.7b) and (4.7c),

$$\tilde{\mathsf{A}}_\ell = \|\delta_{m+m',0}\delta_{m,\ell}\|$$

$$= \begin{cases} N^{-1/2}\displaystyle\sum_{k=0}^{N-1} F_{\ell,2k}\tilde{\mathsf{I}}_k \;, & N \text{ odd} \;, \qquad \ell = 1, 2, \ldots, N-1 \\ N^{-1/2}\displaystyle\sum_{k=0}^{N/2-1} (F_{\ell,2k}\tilde{\mathsf{I}}_k + F_{\ell,2k+1}\tilde{\mathsf{J}}_k) \;, & \begin{cases} N \text{ even} \\ \ell = 1, 2, \ldots, N-1 \\ \ell \neq N/2 \;. \end{cases} \end{cases} \tag{4.9b}$$

As before, we note that $\tilde{\mathsf{A}}_0 = \tilde{\mathsf{E}}_0$ and, for N even, $\tilde{\mathsf{A}}_{N/2} = \tilde{\mathsf{E}}_{N/2}$. We define $\overline{\mathsf{E}}_\ell$ and $\overline{\mathsf{A}}_\ell$ as in (4.8) wit $\tilde{\mathsf{D}}$ and $\tilde{\mathsf{D}}'$ being (4.9a) and (4.9b), respectively.

IV.8 Time inversions

The transformation of the temporal variable in the lattice equation of motion has been thus far generated by H and finite transformations by $\mathsf{G}(t)$. When damping is absent, the equation of motion, being of second order in time, is also invariant under time inversions $t \leftrightarrow -t$. In the space of solutions this is a reversal of the momentum sign which can be represented through the $2N \times 2N$ matrix

$$\mathsf{T} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathsf{TH} = -\mathsf{HT} \;, \quad \mathsf{TG}(t) = \mathsf{G}(-t)\mathsf{T} \;. \tag{4.10a}$$

Correspondingly, in the travelling-wave basis,

$$\overline{\mathsf{T}} = \mathsf{X}^{-1}\mathsf{T}\mathsf{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{4.10b}$$

Time reversal thus exchanges left- and right-travelling waves and, under

similarity transformation, exchanges the two factors of $\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow}$ and of $\mathcal{C}_N^{\rightarrow} \oplus \mathcal{C}_N^{\leftarrow}$.

IV.9 Lie algebras vs rings, conclusion

We would like to offer here a comment upon the construction of finite discrete vs continuous symmetry groups in finite discrete lattice systems. We draw the reader's attention again to the fact that in (4.5) we did not direct our search towards finding the most general transformation $\overline{\mathsf{C}}$ commuting with the diagonal $\overline{\mathsf{G}}(t)$ given in (3.5), as in Ref. 10. The point to recognize is that the $2N \times 2N$ representations of the elements of this group and of its Lie algebra are contained in our ring $\mathcal{C}_N^{\rightarrow} \oplus \mathcal{C}_N^{\leftarrow}$, for they are but (in general non-integer) powers and logarithms of the $2N \times 2N$ representations of the *discrete* $\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow}$ group representations, and hence within its group ring —modulo the identifications which define $\mathcal{C}_N^{\rightarrow} \oplus \mathcal{C}_N^{\leftarrow}$.

Comparing the count of parameters in the full symmetry group S in Ref. 2 with the dimension of $\mathcal{C}_N^{\rightarrow} \oplus \mathcal{C}_N^{\leftarrow}$, we see that they are equal. Moreover, a basis for the Lie algebra of S is provided precisely by (4.9): The $\overline{\mathsf{E}}_{\ell}^{\rightleftharpoons}$ which will be detailed in the next section, generate translations of the single $(\ell, \rightleftharpoons)$-travelling wave, while the $\overline{\mathsf{A}}_{\ell}^{\rightleftharpoons}$ and $\overline{\mathsf{A}}_{N-\ell}^{\rightleftharpoons}$ generate linear combinations of the $(\ell, \rightleftharpoons)$ and $(N-\ell, \rightleftharpoons)$ travelling waves.

It is perhaps a moot point to argue which approach is preferable: (a) the construction of S and its Lie algebra as followed in Ref. 2, or (b) the equivalent construction of the phase-space discrete symmetry $\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow}$ and its group ring (modulo the identifications stemming from the $2N \times 2N$ representation and) leading to $\mathcal{C}_N^{\rightarrow} \oplus \mathcal{C}_N^{\leftarrow}$ as done here. In the latter, we do not leave the realm of discrete groups in the description of discrete systems, while the former uses Lie tecniques familiar from continuous systems. This equivalence seems to imply that the analysis of nondegenerate, discrete, finite linear systems may be done without involving Lie techniques at all, but in the framework of geometric symmetry groups in the travelling-wave basis. The latter become Lie groups in their own right as we let $N \to \infty$ to describe continuous systems, as will be shown in section VI. The question of more-than-two-level degeneracies in discrete systems may help to explain the corresponding features in certain quantum systems [9], but must be shelved for further analysis elsewhere.

V. INVARIANT QUADRATIC FORMS

The initial phase-space configuration of a lattice $\mathsf{f}(0)$ which determines uniquely the subsquent time evolution $\mathsf{f}(t)$ consists of $2N$ in general

complex numbers. Certain *quadratic* functions of the components of $\mathsf{f}(t)$, such as the energy are of importance because (for the undamped cases) they are independent of time, i.e., constants of the motion. Being quadratic, as we shall see, they also define inner products on the solution space, which can be restricted to be positive. We shall be interested in *quadratic* forms $C(\mathsf{f}, \mathsf{g})$, linear in the second argument, and linear or antilinear in the first, i.e., *bilinear* or *sesquilinear* forms. The latter are widely used in the construction of complex Hilbert spaces since when the form is positive $[C(\mathsf{f}, \mathsf{f}) \geqslant 0$ for $\mathsf{f} \neq \mathsf{0}]$ a norm can be defined out of the inner product. For every $\mathsf{f}(t)$ we expect to find no more than $2N$ functionally independent complex constants of the motion.

V.1 Time-invariant quadratic forms

In proposing a set of quadratic forms, bilinear involving $\mathsf{f}^T(t)$ and $\mathsf{g}(t)$, or sesquilinear involving $\mathsf{f}^\dagger(t)$ and $\mathsf{g}(t)$ which are independent of the time variable, the key element is to realize that in the travelling-wave basis, and only there, the time evolution of the components is simply the multiplication by an exponential factor, $\exp(i\omega_m^+ t)$ for right-moving waves, and $\exp(i\omega_m^- t)$ for left-moving ones. [The consideration of *damping* in the lattice, we saw in Subsect. III.7 is a minor variant of the undamped cases; we shall consider only the latter for most of this section.]

When damping is absent, then $\omega_m^{\pm} = \pm\omega_m^e$ where ω_m^e may be real (oscillatory solutions), pure imaginary (exponential solutions) or zero (critical solutions). If we denote by $(\ddagger)$ the adjunction $(\dagger)$ or transposition (T) involution, the most general sesquilinear or bilinear form can be written as

$$C_{(\ddagger)}(\mathsf{f}, \mathsf{g}) = \overline{\mathsf{f}}^{\ddagger}(t)\overline{\mathsf{C}}\overline{\mathsf{g}}(t) = \overline{\mathsf{f}}^{\ddagger}(0)\overline{\mathsf{G}}^{\ddagger}(t)\overline{\mathsf{C}}\overline{\mathsf{G}}(t)\overline{\mathsf{g}}(0) \ . \tag{5.1}$$

In order that this be time-independent for all $\overline{\mathsf{f}}(t)$ and $\overline{\mathsf{g}}(t)$ in the solution space of the lattice equation of motion, it is necessary and sufficient that $\overline{\mathsf{C}}$ be such that

$$\overline{\mathsf{G}}^{\ddagger}(t)\overline{\mathsf{C}}\overline{\mathsf{G}}(t) = \overline{\mathsf{C}} \quad \text{i.e.,} \quad \overline{\mathsf{H}}^{\ddagger}\overline{\mathsf{C}} + \overline{\mathsf{C}}\overline{\mathsf{H}} = 0 \tag{5.2}$$

The $2N \times 2N$ matrices $\overline{\mathsf{C}}$ satisfying (5.2) form a linear vector space which we proceed to identify —as the notation suggests— with $\mathcal{C}_N^{\rightarrow} \oplus \mathcal{C}_N^{\leftarrow}$: We have at our disposition the basis (4.9) and T in (4.11). Following the analysis made in section III, we present in detail the two particular cases

which will inform us of the typical structure of the most general case. The results are summarized in Table I. First:

V.2 Klein-Gordon sesquilinear forms

The discrete Klein-Gordon equation has only oscillatory solutions: $\omega_m^{\pm} = (\omega_m^{\pm})^* = \pm\omega_m^e$. The invariant sesquilinear (S-) forms are obtained by pairing one $(\ell, \rightleftharpoons)$ travelling wave content of a lattice state vector $\mathsf{g}(t)$ with the complex conjugate of the same $(\ell, \rightleftharpoons)$ travelling wave content of another state vector $\mathsf{f}(t)$, as

$$E_{S(\ell,\rightleftharpoons)}(\mathsf{f},\mathsf{g}) = \overline{\mathsf{f}}^{\dagger}\,\overline{E}_{\ell}^{\rightleftharpoons}\,\overline{\mathsf{g}} = \overline{\mathsf{f}}^{*}_{\ell,\rightleftharpoons}\overline{\mathsf{g}}_{\ell,\rightleftharpoons} = [E_{S(\ell,\rightleftharpoons)}\ (\mathsf{g},\mathsf{f})]^* \ , \tag{5.3a}$$

$$A_{S(\ell,\rightleftharpoons)}(\mathsf{f},\mathsf{g}) = \overline{\mathsf{f}}^{\dagger}\,\overline{A}_{\ell}^{\rightleftharpoons}\,\overline{\mathsf{g}} = \overline{\mathsf{f}}^{*}_{\ell,\rightleftharpoons}\overline{\mathsf{g}}_{n-\ell,\rightleftharpoons} = [A_{S(N-\ell,\rightleftharpoons)}(\mathsf{g},\mathsf{f})]^* \ . \tag{5.3b}$$

We have ommited the time argument of the component functions since the expressions are time independent.

V.3 Klein-Gordon bilinear forms

The invariant bilinear (B-) forms are obtained by pairing one $(\ell, \rightleftharpoons)$ travelling wave content with a second $(\ell, \rightleftharpoons)$ *opposite* one, as

$$E_{B(\ell,\rightleftharpoons)}(\mathsf{f},\mathsf{g}) = \overline{\mathsf{f}}^{T}\,\overline{E}_{\ell}^{\rightleftharpoons}\,\overline{T}\overline{\mathsf{g}} = \overline{\mathsf{f}}_{\ell,\rightleftharpoons}\,\mathsf{g}_{\ell,\rightleftharpoons} = E_{B(\ell,\rightleftharpoons)}\ (\mathsf{g},\mathsf{f}) \ , \tag{5.4a}$$

$$A_{B(\ell,\rightleftharpoons)}(\mathsf{f},\mathsf{g}) = \overline{\mathsf{f}}^{T}\,\overline{A}_{\ell}^{\rightleftharpoons}\,\overline{T}\,\overline{\mathsf{g}} = \overline{\mathsf{f}}_{\ell,\rightleftharpoons}\overline{\mathsf{g}}_{N-\ell,\rightleftharpoons} = A_{B(N-\ell,\rightleftharpoons)}(\mathsf{g},\mathsf{f}) \ . \tag{5.4b}$$

V.4 Incompleteness of the set of quadratic forms

The number of independent sesquilinear or bilinear forms is the dimension of the complex vector space $C_N^{\rightarrow} \oplus C_N^{\leftarrow}$, namely $4N-2$ for N odd, or $4N-4$ when N is even. Since $\mathsf{f}(t)$ and $\mathsf{g}(t)$ are together defined by $4N$ complex constants, this means that two or four (for N odd or even) complex quantities are lost in building quadratic forms. There are overall complex multiplicative constants: if we let $\overline{\mathsf{f}}_{\ell,\rightleftharpoons}(t) \mapsto (a_{\rightleftharpoons})^*\,\overline{\mathsf{f}}_{\ell,\rightleftharpoons}(t)$ and $\overline{\mathsf{g}}_{\ell,\rightleftharpoons}(t) \mapsto (a_{\rightleftharpoons})^{-1}\,\overline{\mathsf{g}}_{\ell,\rightleftharpoons}(t)$, none of the sesquilinear forms (5.3) are affected. These $a_{\rightleftharpoons}$ are two ℓ-independent complex constants missed. In addition, when N is even, $\overline{\mathsf{f}}_{\ell,\rightleftharpoons}(t) \mapsto (-1)^{\ell}(b_{\rightleftharpoons})^*\,\overline{\mathsf{f}}_{\ell,\rightleftharpoons}(t)$ and $\overline{\mathsf{g}}_{\ell,\rightleftharpoons}(t) \mapsto$

Table I

Properties of quadratic-invariant forms

Case	Quadratic forms	Basis	Invariance group for $C: \ell \to C: N-\ell$	Metric matrices for the h&i forms $C:(\mathsf{f},\mathsf{g})$		Positivity	$N \to \infty$ limit
Klein-Gordon	Sesquilinear (5.6)	$E^+_{S,\ell}$	$\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow}$	M^{K-}, M^{P-}	(5.15b,c) in (5.15a)	> 0	not proper
		$E^-_{S,\ell}$		M^{A-}	(5.15d) in (5.15a)	$\gtrless 0, \mathsf{f}_{\rightleftharpoons}$	proper
		$A^+_{S,\ell}$	—	—		—	—
		$A^-_{S,\ell}$					
	Bilinear (5.6)	E^+_B	$(\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow})_i$	—		—	—
		E^-_B					
		A^+_B	$(\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow})_d$	M^{K-}, M^{P-}	(5.15b, c) in (5.16)	—	
		A^-_B		M^{A-}	(5.15d) in (5.16)		
Helmholtz	Sesquilinear (5.6) $\lvert\Omega\rvert < m_c$ (5.8) $\lvert\Omega\rvert = m_c$ (5.10) $\lvert\Omega\rvert > m_c$	E^+_S	$\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow}$, $\lvert\Omega\rvert < m_c$	M^{K+}, M^{P+}	(5.17b, c) in (5.15a)	> 0	proper
		E^-_S	$(\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow})_d$, $\lvert\Omega\rvert > m_c$	M^{A+}	(5.17d) in (5.15a)	$\gtrless 0, \mathsf{f}_{\rightleftharpoons}$	not proper
		A^+_S	—, $\lvert\Omega\rvert < m_c$,	—		—	—
		A^-_S	$(\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow})_i$, $\lvert\Omega\rvert > m_c$				
	Bilinear (5.6) $\lvert\Omega\rvert \neq m_c$ (5.8) $\lvert\Omega\rvert = m_c$	E^+_B	$(\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow})_i$	—		—	—
		E^-_B					
		A^+_B	$(\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow})_d$	M^{K+}, M^{P+}	(5.15b,c) in (5.16)	—	
		A^-_B		M^{A+}	(5.15d) in (5.16)		

$(-1)^{\ell}(b_{\rightleftharpoons})^{-1}\ \bar{g}_{\ell,\rightleftharpoons}(t)$ provide for the last two missing constants in sesquilinear forms. For bilinear forms, right- and left-moving partial waves can be multiplied by mutually inverse complex contants. i.e., $\bar{f}_{\ell,\rightleftharpoons}(t) \mapsto d_{\rightleftharpoons}\bar{f}_{\ell,\rightleftharpoons}(t)$, $\bar{g}_{\ell,\rightleftharpoons}(t) \mapsto (d_{\rightleftharpoons})^{-1}\ \bar{g}_{\ell,\rightleftharpoons}(t)$ without affecting the forms; when N is even, we can complete the list as above introducing a factor $(-1)^{\ell}$.

V.5 A basis of invariant forms

The physical meaning of these forms can be clarified in the normal mode basis, using

$$\bar{h}_{\ell,\rightleftharpoons}^{\ \ \pm} = \mp\ M^{1/2}[\omega_{\ell}^{\mp}\bar{h}_{\ell} + i\dot{\bar{h}}_{\ell}]^{\pm}\ , \tag{5.5}$$

where $(\pm)$ is complex conjugation $(*)$ for S-forms and the identity for B-forms. Replacing (5.5) in (5.3a) and (5.4a) we find [referring to S or B through $(\pm)$] the following recognizable linear combinations:

$$E^{+}_{(\pm)\ell}(\mathbf{f},\mathbf{g}) = [E_{(\pm)(\ell,\rightarrow)} + E_{(\pm)(\ell,\leftarrow)}](\mathbf{f},\mathbf{g})$$

$$= \frac{1}{2}M[(\omega_{\ell}^{e})^{2}\bar{f}_{\ell}^{\ \pm}\bar{g}_{\ell} + \dot{\bar{f}}_{\ell}^{\ \pm}\dot{\bar{g}}_{\ell}] = [E^{+}_{(\pm)\ell}(\mathbf{g},\mathbf{f})]^{\pm}\ , \tag{5.6a}$$

$$E^{-}_{(\pm)\ell}(\mathbf{f},\mathbf{g}) = [E_{(\pm)(\ell,\rightarrow)} - E_{(\pm)(\ell,\leftarrow)}](\mathbf{f},\mathbf{g})$$

$$= \frac{1}{2}Mi^{\pm}\omega_{\ell}^{e}(\bar{f}_{\ell}^{\ \pm}\dot{\bar{g}}_{\ell} - \dot{\bar{f}}_{\ell}^{\pm}\bar{g}_{\ell}) = i[iE^{-}_{(\pm)\ell}(\mathbf{f},\mathbf{g})]^{\pm}\ . \tag{5.6b}$$

In a similar way, out of the A-quantities in (5.3b) and (5.4b), we define

$$A^{\pm}_{(\pm)\ell}(\mathbf{f},\mathbf{g}) = \{(5.6\text{a, b}) \text{ with } E \mapsto A,\ \bar{g}_{\ell} \mapsto \bar{g}_{N-\ell}\}\ . \tag{5.6c}$$

The E^{+} and A^{+} have the general form of energies [as recall $M(\omega_{\ell}^{e})^{2}\mu_{\ell}$], while E^{-} and A^{-} have the form of angular momenta. See Table I.

V.6 Positivity of energies and angular momenta

Setting $\mathbf{f} = \mathbf{g}$ in (5.6) we see that $E^{+}_{S,\ell}(\mathbf{f},\mathbf{f}) \geqslant 0$ is positive. By contrast $E_{S,\ell}(\mathbf{f},\mathbf{f}) \geqslant 0$ when $\mathbf{f}$ consists entirely of right-moving waves, while $E^{-}_{S,\ell}(\mathbf{f},\mathbf{f}) \leqslant 0$ when $\mathbf{f}$ consists entirely of left-moving waves. When setting

$\mathbf{f} = \mathbf{g}$, the $E^{+}_{(\pm)\ell}(\mathbf{f},\mathbf{f})$ are seen to be the ℓth normal mode energies of the lattice state $\mathbf{f}(t)$. Indeed, the total energy

$$E_{(\pm)}(\mathbf{f},\mathbf{f}) = \sum_{\ell=1}^{N} E^{+}_{(\pm)\ell}(\mathbf{f},\mathbf{f}) = \frac{1}{2}\mathbf{f}^{\pm}\mathbf{K}\mathbf{f} + \frac{1}{2}\mathbf{M}\dot{\mathbf{f}}^{\pm}\dot{\mathbf{f}}\ , \tag{5.7}$$

is the potential plus kinetic energy of the lattice moving as described by $\mathbf{f}(t)$, E_S is a (real) sesquilinear form, while E_B is bilinear and, for complex $\mathbf{f}(t)$, is in general complex itself. Next (for $\mathbf{f} = \mathbf{g}$) $E^{-}_{S,\ell}$ represents the angular momentum of the ℓth partial wave oscillator in the two real dimensions Re $\bar{f}_{\ell}$ and Im $\bar{f}_{\ell}$; $E^{-}_{B,\ell}$ on the other hand, is identically zero. Together, the E's provide for $2N$ real constants of the motion. Regarding the interpretation of the A's we must remember that the ℓth and $(N-\ell)$th modes, when distinct, have degenerate frequencies and hence rotations in the plane of these two modes is possible; the $A^{\pm}$'s provide the cross terms for energies and angular momenta under $\pi/4$ rotations. When $\mathbf{f} = \mathbf{g}$, they are not all independent, but $[A^{+}_{(\pm)\ell}]^{\pm} = A^{+}_{(\pm),N-\ell}$ and $[A^{-}_{(\pm)\ell}]^{\pm} = i^{\pm}\ iA^{-}_{(\pm),N-\ell}$ as can be ascertained from (5.3b) and (5.4b). In letting ℓ range from 1 to $(N-1)/2$ or $N/2-1$ for N odd or even, we obtain double that number of complex constants of the motion. The total number of real quadratic constants of the motion is therefore $4N-2$ or $4N-4$ for N odd or even.

V.7 Incompleteness of quadratic constants of the motion

The 'missing' quadratic constants of the motion stem from overall phases, as in the discussion following Eq. (5.4). For the sesquilinear constants: two phases, one multiplying right and one multiplying left-travelling waves [plus, if N is even, another two such phases times $(-1)^{\ell}$]. These transformations are not registered by the set of quadratic constants of the motion, their location and classification in the travelling-wave basis has been reasonably straightforward, as they can all be represented by diagonal matrices commuting with those present in (5.3) and (5.4). In the normal mode or elongation-momentum description, they will in general mix configuration and momentum components, and are none too easy to recognize.

V.8 Real solutions

As a special restriction, we should examine the constants of the motion in the case when the initial elongations and momenta in the lattice are

real. Since the evolution operator (2.5) is real, so will be the ensuing lattice solutions. Since for $\mathbf{f}$ real, $\bar{f}^*_m = \bar{f}_{N-m}$ [this is due to the fact that $F_{mn} = F^*_{m,N-n} = F^*_{N-m,n}$], and similarly for the time derivatives, one obtains $\bar{\mathbf{f}}^*_{\ell,\rightleftharpoons} = \bar{\mathbf{f}}_{N-\ell,\rightleftharpoons}$. We conclude thus that for real initial conditions the quadratic forms (5.6) will coalesce as $[C^{\pm}_{(\mp)\,\ell}(\mathbf{f},\mathbf{f})]^* = \pm C^{\pm}_{(\mp),N-\ell}(\mathbf{f},\mathbf{f})$, halving the total number of constants of the motion to $2N-1$ or $2N-2$ for N odd or even. The missing constants are now related to overall phases and multiplication constants on the travelling waves which respect the relation $\bar{\mathbf{f}}^*_{\ell,\rightleftharpoons} = \bar{\mathbf{f}}_{N-\ell,\rightleftharpoons}$, i.e., in terms of the phases used in Subsect. V.4., $a^*_{\rightleftharpoons} = a_{\rightleftharpoons}$ and, if N even, $b^*_{\rightleftharpoons} = b_{\rightleftharpoons}$. The effect of these transformations which leave all quadratic constants of the motion unaltered is to rotate all the $\omega^+_\ell \bar{f}_\ell - \dot{\bar{f}}_\ell$ planes by the same (free) angle, i.e., a time translation. When N is even, the extra free variable (which is *not* connected with the identity transformation) involves time translation followed by the lattice rotation by π. The latter is the only non-trivial central element of the dihedral group, and is present only for N even. Also, sesquilinear and bilinear constant now coalesce through

$$E^+_{B,\ell} = A^+_{S,N-\ell}, \quad E^-_{B,\ell} = A^-_{S,N-\ell} = 0 , \quad A^+_{B,\ell} = E^{\pm}_{S,\ell} .$$

We have been occupied in classifying and describing the constants of the motion for the discrete Klein-Gordon equation in some detail. As in section III, the wave and Helmholtz cases will now introduce exponential and perhaps critical solutions with imaginary and zero frequencies.

V.9 The wave equation case and critical solutions

The undamped wave equation is described in letting the constant κ^2 of the Klein-Gordon equation tend to zero from positive values. The effect of this, as $\omega^{\pm}_0 = \pm\omega^e_0 \to 0$ is to make the $m = 0$ modes and travelling waves go critical, as shown in Eq. (3.8). The sesquilinear and bilinear invariant forms (5.3), (5.4) or (5.6) also have a smooth limit, and only the $\ell = 0$ ones need be examined. Of these, we have only E's, and these are

$$E^+_{(\mp),0}(\mathbf{f},\mathbf{g}) = \frac{1}{2} M \dot{\bar{f}}^{\mp}_0 \dot{\bar{g}}_0 = \frac{1}{2} M N^{-1} (\Sigma_n \dot{f}^{\mp}_n)(\Sigma_{n'} \dot{g}_{n'}) , \tag{5.8a}$$

$$E^-_{(\mp),0}(\mathbf{f},\mathbf{g}) = 0 . \tag{5.8b}$$

Since the Klein-Gordon spring binding each mass to equilibrium has dissappeared, only the kinetic energy of the critical $\ell = 0$ mode remains in (5.8a), while we loose the quadratic form (5.8b). The number of real quadratic constants of the motion (for $\mathbf{f} = \mathbf{g}$) now drops to $4N-4$ for N odd and $4N-6$ for N even. The two new missing quadratic constants are related to the real and imaginary parts of $\bar{f}_0 = N^{-1/2}\Sigma_n f_n$, the average elongation of the masses. A lattice all of whose masses have been displaced by the same amount is indistinguishable from the original one through its quadratic forms alone. We thus have now the extra invariance of the set of constants under the *addition* $\mathbf{f}(t) \mapsto \mathbf{f}(t) + \mathbf{c}$ where $\mathbf{c}$ is an N-vector all of whose components are c. The origin of this property is the fact that for the wave equation interaction operator, $\mathbf{kc} = \mathbf{0}$ i.e. $\Sigma_n K_{nn'} = 0$. The only interaction matrices with a nonzero sum over columns (and rows) are those with $k_0 \neq 0$. Multiplication of the components of $\mathbf{f}(t)$ by phases accounts for the rest of the invariances as described before.

When the elongations and momenta are real, again the number of independent nonzero quadratic constants of the motion is halved to $2N-2$ for N odd and $2N-3$ for N even.

V.10 The Helmholtz case

The discrete Helmholtz equation presents a major difference in that in general there will be real as well as pure imaginary values of ω^e_m. These are separated by a critical value m_c, for which $0 = \mu_{m_c} = \kappa^2 - 4\sin^2(\pi m_c/N)$. Whether or not m_c is actually an integer determines whether or not critical solutions (3.8) exist among the solutions to a particular value of κ^2 in the Helmholtz equation. We shall assume for simplicity that they do not. In any case, $|m| < |m_c|$ (all quantities modulo N in the basic Brillouin range) characterize oscillating solutions for which everything we stated for the Klein-Gordon quadratic constants of the motion continues to hold. The range $|m_c| < |m| \leqslant P(N)$ corresponds to exponential solutions, we must now account for the associated quadratic invariants (5.3)-(5.4). Since for these $\bar{\mathbf{f}}_{\ell,\rightleftharpoons}(t) = \exp(\pm w^e_\ell t)\bar{\mathbf{f}}_{\ell,\rightleftharpoons}(0)$, from (2.3b), we see that *both* sesquilinear and bilinear invariants may be obtained as in (5.4), i.e., through pairing left- and right-'travelling' waves of the same mode. For the bilinear forms we have again (5.4), but for the sesquilinear forms, we have

$$E_{S(\ell,\rightleftharpoons)}(\mathbf{f},\mathbf{g}) = \bar{\mathbf{f}}^{\dagger}\bar{\mathbf{E}}^{\rightleftharpoons}_{\ell}\bar{\mathbf{T}}\bar{\mathbf{g}} = \bar{\mathbf{f}}^*_{\ell,\rightleftharpoons}\bar{\mathbf{g}}_{\ell,\rightleftharpoons} = [E_{S(\ell,\rightleftharpoons)}(\mathbf{g},\mathbf{f})]^* , \tag{5.9a}$$

$$A_{S(\ell,\rightleftharpoons)}(\mathbf{f},\mathbf{g}) = \bar{\mathbf{f}}^{\dagger}\bar{\mathbf{A}}^{\rightleftharpoons}_{\ell}\bar{\mathbf{T}}\bar{\mathbf{g}} = \bar{\mathbf{f}}^*_{\ell,\rightleftharpoons}\bar{\mathbf{g}}_{N-\ell,\rightleftharpoons} = [A_{S(N-\ell,\rightleftharpoons)}(\mathbf{g},\mathbf{f})]^* . \tag{5.9b}$$

The corresponding expressions for (5.6) in terms of normal-mode components are

$$E^{+}_{S,\ell}(\mathsf{f},\mathsf{g}) = [E_{S(\ell,\rightarrow)} + E_{S(\ell,\leftarrow)}](\mathsf{f},\mathsf{g})$$

$$= \frac{1}{2}M[(w^{e}_{\ell})^{2}\tilde{f}^{*}_{\ell}\tilde{g}_{\ell} - \dot{\tilde{f}}^{*}_{\ell}\dot{\tilde{g}}_{\ell}] = [E^{+}_{S,\ell}(\mathsf{g},\mathsf{f})]^{*} \ , \tag{5.10a}$$

$$E^{-}_{S,\ell}(\mathsf{f},\mathsf{g}) = [E_{S(\ell,\rightarrow)} - E_{S(\ell,\leftarrow)}](\mathsf{f},\mathsf{g})$$

$$= \frac{1}{2}Mw^{e}_{\ell}(\tilde{f}^{*}_{\ell}\dot{\tilde{g}}_{\ell} - \dot{\tilde{f}}^{*}_{\ell}\tilde{g}_{\ell}) = -[E^{-}_{S,\ell}(\mathsf{g},\mathsf{f})]^{*} \ , \tag{5.10b}$$

$$A^{\pm}_{S,\ell}(\mathsf{f},\mathsf{g}) = \{(5.10\text{a, b}) \text{ with } E \mapsto A, \tilde{g}_{\ell} \mapsto \tilde{g}_{N-\ell}\} \ . \tag{5.10c}$$

See Table I.

The count of independent and 'missing' quadratic invariants is the same as before, and so is the restriction to real initial conditions.

V.11 'Total energy' in the Helmholtz case

It should be noted that in general the construction of a sesquilinear 'total energy' is possible as a sum of the $E^{+}_{S,\ell}$ over ℓ, but, since we should be summing over both the oscillating and exponential modes, the last equality in (5.7) will not carry over to this case. Instead, it will consist of a sum over ℓ for the positive values of μ_{ℓ} (oscillating solutions) *minus* a sum over ℓ for the negative values of μ_{ℓ} (exponential solutions). The reconstitution of the interaction matrix K in the elongation-momentum basis, is therefore *not* possible. We may (and shall, in the next section) sum *only over the oscillating solutions* and obtain —of course— an invariant quadratic form.

The presence of critical solutions for a certain m_c set ($+|m_c|$ and $-|m_c|$) puts the complex constants $E^{-}_{(\mp),m_c}(\mathsf{f},\mathsf{g})$ to zero. This is now due to the invariance of the remaining set under addition $\mathsf{f}(t) \mapsto \mathsf{f}(t) + \mathsf{c}^{(m_c)}$ where $\mathsf{c}^{(m_c)}$ is a vector with components $c^{(m_c)}_{n} = c^{(m_c)}F_{n,m_c}$ (for any complex constant $c^{(m_c)}$). Again, the origin of this property is that $\mathrm{K}\mathsf{c}^{(\pm m_c)} = 0$ i.e., $\sum_{n} K_{nn'}F_{n,\pm m_c} = 0$.

V.12 The damped wave equation case

There is little new to be added for the damped wave equation, as the procedure for oscillating and exponential solutions follows as for the Helmholtz equation, except that the ranges are reversed, i.e., the former may exist for $|\ell| > |m_c|$ and the latter exist for $|\ell| < |m_c|$. The time-dependent exponents will not cancel out completely, however, and all 'constants of the motion' must decay with a factor of $\exp(-2\Gamma t)$.

V.13 Homogeneous and isotropic quadratic forms

Having accounted for all constants of the motion obtainable from quadratic forms, we can now propose the criterion that, since the lattice dynamics is invariant under the geometric $\mathcal{D}_N$ and the $\mathcal{D}^{\rightarrow}_N \otimes \mathcal{D}^{\leftarrow}_N$ group of phase-space dihedral transformations, the quadratic forms (5.1) which are *invariant* under at least the first group,

$$C_{(\mp)}(\mathsf{f},\mathsf{g}) = C_{(\mp)}(\mathsf{Df},\mathsf{Dg}), \quad \mathsf{D} \in \mathcal{D}_N = (\mathcal{D}^{\rightarrow}_N \otimes \mathcal{D}^{\leftarrow}_N)_d \ , \tag{5.11a}$$

should be especially important. Their value will not depend on which system element is counted as the 'origin' $n = 0$ nor on the direction in which the counting is made. These *homogeneous and isotropic* (*h & i*) *quadratic forms* will be determined by those C satisfying

$$\overline{\mathsf{D}}^{\mp}\,\overline{\mathsf{C}}\,\overline{\mathsf{D}} = \overline{\mathsf{C}} \ , \tag{5.11b}$$

where D belongs to $\mathcal{D}_N$ or, for generality, to $\mathcal{D}^{\rightarrow}_N \otimes \mathcal{D}^{\leftarrow}_N \supset \mathcal{D}_N$. The adjunction and transposition properties of the two $N \times N$ blocks of $\overline{\mathsf{D}}$ are given in (4.7) while the $\overline{\mathsf{C}}$ matrices for the sesquilinear and bilinear forms appear in (5.3), (5.4), (5.6), and (5.9). The analysis of all possibilities leads to the following results for *oscillating* solutions:

$$[E^{\pm}_{S,\ell} + E^{\pm}_{S,N-\ell}](\mathsf{f},\mathsf{g}) \qquad \text{h\&i under} \quad \begin{pmatrix} \mathsf{D} & 0 \\ 0 & \mathsf{D}' \end{pmatrix} \in \mathcal{D}^{\rightarrow}_N \otimes \mathcal{D}^{\leftarrow}_N \ , \tag{5.12a}$$

$$A^{\pm}_{S,\ell}(\mathsf{f},\mathsf{g}) \qquad \text{not h\&i under any} \quad \mathcal{D}_N \subset \mathcal{D}^{\rightarrow}_N \otimes \mathcal{D}^{\leftarrow}_N \ , \tag{5.12b}$$

$$[E^{\pm}_{B,\ell} + E^{\pm}_{B,N-\ell}](\mathsf{f},\mathsf{g}) \quad \text{h\&i under} \quad \begin{pmatrix} \mathsf{D} & 0 \\ 0 & \mathsf{I}_0\mathsf{D}\mathsf{I}_0^{-1} \end{pmatrix} \in (\mathcal{D}^{\rightarrow}_N \otimes \mathcal{D}^{\leftarrow}_N)_i \ , \tag{5.13a}$$

$$[A^{\pm}_{B,\ell} + A^{\pm}_{B,N-\ell}]\,(\mathbf{f}, \mathbf{g}) \quad \text{h\&i under} \begin{pmatrix} \mathrm{D} & 0 \\ 0 & \mathrm{D} \end{pmatrix} \in (\mathcal{D}^{\rightarrow}_N \otimes \mathcal{D}^{\leftarrow}_N)_d \ . \quad (5.13b)$$

In Helmholtz-type equations where *exponential* solutions exist, the sesquilinear forms are built as in (5.9), pairing right- and left-moving waves. This leads to the following results:

$$[E^{\pm}_{S,\ell} + E^{\pm}_{S,N-\ell}](\mathbf{f}, \mathbf{g}) \quad \text{h\&i under} \begin{pmatrix} \mathrm{D} & 0 \\ 0 & \mathrm{D} \end{pmatrix} \in (\mathcal{D}^{\rightarrow}_N \otimes \mathcal{D}^{\leftarrow}_N)_d \ , \quad (5.14a)$$

$$[A^{\pm}_{S,\ell} + A^{\pm}_{S,N-\ell}](\mathbf{f}, \mathbf{g}) \quad \text{h\&i under} \begin{pmatrix} \mathrm{D} & 0 \\ 0 & \mathrm{I_0 D I_0} \end{pmatrix} \in (\mathcal{D}^{\rightarrow}_N \otimes \mathcal{D}^{\leftarrow}_N)_i \ . \quad (5.14b)$$

Bilinear forms do not depend on the oscillatory or exponential nature of the solutions and their h&i properties are given by (5.13) for all cases. See table I.

V.14 Homogeneity and isotropy in time

So much for the h&i properties in the lattice space. Regarding homogeneity in time, the quadratic invariants were built with (5.2) as their defining property; this is the direct analogue of (5.9) for time translations. Time *inversions* are produced through T given in (4.10). In the travelling-wave basis this corresponds to the exchange of right- and left-travelling waves. The $C^{+}_{\cdots}(\mathbf{f}, \mathbf{g})$ will be invariant, as energies are, but the $C^{-}_{\cdots}(\mathbf{f}, \mathbf{g})$ will change sign, as angular momenta do.

The panorama on homogeneous and isotropic quadratic forms and constants of the motion thus configures as follows.

V.15 Klein-Gordon sesquilinear h&i forms

Systems exhibiting oscillatory solutions only, as the discrete Klein-Gordon lattice, will have full $(\mathcal{D}^{\rightarrow}_N \otimes \mathcal{D}^{\leftarrow}_N)$- invariant sesquilinear forms (5.12a). The most general form can be written [regressing through (5.12a), (5.6), and (1.5) for $\tilde{\mathbf{f}} = \mathbf{F}^{-1}\mathbf{f}$] as a linear combination

$$C^{(\mathrm{KG})}_S(\mathbf{f}, \mathbf{g}) = \sum_{\sigma=\pm} \sum_{\ell=1}^{P(N),N} \tilde{c}^{(\sigma)}_{\ell} [E^{\sigma}_{S,\ell} + E^{\sigma}_{S,N-\ell}](\mathbf{f}, \mathbf{g})$$

$$= \frac{1}{2} M \sum_{n=1}^{N} \sum_{n'=1}^{N} \{\dot{f}^*_n M^K(n-n')\dot{g}_{n'} + f^*_n M^P(n-n') g_{n'}$$

$$+ (f^*_n \dot{g}_{n'} - \dot{f}^*_n g_{n'}) M^A(n-n')\}$$

$$= \frac{1}{2} M (\mathbf{f}^{\dagger}\ \dot{\mathbf{f}}^{\dagger}) \begin{pmatrix} \mathrm{M}^P & \mathrm{M}^A \\ -\mathrm{M}^A & \mathrm{M}^K \end{pmatrix} \begin{pmatrix} \mathrm{g} \\ \dot{\mathrm{g}} \end{pmatrix}, \quad (5.15a)$$

where

$$M^K(k) = N^{-1} \sum_{\ell=1}^{N} \tilde{c}^{+}_{\ell} \exp(-2\pi i k\ell/N)$$

$$= N^{-1/2}\, \tilde{c}^{+}_{\ell} = (\mathrm{M}^K)_{n\pm k,n} \ , \quad (5.15b)$$

$$M^P(k) = N^{-1} \sum_{\ell=1}^{N} (\omega^e_{\ell})^2 \tilde{c}^{+}_{\ell} \exp(-2\pi i k\ell/N)$$

$$= M^{-1} N^{-1/2} (\mathrm{K c}^{\dagger})_k = (\mathrm{M}^P)_{n\pm k,n} \ , \quad (5.15c)$$

$$M^A(k) = iN^{-1} \sum_{\ell=1}^{N} \omega^e_{\ell}\, \tilde{q}^{-}\ \omega^e_{\ell} \tilde{c}^{-}_{\ell} \exp(-2\pi k\ell/N)$$

$$= iN^{-1} (v^* \mathrm{c}^{-})_k = (\mathrm{M}^A)_{n+k,n} \ , \quad (5.15d)$$

where $\mathrm{c}^{\pm}$ is the inverse Fourier transform of $\tilde{\mathrm{c}}^{\pm} = \|\tilde{c}^{\pm}_{\ell}\|$, and v the inverse Fourier transform of a 'frequency' vector $\tilde{v} = \|\omega^e_{\ell}\|$. The components of these vectors have been extended from (5.15), where $\ell = 1, 2, \ldots, P(N), N$ to the range $\ell = 1, 2, \ldots, N$ through defining $\tilde{c}^{\pm}_{N-\ell} = \tilde{c}^{\pm}_{\ell}$ and thus the $c^{\pm}$ have the same property: $c^{\pm}_n = c^{\pm}_{N-n}$, i.e., $\mathrm{c}^{\pm} = \mathrm{I_0}\,\mathrm{c}^{\pm}$. Finally, as $\tilde{v} = \mathrm{I_0}\tilde{v}$, we also have $v = \mathrm{I_0} v$. The matrix K in (5.15c) is the interaction matrix of the lattice, Eq. (1.3), given through the symmetric circulating matrix $K_{n,n'} = K_{|n-n'|} = MN^{-1}(v * v)_{n-n'}$, where '$*$' means the finite convolution. The c^{+}-part of (5.15) is a linear combination of terms of

energy type while the c^--part is of angular-momentum type. The total number of dimensions in the space of Klein-Gordon invariant quadratic forms is thus $N + 1$ or $N + 2$ for N odd or even.

V.16 Klein-Gordon h&i bilinear forms

No bilinear forms are invariant under the full phase-space symmetry group $\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow}$, but (5.13b) and (5.13a) are invariant under the geometric diagonal and 'inverted-diagonal' subgroups. If we demand that the forms be invariant at least under the geometric symmetry group, we may keep (5.13b), i.e., we may have the h&i bilinear form (under the $\mathcal{D}_N$ subgroup)

$$C_B^{(\mathrm{KG})}(\mathsf{f},\mathsf{g}) = \sum_{\sigma=\pm}\sum_{\varrho=1}^{P(N),N} \tilde{c}_\varrho^{(\sigma)}[A^\sigma_{B,\varrho} + A^\sigma_{B,N-\varrho}](\mathsf{f},\mathsf{g})$$

$$= \frac{1}{2}M\sum_{n=1}^{N}\sum_{n'=1}^{N}\{\dot{f}_n M^K(n-n')\dot{g}_n + f_n M^P(n-n')\dot{g}_{n'}$$

$$+ (f_n\dot{g}_{n'} - \dot{f}_n g_n)M^A(n-n')\}$$

$$= \frac{1}{2}M(\mathsf{f}^T\dot{\mathsf{f}}^T)\begin{pmatrix}\mathbf{M}^P & \mathbf{M}^A\\ -\mathbf{M}^A & \mathbf{M}^K\end{pmatrix}\begin{pmatrix}\mathsf{g}\\ \dot{\mathsf{g}}\end{pmatrix}. \qquad (5.16)$$

This equals the last expression in (5.15a) with the $\mathbf{M}^K$, $\mathbf{M}^P$ and $\mathbf{M}^A$ as given by (5.15b)-(5.15d). The only change of (5.16) with respect to (5.15a) consists in that we write the components of f instead of those of f*.

V.17 Helmholtz h&i quadratic forms

Systems possessing both oscillatory and exponential solutions separated by a value m_c of the normal-mode index (which does not coincide with an integer, so that critical modes be absent) will have $2[m_c] + 1$ $\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow}$-invariant sesquilinear forms associated to the oscillatory solutions (5.12a), and $N + 1$ or $N + 2$ minus that number of sesquilinear forms (5.14a), corresponding to the exponential solutions (for N odd or even). These forms will be invariant only under the geometric-invariance subgroup $\mathcal{D}_N = (\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow})_d$.

In the same way as (5.15) and (5.16) we may now write, instead of the middle expression in (5.15a),

$$C_S^{(H)}(\mathsf{f},\mathsf{g}) = \sum_{\sigma=\pm}\Bigg[\sum_{|\varrho|<m_c}\tilde{c}_\varrho^{(\sigma)}(E^\sigma_{S,\varrho} + E^\sigma_{S,N-\varrho})(\mathsf{f},\mathsf{g}) + \sum_{|\varrho|>m_c}\tilde{c}_\varrho^{(\sigma)}(E^\sigma_{S,\varrho} + E^\sigma_{S,N-\varrho})(\mathsf{f},\mathsf{g})\Bigg], \qquad (5.17a)$$

and the last expression in the same equation retains form when we define the corresponding M's as

$$M^K(k) = N^{-1}\left(\sum_{|\varrho|<m_c} + \sum_{|\varrho|>m_c}\right)\tilde{c}_\varrho^{+}\exp(-2\pi i\varrho k/N)$$

$$= N^{-1/2}c_k^{+}, \qquad (5.17b)$$

$$M^P(k) = N^{-1}\left(\sum_{|\varrho|<m_c}(\omega_\varrho^e)^2 + \sum_{|\varrho|>m_c}(w_\varrho^e)^2\right)\tilde{c}_\varrho^{+}\exp(-2\pi i\varrho k/N), \qquad (5.17c)$$

$$M^A(k) = iN^{-1}\left(\sum_{|\varrho|<m_c}\omega_\varrho^e - i\sum_{|\varrho|>m_c}w_\varrho^e\right)\tilde{c}_\varrho^{-}\exp(-2\pi i\varrho k/N)$$

$$= iN^{-1}(\upsilon * \mathsf{c}^-)_k. \qquad (5.17d)$$

Equations (5.17b) and (5.17d) are the same as (5.15b) and (5.15d), the latter pair with the novelty that $\tilde{\upsilon} = \|\omega_\varrho^e\|$ is a vector with complex components [recall in (2.3b) that $\omega_\varrho^e = -iw_\varrho^e$, w_ϱ^e real, for $|\varrho| > m_c$]. Equation (5.17c) is different, however: the sum $\Sigma_{\varrho=1}^N(\omega_\varrho^e)^2$ ... for the Klein-Gordon case is here $\Sigma_{\varrho=1}^N|\omega_\varrho^e|^2$ ... and hence no longer expressible simply as $\sim(\mathrm{K}\,\mathsf{c}^+)_k$, as in (5.15c). We noted before that the oscillatory-solution part of the sum in (5.17) is invariant under $\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow}$ while the exponential-solution part has only invariance under the geometric dihedral transformations in $(\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\leftarrow})_d$. If $\mathsf{c}^{\pm}$ is such that $\tilde{c}_\varrho^{\pm} = 0$ for $|\varrho| > m_c$,

the corresponding sesquilinear form (5.17a) will have the larger invariance group.

Regarding bilinear forms invariant at least under $(\mathcal{D}_N^{\rightarrow} \otimes \mathcal{D}_N^{\rightarrow})_d$, the construction (5.16), as for the Klein-Gordon case, applies also for the Helmholtz case:

$$C_B^{(H)}(\mathrm{f}, \mathrm{g}) = C^{(\mathrm{KG})}(\mathrm{f}, \mathrm{g}) \ . \tag{5.18}$$

These results are summarized in table I.

V.18 Positivity revisited

We should examine the positivity properties of the inner products defined through the h&i invariant forms. If $\tilde{c}^+$ in (5.15b)-(5.15d) and (5.17b)-(5.17d) has *positive* components ($\tilde{c}_\varrho^+ \geqslant 0$), then, as also $(\omega_\varrho^e)^2 > 0$ $|\varrho| < m_c$ and $(w_\varrho^e)^2 > 0$, $|\varrho| > m_c$, it follows that the vectors $\|M^K(k)\|$ and $\|M^P(k)\|$ –equivalent to circulating matrices as $M_{n,n'} = M^{\cdot}(n-n')$– are *positive definite* [i.e., $\Sigma_n \Sigma_{n'} h_n^* M_{n,n'}^{\cdot} h_{n'} \geqslant 0$ for all $\|h_n\|$]. The c$^+$-part of the sesquilinear and bilinear invariants (5.15)-(5.18) thus give rise to *positive definite* inner products. Recall the discussion on this point following Eqs. (5.3) and (5.7). By the same token, if $\tilde{c}_\varrho > 0$, we recall that $E_{S,\varrho}^-(\mathrm{f}, \mathrm{f})$ are $\geqslant 0$, or $\leqslant 0$, for f's consisting entirely of right- or left-moving waves, i.e., of functions of the type $\exp i(\omega_m^e t - 2\pi mn/N)$ or $\exp i(-\omega_m^e t - 2\pi mn/N)$. In the theory of the (continuous) Klein-Gordon equation, these are the positive- or negative-energy solutions [11] $E/\hbar = \omega^e$ or $E/\hbar = -\omega^e$, having identified $2\pi mn/N = \hbar^{-1} px$ and conjugated the basis functions.

To sum up: Positive (P) sesquilinear h&i forms are obtained for all cases as energy-like invariants (with summands $\dot{f}_n^* \dot{g}_{n'}$ and $f_n^* g_{n'}$) with the $c_n^+ = c_{N-n}^+$ for parameters involving the absolute value of the interaction matrix eigenvalues. Positive/negative (P/N) sesquilinear h&i forms are obtained for all cases as angular-momentum-like invariants (with summands $f_n^* \dot{g}_{n'} - \dot{f}_n^* g_{n'}$) with the $c_n^- = c_{N-n}^-$ for parameters, involving the oscillatory or exponential solution frequencies, for the subspaces of right-moving (positive-energy)/left-moving (negative-energy) waves. There are $(N+1)/2$ or $(N+2)/2$, for N odd or even, sesquilinear invariants of (P)-type and the same number of (P/N)-type. These we write again as

$$C_S^{\cdot}(\mathrm{f}, \mathrm{g}) = \frac{1}{2} M(\mathrm{f}^\dagger \dot{\mathrm{f}}^\dagger) \begin{pmatrix} \mathrm{M}^P & \mathrm{M}^A \\ -\mathrm{M}^A & \mathrm{M}^K \end{pmatrix} \begin{pmatrix} \mathrm{g} \\ \dot{\mathrm{g}} \end{pmatrix} , \tag{5.19}$$

with the M$^{\cdot}$'s being given by (5.15b)-(5.15d) for the Klein-Gordon case, and (5.17b)-(5.17d) for the Helmholtz case. The two diagonal submatrices M^P and M^K are not independent, and are of (P)-type, while the antidiagonal submatrix M^A is (P/N)-type.

In the next section we shall see how the (P)-and (P/N)-type forms provide analogous results for the continuous systems described by the Klein-Gordon and Helmholtz differential equations.

VI. THE CONTINUUM LIMIT, POINCARE AND EUCLIDEAN INVARIANCE

We shall now let $N \to \infty$ and use the limiting expressions to describe the homogeneous quadratic invariant sesquilinear forms for the true Klein-Gordon and Helmholtz partial differential equations.

VI.1 Recalling coordinates, functions and operators

In order to obtain confortable expressions, we consider $(2N+1)$-dimensional spaces whose components are labelled by the values of the variable

$$q = [2\pi/(2N+1)]^{1/2} n \ , \quad n = -N, -N+1, \ldots, N \ , \tag{6.1}$$

which ranges in $[-q_N, q_N]$, $q_N = N[2\pi/(2N+1)]^{1/2}$ in steps of

$$\Delta q = [2\pi/(2N+1)]^{-1/2} \ . \tag{6.2}$$

It is futhermore convenient to treat functions of q defined in terms of functions of integer n through

$$f(q) = [(2N+1)/2\pi]^{1/4} f_n \ . \tag{6.3}$$

The expressions for operator kernels should be

$$A(q, q') = [(2N+1)/2\pi]^{1/2} A_{n,n'} \tag{6.4}$$

where n and n' determine q and q' through (6.1).

VI.2 The continuum limit

If we consider functions of q as step functions with the value $f(\overline{q})$ in $\overline{q} \in (q - \frac{1}{2}\Delta q,\ q + \frac{1}{2}\Delta q]$, we can speak of those step-functions which, when $N \to \infty$, approach piece-wise differentiable functions uniformly, in the intervals of continuity. For these limit functions, which we denote also by $f(q)$, $q \in \mathcal{R}$ we see that inner products become

$$(\mathrm{f}, \mathrm{g}) = \sum_{n=-N}^{N} f_n^* g_n \xrightarrow[N \to \infty]{} \int_{-\infty}^{\infty} dq\, f(q)^* g(q) \ . \tag{6.5}$$

Here, the matrices $\mathrm{A} = \|A_{n,n'}\|$ become operators A with integral kernels $A(q, q')$ following the general rule of replacing $\Sigma_{n=-N}^{N} \Delta q \cdots \mapsto \int_{-\infty}^{\infty} dq \cdots$. In particular, the Fourier matrix (1.5) becomes [12] the Fourier integral kernel $(2\pi)^{-1/2} \exp(ipq)$ where q and p are related to n and m in (1.5) through (6.1). Operators such as the interaction operator (1.3) do not have a well-defined limit in the above framework, but when applied to any vector f whose components f_n tend to a twice-differentiable function $f(q)$, it has the property of having Kf tend to k_0f i.e., $\|K_{n,n'}\| \mapsto k_0 \|\delta(q - q')\|$. In order to obtain second derivatives [10] we must let any one pth-neighbour interaction spring have its k_p multiplied by a factor $(2N + 1)/2\pi p^2$. We set $p = 1$ henceforth for simplicity. Thus we may write, weakly,

$$\mathrm{K}^{(N)} = k_0 1 - k_1^{(N)} \Delta \xrightarrow[N \to \infty]{} k_0 - k_1 \partial_q^2$$

$$\text{for } k_1^{(N)} = k_1 (2N + 1)/2\pi \ . \tag{6.6}$$

The diagonal form of this interaction operator, Eq. (1.7a), exhibits eigenvalues

$$\tilde{K}(p, p') = \mu(p)\delta(p - p') \ , \quad p, p' \in \mathcal{R} \ , \tag{6.7a}$$

$$\mu(p) = k_0 + k_1 p^2 \ . \tag{6.7b}$$

The last expression is obtained from (1.7b) through putting $2N + 1$ for N, using $k_1^{(N)}$ as in (6.6) and letting $N \to \infty$.

The characterization of right- and left-travelling waves is now done through the continuous index p, and their frequencies $\omega^e(p) = [\mu(p)/M]^{1/2}$ as before divide the waves into oscillatory $[\mu(p) > 0]$ and exponential $[\mu(p) < 0]$. The Klein-Gordon equation $[k_0 = \kappa^2,\ k_1 = 1,\ M = 1]$ exhibits solutions only of the first kind with $\omega^{\pm}(p) = \pm(\kappa^2 + p^2)^{1/2}$. The Helmholtz equation $[k_0 = \kappa^2,\ k_1 = -1,\ M = 1]$ has both oscillatory solutions [for $|p| < \kappa$, $\omega^{\pm}(p) = \pm(\kappa^2 - p^2)^{1/2}$] and exponential ones [for $|p| > \kappa$, $w^{\pm}(p) = \pm(p^2 - \kappa^2)^{1/2}$]. Critical solutions $p = \pm\kappa$ need not concern us here as they represent a set of measure zero in the manifold of solutions.

These two differential equations can be written with an index $\tau = -$ for the Klein-Gordon case, and $\tau = +$ for the Helmholtz case, as

$$[\partial_t^2 + \mathrm{K}^{\tau}]f(q, t) = 0 \ , \quad \mathrm{K}^{\tau} = \kappa^2 + \tau\partial_q^2 \ , \tag{6.8}$$

or, in two-component form as

$$\mathrm{H}^{\tau}\begin{pmatrix} f(q, t) \\ f_t(q, t) \end{pmatrix} = \partial_t \begin{pmatrix} f(q, t) \\ f_t(q, t) \end{pmatrix}, \quad \mathrm{H}^{\tau} = \begin{pmatrix} 0 & 1 \\ -\mathrm{K}^{\tau} & 0 \end{pmatrix} \ . \tag{6.9}$$

VI.3 Sesquilinear h&i invariant forms

The sesquilinear h&i invariant forms may be written as in (5.19),

$$C_S^{\tau}(\mathrm{f}, \mathrm{g}) = \frac{1}{2}\int_{-\infty}^{\infty} dq' \int_{-\infty}^{\infty} dq' \Big(f(q, t)^* f_t(q, t) \Big)$$

$$\begin{pmatrix} M^{P,\tau}(q - q') & M^{A,\tau}(q' - q') \\ -M^{A\tau}(q - q') & M^{K,\tau}(q' - q') \end{pmatrix} \begin{pmatrix} g(q', t) \\ g_t(q', t) \end{pmatrix} \ , \tag{6.10}$$

where the functions $M^{\cdot,\tau}(q - q')$ can be found from (5.15b-d) and (5.17b-d). Indeed, regarding the 'energy'-type C's we have the functions $M^{K\tau}$ and $M^{P,\tau}$. Here, $M^{K,\tau}(q - q')$ is an arbitrary function of its argument whose Fourier transform $\tilde{M}^{K,\tau}(p)$ plays the role, essentially, of $\tilde{c}^{+}(p)$. Out of this, one obtains $M^{P,\tau}(r)$ for the Klein-Gordon case as follows

$$M^{P-}(r) = (\mathrm{K}^{-}M^{K-})(r) = (\kappa^2 - \partial_q^2)M^{K-}(r)$$

$$= (2\pi)^{-1/2}\int_{-\infty}^{\infty} ds\,[\omega(s)]^2 \tilde{M}^{K-}(s)\,e^{irs}\ , \quad [\omega(s)]^2 = \kappa^2 + s^2\ . \tag{6.11a}$$

For the Helmholtz case, it is not K which acts on M^{K+} to produce M^{P+}, but the "absolute value of K" operator whose action is

$$M^{P+}(r) = (2\pi)^{-1/2}\left[\int_{-\kappa}^{\kappa} ds\,(\kappa^2 - s^2)\right.$$

$$\left. + \left(\int_{-\infty}^{-\kappa} \int_{\kappa}^{\infty}\right) ds\,(s^2 - \kappa^2)\right]\ \tilde{M}^{\kappa+}(s)\,e^{irs}$$

$$= (\mathrm{K}^{+}M^{\kappa+}_{<})(r) - (\mathrm{K}^{+}M^{\kappa+}_{>})(r)\ . \tag{6.11b}$$

In the last expression, $M^{K+}(r) = M^{K+}_{<}(r) + M^{K+}_{>}(r)$ is decomposed as a sum of two functions: $M^{K+}_{<}(r)$ whose Fourier transform has support on $(-\kappa, \kappa)$ and $M^{K+}_{>}(r)$ whose Fourier transform has support on the complement of that interval. We shall come back to (6.11) below.

Lastly, for the "angular-momentum-type" of C's we have the function $M^{A\tau}(r)$ in (5.15d), (5.17d) and (6.10). This is an arbitrary function: its Fourier transform $\tilde{M}^{A\tau}(s)$ is the product of $\omega(s)$ with an arbitrary function $\tilde{c}^{-}(s)$. As we pointed out for the finite-dimensional case, all $M^{\cdot\cdot}$ -functions must be *even* functions of their argument.

Regarding positivity, we note that $M^{K\tau}$ and $M^{P\tau}$ are for all cases positive definite i.e., for arbitrary $h(q)$,

$$\int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} dq' h(q)\,\tilde{M}^{\cdot\cdot}(q - q')\,h(q') \geqslant 0\ .$$

Not so $M^{A\tau}$. Indeed, as pointed out before, the corresponding "angular-momentum" invariant form is positive on the subspace of solutions $f(q, t)$ which contain only right-moving (i.e., positive-energy) solutions, and negative for the complement.

VI.4 Square-integrable solutions

Up to this point, then, we have translated the results for discrete finite systems to continuous non-compact ones. In doing so, we must be careful about quantities whose range becomes infinite. As in quantum mechanics, we may regard "good" initial conditions as those which are square-integrable and bounded at $t = 0$. Correspondingly, we shall be interested in invariant homogeneous sesquilinear forms (6.10) which are finite on this space of functions. The proper functions $M^{\cdot\cdot}(r)$ which define the forms must then be bounded integral kernels, and thus they or their Fourier transforms may include up to Dirac δ's. Since $M^{P\tau}$ is obtained from $M^{K\tau}$ through (6.11), we see that $M^{K\tau}(r)$ should be at least twice-differentiable. These appear to be all the restrictions, however.

VI.5 Poincaré and Euclidean invariance

Had we started out to find sesquilinear invariant forms for the continuum Klein-Gordon and Helmholtz equations, one obvious requirement would have been that they be invariant under the symmetry group of geometric transformations which leave the system invariant. For the Klein-Gordon equation we would require invariance under space translations and inversions, time translations and *Lorentz* transformations

$$q \mapsto q' = q\cosh\eta + t\sinh\eta\ , \tag{6.12a}$$

$$t \mapsto t' = q\sinh\eta + t\cosh\eta\ , \quad \eta \in \mathcal{R}\ . \tag{6.12b}$$

For the Helmholtz equation we also have space translations and inversions, time translations, but now also *rotations*

$$q \mapsto q' = q\cos\theta - t\sin\theta\ , \tag{6.13a}$$

$$t \mapsto t' = q\sin\theta + t\cos\theta\ , \quad \theta \in (-\pi, \pi]\ . \tag{6.13b}$$

The full group of geometric transformations in the two cases is that of the two-dimensional *Poincaré* and *Euclidean* invariances, respectively.

For the Helmholtz case this means that the double integration defining the sesquilinear form (6.10) can be performed over any line in the $q - t$ plane. For the Klein-Gordon case, we may relativistically "rotate" the line within the light cone containing the q-axis, as well as translating it in the same plane.

Now, invariance of the sesquilinear forms (6.10) under Lorentz or rotation transformations imply that

$$C_S^\tau(\mathsf{f}, \mathsf{R}^\tau \mathsf{g}) = -C_S^\tau(\mathsf{R}^\tau \mathsf{f}, \mathsf{g}) \ . \tag{6.18}$$

Through integration by parts we can bring the operator entries of R^τ to act on the components of the weight function matrix defining the form for any time t. If (6.18) is valid for all f and g in the spaces considered, the component functions in the metric matrix in (6.10) are subject to

$$(q - q')M^{A\tau}(q - q') = 0 \ , \tag{6.19a}$$

$$(\mathrm{A}^\tau - \mathrm{A}'^\tau)M^{A\tau}(q - q') = 0 \ , \tag{6.19b}$$

$$q'M^{P\tau}(q - q') = -\mathrm{A}^\tau M^{K\tau}(q - q') \ , \tag{6.19c}$$

$$qM^{P\tau}(q - q') = -\mathrm{A}'^\tau M^{K\tau}(q - q') \ , \tag{6.19d}$$

where

$$\mathrm{A}^\tau = -\frac{1}{2}\{\kappa^2 + \tau\partial_q^2 \ , \ q\}_+ \ , \quad \mathrm{A}'^\tau = -\frac{1}{2}\{\kappa^2 + \tau\partial_{q'}^2, q'\}_+ \ , \tag{6.19e}$$

plus boundary conditions which are zero for the spaces of functions where the $M^{\cdot\cdot}$ are bounded integral operator kernels, and $\|\mathsf{f}\|$, $f(q, t)$, etc., are finite, or such that the single integrals in (6.10) over the other's value at infinity, are zero.

VI.9 The Klein-Gordon sesquilinear invariant form

Eqs. (6.19a) and (6.19b) are solved by

$$M^{A\tau}(q - q') = c\delta(q - q') \ . \tag{6.20}$$

For solutions of the Klein-Gordon equation, the only angular-momentum-type of Poincaré invariant sesquilinar form is thus found from (6.20) and (6.10). It is

$$C_S^{A^-}(\mathsf{f}, \mathsf{g}) = i \int_{-\infty}^{\cdot} dq \, [f(q, t)^* g_t(q, t) - f_t(q, t)^* g(q, t)] \ , \tag{6.21}$$

where we have chosen $c = 2i$ for reality. We arrive thus at the well-known [11] expression for the inner product of two positive-energy Klein-Gordon amplitudes. We recall that (6.21) is positive only in that invariant energy (or right-travelling wave) region. The angular-momentum-type translation-invariant for the Helmholtz equation was seen to be unsuitable for Euclidean invariance, so no C_S^{A+} exists.

VI.10 Energy-type sesquilinear invariants

Now, as to the energy-type invariant obtained from $M^{K\tau}$ and $M^{P\tau}$, we must remember that they are also related through Eqs. (6.11). This supplements (6.19c-d) and requires that $M^{K\tau}(q - q')$ be a solution of either equation

$$[r\partial_r^2 + \partial_r - \kappa^2 r]M^{K-}(r) = 0 \quad \text{(Klein-Gordon)}, \tag{6.22a}$$

$$[r\partial_r^2 + \partial_r + \kappa^2 r]M_<^{K+}(r) = 0, \quad \partial_r M_>^{K+}(r) = 0 \quad \text{(Helmholtz)}. \tag{6.22b}$$

These are, respectively, modified Bessel and Macdonald functions, or Bessel and Neumann functions:

$$M^{K-}(r) = aI_0(\kappa r) + bK_0(\kappa r) \ , \tag{6.23a}$$

$$M_<^{K-}(r) = aJ_0(\kappa r) + bY_0(\kappa r) \ , \ M_>^{K+}(r) = c \ . \tag{6.23b}$$

Out of these and (6.11) we find

$$M^{P-}(r) = aI_1(\kappa r)/\kappa r - bK_1(\kappa r)/\kappa r \tag{6.24a}$$

$$M_<^{P+}(r) = aJ_1(\kappa r)/\kappa r + bY_1(\kappa r)/\kappa r \ , \quad M_>^{P+} = -\kappa^2 c \ . \tag{6.24b}$$

All functions, as expected, are even in their arguments.

For the Klein-Gordon case, this type of invariant (6.23a)-(6.24a) is unsuitable since K_0 and K_1 grow without bound at $r \to 0^+$ while I_0 and I_1 grow exponentially for large r. We conclude that no energy-type sesquilinear Poincaré invariant exists for the Klein-Gordon equation solutions, and that (6.21) represents the *only* sesquilinear Poincaré invariant form.

Asking for the invariance of the sesquilinear forms under these groups will yield essentially unique weight functions $M^{\tau\tau}(|q-q'|)$ in (6.10). Note that space inversion and translation is guaranteed by the dependence of $M^{\tau\tau}$ on the absolute value of the difference of the positions, while time invariance was used before in asking for the quantities to be conserved. So it is only Lorentz or rotation invariance (6.12)-(6.13) which may still be demanded. We shall see below that this leads to ordinary differential equations for $M^{K\tau}$ and for $M^{P\tau}$.

VI.6 Time inversions

For the Klein-Gordon equation, the time inversion exchanges positive- and negative-energy solutions, and hence changes the sign of the "angular-momentum" sesquilinear form obtained from the $M^{A\,-}$-terms. This behaviour is expected, so the time-inversion invariance of the equation does not apply to the subspace of physically significant solutions. Rather, the latter are physically significant precisely because the evolution equation does not mix them with the elements of other classes of "unphysical' solution spaces. This feature is one of the basic properties of the diagonal travelling-wave basis: time evolution keeps each wave evolving separately, and restrictions imposed on $\tilde{M}^{\tau\,-}(s)$ as to its support will be respected by the translation-inversion subgroup of the Poincaré group. This is in general not true for the Lorentz subgroup (6.12).

For the Helmholtz equation, time inversions also exchange right- and left-travelling wave subspaces, and consequently change the sign of the $M^{A\,+}$-terms. The difference now lies in the fact that time inversions- together with space inversions- lie in the rotation subgroup (6.13) for $\theta = \pi$. A rotation by that angle changes the sign of the purported $M^{A\,+}$-invariant, which can only qualify as an invariant, hence, if $M^{A\,+}(r) = 0$ in (6.10). Angular-momentum type invariant sesquilinear forms are thus excluded for the Helmholtz case on symmetry arguments alone.

VI.7 Exponential solutions

Note that Eqs. (6.13) for $\theta = \pi/2$ exchange the 'space' and 'time' variables q and t. Under this transformations, exponential solutions, be they increasing or decreasing in the 'old' positive-t direction, will turn into non-square-integrable functions of the 'new' q, which must range over the whole of $\mathcal{R}$ Exponential solutions are thus barred from having properly defined sesquilinear forms. Arbitrary solutions of the Helmholtz equation may be first subject to a projection operator which eliminates exponential solutions and leaves only the oscillatory ones, i.e., those constituted out of travelling waves for the range $p \in (-\kappa, \kappa)$. This in turn is achieved by letting $\tilde{M}^{K\,+}(p)$ have support on this interval. This correspondingly reduces $M^{P\,+}(r)$ in (6.11b) to the first integral term. [In the discrete system, Eq. (5.17a) is simplified to its first summation through $\tilde{c}^{(\sigma)}_{\ell} = 0$ for $|\ell| > m_c$ and similarly for (5.17b) and (5.17c).]

In short: For the Klein-Gordon case, $M^{K\,-}$ and $M^{A\,-}$ are still free, with the restriction to positive-energy solutions, while for the Helmholtz case, only $M^{K\,+}$ is free with the restriction to oscillatory solutions.

VI.8 Lorentz and rotation generators

The requirement of Lorentz or rotation invariance of the sesquilinear forms may be reduced to infinitesimal transformations [5] on the solution phase space (6.9) through the matrix operators

$$\mathsf{R}^{\tau} = \begin{pmatrix} -\tau t\partial_q & q \\ -\frac{1}{2}\{\mathsf{K}^{\tau}, q\}_{+} & -\tau t\partial_q \end{pmatrix} , \tag{6.14}$$

where $\tau = -1$ refers to the Klein-Gordon case and $\tau = +1$ to the Helmholtz case, K^{τ} is given in (6.8), q is the multiplication-by-argument operator and $\{\mathsf{A}, \mathsf{b}\}_{+} = \mathsf{AB} + \mathsf{BA}$ is the anticommutation of A and B.

The properties of R^{τ} under commutation with H^{τ} are

$$[\mathsf{H}^{\tau} - \partial_t, \mathsf{R}^{\tau}] = 0 , \tag{6.15}$$

which assures us that R^{τ} maps solutions of (6.9) into solutions of the same equation. The operator (6.14) has the usual action of Lorentz or rotation generators on functions on the $q-t$ plane. We also can form the Poincaré or Euclidean Lie algebra out of R^{τ}, H^{τ} and the generator of translations

$$\mathsf{S} = \begin{pmatrix} \partial_q & 0 \\ 0 & \partial_q \end{pmatrix} , \tag{6.16}$$

[which is the limit of $\mathsf{R} - 1$ as $N \to \infty$]. Indeed, the commutators are

$$[\mathsf{S}, \mathsf{H}^{\tau}] = 0 , \quad [\mathsf{R}^{\tau}, \mathsf{S}] = -\mathsf{H}^{\tau}, \quad [\mathsf{R}^{\tau}, \mathsf{H}^{\tau}] = \tau\mathsf{S} . \tag{6.17}$$

VI.11 The Helmholtz sesquilinear invariant form

We turn lastly to the Helmholtz equation. The two parts of $M^{K+}(r) = M^{K+}_{<}(r) + M^{K+}_{>}(r)$ satisfy different equations in (6.22b) due to the different signs they have in Eq. (6.11). The $M^{K+}_{<}(r)$ must have a Fourier transform with support on $(-\kappa, \kappa)$ and the $M^{K+}_{>}(r)$ on its complement. Bessel functions $J_\nu(\kappa r)/(\kappa r)^\nu$ satisfy the first requirement (Ref. 13, Eq. 3.753.2 for $\nu = 0$ and its derivative for $\nu = 1$), but the $Y_\nu(\kappa r)/(\kappa r)^\nu$ exhibit the second (Ref. 13, Eq. 3.753.4 for $\nu = 0$ and its derivative for $\nu = 1$). Only the Bessel function part can thus be present in the sesquilinear form.

The only positive Euclidean invariant sesquilinear form for the oscillatory Helmholtz equation solutions is thus

$$C^{E}_{S}{}^{+}(\mathsf{f}, \mathsf{g}) = \frac{1}{2}\int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} dq' \{f_t(q, t)^* J_0(\kappa[q - q'])g_t(q', t) + f(q, t)^*\left[J_1(\kappa[q-q'])/\kappa[q-q']\right] g(q', t)\} . \quad (6.25)$$

This result was found by Wolf [14] and Steinberg [15], but does not seem to have another precedent in the literature.

Finally, for the reasons given above, no energy-type invariant exists for exponential Helmholtz solutions. As a final verification of the correctness of (6.25) it should be noted that the only effect of finite Euclidean rotations on the solutions of the Helmholtz equation is to rotate the p — ω plane, the Fourier transform of the $q - t$ plane used here. As p and ω are constrained to lie on a circle $[\omega(p)]^2 = \kappa^2 - p^2$, oscillatory solutions $|p| < \kappa$ are mapped among themselves under the action of these finite transformations. Actually, if we establish a unitary mapping [5] between the oscillating solution space and the space of $\mathcal{L}^2$ functions on the circle S_1, the sesquilinear form (6.25) may be found simply through the Parseval relation from the usual $\mathcal{L}^2(S_1)$ rotation-invariant inner product [15] on S_1.

VI.12 Bilinear invariant forms

Regarding bilinear invariants, we pick up the results of Subsect. V.15 for the Klein-Gordon equation and those at the end of Subsect. V.16 for the Helmholtz case. We note that they reduce to the form (6.10), but without complex conjugation. For the Klein-Gordon case, all ensuing developments which ask for Lorentz invariance follow unchanged. We

arrive thus at a unique acceptable bilinear form, identical to Eq. (6.21), without complex conjugation (so the i can be removed). It is such, however, that $C^{A-}_{B}(\mathsf{f}, \mathsf{f}) = 0$ for all f.

The Helmholtz case also leads to (6.25), without complex conjugation, as the only acceptable form.

We have been interested in exploring Lie algebras of second- and higher-order differential operators, and their Lie groups of integral transforms. We can build an $SL(2, R)$ group through *deformation* of the geometric Poincaré and Euclidean groups seen here [5]. Clarifying the question of invariant sesquilinear forms is thus a step in setting up $SL(2, R)$ as a group of unitary integral transforms on two-component function spaces associated with partial differential equations of the Klein-Gordon and Helmholtz types.

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RESUMEN*

Se consideran sistemas discretos finitos, relacionados con las ecuaciones de diferencias-diferenciales de Klein-Gordon, de onda amortiguada y de Helmholtz. El operador de evolución de estos sistemas es diagonal en la base de ondas viajeras, donde las propiedades de simetría son evidentes. Se construye el conjunto completo de formas sesquilineales y bilineales invariantes en el tiempo, asociadas a un anillo factor del grupo de simetría del espacio fase. Este enfoque es equivalente a la

construcción de estas formas a partir del álgebra de Lie del grupo de simetría completo del sistema. Las constantes de movimiento asociadas tienen la estructura de energías y momentos angulares. Se examina la homogeneidad ante transformaciones geométricas (diedrales) e inversiones en el tiempo, así como sus propiedades de positividad. Finalmente, al permitir que los elementos del sistema tiendan a un continuo e imponiendo invariancia de Poincaré o euclidea, se obtienen productos internos positivos para el espacio de soluciones de energía positiva de Klein-Gordon y para el espacio de soluciones oscilatorias de Helmholtz.

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A comparison of *S*-matrix expansions for elastic potential scattering. An exactly solvable case

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Two different expansions of the scattering matrix, the direct Mittag-Leffler expansion and a Cauchy expansion involving the outgoing Green function of the problem, are applied to the problem of elastic scattering by a delta shell potential, which is exactly solvable and has resonances for *s*-wave. We study the energy region involving the first three resonances. The comparison favours the Cauchy expansion. The results show that unitarity is essentially preserved.

I. INTRODUCTION

It is well known that sharp resonances in scattering can be related to complex eigenfunctions and are associated with the presence of complex poles of the *S*-matrix of the system.

This has led to the idea of constructing formalisms which represent the scattering function as far as possible in terms of its poles and the complex or resonance states.

Along these lines one should mention the work by Hu [1], who obtained a representation of the *S*-matrix as an infinite product of its zeros and poles such that unitarity of S is preserved. However resonant states do not enter into the scheme.

In relation to expansions of S proper, in past years one finds a number of interesting works. In particular there is the work by Humblet [2] of 1952, who studied a Mittag-Leffler expansion of the scattering function. These early work led some years later, in 1961, to the formulation of a theory of nuclear reactions by Humblet and Rosenfeld [3], based also in a Mittag-Leffler expansion of the scattering or reaction amplitude.

One should also mention the work of 1959 by Peierls [4], who considered a representation of the scattering function via a Cauchy-type of expansion of the quantity $S(k) = e^{2ika}$ the exponential factor being introduced to avoid the divergence of $S(k)$ at large values of the complex mo-