Image methods for constructing Green's functions and eigenfunctions for domains with plane boundaries

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We consider the image problem for domains with plane boundaries. We list all three and two dimensional domains for which the image method yields solutions of the potential problem, and we describe the image arrays generated by these domains in familiar crystallographic terms. One obtains from the group–theoretic description of images two representations for the Dirichlet Green's functions for ∇^2. The first is obtained by summing the unrestricted Green's function over the crystal image structures, and the second is obtained in terms of an eigenfunction expansion using solutions of $\nabla^2\psi = \lambda\psi$ which vanish on the plane boundaries.

I. INTRODUCTION

If a point charge q is at some distance d from a grounded conducting plane, the boundary condition imposed by the plane on the resulting potential may be satisfied by replacing the plane with an "image charge" $-q$ located at a position which is the mirror image location of q. This type of solution was called the "method of images" by its inventor, Sir William Thomson,[1] and is illustrated in Fig. 1.

We have studied the general problem of a solution by images for a point charge in a domain bounded by several grounded conducting planes, with the unexpected result that we are able to list all such domains for which the image solution exists. The possible corners are limited to intersections of three planes and are well known in the theory of regular polyhedra. In each case, the set of image charges at such a corner forms a representation of a finite point group. Additional planes result in an infinite crystal structure of image charges in which the unit cell is the finite group of images at a corner. There are no domains whose boundary consists of more than six planes.

The existence of the group structure yields the surprise that one can determine complete systems of fundamental eigenfunctions of the Laplace operator ∇^2, i.e., solutions of $\nabla^2\psi = \lambda\psi$ which vanish on the boundaries. Moreover, the only classical cases are the eigenfunctions for the box, the square, and the three types of Lamé eigenfunctions.[2]

Given one of our domains there are two ways to represent a Green's function for it, i.e., the potential for a unit charge. One is a direct sum of multipoles determined by a unit cell of images, and the other is an eigenfunction expansion.

In Sec. II we deduce the allowed domains with plane boundaries. In Sec. III we summarize the group theory appropriate to the problem, and we show that reflections in a plane not containing the corner vertex generate an infinite crystal structure. In Sec. IV we show that the existence of the image solution for potentials and Green's functions follows directly from the group structure of the array of image charges. In Sec. V we calculate the image arrays for cylinders and prisms formed by terminating a cylinder with planes normal to the cylinder axis. In Sec. VI we consider the tetrahedral domains, which make essential demands on our group theoretic formalisms. In Sec. VII we consider the icosahedral Möbius corner. In Sec. VIII we display a general formula for eigenfunctions of image domains and we devise a completeness proof. In Sec. IX, X, and XI we display explicit eigenfunctions as well as the Green's function expansions for the more interesting image domains.

In an earlier publication[3] we illustrated the details of some constructions and announced some of our principal results.

II. IMAGE DOMAINS WITH PLANE BOUNDARIES

The image solution exists if the potential of the original charge and its images vanishes on each conducting boundary plane, and no proper image lies in the domain bounded by the conducting planes. We first consider the wedge formed by two intersecting planes, where it is well known that the necessary and sufficient condition for existence of an image solution is that the wedge angle is π/n, with n an integer greater than 1. For a domain bounded by more than two planes, it remains a necessary condition that each pair of intersecting planes meets at π/n. We proceed to find all domains bounded by planes which satisfy this necessary constraint. In succeeding sections we show that this necessary condition is sufficient by constructing the space group that generates the image charge array. This group determines the images completely. Thus existence of the domains we seek

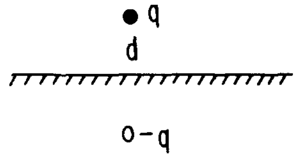

FIG. 1. *Single Plane*. Light and dark circles are charges of opposite sign.

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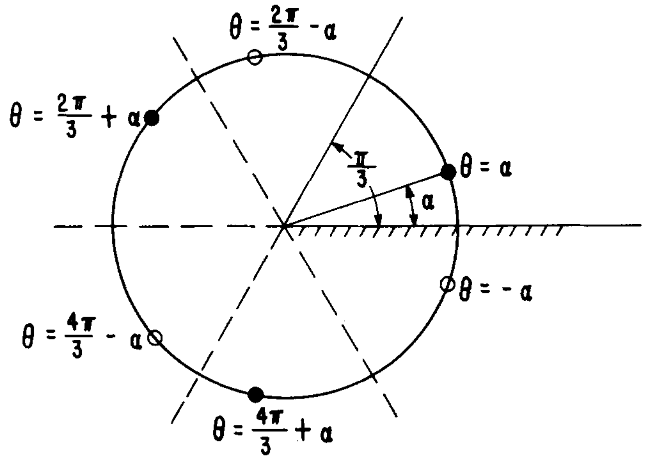


FIG. 2. *The* $\pi/3$*–Wedge*. The array generated is represented by dark and light circles (charges of opposite sign).

will follow from the group structure of the image array. A general domain for which the image method works is called an *image domain*.

A. Intersection of Two Planes

Many texts[4] apply the method of images to a point charge placed between a pair of intersecting planes, where it is easy to show that the image solution exists if and only if the angle between the planes in π/n, with n an integer greater than 1. If n is an integer, there are $2n-1$ image charges as shown in Fig. 2. If n is not an integer, the successive reflections needed to satisfy the boundary condition $V=0$ produce images which lie in the domain $0\leqslant\theta\leqslant\pi/n$. We refer to the domain bounded by planes at an angle π/n as a π/n *wedge*. The case of two parallel planes may be considered as the limit $n\rightarrow\infty$, in which case the number of image charges is infinite.[5] A single plane may be considered as the special case $n=1$.

B. Open Cylinders

Since the interior angles of a polygon with n sides add up to $(n-2)\pi$, the only possible cylindrical cross sections are triangles with angles $(\pi/3|\pi/3|\pi/3)$, $(\pi/2|\pi/4|\pi/4)$, $(\pi/2|\pi/3|\pi/6)$, the rectangle $(\pi/2|\pi/2|\pi/2|\pi/2)$, and an open figure $(\pi/2|\pi/2|0)$, in which two sides meet at infinity. The cylinders are shown in Fig. 4.

C. Corners

If a corner of n planes has its apex at the center of a sphere, the intersection angles between planes are seen to be the interior angles at the corners of a spherical polygon. For a spherical polygon, the sum Σ of the interior angles satisfies $(n-2)\pi<\Sigma<(n+2)\pi$. Simple enumeration shows that the only possible corners have three planes with angles $(\pi/2|\pi/2|\pi/n)$, $(\pi/2|\pi/3|\pi/3)$, $(\pi/2|\pi/3|\pi/4)$, $(\pi/2|\pi/3|\pi/5)$. The spherical triangles associated with such corners are known in the theory of regular polyhedra as the *Möbius triangles*. We shall call such corners *Möbius corners*.

We also note that since the interior angles of an n–sided plane polygon add up to $(n-2)\pi$, the faces of a closed domain with the above corners must be triangles or rectangles.

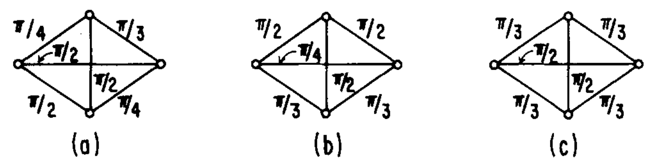


FIG. 3. *Angles*. Angles of intersection for the admissible bounded four sided image domains. With terminology from VI one has: (a) primitive octahedral domain, (b) centered octahedral domain, and (c) large tetrahedral domain.

D. Other Open Domains

With the limitation to corners listed in (C), the only other open domains are cylinders from (B) terminated at one end by a plane perpendicular to the cylinder axis, and a wedge of two planes at an angle π/n intersected by two parallel planes having the π/n intersection as a normal. We find these by the enumeration described in part (E).

E. Closed Domains—4 Faces

Four planes intersect in six lines, each of which is shared by two faces. The only domains are thus tetrahedra with triangular faces. We find the allowed domains by a simple enumeration which consists of taking each corner from (C), intersecting the surfaces with a plane which makes one allowed corner, and then testing the remaining corners. Only three basic tetrahedra emerge. They are described in Fig. 3 by the topology of the corner angles. Fig. 5 shows their con-

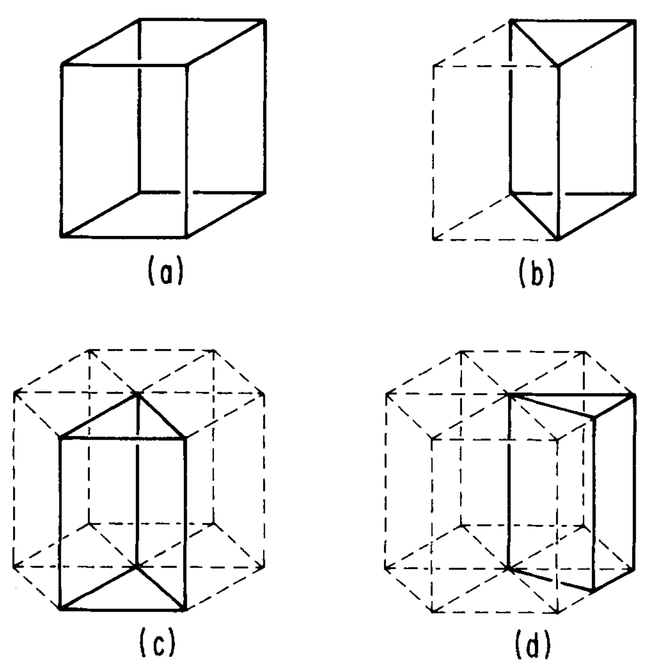


FIG. 4. *Geometric Types*. The bounded prismatic image domains are: (a) rectangular orthohombic domain, (b) $(\pi/2|\pi/4|\pi/4)$–triangular domain, (c) $(\pi/3|\pi/3|\pi/3)$–triangular domain, and (d) $(\pi/2|\pi/3|\pi/6)$–triangular domain.

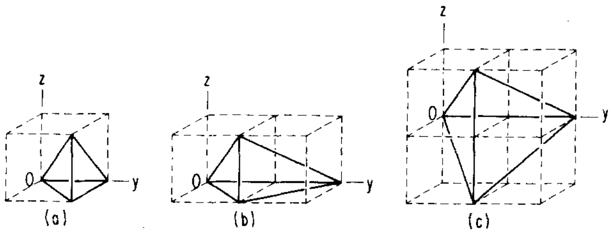


FIG. 5. *Geometric Types.* Cubic constructions show the relationship between the three distinct types of bounded four-sided image domains. Depicted are: (a) primitive octahedral domain, (b) centered octahedral domain, and (c) large tetrahedral domain.

struction by sectioning a cube. We can also arrive at these domains using Descartes' theorem in part (G).

F. Closed Domains—5 Faces

There are no five-sided domains in which each face intersects all the other faces. This would produce 10 lines of intersection; since the number of corners is integer and 2/3 the number of lines, this is impossible. If two planes do not intersect in the surface, this gives 9 lines of intersection which must be the edges of two triangles and three rectangles. The only such domains are the triangular cylinders of part (B) intersected by a pair of parallel planes normal to the cylinder axis. See Fig. 4.

G. Closed Domains—6 or More Faces

Since all planes meet at angles less than π, they form only convex polyhedra. If

$C =$ number of corners,

$E =$ number of edges,

$F =$ number of faces,

Euler's theorem states

$$C + F - E = 2.$$

Since all corners are formed from 3 edges, it follows that $2E = 3C$. Hence

$$C = 2F - 4.$$

Thus, a figure of 6 faces has 8 corners. The sum of the plane angles at a corner is less than 2π. The difference is called the *angular defect*; the corner $(\pi/2|\pi/2|\pi/2)$ has the smallest angular defect, which is $\pi/2$. A theorem of Decartes which can easily be derived from Euler's theorem,[3,6] states that the angular defects sum to 4π for the corners of a convex polyhedron. Hence, we have $C \leqslant 8$, or from Euler's theorem $F \leqslant 6$. For $F = 6$, all corners must be $(\pi/2|\pi/2|\pi/2)$ and the figure is a rectangular parallelipeped. Descartes' theorem, with the condition that an edge angle is shared by two adjacent corners, may be used to derive the results of parts (E) and (F).

The above domains were found by imposing the necessary condition that the angle between any two intersecting planes is π/n. We need to show that the image arrays created by our admissible domains do not contain additional image points which lie inside these domains. We also need to demonstrate that the potential and Green's functions that arise vanish on all the boundaries. As is shown in the following sections, each of the above domains satisfies these conditions. Our necessary condition for a region to be an image domain is thus also sufficient.

III. GROUP THEORY

In order to describe the crystal structures of images, we are fortunate in having at our disposal the language of groups as they occur in solid–state theory and crystallography. In this section we shall recall and elaborate on the necessary group-theoretical formalisms, but for a detailed elementary description of groups we shall refer the reader elsewhere.[7,8,9]

If **G** is a group and **H** and **K** are subgroups, then one defines $\mathbf{HK} = \{\mu\lambda \,|\mu\in\mathbf{H}, \lambda\in\mathbf{K}\}$. If $\mathbf{G} = \mathbf{HK}$ and the subgroups **H** and **K** have only the identity element in common the $\mathbf{G} = \mathbf{HK}$ will be called a *product decomposition*. If $\mathbf{G} = \mathbf{HK}$ is a product decomposition and $\mu\lambda = \lambda\mu$ for all $\mu\in\mathbf{H}$ and all $\lambda\in\mathbf{K}$, then $\mathbf{G} = \mathbf{HK}$ will be called a *direct product decomposition*.

In general, for arbitrary subroups **H** and **K** of **G**, the set $\mathbf{S} = \mathbf{HK}$ will not be a subgroup of **G**. One says that **H** is *normal* (or *invariant*) with respect to **K** if $x^{-1}\mathbf{H}x \subset \mathbf{H}$ for all $x\in\mathbf{K}$. If **H** and **K** are subgroups of **G** and if **H** is normal with respect to **K** then $\mathbf{S} = \mathbf{HK} = \mathbf{KH}$ is a subgroup of **G**. The normality condition is useful for constructing groups, but it should be noted that $\mathbf{S} = \mathbf{HK}$ can be a group without the normality condition. A necessary and sufficient condition for $\mathbf{S} = \mathbf{HK}$ to be a group is that $\mathbf{HK} = \mathbf{KH}$. For a finite group **H**, the number of elements of in **H**, denoted by $n_\mathbf{H}$, is called the *order* of **H**. If $\mathbf{S} = \mathbf{HK}$ is a product decomposition then $n_\mathbf{S} = n_\mathbf{H} n_\mathbf{K}$.

Let **E** be a vector space with inner product $\langle\mathbf{x}|\mathbf{y}\rangle$. A reflection with respect to a plane through the origin is given by the formula

$$\lambda\mathbf{x} = \mathbf{x} - 2\mathbf{a}\langle\mathbf{x}|\mathbf{a}\rangle/\langle\mathbf{a}|\mathbf{a}\rangle \quad (\mathbf{a}\in\mathbf{E}, \mathbf{x}\in\mathbf{E}). \tag{1}$$

The vector **a** is said to be *normal* to the plane which determines λ.

In three dimensions one has the matrix representation

$$\lambda = \begin{bmatrix} 1-2a^2 & -2ab & -2ac \\ -2ab & 1-2b^2 & -2bc \\ -2ac & -2bc & 1-2c^2 \end{bmatrix} \tag{2}$$

when the normal (a,b,c) satisfies $a^2 + b^2 + c^2 = 1$.

For any reflection λ one has the determinant relation $\det(\lambda) = -1$. The *orthogonal group* $\mathrm{O}(n)$ for the vector space **E** is defined to be the set of all linear transformations σ on **E** which leave the inner product invariant, i.e., $\langle\sigma\mathbf{x}|\sigma\mathbf{y}\rangle = \langle\mathbf{x}|\mathbf{y}\rangle$ for all $\mathbf{x},\mathbf{y}\in\mathbf{E}$. It follows that every group generated by reflections in planes through the origin is a subgroup of $\mathrm{O}(n)$.

Two reflections $\lambda\mathbf{x} = \mathbf{x} - 2\mathbf{a}\langle\mathbf{x}|\mathbf{a}\rangle/\langle\mathbf{a}|\mathbf{a}\rangle$ and $\mu\mathbf{x} = \mathbf{x} - 2\mathbf{b}\langle\mathbf{x}|\mathbf{b}\rangle/\langle\mathbf{b}|\mathbf{b}\rangle$ commute if and only if $\langle\mathbf{a}|\mathbf{b}\rangle = 0$ or $\mathbf{a}\times\mathbf{b} = 0$. One infers this from the commutator relation

$$(\lambda\mu - \mu\lambda)\mathbf{x} = 4\langle\mathbf{a}|\mathbf{b}\rangle(\mathbf{x}\times(\mathbf{a}\times\mathbf{b})). \tag{3}$$

Two reflection λ and μ are *perpendicular* if $\langle\mathbf{a}|\mathbf{b}\rangle = 0$ holds for their normals. We have shown a reflection commutes with any perpendicular reflection and itself.

The Möbius corner $(\pi/2|\pi/2|\pi/n)$. For such a Möbius corner one reflection λ is perpendicular to the other two. If **D** is the order-two group generated by λ, and **H** is the group generated by the other two reflections, then perpendicularity implies that $\mathbf{S} = \mathbf{DH}$ is a group and a direct product. In the Schoenflies notation the group **S** is called a *dihedral* group and is denoted by the symbol $\mathbf{D}_{nh}$.

Generation of space groups. A set **L** in a vector space **E** is a *lattice* if **L** contains a set of linearly independent vectors such that every element of **L** can be expressed as an integral combination of these elements. The basis vectors will be called *primitive translation vectors*. The parallelepiped spanned by a set of such vectors is called a *primitive cell*.

The group of integers **Z** is a one-dimensional lattice in the space of real numbers. Henceforth, the space **E** will be a real three-dimensional space, even though this assumption is not formally necessary in this section.

Let **S** be a finite group generated by reflections with respect to planes containing the origin. If we adjoin to **S** a number of reflections with respect to planes not containing the origin, then the group thus generated will be called a *space group*. While the images of a point under **S** will be restricted to the surface of a sphere, the images under the space group can lie infinitely far from the origin.

Hypothesis I. We shall not add to **S** an arbitrary reflection. It is assumed that ξ is a reflection and that the related transformation $\lambda\mathbf{x} = \xi\mathbf{x} - \xi\,\mathbf{O}$, which defines a reflection λ with respect to a plane containing the origin, is an element of the group **S**.

Given this hypothesis about ξ, one writes $\mathbf{a} = \xi\,\mathbf{O}$ and thus ξ is expressible in the form $\xi\mathbf{x} = \lambda\mathbf{x} + \mathbf{a}$ with $\lambda\mathbf{a} = -\mathbf{a}$. Given a point **x** we are now interested in determing all images of **x** under the space group **G** generated by the finite group **S**.

Given $\sigma\in\mathbf{S}$ we now consider a transformation $\mu = \sigma\xi\lambda\sigma^{-1}$. One has $\mu\mathbf{x} = \mathbf{x} + \sigma\mathbf{a}$ and thus μ acts as a *raising operator*. Clearly μ is an element of the space group **G**. One has $\mu^{-1}\mathbf{x} = \mathbf{x} - \sigma\mathbf{a}$ and thus μ^{-1} acts as a *lowering operator*. It follows that $\mu^k\mathbf{x} = \mathbf{x} + k\sigma\mathbf{a}$ is an image of **x** for any integer $k\in\mathbf{Z}$. Let **L** be the integral span of $\{\sigma a|\sigma\in\mathbf{S}\}$.

The pair (**S**,**L**) can now be given a group structure by defining $(\sigma,\mathbf{n})\in(\mathbf{S},\mathbf{L})$ to be a transformation with action

$$(\sigma,\mathbf{n})\mathbf{x} = \sigma\mathbf{x} + \mathbf{n}. \tag{4}$$

The multiplication in (**S**,**L**) is defined by composition of transformations and has the formula

$$(\lambda,\mathbf{n})(\mu,\mathbf{m}) = (\lambda\mu,\lambda\mathbf{m} + \mathbf{n}), \tag{5}$$

and in the context of lattices is called *Seitz* multiplication

It may now be observed that **L** is invariant under **S** and ξ. It follows that all images of **x** under the space group **G** are of the form $(\sigma,\mathbf{n})\mathbf{x} = \sigma\mathbf{x} + \mathbf{n}$ with $\sigma\in\mathbf{S}$ and $\mathbf{n}\in\mathbf{L}$. Indeed, **G** and (**S**,**L**) can be isomorphically identified by assigning ξ to $(\lambda,\mathbf{a})$ and $\sigma\in\mathbf{S}$ to $(\sigma,\mathbf{O})$.

Our notation would suggest that **L** always has the structure of a lattice, but this need not be the case. For example, it is easy to see that the set of real numbers $\{n\sqrt{2} + m|n,m\in\mathbf{Z}\}$ can not be expressed in terms of integral multiples of a single generator.

Hypothesis II. The second hypothesis is that $\{\sigma\mathbf{a}|\sigma\in\mathbf{S}\}$ contains independent vectors such that every other vector in $\{\sigma\mathbf{a}|\sigma\in\mathbf{S}\}$ can be expressed as an integral combination of these vectors.

Under the second hypothesis the set **L** is a lattice.

In order to adjoin to **S** simulataneously two reflections ξ and ξ', it will be assumed that both satisfy Hypothesis I. One sets $\mathbf{a} = \xi\,\mathbf{O}$ and $\mathbf{a}' = \xi'\mathbf{O}$ and one defines **L** to be the integral span of the sets $\{\sigma\mathbf{a}|\sigma\in\mathbf{S}\}\cup\{\sigma\mathbf{a}'|\sigma\in\mathbf{S}\}$. If this larger integral span satisfies Hypothesis II then **L** is a lattice and (**S**,**L**) is the space group generated by $\{\mathbf{S},\xi,\xi'\}$. In this manner, any number of suitable reflections can be adjoined to **S**.

On the assumption that the space group (**S**,**L**) is determined by a lattice, our group (**S**,**L**) will be a space group in the crystalographic sense.[7] The only situation of interest in our theory and in electrostatics is the case where **L** is a Bravais lattice.

IV. IMAGE CRYSTAL STRUCTURES

The images of a point in suitable domains formed from planes form crystal structures in the abstract sense. We shall give an overview of this approach.

Space groups for image domains. One associates a space group to any domain **V** formed by plane surfaces by considering the group **G** generated by reflections with respect to the bounding planes.

If for every $g\in\mathbf{G}$ distinct from the identity and for every $\mathbf{x}\in\mathbf{V}$ the image $g\mathbf{x}$ lies outside of **V**, then **V** is an *image domain*. The group theory section shows that one should be able to represent the space group **G** in the form (**S**,**L**), where **S** is a finite group of reflections and **L** is the lattice which arises through the extension process. However, the fact that **L** is a lattice does not follow from general considerations and needs to be verified through explicit computation. Moreover, it turns out that the proper corner to choose for the generation of **S** is the sharpest corner of the domain. The resulting accounting of images will allow one to deduce that all the domains described in the first section are image domains.

Potentials for image domains. Let **V** be a corner domain or a wedge domain. Let **S** be the associated group of reflections. If a unit charge is placed at $\mathbf{x}\in\mathbf{V}$ then the potential is given by

$$\phi(\mathbf{u}) = \sum_{\sigma\in\mathbf{S}} \det(\sigma)\|\sigma\mathbf{x} - \mathbf{u}\|^{-1}. \tag{6}$$

Let **V** be a general image domain with space group (**S**,**L**). The potential for **V** is then given by

$$\Phi(\mathbf{u}) = \sum_{\mathbf{n}\in\mathbf{L}} \phi(\mathbf{n} + \mathbf{u}), \tag{7}$$

where $\phi(\mathbf{u})$ is the *corner potential* defined by (6). It is a consequence of Seitz multiplication (5) that the sign of the image charge at $(\sigma,\mathbf{n})\mathbf{x}$ is specified by the determinant of σ. When the monopole, dipole or quadrupole moments of the charge distribution $\{\det(\sigma),\sigma\mathbf{x}|\sigma\in\mathbf{S}\}$ vanish, then $\phi(\mathbf{u})$ tends to zero rapidly as **u** gets large. This circumstance allows one to assert that (7) converges absolutely. The explicit determinations of (S,L) will allow one to see this with complete rigor.

The potential satisfies the transformation property

$$\Phi\,((\sigma,\mathbf{n})\mathbf{u}) = \det(\sigma)\Phi\,(\mathbf{u}) \tag{8}$$

for an arbitrary $(\sigma,\mathbf{n})\in(\mathbf{S},\mathbf{L})$.

Vanishing of the potential. One has that $\Phi\,(\mathbf{u}) = 0$ when $\mathbf{u}$ lies on the boundary of $\mathbf{V}$.

The assertion is easily proved. When $\mathbf{u}$ lies on the boundary of $\mathbf{V}$ then $(\sigma,\mathbf{n})\mathbf{u} = \mathbf{u}$, for $(\sigma,\mathbf{n})$ the reflection with respect to the boundary plane containing $\mathbf{u}$. For a reflection one has $\det(\sigma) = -1$. One now computes that $\Phi\,(\mathbf{u}) = \Phi\,((\sigma,\mathbf{n})\mathbf{u}) = -\Phi\,(\mathbf{u})$. Thus $\Phi\,(\mathbf{u}) = 0$.

Interchange of summation and differentiation. One can prove mathematically that if $\mathbf{D}$ is any differential operator with respect to $\mathbf{u}$ then

$$\mathbf{D}\Phi\,(\mathbf{u}) = \sum_{\mathbf{n}\in\mathbf{L}} \mathbf{D}\phi\,(\mathbf{n}+\mathbf{u}) \tag{9}$$

and the derived series converges absolutely.

The differentiation interchange implies that $\Phi\,(\mathbf{u})$ satisfies the Laplace equation

$$\nabla^2\Phi\,(\mathbf{u}) = -4\pi\delta\,(\mathbf{x}-\mathbf{u}), \tag{10}$$

where δ is the Dirac delta function and ∇^2 is the Laplace operator with respect to $\mathbf{u}$.

Interchange of summation and integration. This interchange is not always valid. It is worthwhile recalling the hypotheses for integration and summation interchange. If for a convergent series $\Sigma\phi_n$ of integrable functions the series $\Sigma \int |\phi_n|$ converges, then the interchange $\int \Sigma\, \phi_n = \Sigma \int \phi_n$ is valid. The example we mention is a rare instance where this interchange is not possible and where the problem arises in a natural context.

We shall consider the potential for parallel plates. The function $\|(x-u,y-v,z-w)\|^{-1}$ is the *unrestricted potential* for all space. The difference

$$\phi\,(u,v,w) = \|(x-u,y-v,z-w)\|^{-1} - \|(-x-u,y-v,z-w)\|^{-1}$$

is a special case of the group sum (7). The lattice sum

$$\Phi\,(u,v,w) = \sum_{n\in\mathbf{Z}} \phi\,(2n+u,v,w) \tag{11}$$

is an absolutely convergent series and represents the potential due to a unit charge at (x,y,z) between two conducting parallel plates at $x=0$ and $x=1$. The derived series

$$\frac{\partial\Phi}{\partial u} = \sum_{n\in\mathbf{Z}} \frac{\partial\phi}{\partial u}$$

is also seen to be absolutely convergent. However, if one now considers the surface integral over the whole infinite plane at $x=0$, then term by term integration (up to factor of 2π) yields

$$2(1-x) = \cdots + (-1+1) + (1+1) + (1-1) + \cdots = 2, \tag{12}$$

where the left-hand side is obtained from the correct total charge computation of Zahn,[5] Schockley,[10] and Kittel and Fong.[11] Despite assertions to the contrary by Pleines and Mahajan,[12] there exists no physically meaningful rearrangement of parentheses which will make (12) an identity. In this regard we also note the discussion of Epstein and Smith.[13] In Terras[14] the "method of theta functions" is applied to the parallel plate problem.

V. CYLINDERS AND PRISMS

In this section we will derive the space groups for the admissible cylinders and prisms. This computation will demonstrate that these figures are indeed image domains. If $\mathbf{S} = \mathbf{HK}$ is a product decomposition of a point group then

$$\sum_{\sigma\in S} \det(\sigma) f(\sigma\mathbf{x}) = \sum_{\lambda\in\mathbf{H}} \det(\lambda) \sum_{\mu\in\mathbf{K}} \det(\mu) f(\mu\lambda\mathbf{x}). \tag{13}$$

This decomposition of a group sum underlies our formulas for normal modes. Use of this method to construct efficient codings for potentials is illustrated by (31) and (36). It is for these reasons that in our listings we give point groups in product form, but we also identify these groups with the point groups of crystallography in Schoenflies notation.[7]

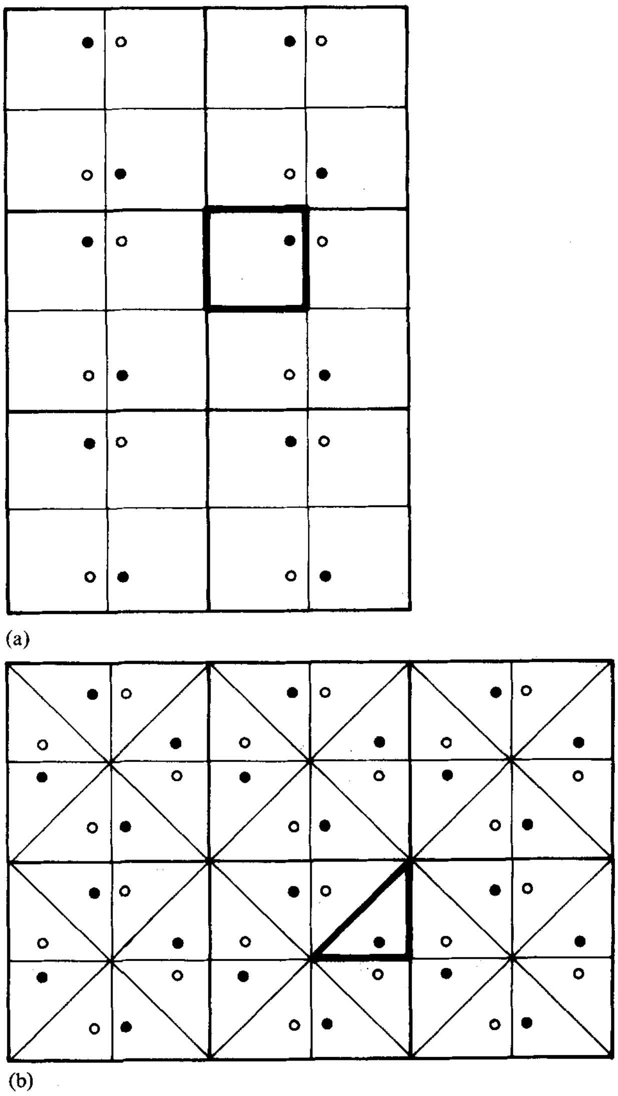


FIG. 6. *Crystal Structure.* (a) A charge in the dark rectangle generates a cluster which is replicated by a rectangular Bravais lattice; (b) a charge in a $(\pi/2|\pi/4|\pi/4)$–triangle generates a cluster which is also replicated by a rectangular Bravais lattice.

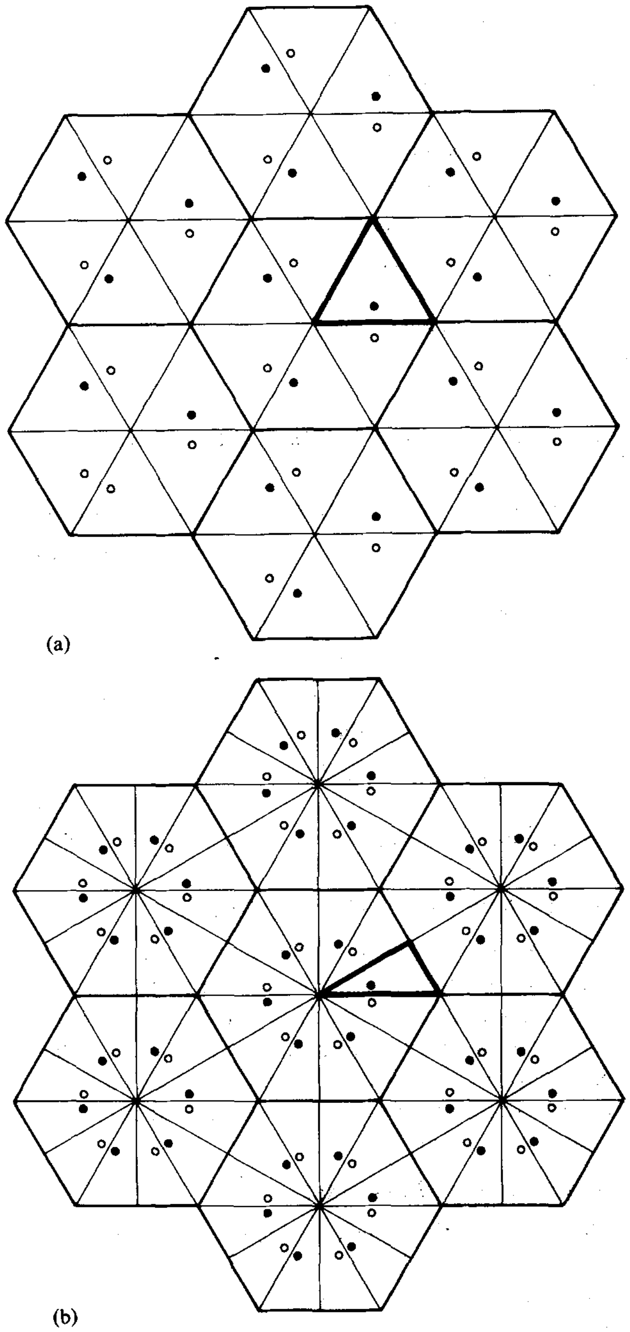


FIG. 7. *Crystal Structure.* (a) A charge in the dark $(\pi/3|\pi/3|\pi/3)$–triangle leads to a hexagonal Bravais lattice; (b) a charge in a $(\pi/2|\pi/3|\pi/6)$–triangle also leads to a hexagonal Bravais lattice.

A. Rectangular and $(\pi/4|\pi/4|\pi/2)$ triangular cross sections

The following notation for matrix generators of reflection groups will be used in this section:

$$\lambda = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \mu = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
$$\eta = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \nu = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{14}$$

1. *The open rectangular cylinder* $\mathbf{V} = \{(x,y,z)/0 \leqslant x \leqslant a, 0 \leqslant y \leqslant b\}$.

The bounding planes through the origin determine reflections λ and μ, and generate the point group

$$\mathbf{S} = \{1,\lambda\}\{1,\mu\} = \{1,\lambda,\mu,\lambda\mu\}, \text{ (Schoenflies } C_{2v}) \tag{15}$$

which we term the *square corner group*. The cylinder is then seen to have space group $(\mathbf{S},\mathbf{L})$, where

$$\mathbf{L} = \{(2am,2bn,0)|m,n\in\mathbf{Z}\}, \tag{16}$$

which is a *rectangular* Bravais lattice. The crystal structure generated by this space group is depicted in Fig. 6(a).

In terms of the unrestricted potential, formula (6) translates into the formulas

$$\begin{aligned}\phi(u,v,w) &= \sum_{\delta\in\mathbf{S}} \det(\sigma)\|\sigma(x,y,z) - (u,v,w)\|^{-1} \\ &= \|(x,y,z) - (u,v,w)\|^{-1} - \|(-x,y,z) - (u,v,w)\|^{-1}. \\ &\quad + \|(-x,-y,z) - (u,v,w)\|^{-1} \\ &\quad - \|(x,-y,z) - (u,v,w)\|^{-1}.\end{aligned} \tag{17}$$

It is easy to see that this is the potential due to a quadrupole and goes to zero as $\|(u,v,w)\|^{-3}$. It follows that

$$\Phi(u,v,w) = \sum_{m\in\mathbf{Z}} \sum_{n\in\mathbf{Z}} \phi(2am + u, 2bn + v, w)$$

converges absolutely. Such a verification would have to be made for every explicit realization of (6) in order to substantiate our claim regarding absolute convergence, but we will leave the remaining verifications for the reader. It is worth noting that we had good success in computer evaluation of this and other lattice sums due to additional cancellation which occurs when summation is carried out over blocks of indices that are invariant under the point group action.

We tabularize the remaining space groups with sparse detail. The data presented is needed to parametrize the normal modes discussed in Sec. VIII. The computations need to be performed in order to finish the formal proof that our admissible regions are indeed image domains as defined in Sec. I.

One should note that the domains are all oriented in such a manner that the sharpest corner is at the origin. The generators of the point groups are the reflections in the bounding planes through the origin. The lattice is generated by the adjoining to the point group the remaining reflections in the bounding planes, through the group extension process described in Sec. III. The geometric constructions of image arrays in Figs. 6 and 7 may be used to good advantage in checking our data.

2. *The closed cylinder* $V = \{(x,y,z)/0 \leqslant x \leqslant a, 0 \leqslant y \leqslant b, 0 \leqslant z\}$.

Generators: λ, μ, η;

$$\mathbf{S} = \{1,\lambda\}\{1,\mu\}\{1,\eta\} \quad \text{(Schoenflies } D_{2h}), \qquad \mathbf{L} = \{(2am,2bn,0)|m,n\in\mathbf{Z}\} \quad \text{[see Fig. 6(a)]}. \tag{18}$$

We shall refer to the frequently occurring point group $\mathbf{S}$ as the *cube corner group*.

3. The rectangular box $V = \{(x,y,z)/0<x\leqslant a,\ 0<y<b,\ 0\leqslant z\leqslant c\}$.

Generators: λ, μ, η;

$$\mathbf{S} = \{1,\lambda\}\{1,\mu\}\{1,\eta\},$$
$$\mathbf{L} = \{(2ak,2bm,2cn)|k,m,n\in\mathbf{Z}\}. \tag{19}$$

4. The $(\pi/2|\pi/4|\pi/4)$ cylinder $V = \{(x,y,z)/0\leqslant y\leqslant x\leqslant a\}$.

Generators: μ, ν; Relations: $\lambda = \nu\mu\nu$

$$\mathbf{S} = \{1,\lambda\}\{1,\mu\}\{1,\nu\} \quad (\text{Schoenflies } C_{4v}),$$
$$\mathbf{L} = \{(2am,2an,0)|m,n\in\mathbf{Z}\} \quad (\text{see Fig. 6(b)}. \tag{20}$$

5. The closed $(\pi/2|\pi/4|\pi/4)$ cylinder $V = \{(x,y,z)/0\leqslant y\leqslant x\leqslant a,\ 0\leqslant z\}$.

Generators: μ, ν, η; Relations: $\lambda = \nu\mu\nu$;

$$\mathbf{S} = \{1,\lambda\}\{1,\mu\}\{1,\nu\}\{1,\eta\} \quad (\text{Schoenflies } D_{4h}),$$
$$\mathbf{L} = \{2am,2an,0)|m,n\in\mathbf{Z}\}. \tag{21}$$

6. The $(\pi/2|\pi/4|\pi/4)$ prism $V = \{(x,y,z)/0\leqslant y\leqslant x\leqslant a,\ 0\leqslant z\leqslant c\}$.

Generators: μ, ν, η Relations: $\lambda = \nu\mu\nu$;

$$\mathbf{S} = \{1,\lambda\}\{1,\mu\}\{1,\nu\}\{1,\eta\},$$
$$\mathbf{L} = \{(2ak,2am,2cn)|k,m,n\in\mathbf{Z}\}. \tag{22}$$

B. Triangular $(\pi/3|\pi/3|\pi/3)$ and $(\pi/2|\pi/3|\pi/6)$ cylinders and prisms

We shall consider the additional matrix generators:

$$\kappa = \begin{bmatrix} 1/2 & \sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \gamma = \begin{bmatrix} -1/2 & \sqrt{3}/2 & 0 \\ \sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{23}$$

1. The open $\pi/3$ cylinder $V = \{(x,y,z)/0\leqslant y/\sqrt{3}\leqslant x,\ y\leqslant(a-x)\sqrt{3}\}$.

Generators: μ, γ;

$$\mathbf{S} = \{1,\mu\gamma,\gamma\mu\}\{1,\mu\} \quad (\text{Schoenflies } C_{3v}),$$
$$\mathbf{L} = \{(3a(n+m)/2,\sqrt{3}a(n-m)/2,0)|k,m,n\in\mathbf{Z}\} \tag{24}$$
[see Fig. 7(a)].

2. The closed $\pi/3$ cylinder $V = \{(x,y,z)/0\leqslant y/\sqrt{3}\leqslant x,\ y\leqslant(a-x)\sqrt{3},\ 0\leqslant z\}$.

Generators: μ, γ, η;

$$\mathbf{S} = \{1,\mu\gamma,\gamma\mu\}\{1,\mu\}\{1,\eta\} \quad (\text{Schoenflies } D_{3h}),$$
$$\mathbf{L} = \{(3a(n+m)/2,\sqrt{3}a(n-m)/2,0)|m,n\in\mathbf{Z}\}. \tag{25}$$

3. The prism $V = \{(x,y,z)/0\leqslant y/\sqrt{3}\leqslant x,\ y\leqslant(a-x)\sqrt{3},\ 0\leqslant z\leqslant c\}$.

Generators: μ, γ, η;

$$\mathbf{S} = \{1,\mu\gamma,\gamma\mu\}\{1,\mu\}\{1,\eta\},$$
$$\mathbf{L} = \{(3a(n+m)/2,\sqrt{3}a(n-m)/2,2kc)|k,m,n\in\mathbf{Z}\}. \tag{26}$$

4. The open $\pi/6$ cylinder $V = \{(x,y,z)/0\leqslant\sqrt{3}y\leqslant x,\ y\leqslant(a-x)\sqrt{3}\}$.

Generators: κ, μ; Relations: $\gamma = \kappa\mu\kappa$, $\lambda = \kappa\mu\kappa\mu\kappa$;

$$\mathbf{S} = \{1,\mu\gamma,\gamma\mu\}\{1,\mu\}\{1,\lambda\} \quad (\text{Schoenflies } C_{6v}),$$
$$\mathbf{L} = \{(3a(n+m)/2,\sqrt{3}a(n-m)/2,0)|m,n\in\mathbf{Z}\} \tag{27}$$
[see Fig. 7(b)].

5. The closed $\pi/6$ cylinder $V = \{(x,y,z)/0\leqslant\sqrt{3}y\leqslant x,\ y\leqslant(a-x)\sqrt{3},\ 0\leqslant z\}$.

Generators: κ, μ, η; Relations: $\gamma = \kappa\mu\kappa$, $\lambda = \kappa\mu\kappa\mu\kappa$;

$$\mathbf{S} = \{1,\mu\gamma,\gamma\mu\}\{1,\mu\}\{1,\lambda\}\{1,\eta\} \quad (\text{Scheonflies } D_{6h}),$$
$$\mathbf{L} = \{3a(n+m),\sqrt{3}a(n-m)/2,0)|m,n\in\mathbf{Z}\} \tag{28}$$

6. The prism $V = \{(x,y,z)/0\leqslant\sqrt{3}y\leqslant x,\ y\leqslant(a-x)\sqrt{3},\ 0\leqslant z\leqslant c\}$.

Generators: κ, μ, η; Relations: $\gamma = \kappa\mu\kappa$, $\lambda = \kappa\mu\kappa\mu\kappa$;

$$\mathbf{S} = \{1,\mu\gamma,\gamma\mu\}\{1,\mu\}\{1,\lambda\}\{1,\eta\},$$
$$\mathbf{L} = \{(3a(n+m)/2,\sqrt{3}a(n-m)/2,2kc)|k,m,n\in\mathbf{Z}\}. \tag{29}$$

VI. THE BOUNDED FOUR-SIDED DOMAINS

Analysis of these domanisn requires more use of group theory and less reliance on geometrical construction. These bounded domains are all tetrahedra, but will be distinguished according to the space groups associated with them. Our three tetrahedra will thus be termed the *large tetrahedral domain*, the *centered octahedral* domain, and the *primitive octahedral* domain.

A. The large tetrahedral domain

The representation considered is $\mathbf{V} = \{(x,y,z)|x\leqslant y,\ z\leqslant x,\ -z\leqslant x,\ x+y\leqslant 2a\}$, and is depicted in Fig. 5(c).

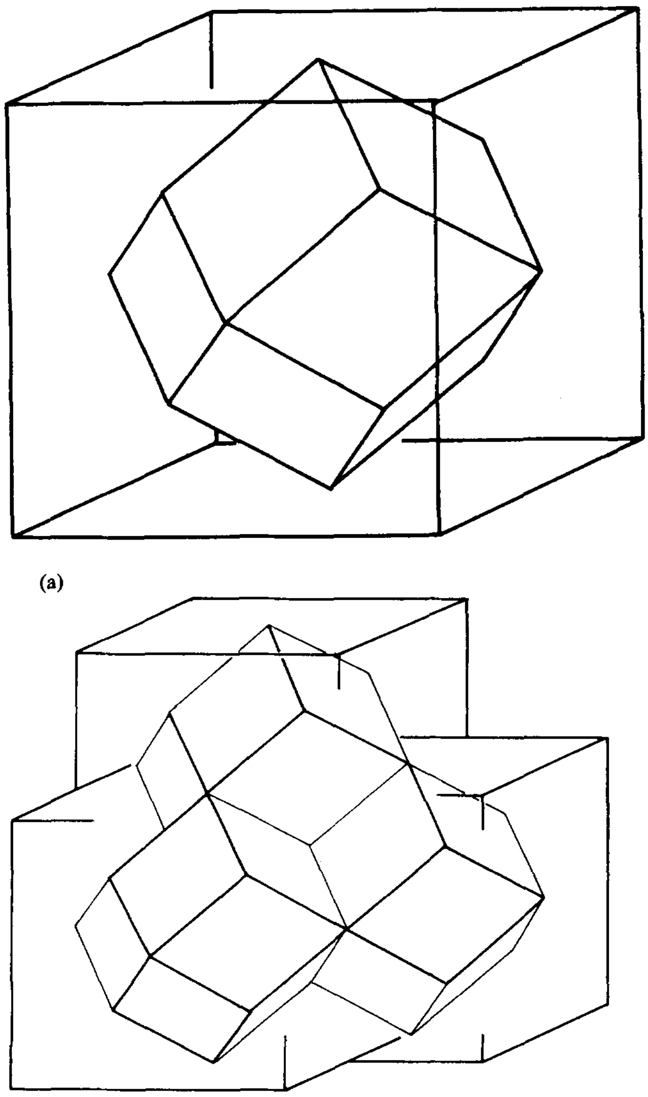
The Möbius corner $(\pi/2,\pi/3,\pi/3)$. This corner generates the *tetrahedral* group. The planes of $\mathbf{V}$ which pass through the origin generate the reflections

$$\lambda = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \ \mu = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$
$$\nu = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix}. \tag{30}$$

One finds that $\lambda\nu(x,y,z) = (-x,y,-z)$ and $\mu\lambda\nu\mu(x,y,z) = (x,-y,-z)$. The elements $\lambda\nu$ and $\mu\lambda\nu\mu$ generate the diagonal group $\mathbf{D}$ of order four, the matrices of determinant unity with diagonal entries plus or minus unity. The effect of $\mathbf{D}$ on (x,y,z) is to generate the images

$$\{(x,y,z),\ (x,-y,-z),\ (-x,-y,z),\ (-x,y,-z)\}.$$

On the other hand, λ and μ generate the permutation



(a)

(b)

FIG. 8. *Symmetric Cell.* (a) Under the action of the tetrahedral group T_h the large tetrahedral domain generates a Wigner–Seitz cell (a rhombic dodecahedron) for the associated cubic F–lattice; (b) the Wigner–Seitz cells stack to fill all space without gaps.

group **P** on three letters. The effect of **P** on (x,y,z) is to generate the images

$$\{(x,y,z), (z,y,x), (y,x,z), (z,x,y), (x,z,y), (y,z,x)\}$$

The group **D** is normal with respect to **P**. It follows that $\mathbf{S} = \mathbf{DP}$ is a group and has order 24. In Schoenflies notation the group **S** is denoted by $\mathbf{T}_h$.

The corner potential. Use of (13) with $f(x,y,z) = \|(x-u, y-v, z-w)\|^{-1}$ allows one to write the potential (6) with the help of a simple sequence of auxiliary functions. One has

$$\begin{aligned} g(u,v,w) &= f(u,v,w) + f(-u,-v,w) \\ &\quad + f(u,-v,-w) + f(-u,v,-w), \\ h(u,v,w) &= g(u,v,w) + g(v,w,u) + g(w,u,v), \qquad (31) \\ \phi(u,v,w) &= h(u,v,w) - h(v,u,w). \end{aligned}$$

In the manipulations of these formulas we made free use of the duality property

$$\sum_{\sigma\in S} \det(\sigma)\|\sigma\mathbf{x} - \mathbf{u}\|^{-1} = \sum_{\sigma\in S} \det(\sigma)\|\mathbf{x} - \sigma\mathbf{u}\|^{-1}.$$

The space group. Reflection across the plane $x + y = 2a$ has the formula $\xi(x,y,z) = (-y,-x,z) + 2a(1,1,0)$. It is this reflection which needs to be adjoined to **S**. One has $(\nu\lambda)\mu(\nu\lambda)(x,y,z) = (-y,-x,z)$ and thus Hypothesis I for space group generation is satisfied. One now needs to examine all the images of $\xi(0,0,0) = 2a(1,1,0)$ under the action of the tetrahedral group. A glance at our decomposition result $\mathbf{S} = \mathbf{DP}$ shows that the listing of the twelve elements $2a(\mp 1, \mp 1, 0)$, $2a(0, \mp 1, \mp 1)$, $2a(\mp 1, 0, \mp 1)$ yields all possible images. Thus Hypothesis II is also satisfied. Let

$$\mathbf{L} = \{2a(i+k, i+j, j+k) \,|\, i,j,k\in\mathbf{Z}\}. \qquad (32)$$

This is a *face–centered cubic Bravais lattice*. The space group for **V** is thus seen to be (**S**,**L**).

The different images of the domain **V** produced by the action of the tetrahedral group **S** are disjoint and do not overlap except at the boundaries. The solid region represented by the union $\mathbf{V}_S = \cup\{\sigma\mathbf{V}|\sigma\in\mathbf{S}\}$ appears in Fig. 8(a), and is called a *Wigner–Seitz cell* for the cubic F–Lattice **L**. The effect of the lattice **L** is to fill all three dimensional space with copies of this cell is a non-overlapping manner as in Fig. 8(b). One thus deduces that the tetrahedral domain **V** is an image domain.

The potential function. If $\phi(u,v,w)$ is the potential (31) for the corner region, then the lattice sum

$$\Phi(u,v,w) = \sum_{i,j,k\in\mathbf{Z}} \phi((u,v,w) + 2a(i+k, i+j, j+k)) \qquad (33)$$

is an absolutely convergent series for the Green's function for the image domain **V**.

B. Centered Octahedral Domain

A representation of this octahedral domain is $\mathbf{V} = \{(x,y,z)|x<y, 0<z<x, x+y<2a\}$. The orientation of this domain is depicted in Fig. 5(b).

The Möbius corner $(\pi/2, \pi/3, \pi/4)$. This corner generates the octahedral group. The planes passing through the origin generate reflections $\lambda(x,y,z) = (z,y,x)$, $\mu(x,y,z) = (y,x,z)$ as in (30), and the reflection $\eta(x,y,z) = (x,y,-z)$, which is not an element of the tetrahedral group. One constructs diagonal elements by noting that $\lambda\eta\lambda(x,y,z) = (-x,y,z)$ and $(\lambda\mu\lambda)\eta(\lambda\mu\lambda)(x,y,z) = (x,-y,z)$. The elements η, $\lambda\eta\lambda$, and $(\lambda\mu\lambda)\eta(\lambda\mu\lambda)$ are mutually orthogonal and generate the cube corner group **D**, which is a diagonal group of order eight. The elements λ and μ generate the same permutation group **P** as occurred in the tetrahedral case. Since **D** is normal with respect to **P** it follows that $\mathbf{S} = \mathbf{DP}$ is a group of order forty-eight.

The space group. One has to add the reflection $\xi(x,y,z) = (-y,-x,z) + 2a(1,1,0)$ to the octahedral group in order to generate the space group. The product decomposition $\mathbf{S} = \mathbf{DP}$ shows that hypothesis I is satisfied. The decomposition also shows that the images of

$\xi(0,0,0) = 2a(1,1,0)$ under the octahedral group are the same as under the tetrahedral group. Thus Hypothesis II is also satisfied and it follows that the space group is given by (**S**,**L**), where **S** is the currently discussed octahedral group and **L** is the previously defined face-centered cubic lattice (32).

The Wigner–Seitz cell $\mathbf{V}_S = \{\sigma\mathbf{V} | \sigma\in\mathbf{S}\}$ is the same as the one that occurred in the tetrahedral case. It follows that **V** is an image domain.

C. Primitive Octahedral Domain

This region has the representation $\mathbf{V} = \{(x,y,z) | x \leqslant y, 0 \leqslant z \leqslant x, y \leqslant a\}$. The orientation of the figure is as in Fig. 5(a). The Möbius corner at the origin generates the octahedral group. The reflection to adjoin is $\xi(x,y,z) = (x, -y,z) + 2a(0,1,0)$. One sees that Hypothesis I is satisfied. The images of $\xi(0,0,0) = 2a(0,1,0)$ under the octahedral group are just the eight vectors $\{\pm 2a(1,0,0), \pm 2a(0,1,0), \pm 2a(0,0,1)\}$. It follows that Hypothesis II is satisfied. We now define

$$\mathbf{L} = \{2a(i,j,k) | i,j,k\in\mathbf{Z}\}, \tag{34}$$

which is a *primitive cubic lattice*. The space group for **V** is thus (**S**,**L**), where **S** is the octahedral group, and **L** is the currently defined lattice (34).

The Wigner–Seitz cell $\mathbf{V}_S = \cup\{\sigma\mathbf{V} | \sigma\in\mathbf{S}\}$ is just the cube $\{(x,y,z) | -a \leqslant x,y,z \leqslant a\}$ and is formed as a union of domains which do not overlap. Moreover, under the action of the lattice **L** all space is filled in a non–overlapping manner with these cubes. It follows that **V** is an image domain.

VII. THE ICOSAHEDRAL POTENTIAL

The Möbius corner $(\pi/2,\pi/3,\pi/5)$. The reflection group generated by this corner is called the *icosahedral group* $\mathbf{Y}_h$. This group does not manifest itself as a crystallographic point group. Nevertheless, the unit cell of some intermetallic compounds, such as $MoAl_{12}$ contains an icosahedral structure.[15,16] The group is best known from the theory of regular polyhedra and was discussed by Möbius[17] and more recently by Coxeter.[6]

We shall obtain an explicit representation by exploiting the relation $\cos(\pi/5) = (\sqrt{5}+1)/4$. Set $\tau = (\sqrt{5}+1)/2$. One notes that $\tau^{-1} = (\sqrt{5}-1)/2$. One now considers the sector $\{(x,y,z) | z \leqslant \tau^{-1}x - \tau y, y \geqslant 0, z \geqslant 0\}$. The sector is depicted in Fig. 9. The reflections associated to the corner have matrix representations μ and η as in (14) and

$$\lambda = \frac{1}{2}\begin{bmatrix} \tau & 1 & \tau^{-1} \\ 1 & -\tau^{-1} & -\tau \\ \tau^{-1} & -\tau & 1 \end{bmatrix}.$$

The elements $\mathbf{K} = \{1, \mu\lambda, \lambda\mu, \lambda\mu\lambda\mu, \mu\lambda\mu\lambda\}$ form a cyclic group of order five and represent rotations through 0, $2\pi/5$, $8\pi/5$, $4\pi/5$, $6\pi/5$ radians. The matrix elements for the non-identity rotations are

$$\mu\lambda = \frac{1}{2}\begin{bmatrix} \tau & 1 & \tau^{-1} \\ -1 & \tau^{-1} & \tau \\ \tau^{-1} & -\tau & 1 \end{bmatrix},$$

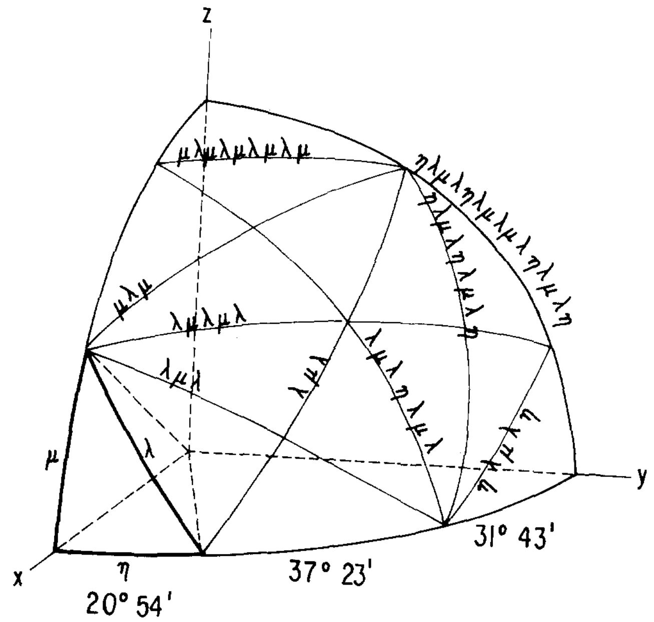


FIG. 9. *Reflection Planes.* Geodesics in the sphere are used to represent the reflection planes in the first octant generated by the icosahedral Möbius corner outlined in the lower left.

$$\lambda\mu = \frac{1}{2}\begin{bmatrix} \tau & -1 & \tau^{-1} \\ 1 & \tau^{-1} & -\tau \\ \tau^{-1} & \tau & 1 \end{bmatrix},$$

$$\mu\lambda\mu\lambda = \frac{1}{2}\begin{bmatrix} 1 & \tau^{-1} & \tau \\ -\tau^{-1} & -\tau & 1 \\ \tau & -1 & -\tau^{-1} \end{bmatrix}, \tag{35}$$

$$\lambda\mu\lambda\mu = \frac{1}{2}\begin{bmatrix} 1 & -\tau^{-1} & \tau \\ \tau^{-1} & -\tau & -1 \\ \tau & 1 & -\tau^{-1} \end{bmatrix}.$$

A calculation yields $\rho\mu\eta\,\rho^2(x,y,z) = (-x,y,-z)$, where $\rho = (\lambda\mu\lambda\mu)\eta(\lambda\mu\lambda)(\eta\lambda\eta)$, for which one has $\rho(x,y,z) = (z,x,y)$. The element ρ generates the cyclic group of order three $\mathbf{P} = \{1, \rho, \rho^2\}$. The diagonal elements μ, $\mu\eta$, $\rho\mu\eta\,\rho^2$ generate the cube corner group **D**, which has order eight. The product $\mathbf{S} = \mathbf{DPK}$ can be shown to be a group, and is the icosahedral group that we have been seeking to define.

The potential for the icosahedral corner is now easy to obtain by using (13). Let $f(u,v,w) = \|(x-u, y-v, z-w)\|^{-1}$. Define

$$\begin{aligned} g(u,v,w) &= f(u,v,w) + f(-u,-v,w) \\ &\quad + f(u,-v,-w) + f(-u,v,-w), \\ h(u,v,w) &= f(u,v,w) + g(v,w,u) + g(w,u,v), \\ k(u,v,w) &= h(u,v,w) - h(u,-v,w), \\ \phi(u,v,w) &= \sum_{\sigma\in\mathbf{K}} k(\sigma(u,v,w)). \end{aligned} \tag{36}$$

The formidable problem of coding a matrix sum with 120 terms has thus been reduced to the problem of coding a matrix sum with 5 terms. The necessary elements of **K** were listed in (35).

VIII. EIGENFUNCTION EXPANSIONS

In this section we shall discuss normal modes for image domains. We also consider the abstract aspects of Green's function expansions in normal modes for the cylindrical image domains and the bounded image domains. We omit the famous parallel plate problem which was considered by Fong[11] and Jackson.[18]

The principal problem is to parametrize complete systems of normal modes. Because normal modes occur in the description of waveguides and cavity resonators, this aspect of the problem is useful for its own sake. The Dirichlet normal modes for the plane $(\pi/3|\pi/3|\pi/3)$ and $(\pi/2|\pi/3|\pi/6)$ triangles appeared already in the treatise of Lamé,[2] which, however, contained no proof of completeness. After years of controversy the completeness problem was settled by C. G. Nooney.[19] Our own completeness proof is based on group-theoretic methods and is short and novel and applies to the Lamé normal modes as well as our own varieties and is by far the most significant contribution of this section.

Normal Modes. We shall consider image domains in two or three dimensions, but most arguments are formal and apply quite generally. Let $\mathbf{V}$ be an image domain with space group $(\mathbf{S},\mathbf{L})$. Let

$$\phi_{\mathbf{v}}(\mathbf{u}) = \sum_{\sigma\in\mathbf{S}} \det(\sigma) e^{-2\pi i\langle \mathbf{v}|\sigma\mathbf{u}\rangle}, \tag{37}$$

where $\mathbf{u}$ and $\mathbf{v}$ are elements of the same underlying vector space $\mathbf{E}$.

We shall call $\phi_{\mathbf{v}}(\mathbf{u})$ a *Dirichlet normal mode* for $\mathbf{E}$.

It is easy to see that

$$\nabla^2\phi_{\mathbf{v}}(\mathbf{u}) = -4\pi^2\langle \mathbf{v}|\mathbf{v}\rangle\phi_{\mathbf{v}}(\mathbf{u}), \tag{38}$$

where ∇^2 is the Laplace operator with respect to $\mathbf{u}$. It follows that our terminology is appropriate.

We shall consider the symmetric cell $\mathbf{V}_S = \cup\{\sigma\mathbf{V}|\sigma\in\mathbf{S}\}$. One sees from the preceding sections that in every instance $\mathbf{E} = \{\mathbf{V}_S + \mathbf{n}|\mathbf{n}\in\mathbf{L}\}$ and that this union is formed in a non-overlapping manner. It follows that an arbitrary function $f(\mathbf{u})$ on $\mathbf{V}$ can be extended to a function on all space by $f(\sigma\mathbf{u}+\mathbf{n}) = \det(\sigma)f(\mathbf{u})$ for $\mathbf{u}\in\mathbf{V}$. This extension of $f(\mathbf{u})$ to all space is called the *alternating extension*. If $f(\mathbf{u})$ is continuous and vanishes on the boundary of $\mathbf{V}$ then the alternating extension is a continuous function on all space.

The lattice $\mathbf{L}$ need not have the same dimension as $\mathbf{E}$. We thus consider the space $\mathbf{F}$ spanned by $\mathbf{L}$ in $\mathbf{E}$. The *dual* of $\mathbf{L}$ is defined to be a lattice in $\mathbf{F}$ defined by

$$\mathbf{L}' = \{\mathbf{m}\in\mathbf{F}|\langle\mathbf{m}|\mathbf{n}\rangle\in\mathbf{Z}, \text{ for all } \mathbf{n}\in\mathbf{L}\}. \tag{39}$$

When $\mathbf{n}\in\mathbf{L}$ and $\mathbf{m}\in\mathbf{L}'$ then one has

$$\phi_{(\sigma,\mathbf{n})\mathbf{m}}(\mathbf{u}) = \phi_{\mathbf{m}}((\sigma,\mathbf{n})\mathbf{u}) = \det(\sigma)\phi_{\mathbf{m}}(\mathbf{u}). \tag{40}$$

These relations show that $\phi_{\mathbf{m}}(\mathbf{u}) = 0$ when either $\mathbf{u}$ or $\mathbf{m}$ lies on the boundary of $\mathbf{V}$.

Any $\mathbf{L}$-periodic function $g(\mathbf{u})$ on $\mathbf{F}$ can be expanded as a Fourier series[20] through

$$g(\mathbf{u}) = \frac{1}{v(\mathbf{R})}\sum_{\mathbf{m}\in\mathbf{L}'}\hat{g}(\mathbf{m})e^{2\pi i\langle\mathbf{m}|\mathbf{u}\rangle}, \tag{41}$$

where

$$\hat{g}(\mathbf{m}) = \int_{\mathbf{R}} g(\mathbf{u})e^{-2\pi i\langle\mathbf{m}|\mathbf{u}\rangle}\,\mathbf{du},$$

and where $v(\mathbf{R})$ is the volume of a primitive cell $\mathbf{R}$ in $\mathbf{L}$, and where the integration $\mathbf{du}$ is carried out in $\mathbf{F}$.

Bounded Image Domains. Let $\mathbf{V}$ be a bounded image domain with space group $(\mathbf{S},\mathbf{L})$ and let $g(\mathbf{u})$ be a function which is continuous on $\mathbf{V}$ and vanishes on the boundary of $\mathbf{V}$. If we now consider the alternating extension of $g(\mathbf{u})$ to $\mathbf{E}$ then (41) yields

$$g(\mathbf{u}) = \frac{1}{n_S v(\mathbf{R})}\sum_{\mathbf{m}\in\mathbf{L}'}\hat{g}(\mathbf{m})\sum_{\sigma\in S}\det(\sigma)e^{2\pi i\langle\mathbf{m}|\sigma\mathbf{u}\rangle},$$

which in terms of (37) becomes

$$g(\mathbf{u}) = \frac{1}{n_S v(\mathbf{R})}\sum_{\mathbf{m}\in\mathbf{L}'} g(\mathbf{m})\phi^*_{\mathbf{m}}(\mathbf{u}). \tag{42}$$

If $\mathbf{m}\in\mathbf{L}'$ then one has

$$\int_{\mathbf{V}} g(\mathbf{u})\phi_{\mathbf{m}}(\mathbf{u})d\mathbf{u} = \int_{\cup\{\sigma\mathbf{V}|\sigma\in\mathbf{S}\}} g(\mathbf{u})e^{-2\pi i\langle\mathbf{m}|\mathbf{u}\rangle}\,d\mathbf{u}$$
$$= \int_{\mathbf{R}} g(\mathbf{u})e^{-2\pi i\langle\mathbf{m}|\mathbf{u}\rangle}\,d\mathbf{u}, \tag{43}$$

where $\mathbf{R}$ is a primitive cell in $\mathbf{L}$. The change in the domain of integration from $\cup\{\sigma\mathbf{V}|\sigma\in\mathbf{S}\}$ is permissible in every one of our explicit constructions.

Define $[\mathbf{n}] = \{\sigma\mathbf{n}|\sigma\in\mathbf{S}\}$. Two classes $[\mathbf{n}]$ and $[\mathbf{m}]$ have either no elements in common or are the same. Let $\mathbf{L(S)}$ denote a selection of parameter elements in the dual $\mathbf{L}'$ obtained by choosing one element from each maximal equivalence class. In actual fact, $\mathbf{L(S)}$ may be obtained by choosing those elements of $\mathbf{L}'$ which lie properly in the interior of the sector that defines $\mathbf{S}$, as illustrated in Fig. 10.

For $\mathbf{n}$, $\mathbf{m}\in\mathbf{L(S)}$ one has that

$$\int_{\mathbf{V}}\phi_{\mathbf{m}}(\mathbf{u})\phi^*_{\mathbf{n}}(\mathbf{u})\,d\mathbf{u} = \begin{cases} 0 & [\mathbf{n}]\neq[\mathbf{m}] \\ v(\mathbf{R}) & [\mathbf{n}]=[\mathbf{m}]. \end{cases} \tag{44}$$

The normal mode expansion is thus summarized by

$$g(\mathbf{u}) = \frac{1}{v(\mathbf{R})}\sum_{\mathbf{m}\in\mathbf{L(S)}}\hat{\mathbf{g}}(\mathbf{m})\phi^*_{\mathbf{m}}(\mathbf{u}),$$

where

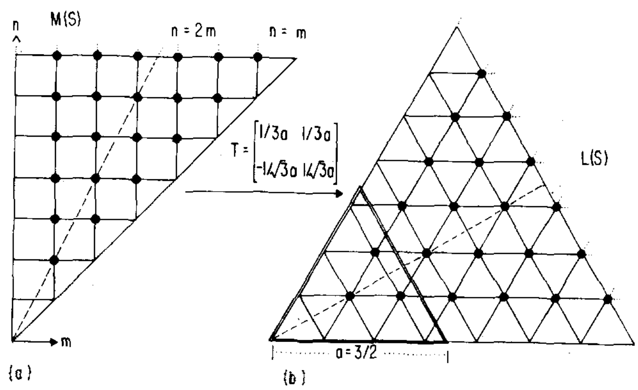


FIG. 10. *Index Sets.* (a) The standard index set, the sector $\mathbf{M(S)}$, parametrizies the normal modes, for the $(\pi/3|\pi/3|\pi/3)$–triangle; (b) the natural parameter set $\mathbf{L(S)}$ is a sector with a simple relationship to the $(\pi/3|\pi/3|\pi/3)$–domain.

$$\hat{g}(\mathbf{m}) = \int_{\mathbf{V}} g(\mathbf{u})\phi_{\mathbf{m}}(\mathbf{u})\, d\mathbf{u}. \quad (45)$$

Since $g(\mathbf{u})$ was an arbitrary function on $\mathbf{V}$ with the homogeneous boundary condition $g(\mathbf{u}) = 0$, the above demonstrates completness of the Dirichlet normal modes. Neumann normal modes can be defined by the symmetric sums $\psi_{\mathbf{v}}(\mathbf{u}) = \Sigma_{\sigma\in\mathbf{S}} e^{-2\pi i\langle\mathbf{v}|\sigma\mathbf{u}\rangle}$. A demonstration of completeness can be obtained through the use of symmetric extensions of a function on $\mathbf{V}$.

Green's Functions for Bounded Image Domains. Let $\mathbf{V}$ be a bounded image domain with space group $(\mathbf{S},\mathbf{L})$. Let $\Phi(\mathbf{u}) = G(\mathbf{x},\mathbf{u})$ be the Green's function for $\mathbf{V}$, i.e., the potential for a unit charge at $\mathbf{x}$. Computing as in Jackson[18] one obtains the eigenfunction expansion. One has

$$\Phi(\mathbf{u}) = [\pi v(\mathbf{R})]^{-1} \sum_{\mathbf{m}\in\mathbf{L}(\mathbf{S})} \langle\mathbf{m}|\mathbf{m}\rangle^{-1}\phi_{\mathbf{m}}(\mathbf{x})\,\overline{\phi_{\mathbf{m}}(\mathbf{u})}\,. \quad (46)$$

Set $\alpha_{\mathbf{m}}(\mathbf{u}) = [\phi_{\mathbf{m}}(\mathbf{u}) + \phi_{-\mathbf{m}}(\mathbf{u})]/2$ and $\beta_{\mathbf{m}}(\mathbf{u}) = [\phi_{\mathbf{m}}(\mathbf{u}) - \phi_{-\mathbf{m}}(\mathbf{u})]/2i$. One has $\nabla^2\alpha_{\mathbf{m}}(\mathbf{u}) = -4\pi^2\langle\mathbf{m}|\mathbf{m}\rangle\alpha_{\mathbf{m}}(\mathbf{u})$ and $\nabla^2\beta_{\mathbf{m}}(\mathbf{u}) = -4\pi^2\langle\mathbf{m}|\mathbf{m}\rangle\beta_{\mathbf{m}}(\mathbf{u})$. Thus $\alpha_{\mathbf{n}}(\mathbf{u})$ and $\beta_{\mathbf{n}}(\mathbf{u})$ are real eigenfunctions of the Laplace operator, which vanish on the boundary of $\mathbf{V}$, and will be called the *real Dirichlet normal modes* for $\mathbf{V}$. One sees that

$$\Phi(\mathbf{u}) = [\pi v(\mathbf{R})]^{-1} \sum_{\mathbf{m}\in\mathbf{L}(\mathbf{S})} \frac{[\alpha_{\mathbf{m}}(\mathbf{x})\alpha_{\mathbf{m}}(\mathbf{u}) + \beta_{\mathbf{m}}(\mathbf{x})\beta_{\mathbf{m}}(\mathbf{u})]}{\langle\mathbf{m}|\mathbf{m}\rangle}. \quad (47)$$

It follows that $\{\alpha_{\mathbf{m}}(\mathbf{u})|\mathbf{m}\in\mathbf{L}(\mathbf{S})\}\cup\{\beta_{\mathbf{m}}(\mathbf{u})|\mathbf{m}\in\mathbf{L}(\mathbf{S})\}$ forms a complete set, but it should be pointed out that this listing may contain duplications due to additional relations.

We will now explain why most three-dimensional Dirichlet normal modes are purely imaginary for three-dimensional image domains. One has the relations $\alpha_{\mathbf{m}}(\sigma\mathbf{u}) = \det(\sigma)\alpha_{\mathbf{m}}(\mathbf{u})$ and $\beta_{\mathbf{m}}(\sigma\mathbf{u}) = \det(\sigma)\beta_{\mathbf{m}}(\mathbf{u})$ for $\sigma\in\mathbf{S}$. If inversion is an element of $\mathbf{S}$, i.e., if $-\mathbf{n}$ can be obtained from $\mathbf{n}$ by a group operation in $\mathbf{S}$, then $\alpha_{-\mathbf{n}}(\mathbf{u}) = -\alpha_{\mathbf{m}}(\mathbf{u})$. However, the defining condition implies that $\alpha_{\mathbf{m}}(\mathbf{u}) = \alpha_{-\mathbf{m}}(\mathbf{u})$. It follows that $\alpha_{\mathbf{m}}(\mathbf{u}) = 0$ whenever inversion is an element of $\mathbf{S}$.

Lattices of the form $\mathbf{Z}, \mathbf{Z}\times\mathbf{Z}, \mathbf{Z}\times\mathbf{Z}\times\mathbf{Z},\cdots$ are called *standard lattices*. In practice it is desirable to index the eigenfunctions on a standard lattice. Let $\mathbf{M}$ be a standard lattice. Let $\mathbf{T}$ be an invertible linear map which transforms $\mathbf{M}$ into $\mathbf{L}'$. One sets

$$\phi_{\mathbf{T}(\mathbf{m})}(\mathbf{u}) = \alpha_{\mathbf{m}}(\mathbf{u}) + i\alpha_{\mathbf{m}}(\mathbf{u}). \quad (48)$$

Our explicit expansions adhere to this notation. The parameter set for the real and imaginary parts $\alpha_{\mathbf{m}}(\mathbf{u})$ and $\beta_{\mathbf{m}}(\mathbf{u})$ then is $\mathbf{M}(\mathbf{S}) = \{\mathbf{m}\in\mathbf{M}|\mathbf{T}(\mathbf{m})\in\mathbf{L}(\mathbf{S})\}$. The relationship between $\mathbf{M}(\mathbf{S})$ and $\mathbf{L}(\mathbf{S})$ for the $(\pi/3|\pi/3|\pi/3)$ cylinder is illustrated in Fig. 10.

Green's Functions for Cylinder Domains. Let $\{\phi_{\mathbf{a}}(u,v)|\mathbf{a}\in\mathbf{I}\}$ be a complete set of orthonormal Dirichlet normal modes with respect to the Laplace operator $\partial^2/\partial u^2 + \partial^2/\partial v^2$ on a bounded plane domain $\mathbf{D}$. With respect to such a system any continuous function $f(u,v)$ on $\mathbf{D}$ which vanishes on the boundary has the expansion

$$f(u,v) = \sum_{\mathbf{a}\in\mathbf{I}} \hat{f}(\mathbf{a})\phi_{\mathbf{a}}(u,v), \quad (49)$$

where

$$\hat{f}(\mathbf{a}) = \int_{\mathbf{D}} f(u,v)\phi_{\mathbf{a}}(u,v)\, du\, dv.$$

Let $\Phi(u,v,w) = G(x,y,z|u,v,w)$ be the Green's function for a perpendicular cylinder with cross section $\mathbf{D}$. Computing as in Jackson[18] one obtains the expansion

$$\Phi(u,v,w) = 2\pi \sum_{\mathbf{a}\in\mathbf{I}} \frac{\exp(-\lambda_{\mathbf{a}}^{1/2}|z-w|)}{\lambda_{\mathbf{a}}^{1/2}}\phi_{\mathbf{a}}(x,y)\phi^*_{\mathbf{a}}(u,v), \quad (50)$$

where the eigenvalue $\lambda_{\mathbf{a}}$ corresponds to $\nabla^2\phi_{\mathbf{a}}(u,v) = -\lambda_{\mathbf{a}}\phi_{\mathbf{a}}(u,v)$.

IX. FORMULAS FOR CYLINDERS

The case of the rectangular cylinder is a well-known classical case,[21] but the remaining formulas are expressed in terms of our versions of the Lamé normal modes.

A. The Rectangular Cylinder $\mathbf{V} = \{(x,y,z)/0\leqslant x\leqslant a, 0\leqslant y\leqslant b\}$

$$\Phi(u,v,w) = \frac{1}{2ab}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} \times\frac{\exp\{-\pi[(m/a)^2+(n/b)^2]^{1/2}|z-w|\}}{[(n/a)^2+(n/b)^2]^{1/2}} \times\alpha_{m,n}(x,y)\alpha_{m,n}(u,v), \quad (51)$$

where

$$\alpha_{m,n}(u,v) = 4\sin(\pi mu/a)\sin(\pi nv/b). \quad (52)$$

With the parameter set $\mathbf{M}(\mathbf{S}) = \{(m,n)|m\geqslant 1, n\geqslant 1\}$ one has a complete set of Dirichlet normal modes for the square $\{(x,y)|0\leqslant x\leqslant a, 0\leqslant y\leqslant b\}$.

B. The $\pi/4$–Triangular Cylinder $\mathbf{V} = \{(x,y,z)/0\leqslant y\leqslant x\leqslant a\}$

$$\Phi(u,v,w) = \frac{1}{2a}\sum_{n=2}^{\infty}\sum_{m=1}^{n-1} \times\frac{\exp[-\pi a^{-1}(m^2+n^2)^{1/2}|z-w|]}{(m^2+n^2)^{1/2}} \times\alpha_{m,n}(x,y)\alpha_{m,n}(u,v), \quad (53)$$

where

$$\alpha_{m,n}(u,v) = 4\begin{vmatrix}\sin(\pi mu/a) & \sin(\pi mv/a)\\ \sin(\pi nu/a) & \sin(\pi nv/a)\end{vmatrix}. \quad (54)$$

With the parameter set $\mathbf{M}(\mathbf{S}) = \{(m,n)|0<m<n\}$ these Dirichlet normal modes form a complete set.[21]

C. The $\pi/6$–Cylinder $\mathbf{V} = \{(x,y,z)|0\leqslant\sqrt{3}y\leqslant x, y\leqslant(a-x)\sqrt{3}\}$

$$\Phi(u,v,w) = \frac{1}{\sqrt{3}a}\sum_{n=3}^{\infty}\sum_{m=[n/2]+1}^{n-1} \times\frac{\exp[-(4\pi/3a)|z-w|(n^2-mn+m^2)^{1/2}]}{(n^2-mn+m^2)^{1/2}} \times\alpha_{m,n}(x,y)\alpha_{m,n}(u,v), \quad (55)$$

where $[x]$ denotes the greatest integer less than or equal to x, and where

$$\alpha_{m,n}(u,v) = 4[\sin(2\pi(n+m)u/3a)\sin(2\pi(n-m)v/\sqrt{3}a) - \sin(2\pi(2n-m)u/3a)\sin(2\pi mv/\sqrt{3}a) - \sin(2\pi(n-2m)u/3a)\sin(2\pi nv/\sqrt{3}a)]. \quad (56)$$

With the parameter set $\mathbf{M(S)} = \{(m,n)|0<m<n<2m\}$ one has a complete set of Dirichlet normal modes.

D. The $\pi/3$–Cylinder $\mathbf{V} = \{(x,y,z)/0<y<\sqrt{3}x, y\leqslant(a-x)\sqrt{3}\}$

$$\Phi(u,v,w) = \frac{1}{\sqrt{3}a}\sum_{n=2}^{\infty}\sum_{m=1}^{n-1} \times \frac{[(-4\pi/3a)|z-w|(n^2-mn+m^2)^{1/2}]}{(n^2-mn+m^2)^{1/2}} \times \phi_{(m,n)}(x,y)\phi^*_{(m,n)}(u,v), \quad (57)$$

where $\phi_{(m,n)} = \alpha_{m,n} + i\beta_{m,n}$, and where

$$\alpha_{m,n}(u,v) = 2[\sin(2\pi(n+m)u/3a)\sin(2\pi(n-m)v/\sqrt{3}a) - \sin(2\pi(2n-m)u/3a)\sin(2\pi mv/\sqrt{3}a) - \sin(2\pi(n-2m)u/3a)\sin(2\pi nv/\sqrt{3}a)], \quad (58)$$

$$\beta_{m,n}(u,v) = 2[\sin(2\pi(n+m)u/3a)\cos(2\pi(n-m)v/\sqrt{3}a) - \sin(2\pi(2n-m)u/3a)\cos(2\pi mv/\sqrt{3}a) - \sin(2\pi(n-2m)u/3a)\cos(2\pi nv/\sqrt{3}a)].$$

With the parameter set $\mathbf{M(S)} = \{(m,n)|0<m<n, m,n\in\mathbf{Z}\}$ the complex functions $\phi_{(m,n)}$ form a complete set of Dirichlet normal modes. The relationship between $\mathbf{L(S)}$ and $\mathbf{M(S)}$ is depicted in Fig. 10, which also allows one to infer the additional relations in the real modes. One may thus write

$$\Phi(u,v,w) = \frac{2}{3a}\sum_{n=1}^{\infty}\frac{1}{n}\exp\Big(-\frac{4\pi n}{a\sqrt{3}}|z-w|\Big) \times\beta_{n,2n}(x,y)\beta_{n,2n}(u,v) + \frac{2}{\sqrt{3}a}\sum_{n=3}^{\infty}\sum_{m=[n/2]+1}^{n-1} \times\exp\frac{[-(4\pi/3a)|z-w|(n^2-mn+m^2)^{1/2}]}{(n^2-mn+m^2)^{1/2}} \times\Big(\alpha_{m,n}(x,y)\alpha_{m,n}(u,v)+\beta_{m,n}(x,y)\beta_{m,n}(u,v)\Big). \quad (59)$$

X. FORMULAS FOR PRISMS

A. The Rectangular Box

$\mathbf{V} = \{(x,y,z)/0\leqslant x\leqslant a, 0\leqslant y\leqslant b, 0\leqslant z\leqslant c\}$

$$\Phi(u,v,w) = \frac{1}{2\pi abc}\sum_{k=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} \times\frac{\beta_{k,m,n}(x,y,z)\beta_{k,m,n}(u,v,w)}{(k/a)^2+(m/b)^2+(n/c)^2}, \quad (60)$$

where

$$\beta_{k,m,n}(u,v,w) = -8\sin(\pi ku/a)\sin(\pi mv/b)\sin(\pi nw/c). \quad (61)$$

With the parameter set $\mathbf{M(S)} = \{(k,m,n)|k\geqslant1, m\geqslant1, n\geqslant1, k,m,n\in\mathbf{Z}\}$, one has a complete set of Dirichlet normal modes for the box. It should be noted that the expansion reported in Courant and Hilbert[22] is flawed, but the formula is very classical and appears in Jackson.[18]

B. The $\pi/4$ Prism $\mathbf{V} = \{(x,y,z)/0\leqslant y\leqslant x\leqslant a, 0\leqslant z\leqslant b\}$

$$\Phi(u,v,w) = \frac{1}{2\pi a^2 b}\sum_{n=1}^{\infty}\sum_{k=2}^{\infty}\sum_{m=1}^{k-1} \times\frac{\beta_{k,m,n}(x,y,z)\beta_{k,m,n}(u,v,w)}{(k/a)^2+(m/a)^2+(n/b)^2}, \quad (62)$$

where

$$\beta_{k,m,n}(u,v,w) = -8\begin{vmatrix}\sin(\pi ku/a) & \sin(\pi kv/a)\\ \sin(\pi mu/a) & \sin(\pi mv/a)\end{vmatrix}\sin(\pi nw/b). \quad (63)$$

With the parameter set $\mathbf{M(S)} = \{(k,m,n)|1\leqslant m\leqslant k-1, 1\leqslant n\}$ one has a complete listing for these normal modes.

C. The $\pi/6$ Prism $\mathbf{V} = \{(x,y,z)/0<\sqrt{3}y\leqslant x, y\leqslant(a-x)\sqrt{3}, 0\leqslant z\leqslant c\}$

$$\Phi(u,v,w) = \frac{1}{12\sqrt{3}\pi a^2 c}\sum_{k=1}^{\infty}\sum_{n=2}^{\infty}\sum_{m=[n/2]+1}^{n=1} \times\frac{\beta_{k,m,n}(x,y,z)\beta_{k,m,n}(u,v,w)}{[(m^2-mn+n^2)/(3a)^2]+[k^2/(4c)^2]}, \quad (64)$$

where $\beta_{k,m,n}(u,v,w) = 2\alpha_{m,n}(u,v)\sin(\pi kw/c)$, with $\alpha_{m,n}(u,v)$ defined by (56). One obtains a complete set of real Dirichlet normal modes with the parameter set $\mathbf{M(S)} = \{(k,m,n)|k\geqslant1, 0<m<n<2m\}$.

D. The $\pi/3$ Prism $\mathbf{V} = \{(x,y,z)/0\leqslant y\leqslant\sqrt{3}x, y\leqslant(a-x)\sqrt{3}, 0\leqslant z\leqslant c\}$

$$\Phi(u,v,w) = \frac{1}{12\sqrt{3}\pi a^2 c}\sum_{k=1}^{\infty}\sum_{n=2}^{\infty}\sum_{m=1}^{n-1}\frac{\phi_{(k,m,n)}(x,y,z)\ \phi^*_{(k,m,n)}(u,v,w)}{[n^2-mn+m^2)/(3a)^2]+[k^2/(4c)^2]}$$

$$= \frac{1}{12\sqrt{3}\pi a^2 c}\sum_{k=1}^{\infty}\sum_{m=1}^{\infty}\frac{\alpha_{k,m,2m}(x,y,z)\alpha_{k,m,2m}(u,v,w)}{[n^2/3a^2]+[k^2/(4c)^2]} + \frac{1}{6\sqrt{3}\pi a^2 c}\sum_{k=1}^{\infty}\sum_{n=2}^{\infty}\sum_{m=[n/2]+1}^{n-1}\left[\frac{\alpha_{k,m,n}(x,y,z)\alpha_{k,m,n}(u,v,w)+\beta_{k,m,n}(x,y,z)\beta_{k,m,n}(u,v,w)}{[(n^2-mn+m^2)/(3a)^2]+[k^2/(4c)^2]}\right], \quad (65)$$

where $\phi_{(k,m,n)} = \alpha_{k,m,n} + i\beta_{k,m,n}$ and where $\alpha_{k,m,n}(u,v,w) = 2\beta_{m,n}(u,v)\sin(\pi kw/c)$, and $\beta_{k,m,n}(u,v,w) = 2\alpha_{m,n}(u,v) \times \sin(\pi kw/c)$, with $\alpha_{m,n}$ and $\beta_{m,n}$ as in (58). The parameter set $\mathbf{M(S)} = \{(k,m,n)|k\geqslant 1, 0<m<n\}$ determines a complete orthogonal set of the complex modes.

XI. FORMULAS FOR THE TETRAHEDRA

Our most novel formulas appear in this section. The derivation of the normal modes for these domains makes essential use of our group–theoretic approach. In these cases it is even hard to depict and generate the image crystal structures through geometric constructions.

A. Primitive Octahedral Domain $V = \{(x,y,z)/x\leqslant y,\ 0\leqslant z\leqslant x,\ y\leqslant a\}$

$$\Phi(u,v,w) = \frac{1}{2\pi a}\sum_{m=3}^{\infty}\sum_{k=2}^{m-1}\sum_{n=1}^{k-1}\frac{\beta_{k,m,n}(x,y,z)\,\beta_{k,m,n}(u,v,w)}{(k^2+m^2+n^2)}, \tag{66}$$

where

$$\beta_{k,m,n})(u,v,w) = -8\begin{vmatrix}\sin(\pi ku/a) & \sin(\pi kv/a) & \sin(\pi kw/a)\\ \sin(\pi mu/a) & \sin(\pi mv/a) & \sin(\pi mw/a)\\ \sin(\pi nu/a) & \sin(\pi nv/a) & \sin(\pi nw/a)\end{vmatrix}. \tag{67}$$

The above Dirichlet normal modes form a complete set with the parameter set $\mathbf{M(S)} = \{(k,m,n)|0<n<k<m\}$.

B. Centered Octahedral Domain $V = \{(x,y,z)/x\leqslant y,\ 0\leqslant z\leqslant x,\ x+y\leqslant 2a\}$

$$\Phi(u,v,w) = \frac{1}{\pi a}\sum_{k=4}^{\infty}\sum_{n=[(k+3)/2]}^{k-1}\sum_{m=k-n+1}^{n-1}\frac{\beta_{k,m,n}(x,y,z)\,\beta_{k,m,n}(u,v,w)}{3(k^2+m^2+n^2)-2(km+kn+mn)} \tag{68}$$

where

$$\beta_{k,m,n})(u,v,w) = -8\begin{vmatrix}\sin(\pi u(k+m-n)/2a) & \sin(\pi v(k+m-n)/2a) & \sin(\pi w(k+m-n)/2a)\\ \sin(\pi u(k-m+n)/2a) & \sin(\pi v(k-m+n)/2a) & \sin(\pi w(k-m+n)/2a)\\ \sin(\pi u(-k+m+n)/2a) & \sin(\pi v(-k+m+n)/2a) & \sin(\pi w(-k+m+n)/2a)\end{vmatrix}. \tag{69}$$

One obtains a complete orthogonal set with $\mathbf{M(S)} = \{(k,m,n)|1\leqslant m<n<k<m+n\}$.

C. Large Tetrahedral Domain $V = \{(x,y,z)/x\leqslant y,\ -x\leqslant z\leqslant x,\ x+y\leqslant 2a\}$

$$\begin{aligned}\Phi(u,v,w) &= \frac{1}{\pi a}\sum_{k=3}^{\infty}\sum_{n=2}^{k-1}\sum_{m=1}^{n-1}\frac{\phi_{(k,m,n)}(x,y,z)\,\phi^*_{(k,m,n)}(u,v,w)}{3(k^2+m^2+n^2)-2(km+kn+mn)},\\ &= \frac{1}{4\pi a}\sum_{n=2}^{\infty}\sum_{m=1}^{n-1}\frac{\alpha_{m+n,m,n}(x,y,z)\alpha_{m+n,m,n}(u,v,w)}{m^2+n^2} + \frac{2}{\pi a}\sum_{k=4}^{\infty}\sum_{n=[(k+3)/2]}^{k-1}\sum_{m=k-n+1}^{n-1}\\ &\quad\times\frac{\alpha_{k,m,n}(x,y,z)\alpha_{k,m,n}(u,v,w)+\beta_{k,m,n}(x,y,z)\,\beta_{k,m,n}(u,v,w)}{3(k^2+m^2+n^2)-2(km+kn+mn)},\end{aligned} \tag{70}$$

where

$$\alpha_{k,m,n}(u,v,w) = 4\begin{vmatrix}\cos(\pi u(k+m-n)/2a) & \cos(\pi v(k+m-n)/2a) & \cos(\pi w(k+m-n)/2a)\\ \cos(\pi u(k-m+n)/2a) & \cos(\pi v(k-m+n)/2a) & \cos(\pi w(k-m+n)/2a)\\ \cos(\pi u(-k+m+n)/2a) & \cos(\pi v(-k+m+n)/2a) & \cos(\pi w(-k+m+n)/2a)\end{vmatrix}, \tag{71}$$

and $\beta_{k,m,n}(u,v,w)$ is as in (71), except that cos is replaced by the sin. A complete set of orthogonal complex modes $\phi_{k,m,n} = \alpha_{k,m,n} + i\beta_{k,m,n}$ is obtained with $\mathbf{M(S)} = \{(k,m,n) = |1\leqslant m<n<k\}$.

XII. SUMMARY

We have determined all the domains bounded by linear planes for which the image method determines the solution of the potential problem. In the applications one considers such domains to have conducting walls. The domains are listed in Table I, together with the point group and lattice which determine the crystal structure of the images. The lattice parameters are given in the text, as are the Green's functions associated with each domain. Solutions for the wedge and rectangular prism are in the existing literature.[4,18] For the Green's functions we have numerically evaluated the Coulomb sums as well as the eigenfunction expansions, which required special summation methods, and we found numerical agreement. We found the partial Coulomb sums over invariant sets of indices to be rapidly convergent when three-dimensional lattices were involved, and to be moderately rapidly convergent for two-dimensional lattices, but we have refrained from including our mathematical esti-

TABLE I. Image domains

Domain	Schoenflies corner group	Lattice
Parallel Plates	C_{1v}	(1 dim)
π/n–Wedge	C_{nv}	None
$(\pi/2,\pi/2,\pi/n)$–Corner	D_{nh}	None
$(\pi/2,\pi/3,\pi/3)$–Corner	T_h	None
$(\pi/2,\pi/3,\pi/4)$–Corner	O_h	None
$(\pi/2,\pi/3,\pi/5)$–Corner	Y_h	None
Open Channel	C_{2v}	(1 dim)
Prismatic Wedge	D_{nh}	(1 dim)
Open Rectangular Cylinder	C_{2v}	Primitive rectangular (square if 2 sides equal)
Closed Rectangular Cylinder	D_{2h}	Primitive rectangular (square if 2 sides equal)
Rectangular Prism	D_{2h}	Primitive orthorhombic (tetrahgonal or cubic if equal sides)
Open $\pi/4$–Triangular Cylinder	C_{4v}	Square
Closed $\pi/4$–Triangular Cylinder	D_{4h}	Square
$\pi/4$–Triangular Prism	D_{4h}	Primitive tetragonal (cubic if equal sides)
Open $\pi/3$–Triangular Cylinder	C_{3v}	Hexagonal (2 dim)
Closed $\pi/3$–Triangular Cylinder	D_{3h}	Hexagonal (2 dim)
$\pi/3$–Triangular Prism	D_{3h}	Hexagonal (3 dim)
Open $\pi/6$–Triangular Cylinder	C_{6v}	Hexagonal (2 dim)
Closed $\pi/6$–Triangular Cylinder	D_{6h}	Hexagonal (2 dim)
$\pi/6$–Triangular Prism	D_{6h}	Hexagonal (3 dim)
Tetrahedral Domain	T_h	Face centered cubic
Primitive Octahedral Domain	O_h	Primitive cubic
Centered Octahedral Domain	O_h	Face centered cubic

mates on the rates of convergence of these sums in this paper.

The eigenfunctions that we have displayed also arise in a number of other boundary value problems, such as those connected with cavity resonators and waveguides, but these problems also require the Neumann normal modes, which, as we indicated, can be defined with symmetric sums.

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