Vector difference calculus for physical lattice models

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A vector difference calculus is developed for physical models defined on a general triangulating graph $\mathcal{G}$, which may be a regular or an extremely irregular lattice, using discrete field quantities roughly analogous to differential forms. The role of the space Λ^p of p-forms at a point is taken on by the linear space generated at a graph vertex by the geometrical p-simplices which contain it. The vector operations divergence, gradient, and curl are developed using the boundary ∂ and coboundary d. Dot, cross, and scalar products are defined in such a way that discrete analogs of the vector integral theorems, including theorems of Gauss-Ostrogradski, Stokes, and Green, as well as most standard vector identities hold exactly, not as approximations to a continuum limit. Physical conservation laws for the models become theorems satisfied by the discrete fields themselves. Three discrete lattice models are constructed as examples, namely a discrete version of the Maxwell equations, the Navier-Stokes equation for incompressible flow, and the Navier linearized model for a homogeneous, isotropic elastic medium. Weight factors needed for obtaining quantitative agreement with continuum calculations are derived for the special case of a regular triangular lattice. Green functions are developed using a generalized Helmholtz decomposition of the fields. [S1063-651X(99)09801-3]

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I. INTRODUCTION

This paper concerns discrete representation of continuous field quantities that appear, for example, in quantum mechanics, continuum mechanics, electromagnetism, or transport theory. In particular, it presents an analog of vector differential calculus, not an approximation to it, which acts directly on the discrete models. Although the paper is not primarily about numerical methods, the numerical treatment of continuum problems forms a convenient logical starting point, thus the first part of the Introduction is framed in this context.

For computing field quantities one may choose to divide space into cells and make some finite difference [1,2] or finite element approximation [3]. This replaces the partial differential equations (PDEs) governing the fields by matrix equations. Another way to accomplish this is to expand the fields in a basis of localized functions. Usually, the main point of the matrix equations is that their solutions should approximate, in some well-defined sense, the solutions of the original PDEs. However, sometimes what is called for is a simple lattice model that preserves qualitative features of the phenomenon, but which need not be an accurate numerical approximation to the original PDEs. This kind of model approximation is most useful if the qualitative properties of the solution to the original problem are not known in certain limits, and if one has reason to suppose the solutions of the discrete model will behave similarly. It is particularly attractive when spatial boundary conditions are very complicated, as in the case for fluid motion inside the pore cavities of a porous material or quantum-mechanical transport in a glassy structure.

Lattice models of this type are used routinely for scalar fields obeying, e.g., the Schrödinger equation or diffusion equation on spatially complex structures. Vector or tensor fields can be treated in similar fashion with indices accounting for field components. However, the resulting formalism is more complicated. Boundary conditions mix the field components, and the mixing is worse when the equations are nonlinear and hence couple field components together at each point in space. The conceptual simplicity of matrix calculations erodes as the number of indices increases. The task of deriving properties of the discrete models becomes more and more daunting if at some point all the subscripts must be unpacked and all the details taken into account. One prefers to keep as much conceptual simplicity as possible, even when addressing a high level of detail. For continuum calculations, vector and tensor operations can often be performed without explicit reference to individual components. The use of differential forms [4,5], for example, makes this particularly convenient. However, if the discrete models arise only as approximations to the PDEs, one cannot do precise calculations on the lattice using tools developed for the continuum.

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The current paper presents a lattice formulation of vector calculus with which one can rewrite systems of PDEs for physical phenomena as systems of difference equations on a graph which serves as a quadrature grid. Some combinatorial aspects of the theory of differential forms are adapted for use on the graph with little mention of metric properties for the time being. The treatment is topological in the sense that it derives from adjacency rather than detailed geometry, and algebraic or combinatorial rather than metric or measure theoretic properties are of primary concern. Therefore, one arrives at lattice models for a physical phenomenon which, like the Ising model, attempt to capture its qualitative features without including details that may or may not be important but which detract from conceptual simplicity. It is possible to reintroduce the proper metric content by means of quadrature weights. This results in numerical methods related to the popular finite difference [1,2] (see Sec. VII), finite element [3], or lattice gas methods [6].

Scalar and vector fields are placed on equal footing, one that does not depend on space outside the graph itself. Vector fields are defined with respect to an intrinsic local basis with no reference to direction in the external space. This is novel since a vector field assigns a vector to each point in space, and normally a vector is defined by its magnitude and direction.

Calculations take place on the simplicial complex defined by a graph. The graph is a triangulation, meaning that it divides three-dimensional space into tetrahedral cells or 3-simplices that can share triangular faces (2-simplices), edges (1-simplices), or vertices (0-simplices). Graph vertices or lattice sites are points in the discrete space. The graph with the set of all simplices is the simplicial complex. The homology theory of simplicial complexes [7–9] can be thought of as a model approximation that forestalls confronting some of the subtleties of manifolds [10]. Here we adopt a similar position toward the relation between discrete and continuous physical models.

Continuum vector calculus makes use of a set of basis vectors at each point. The basis vectors are in general different at different points, such as $\hat{r}$ and $\hat{\theta}$ of polar coordinates. In the lattice development, the role of the set of basis vectors at a given point is taken on by the set of elementary geometrical simplices, i.e., bonds, triangles, and tetrahedra that include a given site. For each value of p from 0 to 3, the set of all p-simplices on the graph is a basis for the real vector space we shall call the space of p-fields. Discrete p-field variables of four types are introduced, corresponding in the continuous case to differential 0-, 1-, 2-, and 3-forms. Roughly speaking, the discrete analogs to space Λ^p at a particular point in the theory of differential forms [5] are the vector spaces generated by the set of p-simplices containing a particular graph vertex. As in the theory of differential forms, the field quantities of the discrete theory divide naturally into types corresponding to scalar, vector, pseudovector, and pseudoscalar fields. The prefix *pseudo* implies a classification with respect to a graph parity operation to be discussed presently.

Think of the set $\{(i)\}$ of 0-simplices, where i indexes graph vertices or lattice sites, as a geometrical basis set for representing scalar fields. This is similar to the convention of expanding scalar functions approximately in a set of localized basis functions. For our purposes, a 0-field or scalar field will be a vector

$$\phi=\sum_{[i]}(i)\phi_i \tag{1}$$

in the space where the set of 0-simplices forms a basis. The variable ϕ_i is as usual the strength of the field ϕ at point i, analogous to field strength $\phi(x)$ in continuous space. Likewise, 1-, 2- and 3-fields are vectors,

$$\alpha=\sum_{[i,j]}(i,j)\alpha_{ij},$$

$$\beta=\sum_{[i,j,k]}(i,j,k)\beta_{ijk}, \tag{2}$$

$$\gamma=\sum_{[i,j,k,l]}(i,j,k,l)\gamma_{ijkl},$$

in the spaces where the oriented 1-, 2-, or 3-simplices, respectively, form a basis. The oriented 1-simplex (i,j) is a basis vector oriented along the bond from vertex i to vertex j. Likewise the ordered triple (i,j,k) is a right-hand oriented 2-simplex, or triangle, containing vertices i, j, and k. One can associate with it a basis vector normal to the triangle in the right-handed direction. Interchanging vertices merely changes sign, so that if $\mathcal{P}$ is a permutation,

$$(\mathcal{P}(i),\mathcal{P}(j),\mathcal{P}(k),\ldots,\mathcal{P}(n))=\mathrm{sgn}(\mathcal{P})\quad(i,j,k,\ldots,n), \tag{3}$$

where $\mathrm{sgn}(\mathcal{P})$ is ± 1 depending on whether $\mathcal{P}$ is even or odd. Field components such as α_{ij}, β_{ijk}, or γ_{ijkl} are therefore antisymmetric with respect to index permutation. The summations include each simplex only once. Thus the square bracket $[\cdots]$ denotes one representative of an equivalence class related by exchange of indices.

Renumbering the vertex set of $\mathcal{G}$ is a formal symmetry which cannot have physical consequences. Reversing the vertex ordering changes the sign of p-simplices with odd p, so it changes the sign of the components for p-fields with $p=1$ and 3. Thus by analogy with the parities of continuum fields with respect to coordinate inversion, we classify the basic p-field quantities as 0-fields (scalars), 1-fields (polar vectors), 2-fields (axial vectors), and 3-fields (pseudoscalars). Evidently these discrete quantities bear some resemblance to the continuum fields, although simplified.

The theory is constructed in such a way that certain integral theorems, particularly the generalized Stokes theorems, and many of the standard vector identities hold true exactly in the discrete case. Since it is a topological theory, independent of deformations, the difference operators on arbitrary, nonregular graphs need not correspond to particular differential operators in the external space. Of course for regular triangulations (e.g., triangular lattice) one often finds such a correspondence generated naturally by Taylor expansion.

In any event, the discrete reformulation of the PDEs of any continuum model results in a discrete model that is in many ways much simpler and corresponds at least topologically to the original physics. Often the interesting phenom-

ena induced by constrained geometry are topological in origin. In such cases the formalism provides finite difference models that satisfy the proper integral constraints or conservation rules exactly, not only in the continuum limit. These conservation laws ensure the models must exhibit certain qualitatively correct behaviors. In some cases, they also prevent what would otherwise be numerically unstable behavior of solution methods.

The current paper is organized in the following way. Section II is a review of the properties of the boundary ∂ and coboundary d. The discrete analogs of the generalized Stokes theorems, including Stokes' theorem, the divergence theorem, and the fundamental theorem of calculus, are derived in Sec. III from the duality between ∂ and d. These theorems motivate the definitions of divergence, gradient, and curl given in Sec. IV (see Fig. 1). In Sec. V, the scalar and vector products of combinations of p-fields are defined in such a way as to permit derivation of a reasonably complete set of vector identities for p-fields, each of which has a precise continuum analog. Nonassociativity arising from nonlocality of products is discussed. Three examples of discrete lattice models are developed in Sec. VI. These are the lattice versions of Maxwell's electrodynamic equations, the Navier-Stokes equation for incompressible flow, and the Navier linearized model for a homogeneous, isotropic elastic medium. Section VII shows how to determine the quadrature weights necessary for obtaining quantitative agreement with the continuum calculations. These weights are evaluated for the special case of the triangular lattice. The Helmholtz decomposition of a general p-field is treated in some detail in Sec. VIII in connection with the orthogonal pair of operators ∂d and $d\partial$. Section IX is a summary discussion of the main results.

II. BOUNDARY AND COBOUNDARY

The vector difference models of interest are defined on the simplicial complex of graph $\mathcal{G}$ using the fields described above. Two vertices n and m appear in a 1-simplex (m,n) if they are adjacent in $\mathcal{G}$, which we denote $n@m$. Similarly, (l,m,n) or (k,l,m,n) are 2- or 3-simplices if the vertices involved are adjacent in pairs. The graph adjacency matrix H, with entry $H_{mn}=1$ if $n@m$ and 0 otherwise, determines the entire simplicial complex of $\mathcal{G}$.

The boundary [8] ∂_p is a linear map from the space $\mathcal{C}_p$ of p-simplices to $\mathcal{C}_{p-1}$. Its action on a simplex, which corresponds to taking the oriented boundary, is defined by

$$\begin{aligned}\partial_0(n)&=0,\\ \partial_1(m,n)&=(n)-(m),\\ \partial_2(l,m,n)&=(m,n)-(l,n)+(l,m),\\ \partial_3(k,l,m,n)&=(l,m,n)-(k,m,n)+(k,l,n)-(k,l,m).\end{aligned}\tag{4}$$

The rule is to drop each vertex successively and let the sign $\pm$ depend on whether the position of the deleted vertex is odd or even. The result in each case is an oriented boundary. If (m,n) is the directed bond from m to n, its boundary is the final minus the initial point, and if (l,m,n) is an oriented triangle, its boundary is the sequence of oriented bonds $(l,m)+(m,n)+(n,l)$. This is the usual, right-hand boundary orientation. Note, however, that the boundary of (k,l,m,n) is oriented such that (l,m,n) is positive outward, but (k,l,m) is oriented positive inward, i.e., toward vertex n. When the rank p is clear from the context, the subscript of ∂_p will be suppressed and we speak loosely of the boundary map ∂. Sometimes, however, it is best to keep careful track of p.

The action of ∂ on a field is found from linearity by distributing and letting it act on each basis simplex. For example, if β is the generic 2-field presented above,

$$\begin{aligned}\partial\beta&=\sum_{[l,m,n]}\beta_{lmn}\partial(l,m,n)\\ &=\sum_{[l,m,n]}\beta_{lmn}[(m,n)-(l,n)+(l,m)],\end{aligned}\tag{5}$$

where of course ∂ means in this case ∂_2. Notice that the boundary ∂ is defined without explicit reference to the structure of $\mathcal{G}$, i.e., without reference to H.

The coboundary d_p is a linear map from $\mathcal{C}_p$ to $\mathcal{C}_{p+1}$. It is adjoint to ∂_p in a certain sense to be discussed in Sec. III. In contrast to the case of ∂_p, the definition of the coboundary [8] d_p refers to $\mathcal{G}$ explicitly. Applying d_p to a p-simplex σ results in a sum of $(p+1)$-simplices, the boundary of each of which contains $+\sigma$. The sign is important. When the context makes p unambiguous, the subscript can be suppressed, and we speak of the coboundary map d, a shorthand notation similar to the use of ∂ for boundary. When the p subscripts are suppressed in an expression containing ∂ or d, the most general value of p consistent with the rest of the expression can be assumed. Thus let

$$d(k,l,\ldots,m)=\sum_{j@[k,l,\ldots,m]}(j,k,l,\ldots,m),\tag{6}$$

where the sum is over vertices j adjacent to each vertex in $[k,l,\ldots,m]$. Such vertices are characterized by $H_{jk}H_{jl}\cdots H_{jm}=1$.

As with ∂, the action of d on a field is induced by its action on the simplex bases. Thus if ϕ is a generic 0-field or scalar, then

$$\begin{aligned}d\phi&=\sum_{[n]}\phi_n d(n)=\sum_{[n]}\phi_n\sum_{m@n}(m,n)\\ &=\sum_{[m,n]}(\phi_n-\phi_m)(m,n).\end{aligned}\tag{7}$$

If (m,n) is a unit vector directed along the bond from m to n, the 1-field $d\phi$ is a difference gradient of ϕ.

The divergence of a 1-field is obtained with ∂. One has

$$\begin{aligned}\partial\alpha&=\sum_{[m,n]}\alpha_{mn}\partial(m,n)=\sum_{[m,n]}\alpha_{mn}[(n)-(m)]\\ &=\sum_{[n]}(n)\sum_{m@n}\alpha_{mn}.\end{aligned}\tag{8}$$

The coefficient of (m) is *minus* the difference divergence of α at point m, since it is the Kirchhoff sum of currents flow-

ing *into* the vertex m. Thus when ϕ is a 0-field, $d\phi = \text{grad}\,\phi$, and when α is a 1-field, $\partial\alpha = -\text{div}\alpha$. Putting these together gives the Laplacian operator for scalar fields, $\nabla^2\phi = \text{div}(\text{grad}\,\phi) = -\partial d\phi$, or

$$-\partial d\phi = -\sum_n (n) \sum_{m@n} (\phi_n - \phi_m) = \nabla^2\phi. \tag{9}$$

This intrinsic definition of the Laplacian for a discrete scalar field is identical to the one motivated physically by diffusion in the following way [11]. First the gradient is defined in relation to Fick's law. Thus the flux of material diffusing along a bond is assumed proportional to the difference $\phi_m - \phi_n$ in concentration between the two ends. Then Kirchhoff's current sum applied to vertex m defines divergence as current out minus current in. The difference operator ∇^2 constructed for the diffusion equation can be transplanted to any other discrete scalar equation, such as the Schrödinger equation [12]. Therefore, even for an irregular graph on which the discrete operators do not correspond by Taylor expansion to the continuum case, they can have topological meaning like that given by diffusion to the scalar Laplacian.

An essential property shared by ∂ and d is that, when applied twice to any field ψ, they annihilate it. In other words, $d^2\psi = 0$ and $\partial^2\psi = 0$ for any ψ, which means of course that if ψ is any p-field, $\partial_{p-1}\partial_p\psi = 0$ and $d_{p+1}d_p\psi = 0$. These equalities are obtained from direct computation applied to a basis simplex. They are essential for the analogy to the continuum vector calculus since, as will develop below, they force the curl of a gradient or the divergence of a curl to vanish.

To arrive at a difference ∇^2 for vector quantities, one needs an intrinsic notion of curl. It is convenient to develop this in relation to a generalized Stokes theorem, which is the subject of the following section.

III. STOKES THEOREMS

Definitions of other vector operators are motivated by the generalized Stokes theorems, which include Green's theorem, the Gauss-Ostrogradski divergence theorem, and Stokes' theorem in three dimensions. Divergence and curl are defined heuristically in the continuous case using the divergence theorem and Stokes' theorem applied to a region of diameter ϵ, in the limit $\epsilon \to 0$. Our approach is not to approximate the continuous case, but to construct discrete analogs to the integral theorems. As a byproduct, these reduce to the usual integral theorems in the limit of small lattice spacing for sufficiently regular lattices. But the discrete theorems hold exactly for any $\mathcal{G}$ without regard to a limit. The strategy is to use the discrete Stokes theorems to construct vector difference operators.

The discrete analog of an oriented arc or contour from a to b is an ordered set $\mathcal{C}$ of edges (1-simplices) such that the first vertex of the first edge is a, the second vertex of the last edge is b, and the second vertex of each edge in between is the first vertex of the next edge. In other words, it is an oriented polygonal path. For simplicity, suppose $\mathcal{C}$ does not intersect itself, so it forms a self-avoiding walk. Associated with $\mathcal{C}$ is the 1-field or 1-chain C defined by the sum

$$C = \sum_{(m,n)\in\mathcal{C}} (m,n). \tag{10}$$

The analog of a contour integral of the 1-field α is

$$\langle \alpha, C\rangle = \sum_{(m,n)\in\mathcal{C}} \alpha_{mn}, \tag{11}$$

where the left-hand side is the inner product, defined by $\langle (k,l),(m,n)\rangle = \delta_{km}\delta_{ln} - \delta_{kn}\delta_{lm}$, of α with C.

Now consider $\langle d\phi, C\rangle$, where ϕ is any scalar field,

$$\langle d\phi, C\rangle = \sum_{(m,n)\in\mathcal{C}} (\phi_n - \phi_m) = \phi_b - \phi_a. \tag{12}$$

Because of the definition of $\mathcal{C}$, the amplitudes cancel in pairs, except for the first and last. Since $\partial C = (b) - (a)$, one sees that

$$\langle d\phi, C\rangle = \langle \phi, \partial C\rangle, \tag{13}$$

where the inner product $\langle \phi, \psi\rangle$ of two 0-fields indicated on the right-hand side is defined by $\langle (m),(n)\rangle = \delta_{mn}$.

The result $\langle d\phi, C\rangle = \langle \phi, \partial C\rangle$ is analogous to the fundamental theorem of calculus, which is a special case of the generalized Stokes theorem $\langle d\psi, \Omega\rangle = \langle \psi, \partial\Omega\rangle$, where Ω is a p-chain expressing content (i.e., the oriented length, area, or volume) of some portion of $\mathcal{G}$, and ψ is a $(p-1)$-field. The Stokes theorem is actually a special case of a more general adjoint relation [8] deriving from the definitions of ∂ and d, namely

$$\langle d\lambda, \mu\rangle = \langle \lambda, \partial\mu\rangle, \tag{14}$$

for any p-field λ and $(p+1)$-field μ. To develop the Stokes theorem based on this general relation we begin with the case where ψ is a 1-field and Ω is a 2-chain representing an oriented surface. The discrete analog $\mathcal{S}$ of an oriented surface is a contiguous set of triangles sharing edges and oriented so that internal boundaries cancel. Of course, $\mathcal{S}$ need not be planar. It could as well be any surface in $\mathcal{G}$. The oriented area is represented by S and the corresponding boundary by ∂S. Therefore the surface is tiled with oriented triangular facets. Define

$$S = \sum_{(l,m,n)\in\mathcal{S}} (l,m,n). \tag{15}$$

One sees that ∂S corresponds to the usual oriented boundary curve. Likewise if the outward oriented volume or 3-simplex content of a region $\mathcal{V}$ of $\mathcal{G}$ is

$$V = \sum_{(k,l,m,n)\in\mathcal{V}} (k,l,m,n) \tag{16}$$

with oriented boundary ∂V and β is any 2-field, one finds $\langle d\beta, V\rangle = \langle \beta, \partial V\rangle$, which is the divergence theorem. Thus, combining every case, we have the Stokes theorem

$$\langle d\psi, \Omega\rangle = \langle \psi, \partial\Omega\rangle. \tag{17}$$

The dual correspondence between points and volumes and between lines and planes plays a role quite similar to the

Hodge star duality in the theory of differential forms [5]. If $\mathcal{G}$ is embedded in three dimensions, the cells or 3-simplices are associated pairwise by shared faces in the same way vertices are associated pairwise by the edges joining them. The dual graph $\star\mathcal{G}$, the vertices of which are the 3-simplices of $\mathcal{G}$, must be augmented by an external point to represent the region external to $\mathcal{G}$, and even after augmentation $\star\mathcal{G}$ does not correspond to a triangulation. Although the duality between ∂ and d can often be visualized easily in terms of $\star\mathcal{G}$, one should note that the simplices actually dealt with are always those of $\mathcal{G}$. We use this duality to generalize Stokes theorem somewhat further and arrive at a complete set of vector operators.

The divergence theorem derived above for 2-fields makes use of the 3-simplex content V of a region $\mathcal{V}$ of $\mathcal{G}$. But in view of duality one could as well fill $\mathcal{V}$ with vertices and consider the 1-simplex content

$$\star V=\sum_{n\in\mathcal{V}}(n). \tag{18}$$

Then the coboundary is

$$d\star V=\sum_{n\in\mathcal{V}}\sum_{m@n}(m,n). \tag{19}$$

Since (m,n) points from m to n, the coboundary is directed inward rather than outward. Hence, if α is a 1-field,

$$\langle\partial\alpha,\star V\rangle=\langle\alpha,d\star V\rangle. \tag{20}$$

This is the dual of the divergence theorem. Since $d\star V$ is oriented inward, one arrives once again at $-\partial\alpha=\mathrm{div}\alpha$.

An oriented 1-chain content can be assigned likewise to a surface $\mathcal{S}$ by counting the oriented bonds or 1-simplices that pierce $\mathcal{S}$. In this case $\mathcal{S}$ may be thought of not as a subset of $\mathcal{G}$ but as a curved surface passing through $\mathcal{G}$ in such a way as to sever all bonds attaching $\mathcal{V}$ to the rest of $\mathcal{G}$. This is consistent of course with our handling of the coboundary $d\star V$. Hence let

$$\star S=\sum_{(m,n)\in\mathcal{S}}(m,n). \tag{21}$$

So S is the sum over all bonds piercing $\mathcal{S}$ in a sense chosen as positive. Thus,

$$d\star S=\sum_{(m,n)\in\mathcal{S}}\sum_{l@[m,n]}(l,m,n), \tag{22}$$

so that the right-hand side of

$$\langle\partial\beta,\star S\rangle=\langle\beta,d\star S\rangle \tag{23}$$

receives unbalanced contributions only when the curve bounding $\mathcal{S}$ passes through a triangle (l,m,n). This result is the dual Stokes theorem in three dimensions for 2-fields.

In the same way, if $\star C$ is the 3-simplex content of a curve $\mathcal{C}$ defined by a string of oriented tetrahedra through which $\mathcal{C}$ passes, and γ is any 3-field, we have

$$\langle\partial\gamma,\star C\rangle=\langle\gamma,d\star C\rangle, \tag{24}$$

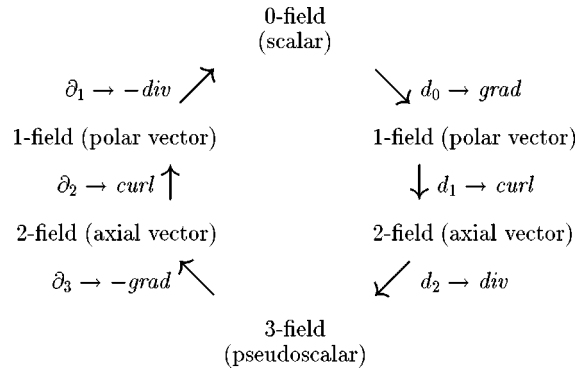

FIG. 1. Correspondence between differential operators and boundary and coboundary maps.

which is dual to the fundamental theorem of calculus. Combining results, we have the dual Stokes theorem:

$$\langle\partial\psi,\star\Omega\rangle=\langle\psi,d\star\Omega\rangle. \tag{25}$$

IV. VECTOR OPERATORS

The relation $\langle d\alpha,S\rangle=\langle\alpha,\partial S\rangle$ identifies $d\alpha$ as curlα when α is a 1-field. There is a simple geometrical meaning. Suppose α contains the 1-simplex (q,r). The coboundary $d\alpha$ contains $d(q,r)$ which is a sum over oriented triangles, the normal vectors of which circulate about (q,r) right-handedly. The coefficient of (m,n,p) in $d\alpha$ is $\alpha_{np}+\alpha_{pm}+\alpha_{mn}$, which is the limiting form of the right-hand circulation of α around (m,n,p). The identity $d^2\phi=0$ for an arbitrary 0-field ϕ corresponds to curl(gradϕ)$=0$.

The identity $\langle d\beta,V\rangle=\langle\beta,\partial V\rangle$ implies that $d\beta$ is divβ when β is a 2-field in the following way. First consider an arbitrary 2-simplex (p,q,r) in β. For simplicity suppose it is in the interior of $\mathcal{G}$. The coboundary $d(p,q,r)$ contains exactly two oriented tetrahedra, (n_1,p,q,r) and (n_2,p,q,r). Both appear with positive sign in $d(p,q,r)$, so one of them, say (n_1,p,q,r), is oriented positive outward and the other (n_2,p,q,r) inward. Thus the coefficient in $d\beta$ of an arbitrary 3-simplex (n,p,q,r) oriented outward is $\beta_{pqr}+\beta_{rqn}+\beta_{npr}+\beta_{qpn}$, which is the sum of the 2-vector currents outward. Divergence is the limiting form of the net outward flux. The identity $d^2\alpha=0$ for α a 1-field corresponds to div(curlα) $=0$. From the dual Stokes theorem one finds also that $-\partial\gamma$ is the gradient of the 3-field γ and, from Stokes theorem, that $\partial\beta$ is curlβ for a 2-field.

The vector difference operators in terms of ∂ and d are summarized schematically in Fig. 1. From the vector identity curl(curl$\vec{A}$)$=$grad(div$\vec{A}$)$-\nabla^2\vec{A}$, we find that the Laplacian for α either a 1- or a 2-field is

$$\nabla^2\alpha=-(d\partial+\partial d)\alpha. \tag{26}$$

The Laplacian for 3-fields, which are pseudoscalars, is $\nabla^2\gamma=-d\partial\gamma$. In summary, the Laplacian operator for a general p-field is

$$\nabla^2=-(d\partial+\partial d). \tag{27}$$

We shall see in Sec. VIII that the two operators ∂d and $d\partial$ when acting on all of $\mathcal{G}$ are each Hermitian with non-

negative eigenvalues, so that the eigenvalues of ∇^2 are nonpositive. Addition of the quadrature weights needed to make the combinatorial framework into a *bona fide* numerical method, as discussed in Sec. VII, introduces positive constants a and b so that $\nabla^2=-(ad\partial+b\partial d)$, which has all the same qualitative properties.

V. VECTOR IDENTITIES

The program of this section is to construct vector difference identities as similar as possible to those of vector calculus. The way to do this is to make judicious choices for definitions of the various scalar, dot, and cross products of p-fields so as to force each identity, taking the identities in order of increasing complexity and the fields in order, generally, of increasing p. In many cases alternative identities exist which provide an internal consistency check. In the end, for identities involving products of three or more fields, it is impossible to match all the continuum identities, because the nonlocality of the p-simplex basis makes these products behave differently. This is seen to be a necessary consequence of the discrete formulation.

Applying d and ∂ equivalents of divergence, gradient, and curl to properly chosen products leads directly to difference analogs of the familiar identities of vector calculus. The products are expressible in terms of either the field components or products of basic simplices. The differential identities of vector calculus are

$$\vec{\nabla}(fg)=f\vec{\nabla}g+g\vec{\nabla}f, \tag{28}$$

$$\vec{\nabla}\cdot(f\vec{A})=f(\vec{\nabla}\cdot\vec{A})+\vec{A}\cdot\vec{\nabla}f, \tag{29}$$

$$\vec{\nabla}\times(f\vec{A})=f(\vec{\nabla}\times\vec{A})-\vec{A}\times\vec{\nabla}f, \tag{30}$$

$$\vec{\nabla}(\vec{A}\cdot\vec{B})=(\vec{A}\cdot\vec{\nabla})\vec{B}+(\vec{B}\cdot\vec{\nabla})\vec{A} +\vec{A}\times(\vec{\nabla}\times\vec{B})+\vec{B}\times(\vec{\nabla}\times\vec{A}), \tag{31}$$

$$\vec{\nabla}\cdot(\vec{A}\times\vec{B})=\vec{B}\cdot(\vec{\nabla}\times\vec{A})-\vec{A}\cdot(\vec{\nabla}\times\vec{B}), \tag{32}$$

$$\vec{\nabla}\times(\vec{A}\times\vec{B})=\vec{A}(\vec{\nabla}\cdot\vec{B})-\vec{B}(\vec{\nabla}\cdot\vec{A}) +(\vec{B}\cdot\vec{\nabla})\vec{A}-(\vec{A}\cdot\vec{\nabla})\vec{B}. \tag{33}$$

Corresponding scalar and vector products, for both 1- and 2-fields, are deduced systematically, starting from the differential identities, by substituting the difference representation for each term and using the correspondence between the vector differential and difference operators. By isolating the residual terms in the difference expression, the definition required for each type of product is determined hierarchically.

We denote 0-fields by ϕ and ψ, 1-fields by α and σ, 2-fields by β and δ, and 3-fields by γ and λ. The natural definition for scalar-scalar multiplication is

$$\phi\psi=\sum_{[m]}\phi_m\psi_m(m). \tag{34}$$

Applying the difference gradient d_0 yields

$$d_0(\phi\psi)=\sum_{[m,n]}\frac{1}{2}(\phi_m+\phi_n)(\psi_n-\psi_m)(m,n) +\sum_{[m,n]}\frac{1}{2}(\psi_m+\psi_n)(\phi_n-\phi_m)(m,n). \tag{35}$$

Since $d_0\phi=\Sigma_{[m,n]}(\phi_n-\phi_m)(m,n)$, the form of the gradient of $\phi\psi$ prompts the definition of 0-field–1-field scalar multiplication,

$$\phi\alpha=\sum_{[m,n]}\frac{1}{2}(\phi_m+\phi_n)\alpha_{mn}(m,n), \tag{36}$$

which reduces $d_0(\phi\psi)$ to

$$d_0(\phi\psi)=\phi(d_0\psi)+\psi(d_0\phi), \tag{37}$$

the 0-field equivalent of Eq. (28). This example illustrates the general approach.

The 1-field equivalent of the identity Eq. (29) is obtained from applying $-\partial_1$ to the definition Eq. (36),

$$-\partial_1(\phi\alpha)=-\partial_1\left[\sum_{[m,n]}\frac{1}{2}(\phi_m+\phi_n)\alpha_{mn}(m,n)\right]. \tag{38}$$

Carrying out the operation on the right-hand side yields

$$-\partial_1(\phi\alpha)=\sum_{[m]}\phi_m\left[\sum_{n@m}\alpha_{mn}\right](m) +\sum_{[m]}\left[\sum_{n@m}\frac{1}{2}(\phi_n-\phi_m)\alpha_{mn}\right](m). \tag{39}$$

Utilizing Eq. (34) for scalar-scalar multiplication and defining the dot product for 1-fields as

$$\alpha\cdot\sigma=\sum_{[m]}\frac{1}{2}\left[\sum_{n@m}\alpha_{mn}\sigma_{mn}\right](m) \tag{40}$$

reduces $-\partial_1(\phi\alpha)$ to

$$-\partial_1(\phi\alpha)=\phi(-\partial_1\alpha)+\alpha\cdot d_0\phi. \tag{41}$$

This is the 1-field equivalent of the vector identity Eq. (29). The dot product defined in Eq. (40) has the necessary symmetry and linearity, together with the property that $\alpha\cdot\alpha=0$ if and only if $\alpha=0$.

Applying d_1 to $\phi\alpha$ results in

$$d_1(\phi\alpha)=\sum_{[l,m,n]}\frac{1}{3}(\phi_l+\phi_m+\phi_n)(\alpha_{mn}-\alpha_{ln}+\alpha_{lm})(l,m,n)$$
$$+\sum_{[l,m,n]}\frac{1}{6}\{[(\phi_n-\phi_l)+(\phi_m-\phi_l)]\alpha_{mn}-[(\phi_l-\phi_m)+(\phi_n-\phi_m)]\alpha_{ln}$$
$$+[(\phi_l-\phi_n)+(\phi_m-\phi_n)]\alpha_{lm}\}(l,m,n). \tag{42}$$

The first sum suggests taking the definition of 0-field–2-field scalar multiplication as

$$\phi\beta=\sum_{[l,m,n]}\frac{1}{3}(\phi_l+\phi_m+\phi_n)\beta_{lmn}(l,m,n), \tag{43}$$

which continues the pattern in Eqs. (34) and (36) of spreading the scalar amplitude out equally over the vector components. Reorganizing the second sum on the right-hand side of Eq. (42) and comparing to Eq. (30) implies that the equivalent vector product for 1-fields must be

$$\alpha\times\sigma=\sum_{[l,m,n]}\frac{1}{6}[(\alpha_{ln}+\alpha_{lm})\sigma_{mn}-(\alpha_{ml}+\alpha_{mn})\sigma_{ln}+(\alpha_{nl}+\alpha_{nm})\sigma_{lm}](l,m,n). \tag{44}$$

Then using $d_1\alpha$ and $d_0\phi$ simplifies Eq. (42) for $d_1(\phi\alpha)$ to

$$d_1(\phi\alpha)=\phi(d_1\alpha)-\alpha\times d_0\phi, \tag{45}$$

a form equivalent to that of the identity Eq. (30). The cross product Eq. (44) of two 1-fields is antisymmetric and gives a 2-field, as required by parity.

Applying d_2 and ∂_2 separately to definition Eq. (43) for $\phi\beta$ induces difference identities equivalent to Eqs. (29) and (30) for 2-fields. Thus d_2 acting on $\phi\beta$ yields

$$d_2(\phi\beta)=\sum_{[k,l,m,n]}\frac{1}{4}(\phi_k+\phi_l+\phi_m+\phi_n)(\beta_{lmn}-\beta_{kmn}+\beta_{kln}-\beta_{klm})(k,l,m,n)+\sum_{[k,l,m,n]}\frac{1}{12}[(\phi_l+\phi_m+\phi_n-3\phi_k)\beta_{lmn}$$
$$-(\phi_k+\phi_m+\phi_n-3\phi_l)\beta_{kmn}+(\phi_k+\phi_l+\phi_n-3\phi_m)\beta_{kln}-(\phi_k+\phi_l+\phi_m-3\phi_n)\beta_{klm}](k,l,m,n). \tag{46}$$

Using the component expressions for $d_2\beta$ and $d_0\phi$ and defining 0-field–3-field scalar multiplication so as to spread the scalar amplitudes out equally over the pseudoscalar tetrahedra,

$$\phi\gamma=\sum_{[k,l,m,n]}\frac{1}{4}(\phi_k+\phi_l+\phi_m+\phi_n)\gamma_{klmn}(k,l,m,n), \tag{47}$$

suggests defining the 1-field–2-field dot product as

$$\alpha\cdot\beta=\sum_{[k,l,m,n]}\frac{1}{12}[(\alpha_{kl}+\alpha_{km}+\alpha_{kn})\beta_{lmn}-(\alpha_{lk}+\alpha_{lm}+\alpha_{ln})\beta_{kmn}+(\alpha_{mk}+\alpha_{ml}+\alpha_{mn})\beta_{kln}$$
$$-(\alpha_{nk}+\alpha_{nl}+\alpha_{nm})\beta_{klm}](k,l,m,n), \tag{48}$$

which reduces $d_2(\phi\beta)$ to

$$d_2(\phi\beta)=\phi(d_2\beta)+\beta\cdot d_0\phi. \tag{49}$$

The latter is the 2-field equivalent of vector identity Eq. (29). Thus the dot product of a 1- and a 2-field is a 3-field, which is consistent with the fact that a continuum vector dotted into a pseudovector gives a pseudoscalar.

Similarly, applying ∂_2 to $\phi\beta$ gives

$$\partial_2(\phi\beta)=\sum_{[m,n]}\frac{1}{2}(\phi_m+\phi_n)\left[\sum_{l@(m,n)}\beta_{lmn}\right](m,n)$$
$$+\sum_{[m,n]}\frac{1}{6}\left[\sum_{l@(m,n)}(2\phi_l-\phi_m-\phi_n)\beta_{lmn}\right](m,n). \tag{50}$$

Then recognizing $\partial_2\beta$, $d_0\phi$, and $\phi\alpha$ and defining

$$\alpha\times\beta=\sum_{[m,n]}\frac{1}{6}\left[\sum_{l@(m,n)}(\alpha_{ml}+\alpha_{nl})\beta_{lmn}\right](m,n), \tag{51}$$

one arrives at

$$\partial_2(\phi\beta)=\phi(\partial_2\beta)-\beta\times d_0\phi, \tag{52}$$

which is equivalent to Eq. (30).

From the formulas for $d_1\alpha$, $\alpha\times\sigma$, and $\alpha\cdot\beta$, it is easily seen that

$$d_2(\alpha\times\sigma)=\sigma\cdot d_1\alpha-\alpha\cdot d_1\sigma, \tag{53}$$

a 1-field–1-field difference equivalent to Eq. (32) for the divergence of a cross product.

Finally, to obtain a discrete form of $(\vec{v}\cdot\vec{\nabla})\vec{u}$, which appears in the convective derivative $D/Dt=\partial/\partial t+\vec{v}\cdot\vec{\nabla}$ of a vector, for example, it is convenient to begin by adding differential identities Eqs. (31) and (33). This gives

$$\begin{aligned}\vec{\nabla}(\vec{A}\cdot\vec{B})+\vec{\nabla}\times(\vec{A}\times\vec{B})&\\ =2(\vec{B}\cdot\vec{\nabla})\vec{A}+\vec{A}\times(\vec{\nabla}\times\vec{B})+\vec{B}\times(\vec{\nabla}\times\vec{A})&\\ +\vec{A}(\vec{\nabla}\cdot\vec{B})-\vec{B}(\vec{\nabla}\cdot\vec{A}).&\end{aligned} \tag{54}$$

Each term has a difference equivalent already determined, except $(\vec{B}\cdot\vec{\nabla})\vec{A}$. Thus, the equivalent difference form is

$$\begin{aligned}(\sigma\cdot\vec{\nabla})\alpha=\frac{1}{2}[\partial_2(\alpha\times\sigma)+d_0(\alpha\cdot\sigma)-\alpha\times d_1\sigma&\\ -\sigma\times d_1\alpha+\alpha(\partial_1\sigma)-\sigma(\partial_1\alpha)].&\end{aligned} \tag{55}$$

A special case of interest is $v\cdot(\vec{\nabla}v)=(1/2)d(v\cdot v)-v\times(dv)$, which appears in the Navier-Stokes equation for the velocity 1-field v. If an explicit formula for components is required, substitute the component expansion for each term and simplify the summations using the adjacency matrix H. This gives

$$\begin{aligned}\frac{1}{4}\sum_{[m,n]}\sum_{l}\Big\{&H_{lm}[\sigma_{mn}\alpha_{ml}-\sigma_{ml}(\alpha_{mn}+\alpha_{ml})]\\ &+H_{ln}[\sigma_{mn}\alpha_{nl}-\sigma_{nl}(\alpha_{mn}-\alpha_{nl})]\\ &+\frac{1}{3}H_{lm}H_{ln}[\sigma_{ml}(2\alpha_{ml}-\alpha_{nl})+\sigma_{nl}(\alpha_{ml}-2\alpha_{nl})\\ &-2\sigma_{mn}(\alpha_{ml}+\alpha_{nl})]\Big\}(m,n),\end{aligned} \tag{56}$$

where the summation over l can extend over all 0-simplices since the adjacency matrix H vanishes for nonadjacent index pairs.

The rules equivalent to scalar multiplication, scalar products, and vector products introduced above can be generated in an alternative way by defining the corresponding products of basis simplices. This is simplified by introducing the inner products. Note, however, that each of the following formulas assumes that the ordered sets of indices listed do indeed represent simplices of $\mathcal{G}$. Otherwise the inner product should be zero. To guarantee this, each ordered p-tuple can be multiplied by appropriate entries of the adjacency matrix H. Thus, (k,l,m) can be replaced by $H_{kl}H_{lm}H_{mk}(k,l,m)$ to ensure it does represent a simplex. The formulas as listed handle the sign changes due to vertex order, unless otherwise noted. Thus

$$\langle(m),(n)\rangle=\delta_{mn}, \tag{57}$$

$$\langle(k,l),(m,n)\rangle=\det\begin{bmatrix}\delta_{km}&\delta_{kn}\\ \delta_{lm}&\delta_{ln}\end{bmatrix}, \tag{58}$$

or in general

$$\langle(k,\ldots,l),(m,\ldots,n)\rangle=\det\begin{bmatrix}\delta_{km}&\cdots&\delta_{kn}\\ \vdots&\ddots&\vdots\\ \delta_{lm}&\cdots&\delta_{ln}\end{bmatrix}. \tag{59}$$

The equivalent of scalar multiplication $\phi\psi=\Sigma_{[m]}\phi_m\psi_m(m)$ can be rewritten, using the simplex basis set of the fields and the inner product rule, as

$$\langle(l)(m),(n)\rangle=\delta_{ln}\delta_{mn}=\langle(l),(n)\rangle\langle(m),(n)\rangle. \tag{60}$$

Thus, with $\phi=\Sigma_{[l]}\phi_l(l)$ and $\psi=\Sigma_{[m]}\psi_m(m)$,

$$\begin{aligned}\langle\phi\psi,(n)\rangle&=\sum_{[l]}\sum_{[m]}\phi_l\psi_m\langle(l)(m),(n)\rangle\\ &=\sum_{[l]}\sum_{[m]}\phi_l\psi_m\delta_{ln}\delta_{mn}=\phi_n\psi_n,\end{aligned} \tag{61}$$

similarly the product $\phi\alpha$ can be rewritten in terms of the simplex basis sets and inner product as

$$\begin{aligned}\langle(j)(k,l),(m,n)\rangle&=\frac{1}{2}(\delta_{jk}+\delta_{jl})(\delta_{km}\delta_{ln}-\delta_{kn}\delta_{lm})\\ &=\frac{1}{2}[\langle(j),(k)\rangle+\langle(j),(l)\rangle]\langle(k,l),(m,n)\rangle.\end{aligned} \tag{62}$$

So, with $\phi=\Sigma_{[j]}\phi_j(j)$ and $\alpha=\Sigma_{[k,l]}\alpha_{kl}(k,l)$,

$$\langle\phi\alpha,(m,n)\rangle=\sum_{[j]}\sum_{[k,l]}\phi_j\alpha_{kl}\langle(j)(k,l),(m,n)\rangle. \tag{63}$$

Substituting for the inner product and assuming, for purposes of summation, that the pair (m,n) represents a properly ordered simplex,

$$\langle\phi\alpha,(m,n)\rangle=\frac{1}{2}(\phi_m+\phi_n)\alpha_{mn}. \tag{64}$$

The products $\phi\beta$ and $\phi\gamma$ rewritten in terms of simplex basis and inner product are

$$\langle (h)(i,j,k),(l,m,n)\rangle = \frac{1}{3}\left[\langle (h),(i)\rangle + \langle (h),(j)\rangle + \langle (h),(k)\rangle\right]\langle (i,j,k),(l,m,n)\rangle, \tag{65}$$

$$\langle (f\,)(g,h,i,j),(k,l,m,n)\rangle = \frac{1}{4}\left[\langle (f\,),(g)\rangle + \langle (f\,),(h)\rangle + \langle (f\,),(i)\rangle + \langle (f\,),(j)\rangle\right]\langle (g,h,i,j),(kl,m,n)\rangle. \tag{66}$$

By applying the same treatment to the scalar and vector products, respectively, one obtains

$$\langle (j,k)\cdot(l,m),(n)\rangle = \frac{1}{2}[\langle (j),(n)\rangle + \langle (k),(n)\rangle]\langle (j,k),(l,m)\rangle, \tag{67}$$

$$\langle (h,i)\times(j,k),(l,m,n)\rangle = \frac{1}{6}\{[\langle (h),(j)\rangle + \langle (i),(j)\rangle]\langle (h,i,k),(l,m,n)\rangle - [\langle (h),(k)\rangle + \langle (i),(k)\rangle]\langle (h,i,j),(l,m,n)\rangle\}, \tag{68}$$

$$\langle (f,g)\cdot(h,i,j),(k,l,m,n)\rangle = \frac{1}{12}\{[\langle (g),(h)\rangle + \langle (g),(i)\rangle + \langle (g),(j)\rangle]\langle (f,h,i,j),(k,l,m,n)\rangle - [\langle (f\,),(h)\rangle + \langle (f\,),(i)\rangle + \langle (f\,),(j)\rangle]\langle (g,h,i,j),(k,l,m,n)\rangle\}, \tag{69}$$

$$\langle (h,i)\times(j,k,l),(m,n)\rangle = \frac{1}{6}\{[\langle (h,i),(l,j)\rangle - \langle (h,i),(j,k)\rangle]\langle (k,l),(m,n)\rangle + [\langle (h,i),(j,k)\rangle - \langle (h,i),(k,l)\rangle]\langle (l,j),(m,n)\rangle + [\langle (h,i),(k,l)\rangle - \langle (h,i),(l,j)\rangle]\langle (j,k),(m,n)\rangle\}. \tag{70}$$

The geometrical meaning of the dot and cross products of 1- and 2-fields is interesting. Equation (67) shows that the dot product of 1-simplices is purely local, in that $(j,k)\cdot(l,m)$ is zero unless the two bonds coincide, and if they do the result is ± 1 depending on relative sense.

The cross product of two 1-fields generated by Eq. (68) is slightly less local, since $(h,i)\times(l,m)$ is nonzero whenever the two bonds form two sides of a triangle. If the orientation of the two directed bonds is head to tail, then the result is the completed 2-simplex oriented consistently with the bond directions, or in other words the two bonds form part of the oriented boundary of the 2-simplex. On the other hand, if the two 1-simplices meet head to head or join tail to tail, then the right-hand rule applies. One can always reduce a nonzero product to a standard case by permuting indices and keeping track of the sign. The nonlocality of the product is manifest in the involvement in the product of an extra bond, the third leg of the 2-simplex triangle in the product.

As seen in Eq. (69), the dot product of a 1-field with a 2-field is a 3-field. This is necessary since the contraction of a vector with a pseudovector must yield a pseudoscalar. In the continuum formulation this is so because of parity with respect to space inversion. In the discrete calculus it is required due to parity with respect to reversal of the vertex collating sequence. Nonlocality results again from the introduction of bonds for completion of the 3-simplex. When the 1-simplex (f,g) does not intersect (h,i,j) the product is zero. The product is also zero if the bond (f,g) lies completely on the boundary of (h,i,j), which is the discrete analog of orthogonality between 1- and 2-fields. Otherwise, the product is $+(f,h,i,j)$ if the bond intersects the triangle at $g=h$, thus making an oriented polygonal path from f to h to i to j. Other cases can be computed by permuting the indices and keeping track of the sign. Similarly, Eq. (70) shows that the cross product of a 1-field with a 2-field gives a 1-field, as again is required by consideration of parity.

As mentioned above, a product of three or more field quantities is generally not analogous to the continuum counterpart. This arises due to nonlocality of multiplication. Thus the cyclical invariance of the scalar triple product, $\vec{A}\cdot(\vec{B}\times\vec{C})$, does not hold, nor does the identity $\vec{A}\times(\vec{B}\times\vec{C}) = \vec{B}(\vec{A}\cdot\vec{C}) - \vec{C}(\vec{A}\cdot\vec{B})$. For example, consider the triple product $P=(1,2)\cdot[(2.3)\times(3,4)]$, where (1,2,3,4) is an oriented 3-simplex. The value of the triple product is well defined, using the rules derived above, and it is the simplex (1,2,3,4) itself. However, if the multiplicands are permuted in cyclic order, one has, for example, $(2,3)\cdot[(3,4)\times(1,2)]$, and this product is strictly zero, since the bonds (3,4) and (1,2) are disjoint, representing skew edges of the tetrahedron. This failure is due to nonlocality of the products. In continuous space one can translate vectors at different points, by means of a connection recipe, and compare them at the same point. In the discrete case the tangent spaces at adjacent points overlap but not completely. This difference stemming from nonlocality is characteristic of a discrete formulation and is unavoidable in vector identities containing three or more vectors. This has to be taken into account when using the vector difference formalism, although at this point it does not appear to be a very serious drawback.

We note that the scalar, dot, and cross products of p-fields defined above must relate to the cap and cup products of simplicial homology theory. [8] The vector identities could be induced by representing the continuous fields as differential forms [5] and then comparing the Leibnitz rule for exterior differentiation of the wedge product of differential forms to the boundary formula for the cup product, as reflected in

Eqs. (41) and (52), and the coboundary formula for the cap product, as in Eqs. (37), (45), (41), and (53). However, the route we have chosen seems to us more natural and better motivated.

Thus we have been able to construct identities involving 0-, 1-, and 2-fields that are exact analogs for most of the corresponding differential identities of vector calculus. In the next section, we illustrate how to use them to construct physical models.

VI. PHYSICAL MODELS ON LATTICES

As examples of physical lattice models, we construct difference forms of the Maxwell electromagnetic theory, the Navier-Stokes equation for solenoidal (i.e., incompressible) flow, and the Navier linearized equation of motion for an isotropic elastic medium. The first example is developed in more detail to show application of the difference calculus for deriving model properties. Similar manipulations can be made for the other two models to obtain energy transport expressions. The main point of each example is to illustrate the use of the formalism for constructing a lattice model.

A. Lattice electromagnetism

As a first example we develop a discrete Maxwell electromagnetic theory on a general graph. Though austere, the formulation shares interesting properties with the familiar PDEs of electromagnetism.

One can see the bonds of $\mathcal{G}$ as conducting wires. Thus we choose charge ρ to be a 0-field on vertices acting as capacitors, and current J to be a 1-field associated with bonds acting as wires. Let time t remain continuous, so that charge conservation results in an equation of continuity

$$-\partial J+\dot{\rho}=0, \tag{71}$$

where the dot indicates time derivative d/dt. The Maxwell difference equations become

$$\partial E=-\rho, \tag{72}$$

$$dB=0, \tag{73}$$

$$dE+\dot{B}=0, \tag{74}$$

$$\partial B-\dot{E}=J. \tag{75}$$

Evidently in this formulation the electric field E is a 1-field and the magnetic field B is a 2-field.

One cannot conclude that $dB=0$ implies $B=dA$. For general $\mathcal{G}$, $B=dA+\Gamma$, where Γ has a vanishing coboundary, so that B consists of a curl and a globally circulating part Γ with a vanishing local curl. This corresponds roughly to a B field forming closed loops within the space such that field lines thread around a handle. Thus, for example, $\mathcal{G}$ could be the space inside a toroidal solenoid. If we exclude this possibility, so that $B=dA$, then $d(E+\dot{A})=0$ shows $E=-\dot{A}-d\phi+\Lambda$, where Λ with vanishing coboundary also represents a kind of global circulation. In other words, Λ is a static electric field contribution with closed loops. It is not a static solution of Maxwell's PDEs and would correspond to a time varying magnetic flux in space outside the graph through a handle of $\mathcal{G}$. If we exclude this possibility as well, $E=-\dot{A}-d\phi$. We refer to the dropping of Γ and Λ as Helmholtz conditions. The topic of fields such as Γ and Λ will be taken up in detail in the following section.

One finds wave equations for E and B from the Maxwell equations:

$$-(d\partial+\partial d)E-\ddot{E}=\dot{J}+d\rho, \tag{76}$$

$$-(d\partial+\partial d)B-\ddot{B}=dJ. \tag{77}$$

These correspond to the usual wave equations with source terms. It is important to bear in mind, however, that they are not approximations to continuum wave equations but follow rigorously from the discrete model.

With Helmholtz conditions one can derive coupled wave equations for the gauge potentials (ϕ,A). With the Lorentz condition $\dot{\phi}-\partial A=0$ these decouple to give

$$-(d\partial+\partial d)\phi-\ddot{\phi}=-\rho, \tag{78}$$

and

$$-(d\partial+\partial d)A-\ddot{A}=-J. \tag{79}$$

One obtains a discrete version of the Poynting theorem from the lattice field equations using the vector identities proven in the preceding section. Transfer from the field to charged matter is $E\cdot J$. Eliminating J using the inhomogeneous equation $\partial B=J+\dot{E}$ gives

$$J\cdot E=E\cdot\partial B-E\cdot\dot{E}. \tag{80}$$

In view of the vector identity for the boundary of a cross product of a 1-field E and a 2-field B,

$$-\partial(E\times B)=B\cdot dE-E\cdot\partial B, \tag{81}$$

one has

$$J\cdot E=B\cdot dE+\partial(E\times B)-E\cdot\dot{E}. \tag{82}$$

Then using the lattice Maxwell equation for coboundary of E yields the discrete Poynting theorem

$$J\cdot E=\partial S-\dot{U}, \tag{83}$$

where S is the Poynting vector 1-field

$$S=E\times B \tag{84}$$

and U is the field energy

$$U=\frac{1}{2}(E\cdot E+B\cdot B). \tag{85}$$

Interpretation of S as electromagnetic energy flux, and indeed of U as field energy in the model, would at first seem more difficult than for continuum fields because of multiple connectedness. But this is not the case. Consider an arbitrary, simply connected $\star V$ in $\mathcal{G}$. One has

$$\langle \partial S, \star V \rangle = \langle S, d\star V \rangle = \langle J \cdot E, \star V \rangle + \frac{d}{dt} \langle U, \star V \rangle. \quad (86)$$

Because the coboundary of $\star V$ is oriented inward, one would like to conclude, topological subtleties not withstanding, that the inward Poynting flux $\langle S, d\star V \rangle$ equals the rate of energy transfer out of the field to the charged matter in $\star V$, plus the rate of increase of the integral of U within $\star V$. When $\star V$ includes all vertices in $\mathcal{G}$, then there is no coboundary and the two volume integrals cancel. This helps identify U with the field energy. Thus for an arbitrary $\star V$ one arrives at the usual interpretation of the surface integral of S as electromagnetic energy flux. So in general one may surmise that for any orientable surface, not necessarily closed, the electromagnetic energy flux is given by a similar surface integral. The difficulty in making this identification rigorously, just as in the continuum case, is that the Poynting theorem only gives the energy flux modulo quantities that always integrate to zero over any closed surface, i.e., over any $d\star V$.

The discrete Poynting theorem is a good example of a conservation theorem that holds exactly for the discrete model, not just as an approximation to the continuum result. It can be used to implement computational strategies or derive further results. It is a constraint that will be satisfied exactly.

Electromagnetic theory really requires all three spatial dimensions. For fluid motion or some electrostatics problems, two dimensions is sufficient, so that the regular triangular lattice can be used. Unfortunately there is no regular triangulation of three-dimensional space. However, any triangulation will suffice. One can use a triangulation based on a subdivision of the NaCl lattice structure. Thus lattice points are of two inequivalent types occupying interpenetrating fcc lattices. Bonds connect type 1 sites to each nearest type 1 or type 2 site, and type 2 sites to each neighboring type 1 site only. The triangulation then consists of two types of tetrahedra, one regular and one rectangular, and the lattice resembles the face centered hypercubic one used for lattice gas simulations [6].

Consider any cluster subset of the lattice, perhaps a cube or perhaps a percolation cluster. Suppose the boundary of the cluster is a perfect conductor and inside is hollow, and that one needs to know the electromagnetic modes inside. Call the cluster $\mathcal{V}$, its conducting boundary $b=\partial\mathcal{V}$, and its hollow interior a.

On the conductor J_b and ρ_b adjust to keep $E_b=0$ and $\dot{B}_b=0$. The 1- and 2-fields E_b and $\dot{B}_b$ are analogs of $\vec{E}_{\|}$ and $\partial B_{\perp}/\partial t$. In the cavity, $J_a=0$ and $\rho_a=0$. Thus for normal modes one has

$$[\partial d]_{aa} E_a = \omega^2 E_a \quad (87)$$

and

$$[d\partial]_{aa} E_a = 0, \quad (88)$$

where the subscripts indicate that the matrices are first computed for the whole cluster and then projected onto a. The second equation ensures that no charge density appears in the cavity. With E_a one can compute both the magnetic field B_a and the surface charge and current densities ρ_b and J_b, etc.

B. Incompressible Navier-Stokes equations

The point of this subsection is to construct a nonlinear lattice model representing the flow of an incompressible fluid. The model should exhibit physical behavior including turbulence.

For incompressible flow, the Navier-Stokes equation for the velocity field is

$$\rho \frac{\partial \vec{v}}{\partial t} + \rho \vec{v} \cdot \vec{\nabla} \vec{v} = -\vec{\nabla} p + \mu \nabla^2 \vec{v}, \quad (89)$$

where ρ is the fluid density and μ is the viscosity, with the constraint that $\vec{\nabla} \cdot \vec{v} = 0$. Transcription of the nonlinear, inertial term into the lattice formulation is accomplished using the vector identity $v \cdot \vec{\nabla} v = \frac{1}{2} d(v \cdot v) - v \times (dv)$, derived above for a 1-field, to obtain

$$\rho \dot{v} + \frac{\rho}{2} d(v \cdot v) - \rho v \times (dv) = -dp - \mu \partial dv, \quad (90)$$

with the constraint

$$\partial v = 0 \quad (91)$$

expressing incompressibility. It is not convenient to integrate the lattice model forward in time as it stands, since the pressure is not known initially and because nonzero divergence introduced from any source is amplified in solving the equations and tends to diverge. To overcome this problem, a vector potential ψ (corresponding to the stream function) may be introduced so that $v = \partial\psi$. In this way, Eq. (91) is satisfied identically on the lattice. The stream function ψ is a 2-field. Since ψ is expanded in a basis of 2-simplices, the corresponding velocity 1-field consists of a sum of loop currents, and hence has zero Kirchhoff divergence automatically at each point. In other words, the computation takes place in a strictly divergence-free subspace of $\mathcal{C}_1$.

It is also convenient to introduce the 2-field $\omega = dv$ corresponding to the curl of the velocity, thus defining the vorticity. Applying the coboundary map to Eq. (90) and taking the constancy of ρ into account, it follows that

$$\rho d\dot{v} - \rho d[v \times (dv)] = -\mu d \partial dv, \quad (92)$$

i.e.,

$$\rho \dot{\omega} - \rho d(\partial\psi \times \omega) = -\mu d \partial \omega, \quad (93)$$

augmented by the equation expressing ω as the Laplacian of the stream function

$$\omega = d\partial\psi. \quad (94)$$

The solution of an incompressible flow problem on the lattice implies the solution of the coupled systems of Eqs. (93) and (94) for ω and ψ analogous to the continuous formulation [13]. As in Sec. VI A above for the difference Maxwell equations, integral conservation theorems can be obtained readily from the discrete formulation of the field equations. For example, consider the case of an inviscid (Eulerian) flow for which $\mu = 0$. In this case the vorticity equation simplifies to $\dot{\omega} = d(\partial\psi \times \omega)$. By taking the coboundary it follows that

$d\dot{\omega}=0$. Therefore, if V is the oriented 3-simplex content of a region $\mathcal{V}$ of a graph $\mathcal{G}$, it follows that $\langle d\dot{\omega},V\rangle=0=\langle\dot{\omega},\partial V\rangle$, therefore $\langle\omega,\partial V\rangle$ is constant, which corresponds to one consequence of the Kelvin theorem for inviscid flows.

C. Discrete model of elastic medium

From the Navier linearized model for an isotropic, homogeneous elastic medium

$$\rho\frac{\partial^2\vec{u}}{\partial t^2}=\mu\nabla^2\vec{u}+(\mu+\lambda)\vec{\nabla}(\vec{\nabla}\cdot\vec{u})+\vec{f}, \tag{95}$$

where u is the displacement field, ρ is the density, λ and μ are the Lamé constants, and $\vec{f}$ is a body force density, follows the lattice representation

$$\rho\ddot{u}=-[(2\mu+\lambda)d\partial+\mu\partial d]u+f. \tag{96}$$

Although the continuum model is for a homogeneous isotropic medium, the discrete model can be made very heterogeneous by choosing heterogeneous boundary conditions. The discrete elastic model can be developed on an arbitrary triangulating graph, such as a fattened percolation cluster. The simplest $u=0$ conditions on the boundary surface represent an elastic medium inside a cavity with fixed walls, similar to the boundary conditions for the electromagnetic cavities described above.

We consider briefly a comparison between cavity modes arising from the scalar Helmholtz equation and those arising from the electromagnetic or from the elastic vector model. Either the electromagnetic or the elastic problems are sometimes modeled by a scalar Helmholtz equation [14]. Taking zero field at the boundary for each case, the characteristic equations are

$$[\partial_2 d_1]_{aa}E_a=\omega^2E_a \tag{97}$$

for the electromagnetic,

$$[(2\mu+\lambda)d_0\partial_1+\mu\partial_2 d_1]_{aa}u_a=\omega^2u_a \tag{98}$$

for the elastodynamic, and

$$[\partial_1 d_0]_{a,a}\phi_a=\omega^2\phi_a \tag{99}$$

for the scalar Helmholtz equation. Ignoring the projection onto the cavity interior a, and taking into account the isomorphism between the scalar fields and the gradientlike vector fields, which is discussed in detail in Sec. VIII, it would seem that the operators ∂d and $d\partial$ of the elastodynamic case contribute electromagneticlike and scalar-Helmholtz-like character to the spectrum. The electromagnetic modes are primarily torsional, while the scalar modes relate simply to the compressional modes of vibration. In the case of a percolation cluster, or in any case where the boundary effects dominate, the separation does not hold, since ∂d and $d\partial$ do not remain orthogonal when projected onto a. Notice that the physical range of the Lamé constants is limited by the requirements that both μ and $\frac{2}{3}\mu+\lambda$ be non-negative. Thus the elastodynamic model is essentially bounded away from pure Helmholtz behavior. Introduction of quadrature weights does not remove this qualitative difference. The discrete lattice formulation i.e., Eqs. (97)–(99), delineates rather well the differences among the three types of cavity modes involving the scalar Helmholtz equation and electromagnetic and linear elastic models. This difference stems from the different admixture in each of the operators $[\partial_2 d_1]_{aa}$,$[(2\mu+\lambda)d_0\partial_1+\mu\partial_2 d_1]_{aa}$,$[\partial_1 d_0]_{aa}$, of the two distinct spectral contributions, one from the equivalent pair $\partial_1 d_0$, $d_0\partial_1$, and the other from $\partial_2 d_1$, accounting also for the boundary conditions. These spectral differences correlate with different van Hove singularities in the case of regular periodic lattices, and may correlate with different qualitative behavior (e.g., scaling behavior) in the case of highly disordered structures such as percolation clusters at the critical threshold.

VII. COMMENT ON NUMERICS

The current formulation should not be considered a numerical method, to be compared, for example, with finite element methods. Rather, it is a mathematical model of vector calculus itself, one in which there is a discrete counterpart for each of the integral theorems and most vector identities. By determination of quadrature weights appropriate to particular lattice types, as illustrated in this section for the triangular lattice, the formalism can accommodate a finite-difference-like numerical method. It can be adapted for use with other numerical methods as well.

A practical numerical method requires a recipe for transcribing back and forth between discrete and continuous field quantities and between difference and differential operators. The main ingredient is a set of weights chosen consistently in the following sense. If one projects the continuum field equations to get a difference system on the lattice and solves the difference system, the result should match the continuum solutions up to terms that vanish with the lattice spacing. One can generate such a correspondence by projecting and averaging over a suitably chosen cell centered on each vertex or lattice site. Consistency fixes the values of the weights that define two operators for each field type. In this section we treat the two-dimensional triangular lattice for which there are no 3-fields, and 2-fields take on the role of pseudoscalars.

Let a be the distance between sites on the triangular lattice. An averaging cell at vertex i is a system of p-simplices, for $p=0$, 1, or 2 centered at i, equipped with each of the sets of information, $\mathcal{S}_i^{(p)}$, $\mathcal{E}_i^{(p)}$, and $\mathcal{X}_i^{(p)}$, where p pertains to the simplex type. $\mathcal{S}_i^{(p)}$ is the set of p-simplices associated with the cell of i. $\mathcal{E}_i^{(p)}=\{\vec{e}_\alpha^{(p)}\}$ is a set of basis vectors and $\mathcal{X}_i^{(p)}$ is the set of baricentric coordinates associated with the simplices of $\mathcal{S}_i^{(p)}$. The choice of these sets is to some extent arbitrary, since averaging can be affected in different ways on the same lattice. We make it in such a way as to achieve a site-independent correspondence between lattice and continuum operators in the limit $a\to 0$.

A suitable averaging cell is indicated in Fig. 2(a). The set $\mathcal{S}_i^{(0)}$ contains only the site i which is associated with the zero-dimensional basis vector $\vec{e}_1^{(0)}=1$ and baricentric coordinates $\vec{x}_i^{(0)}=\vec{x}_i$. The set $\mathcal{S}_i^{(1)}$ contains the six 1-simplices (i,j) with $i@j$, the basis $\mathcal{E}_i^{(1)}$ contains six unit vectors $\vec{e}_\alpha^{(1)}=(\cos(2\pi\alpha/6),\sin(2\pi\alpha/6))$, $\alpha=0,\ldots,5$ pointing toward neighboring sites as illustrated, and the set $\mathcal{X}_i^{(1)}$ contains the

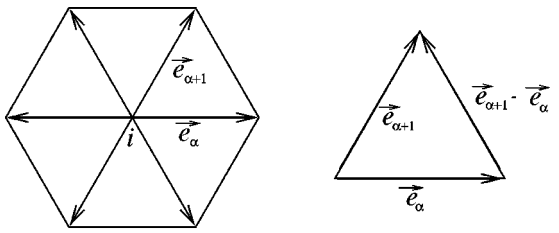

FIG. 2. (a) Averaging unit cell used for the triangular lattice. (b) Generic 2-simplex belonging to $\mathcal{S}_i^{(2)}$.

six bond-center coordinates $\vec{x}_{i\alpha}^{(1)}=\vec{x}_i+a\vec{e}_\alpha^{(1)}/2$. $\mathcal{S}_i^{(2)}$ contains the six 2-simplices built with neighboring sites j and k chosen to make (i,j,k) right-hand oriented so the associated $\mathcal{E}_i^{(2)}$ contains six vectors of the form $\vec{e}_\alpha^{(2)}=2(\vec{e}_\alpha^{(1)}\times\vec{e}_{\alpha+1}^{(1)})/\sqrt{3}$ and $\mathcal{X}_i^{(2)}$ is comprised of the triangle baricenters $\vec{x}_{i\alpha}^{(2)}=\vec{x}_i+a(\vec{e}_\alpha^{(1)}+\vec{e}_{\alpha+1}^{(1)})/3$. To simplify notation, let $v_{i\alpha}$ represent the 1-field component v_{ij} for $\vec{e}_\alpha^{(1)}$ along the bond (i,j), and $\beta_{i\alpha}$ represent the 2-field component β_{ijk} for $\vec{e}_\alpha^{(2)}$ oriented along the normal of (i,j,k). Notice the averaging cell is chosen symmetrically around site i so that, for this regular lattice example, the sums $E_m^{(1)}=\Sigma_\alpha e_{\alpha m}^{(1)}$ and $E_{mn}^{(2)}=\Sigma_\alpha e_{\alpha m}^{(1)}e_{\alpha n}^{(1)}$ of vector components give 0 and $3\delta_{mn}$, respectively [6]. The importance of these isotropy conditions will become clear presently.

Discrete field quantities are obtained by projecting continuous fields onto the lattice. Let $\phi(\vec{x})$ and $\vec{v}(\vec{x})$ be continuum scalar and polar vector fields, respectively, and let $\vec{\beta}(\vec{x})=\beta(\vec{x})\hat{z}$ be an axial vector field oriented normal to the surface. Components of the corresponding discrete fields are

$$\begin{aligned}\phi_i&=\phi(\vec{x}_i^{(0)})\cdot\vec{e}_1^{(0)},\\ v_{i\alpha}&=\vec{v}(\vec{x}_{i\alpha}^{(1)})\cdot\vec{e}_\alpha^{(1)},\\ \beta_{i\alpha}&=\vec{\beta}(\vec{x}_{i\alpha}^{(2)})\cdot\vec{e}_\alpha^{(2)},\end{aligned}\tag{100}$$

where the first equation reduces to $\phi_i=\phi(\vec{x}_i)$. The general projection procedure is $u_{i\alpha}=\Pi_i^{(p)}[u]=u(\vec{x}_i^{(p)})\cdot\vec{e}_\alpha^{(p)}$ for any p-field u.

To compare respective products and operators it becomes necessary to transport discrete vector field components, defined naturally on bonds or triangular plaquettes, back to the lattices sites. This is done by averaging. In a limited sense one can view it as comparing the discrete fields with continuous ones, as long as comparison takes place at a lattice site. Thus one wants to compare the continuum scalar, polar-vector, and axial-vector fields $\phi(\vec{x}_i)$, $\vec{v}(\vec{x}_i)$, and $\vec{\beta}(\vec{x}_i)$ evaluated at vertex i with the average values

$$\begin{aligned}\mathcal{A}_i^{(0)}[\phi]&=\phi_i\vec{e}_\alpha^{(0)},\\ \mathcal{A}_i^{(1)}[v]&=\frac{1}{3}\sum_\alpha v_{i\alpha}\vec{e}_\alpha^{(1)},\\ \mathcal{A}_i^{(2)}[\beta]&=\frac{1}{6}\sum_\alpha \beta_{i\alpha}\vec{e}_\alpha^{(2)},\end{aligned}\tag{101}$$

of the discrete fields. The numerical factors are lattice dependent, the values given being the ones for the triangular lattice. Thus, the first consistency condition is that

$$u(\vec{x}_i)=\mathcal{A}_i^{(p)}[\Pi_i^{(p)}[u]]+O(a),\tag{102}$$

for sufficiently well behaved continuum field $u(\vec{x})$ at each vertex i.

Vector difference operators divergence, gradient, and curl defined in Sec. IV are linear mappings $\psi:\mathcal{C}_p\to\mathcal{C}_q$, while the scalar, dot, and cross products defined in Sec. V are linear mappings from the Cartesian product $\psi:\mathcal{C}_p\times\mathcal{C}_q\to\mathcal{C}_r$, for appropriate choices of ranks p, q, and r. The form of ψ in each case is fixed by combinatorics. Let Ψ be the corresponding map defining a differential operator or product on continuous fields. Its definition comes from standard vector calculus. Thus for consistency of operators

$$\mathcal{A}_i^{(q)}[\psi(u)]=a^\gamma\frac{1}{\lambda_\psi}\Psi(u(\vec{x}_i))+O(a^{\gamma+1}),\tag{103}$$

where γ is the order of differentiation and the constant λ_ψ is independent of the vertex i and is characteristic of the lattice and the operator. The discrete field u on the left side is projected pointwise $u_i=\Pi_i^{(q)}[u]$ from the continuous field $u(\vec{x})$ on the right. Similarly for products

$$\mathcal{A}_i^{(r)}[\psi(u_1,u_2)]=\frac{1}{\lambda_\psi}\Psi(u_1(\vec{x}_i),u_2(\vec{x}_i))+O(a).\tag{104}$$

Consistency criteria Eqs. (102)–(104) determine the proportionality constants for transferring continuum field equations into the discrete formulation.

With the averaging cell the usual operators and products encountered in field theory are consistent. Table I lists the correspondences with associated scale factors. The technique for computing these factors is to Taylor expand and truncate to the relevant order. For the sake of completeness we derive some of the tabulated results.

Consider the dot products of 1-fields. Valuable simplification results from using the abbreviation $\vec{e}_\alpha$ for $\vec{e}_\alpha^{(1)}$. It follows from the definition Eq. (40) that

$$\begin{aligned}\mathcal{A}_i^{(0)}[v\cdot w]&=\frac{1}{2}\sum_\alpha v_{i\alpha}w_{i\alpha}\\ &=\frac{1}{2}\sum_{\alpha,h,k} v_h(\vec{x}_i+a\vec{e}_\alpha)w_k(\vec{x}_i+a\vec{e}_\alpha)e_{\alpha h}e_{\alpha k}\\ &=\frac{1}{2}\sum_{h,k} v_h(\vec{x}_i)w_k(\vec{x}_i)\sum_\alpha e_{\alpha h}e_{\alpha k}+O(a).\end{aligned}$$

As a consequence of the isotropy conditions, it follows that

$$\begin{aligned}\mathcal{A}_i^{(0)}[v\cdot w]&=\frac{3}{2}\sum_h v_h(\vec{x}_i)w_h(\vec{x}_i)+O(a)\\ &=\frac{3}{2}\vec{v}(\vec{x}_i)\cdot\vec{w}(\vec{x}_i)+O(a),\end{aligned}\tag{105}$$

TABLE I. Correspondence between lattice and continuum operators showing appropriate scale factors.

	Operator	Meaning	Continuum quantity	Scale factor λ
1	$v\cdot w$	scalar product of vectors	$\vec{v}\cdot\vec{w}$	2/3
2	$v\times w$	cross product of vectors	$\vec{v}\times\vec{w}$	$4/\sqrt{3}$
3	$v\times\beta$	cross product of planar and axial vectors	$\vec{v}\times\vec{\beta}$	$\sqrt{3}$
4	$d_0\phi$	gradient of a scalar field	$\vec{\nabla}\phi$	1
5	$-\partial_1 v$	divergence of a vector field	$\vec{\nabla}\cdot\vec{v}$	2/3
6	$d_1 v$	curl of a vector field	$\vec{\nabla}\times\vec{v}$	$4/\sqrt{3}$
7	$\partial_2\beta$	curl of an axial vector	$\vec{\nabla}\times\vec{\beta}$	$\sqrt{3}$
8	$-\partial_1 d_0\phi$	Laplacian of a scalar field	$\nabla^2\phi$	2/3
9	$d_0(v\cdot v)$	gradient of the square modulus	$\nabla\lvert\vec{v}\rvert^2$	2/3
10	$v\times d_1 v$	cross product of $\vec{v}$ and its curl	$\vec{v}\times\vec{\nabla}\times\vec{v}$	4
11	$-d_0\partial_1 v$	gradient of the divergence	$\vec{\nabla}(\vec{\nabla}\cdot\vec{v})$	2/3
12	$\partial_2 d_1 v$	curl-curl of a vector field	$\vec{\nabla}\times\vec{\nabla}\times\vec{v}$	4

and therefore the scaling factor equals $\lambda=2/3$.

The cross product of two 1-fields is a 2-field, the components of which are given by Eq. (44). By definition [see Fig. 2(b)]

$$(v\times w)_{i\alpha}=\frac{1}{6}\,v_{i\alpha}\{w_{i,\alpha+1}+\vec{w}[\vec{x}_i+a(\vec{e}_\alpha+\vec{e}_{\alpha+1})/2]\cdot(\vec{e}_{\alpha+1}-\vec{e}_\alpha)\}-\frac{1}{6}\,\vec{v}[\vec{x}_i+a(\vec{e}_\alpha+\vec{e}_{\alpha+1})/2]\cdot(\vec{e}_{\alpha+1}-\vec{e}_\alpha)[w_{i\alpha}+w_{i,\alpha+1}]$$

$$+\frac{1}{6}\,v_{i,\alpha+1}\{\vec{w}[\vec{x}_i+a(\vec{e}_\alpha+\vec{e}_{\alpha+1})/2]\cdot(\vec{e}_{\alpha+1}-\vec{e}_\alpha)-w_{i\alpha}\}=\frac{1}{2}\,(v_{i\alpha}w_{i,\alpha+1}-v_{i,\alpha+1}w_{i\alpha})+O(a).$$

Therefore, by making use of Eq. (101),

$$\mathcal{A}_i^{(2)}[v\times w]=\frac{1}{12}\sum_{h,k}v_h(\vec{x}_i)w_k(\vec{x}_i)\sum_\alpha\,(e_{\alpha h}e_{\alpha+1,k}-e_{\alpha+1,h}e_{\alpha k})+O(a)=\frac{1}{12}\sum_{h,k}v_h(\vec{x}_i)w_k(\vec{x}_i)Q_{hk}+O(a),\qquad(106)$$

where the tensor $Q_{hk}=3\sqrt{3}\varepsilon_{hk}$ with ε_{hk} the Levi-Civita antisymmetric symbol. Therefore

$$\mathcal{A}_i^{(2)}[v\times w]=\frac{\sqrt{3}}{4}\,\vec{v}(\vec{x}_i)\times\vec{w}(\vec{x}_i)+O(a).\qquad(107)$$

By analogous calculation for the cross product of a 1-field v and of a 2-field β defined by Eq. (51), one obtains

$$\mathcal{A}_i^{(1)}[v\times\beta]=\frac{1}{\sqrt{3}}\,\vec{v}(\vec{x}_i)\times\vec{\beta}(\vec{x}_i)+O(a)\qquad(108)$$

and thus the corresponding scale factor $\lambda=\sqrt{3}$.

Now consider the first-order differential operators (lines 4–7 of Table I). If ϕ is a 0-field, the local average of $d_0\phi$ on the unit cell yields

$$\mathcal{A}_i^{(1)}[d_o\phi]=\frac{1}{3}\sum_\alpha\,[\phi(\vec{x}_i+a\vec{e}_\alpha)-\phi(\vec{x}_i)]\vec{e}_\alpha$$

$$=\frac{a}{3}\sum_j\,\left.\frac{\partial\phi(\vec{x})}{\partial x_j}\right|_{\vec{x}=\vec{x}_i}\sum_\alpha\,e_{\alpha j}\vec{e}_\alpha+O(a^2).\qquad(109)$$

Applying the second isotropy property, it follows that $\mathcal{A}_i^{(1)}[d_o\phi]=a\nabla\phi(\vec{x}_i)+O(a^2)$, so the scale factor is $\lambda=1$. Similarly, for the lattice analog ∂_1 of the divergence applied to a 1-field v one finds from the definition of the boundary that

$$\mathcal{A}_i^{(0)}[-\partial_1 v]=\sum_\alpha\,v_\alpha^i=\sum_\alpha\,\vec{v}(\vec{x}_i+a\vec{e}_\alpha/2)\cdot\vec{e}_\alpha$$

$$=\frac{a}{2}\sum_{jk}\,\left.\frac{\partial v_j(\vec{x})}{\partial x_k}\right|_{\vec{x}=\vec{x}_i}\times\sum_\alpha\,e_{\alpha j}e_{\alpha k}+O(a^2),\qquad(110)$$

and therefore $\mathcal{A}_i^{(0)}[-\partial_1 v]=(3a/2)\nabla\cdot\vec{v}(\vec{x}_i)+O(a^2)$. The correspondence summarized in Table I between the other lattice operators and continuum ones is obtained from the same sort of elementary algebra and Taylor expansion. This correspondence defines quantitatively the lattice analogs of a given set of continuum field equations. For example, the lattice analog of the incompressible Navier-Stokes equation on a triangular lattice equipped with the averaging recipe developed in this section, including necessary proportionality constants, is given by

$$\rho\dot{v}+\frac{\rho}{3a}d(v\cdot v)-\frac{4\rho}{a}v\times dv=-\frac{1}{a}dp-\frac{4\mu}{a^2}\partial dv. \quad (111)$$

The solution of this equation can thus be compared quantitatively in the limit $a\to 0$ with the solution of the continuum Navier-Stokes equation.

The analysis developed above connecting difference and differential operators for the triangular lattice can be carried out with some modifications for nonuniform lattices. This topic is outside the scope of the current paper and will be discussed elsewhere.

VIII. OPERATORS AND HELMHOLTZ REPRESENTATION

Some properties of $\partial d=\partial_{p+1}d_p$ and $d\partial=d_{p-1}\partial_p$ pertain to the Helmholtz representation of a general vector field as the sum of a gradient plus a curl, or to topological properties of $\mathcal{G}$. Both operators are Hermitian, since $\langle\partial du,v\rangle=\langle du,dv\rangle=\langle u,\partial dv\rangle$ and $\langle d\partial u,v\rangle=\langle\partial u,\partial v\rangle=\langle u,d\partial v\rangle$. In fact, the latter equations also show that the eigenvalues of both ∂d and $d\partial$ are non-negative, which proves, as promised in Sec. III, that the eigenvalues of ∇^2 are nonpositive. Operators ∂d and $d\partial$ are orthogonal, meaning that $(\partial d)(d\partial)=\partial d^2\partial=0$ and $(d\partial)(\partial d)=d\partial^2 d=0$, and hence commute *a fortiori*. An orthonormal basis of simultaneous eigenvectors of ∂d and $d\partial$ generates $\mathcal{C}_p$. Choosing an arbitrary element $\hat{e}$ of the basis, one sees from orthogonality of the operators that either $\partial d\hat{e}=0$ or $d\partial\hat{e}=0$ or both.

The null space, or kernel, of ∂d has a simple physical meaning. Observe that $du=0$ everywhere if and only if $\partial du=0$ everywhere. To see this, consider $\langle\partial du,u\rangle=\langle du,du\rangle$. If the left-hand side is zero, then du is zero because its norm is zero. The reasoning in the other direction is obvious. Note, however, that if $\partial du=0$ only on some subspace Ω of $\mathcal{C}_p$, one cannot conclude that $du=0$ in Ω. The relation holds only when $\partial du=0$ on every p-simplex of $\mathcal{G}$. Therefore, the null space of ∂d is the space of p-fields with vanishing coboundary. For $p=0$, 1, or 2 this means fields with vanishing gradient, curl, or divergence, respectively. Similarly one can see *mutatis mutandis* that the null space of $d\partial$ is the space of p-fields with vanishing boundary. For $p=1$, 2, or 3 this means fields with vanishing divergence, curl, or gradient, respectively.

The coboundary d_p generates an isomorphism between the space p-fields with nonvanishing coboundary and the space of $(p+1)$-fields with nonvanishing boundary. Suppose $\partial du=\lambda u$ with $\lambda\neq 0$. Then

$$(d\partial)du=d(\partial d)u=\lambda(du), \quad (112)$$

so that du is an eigenvector of $d\partial$ with the same eigenvalue λ. If u is normalized, then

$$\langle du,du\rangle=\langle u,\partial du\rangle=\lambda. \quad (113)$$

Thus the corresponding normalized eigenvector of $d\partial$ is $du/\sqrt{\lambda}$. The same isomorphism can be built in the other direction using ∂_{p+1}.

Quite often for linear problems in k dimensions the solution space separates naturally into at most k fundamental parts, perhaps coupled by boundary conditions. Each part corresponds to an operator pair $\partial_p d_{p-1}$, $d_{p-1}\partial_p$ for p from 1 to k. In physical terms, for $k=2$ (or $k=3$) the isomorphisms developed above imply two (or three) correspondences, one between scalar potentials and gradient fields (or between pseudoscalar potential and gradient pseudovector fields) and one between solenoidal vector and solenoidal pseudovector fields. In the latter case, either one can be the vector potential for the other. Each of these is really the same sort of correspondence between the different field representations of essentially the same aspect of the problem, corresponding to operators with the same spectrum. The correspondence is an exact isomorphism between p-fields and $(p-1)$-fields representing basically the same thing, and either d or ∂ gives a concrete representation for the isomorphism.

Consider now the remaining subspace of $\mathcal{C}_p$, the p-fields with zero boundary and zero coboundary, or the overlap of the kernels of $\partial_{p+1}d_p$ and $d_{p-1}\partial_p$. These have simple, topological meaning. Since $\partial^2=0$, it is clear that the image im ∂_{p+1} is a subspace of the null space ker ∂_p. The homology group $\mathcal{H}_p$ for $\mathcal{G}$ with respect to the complex numbers is the quotient ker ∂_p/im ∂_{p+1}, or the null space of ∂_p modulo the image space of ∂_{p+1}. Thus it represents the set of p-fields which have zero boundary, but not because they are themselves boundaries of $(p+1)$-fields. For example, suppose $\mathcal{G}$ is a rhomboidal section of triangular lattice with periodic boundary conditions, i.e., the surface of a torus. Then it is clear that two closed polygonal paths, each traversing $\mathcal{G}$ in one of its two independent periodic directions, belong to $\mathcal{H}_1$. Since the coefficients are complex numbers, $\mathcal{H}_p$ is isomorphic to the orthogonal complement of im ∂_{p+1} in ker ∂_p. A properly chosen basis for $\mathcal{H}_1$, for example, would correspond to the independent periods or circuits in $\mathcal{G}$. The pth Betti number b_p is the dimension of $\mathcal{H}_p$.

If u is not in im ∂_{p+1}, then there is no v in $\mathcal{C}_{p+1}$ such that $\partial_{p+1}v=u$. Therefore, in view of the isomorphism generated by d_p between p-fields with nonzero coboundary and $(p+1)$-fields with nonzero boundary, it follows that $\partial_{p+1}d_p u=0$ or $d_p u=0$, so $u\in\ker d_n$. Hence if u is in ker ∂_p but not im ∂_{p+1}, then both $\partial_p u=0$ and $d_p u=0$. The steps are reversible, so $\mathcal{H}_p$ is the space of p-fields annihilated by both ∂ and d. These p-fields correspond in the continuum formulation to the set fields of a given type with constant coefficients in an infinite, simply connected space with Cartesian coordinates. But they extend the concept, in a coordinate-free way, to p-fields in the multiply connected case. One could refer to them as constant p-fields. The Betti number b_p is the number of independent, qualitatively different constant p-fields, or the dimension of the space of p-fields with both zero boundary and zero coboundary. In $k=2$ or 3 dimensions, the physical meaning of the constant fields is clear. For $p=1$ or 2, the constant fields represent global circulations around handles of the space. For $p=0$ or 3, they represent independent stationary states of diffusion, hence the number of disconnected parts of $\mathcal{G}$. However, whereas for $p=0$ connectedness is determined by $\mathcal{G}$ or H, it is in the case of $p=3$ determined by $\star\mathcal{G}$ with corresponding adjacency matrix $\star H$ defined by the action $d_2\partial_3$ on $\mathcal{G}$.

Collecting results, we find that the general Helmholtz representation of an arbitrary p-field u is

$$u = d\phi + \partial\psi + c, \tag{114}$$

where u is any element of $\mathcal{C}_p$, and once u is given, c is a unique member of $\mathcal{H}_p$, and ϕ and ψ belonging to $\mathcal{C}_{p-1}$ and $\mathcal{C}_{p+1}$, respectively, are potential fields. The potential ϕ is free to vary by $\delta\phi \in \ker d$ and ψ is free to vary by $\delta\psi \in \ker \partial$, but $c \in \mathcal{H}$ is fixed. To see this, consider

$$u = d(\phi + \delta\phi) + \partial(\psi + \delta\psi) + (c + \delta c). \tag{115}$$

Thus

$$d\,\delta\phi + \partial\,\delta\psi + \delta c = 0. \tag{116}$$

But $d\,\delta\phi = 0$ and $\partial\,\delta\psi = 0$ everywhere. Hence $\delta c = 0$ and c must be unique.

Consider an arbitrary linear operator which is a rather general function of ∂d and of $d\partial$. Examples appear in the lattice Helmholtz equation for arbitrary p, the electromagnetic model, the elastodynamic model and the lattice Navier-Stokes equation in the Stokes limit of low Reynolds number where the inertial term is neglected, as well as the linear Timoshenko equation and many other physical models. When the function $f(\partial d, d\partial)$ can be defined by simultaneous diagonalization of the two matrices, so that, for example, $f(x,y)$ is not singular on the lines $(x,0)$ or $(0,y)$ or for any pair (x,y) of eigenvalues, then due to orthogonality of ∂d and $d\partial$,

$$f(\partial d, d\partial) = f(\partial d, 0) + f(0, d\partial) - f(0,0). \tag{117}$$

This is a rather striking simplification since $f(x,y)$ can be quite general. For example, by expanding one sees that $(\partial d + d\partial + K)^2 = (\partial d + K)^2 + (d\partial + K)^2 - K^2$.

As an application, we obtain Green functions for a linear lattice model of the form

$$Du - f(\partial d, d\partial)u = F, \tag{118}$$

where D is polynomial in the time derivative d/dt and F is a general source term. Laplace or Fourier transforming leads one to consider the resolvent or transfer matrix

$$G_f(z) = [z - f(\partial d, d\partial)]^{-1}, \tag{119}$$

defined for z outside the spectrum. Thus

$$G_f(z) = G_a(z) + G_b(z) - \frac{1}{z - f(0,0)}, \tag{120}$$

where

$$G_a(z) = [z - f(\partial d, 0)]^{-1}, \tag{121}$$

$$G_b(z) = [z - f(0, d\partial)]^{-1}. \tag{122}$$

The latter two expressions are again defined in the usual way by the canonical, diagonal forms of ∂d and $d\partial$. When $f(x,y)$ is a rational function, we have shown [15] how to obtain them as closed formulas in terms of the fundamental resolvents

$$G_{\partial d}(z) = [z - \partial d]^{-1}, \tag{123}$$

$$G_{d\partial}(z) = [z - d\partial]^{-1}. \tag{124}$$

Moreover, since $(d\partial)^n = d(\partial d)^{n-1}\partial$, one has

$$G_{d_{p-1}\partial_p} = \frac{1}{z} + \frac{1}{z^2}\, d_{p-1} G_{\partial_p d_{p-1}}(z)\partial_p. \tag{125}$$

The latter equation applies the isomorphism generated by d_{p-1} or ∂_p to transfer from one equivalent space to another. Green functions for boundary value problems pertaining to the original equation are matrix entries of $G_f(z)$. The boundary conditions that we have not addressed so far can be included by adding terms to correct $G_f(z)$ at the boundary of the region of interest [16,12].

Thus the solution to boundary value problems involving a rather broad class of linear operators can be solved using three or fewer families of fundamental Green functions, each corresponding to either of the two operators $G_{\partial d}(z)$ or $G_{d\partial}(z)$. These in turn can be computed once and for all for a given type of lattice, on in general for a given triangulating graph $\mathcal{G}$. Boundary conditions can be modified by making local modifications, and even in the case of nonlinear models the Green functions are useful for developing a systematic perturbation theory.

IX. SUMMARY

We have shown that with the proper choice of definition of the dot, cross, and scalar multiplication between pairs of p-fields for different combinations of p, it is possible to make a discrete vector calculus, with ∂ and d acting as divergence, gradient, and curl, which has all the integral theorems and most of the vector identities of the vector differential calculus. Generalized Stokes theorems satisfied by p-fields for each p are derived in Sec. III from the duality between ∂ and d. Interpretations of the boundary $\partial\Omega$ of a region Ω of $\mathcal{G}$ and coboundary $d\star\Omega$ of $\star\Omega$ are discussed there in some detail. The correspondence deduced from these integral theorems between the vector operators and the boundary and coboundary is summarized in Fig. 1. A set of vector identities in the difference formulation is obtained in Sec. V, together with the explicit formulas in terms of components.

It is possible using this difference calculus to construct systems of difference equations or differential difference equations on a rather general lattice which is forced to have many of the qualitative behaviors of the analogous system of PDEs. Certain behaviors of the continuous and the corresponding discrete models, whether linear or nonlinear, are locked together topologically by the analogy in formal structure, i.e., they must satisfy analogous conservation laws exactly. In principle one can analyze these models, formally and numerically, on structures of arbitrary complexity. It is possible to derive theoretical results without reference to individual field components or the explicit structure of $\mathcal{G}$.

Where the vector difference formalism comes into play is in the process of manipulating and solving the discrete model. It provides a discrete counterpart to each vector calculus operation, and hence to every conserved quantity or first integral, e.g., the Nötherian invariants, and every solution strategy of the continuum model. These are exact, not

approximations that hold in the continuum limit. Hence we have seen discrete analogs to the Poynting vector and the electromagnetic energy density in the case of the lattice Maxwell equations, which satisfy exactly a discrete analog to the Poynting theorem. For fluids we have seen a special case of the Kelvin circulation theorem. Similar integral relations hold for other kinds of models. We consider this, rather that numerical efficiency, to be the point of the difference calculus. Existence of analogs to the conservation laws, etc., leads one to expect that the behavior of the discrete models will often be qualitatively similar to that of the continuous ones.

To show that the formalism can in fact be adapted to a numerical method, we have derived the scale factors or weights necessary to get quantitative correspondence between PDEs for continuous fields in two dimensions and a set of difference equations on a triangular lattice. This illustrates one of many possible numerical methods compatible with the difference calculus.

We have shown that p-fields for each p partition naturally into three classes related to the spectra of ∂d and $d\partial$, which share eigenvectors. These operators correspond to curl and gradient divergence in different ways, depending on p. The mutual eigenbasis partitions into sets, corresponding to the different p-field classes. The first is the set annihilated by $d\partial$ but not by ∂d, the second is the set annihilated by ∂d but not $d\partial$, and the third is annihilated by both. This corresponds to a Helmholtz representation $u = d\phi + \partial\psi + c$, as discussed in Sec. VIII, where the terms in the expansion of general p-field u each belong to one of the three classes. Thus Green functions for very general linear models can be found from the basic lattice Green functions discussed in Sec. VIII, and these in turn can be found once and for all for a given $\mathcal{G}$.

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