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Triangle lattice Green functions for vector fields

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Abstract

All the identities and integral theorems of vector calculus are contained in the calculus of differential forms. The analogy between the exterior calculus of forms and the homology theory of a cell complex yields discrete lattice models for an array of interesting physical phenomena. These models, based on arbitrary combinations of coupled scalar and polar or axial vector field quantities, can be manipulated as conveniently as the standard scalar tight-binding models. We develop Green functions (GFs) for an infinite hierarchy of such models expressed using the four fundamental operators of the triangle lattice. The triangle lattice is distinguished among two-dimensional grid types for having the highest possible isotropy. Closed formulae are derived for GFs of the scalar and vector models that belong to a hierarchy generated by the four fundamental operators of the triangle family of lattices. The particular example of lattice electromagnetism coupled to an elastic distortion field is treated in detail. Topological properties not dependent upon symmetry split the response functions into plasmon- and polariton-like parts. Since the fundamental vector operators of the triangle lattice are related simply to adjacency matrices of the Kagomé lattice, scalar GFs for this lattice are found also as a byproduct.

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1. Introduction

This paper concerns lattice Green functions (GFs) for vector fields. These are developed in a discrete version of vector calculus introduced recently. It is based on an analogy between differential forms and simplicial homology theory in which the roles of the differential operators divergence, gradient and curl are taken on by the boundary ∂ and coboundary $\partial^\dagger$ maps [1]. In the process of calculating GFs for the vector fields on the triangle lattice, we also extend the set of lattices for which scalar GFs are known in terms of elliptic integrals to include the Kagomé lattice, depicted in figure 1.

The lattice vector calculus described in [2] places vector and scalar fields on an equal, geometrical footing. With it, linear or nonlinear physical models become systems of finite difference equations on a triangulating lattice. One can then treat vector or tensor fields with a formal apparatus quite similar to that of differential forms [3] in the continuum case.

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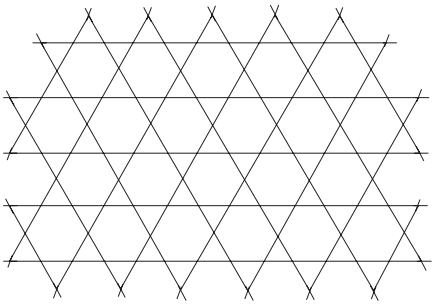

Figure 1. The Kagomé lattice.

For our purposes, lattice GFs are entries of a resolvent matrix

$$G(H;z) = (z\,I - H)^{-1} \tag{1.1}$$

defined for z outside the spectrum of H, which is a difference operator for some physical phenomenon. The operator H could be a model Hamiltonian for lattice vibrations, spin waves or independent electrons. We focus mainly on vector field operators. The most general lattice dealt with by the new formalism is a rather general graph (simplicial complex) with the graph vertex set serving as index set for H and the identity I. However, the work reported below concerns the family of regular planar lattices with three- or sixfold symmetry.

Use of the GFs for introducing sources, changing boundary conditions of linear equations or for developing a perturbation hierarchy in nonlinear problems is quite similar in the case of discrete vector fields to their use for the scalar case. Usually the GFs are the physical response functions. Non-perturbative methods such as renormalization make use of GFs also.

During the early 1970s several exact results were obtained for GFs in the case where H is a discrete form of the scalar Laplacian operator based on nearest-neighbour differences [4,10]. The GFs are combinations of integrals which in the cases of the square and triangle lattice families reduce to complete elliptic integrals. The general triangle lattice family includes also the honeycomb and other lattices. Horiguchi showed how the GFs of the honeycomb lattice, constructed from two interpenetrating triangle lattices with nearest-neighbour interaction, can be written in terms of those of the triangle lattice and thus also in terms of the complete elliptic integrals of the first and second kinds [9]. Horiguchi and Chen [10] expressed the GFs of a diced lattice, built on three interpenetrating triangle lattices with nearest-neighbour interactions of strengths 1 and γ, in terms of the triangle lattice GFs.

In section 2 we introduce notation, some homology theory is reviewed and some of the formalism of [2] is outlined. In particular, the maps ∂ and $\partial^\dagger$ on which the subsequent development rests are discussed in some detail. To demonstrate transcription of a physical model into the discrete formalism, an example of electromagnetism in a polarizable medium is developed. The fundamental operators of the forms $\partial\partial^\dagger$ and $\partial^\dagger\partial$ and their GFs are discussed in section 3. We show how to use these to reduce GFs of a rather general linear model. Reduction of the GFs for the electromagnetic example given in section 2 in terms of GFs of the fundamental operators is presented in some detail. Generating functions for the fundamental GFs are introduced in section 4. Their use for finding relationships between scalar and vector GFs and for computing the GFs is illustrated by examples. Section 5 lists the diagonal GFs in terms of elliptic integrals. The conclusion contains notes on GFs with more general boundary conditions and some observations on the relation between the scalar and the vector GFs on the triangle family of lattices. A complete table of scalar and vector GFs for the triangle lattice, and scalar GFs for the Kagomé and the honeycomb lattices, is presented in appendix A.

2. Vector difference calculus

We introduce notation and review some simplicial homology theory (see also [2]). Consider first a general region in three-dimensional space. To construct a formalism for vector fields, the space is represented by a triangulating graph, regular or not, on which points in the space are graph vertices. The graph defines a simplicial complex on which calculations are carried out. The vertices (0-simplices), oriented bonds (1-simplices), triangles (2-simplices) and tetrahedra (3-simplices) of the complex serve as a bases for quantities analogous to scalar, polar vector, axial vector and pseudoscalar fields. A p-field is represented as a formal sum over all p-simplices of the complex. What we shall call p-fields are in standard nomenclature p-chains (and p-cochains) with real or complex coefficients [1]. The coefficients correspond to the field strengths or field components in the continuum case. We use the notations (i), (i, j), (i, j, k) and (i, j, k, l) for 0-, 1-, 2- and 3-simplices, respectively. If (i, j, k) is a 2-simplex, then vertices i, j and k must be mutually adjacent. Each p-simplex is oriented, so interchanging a vertex pair changes the sign, hence for example $(i, k, j) = -(i, j, k)$. Thus (i, j, k) is a right-hand oriented triangular plaquette, while (i, j) is a directed edge or bond from i to j. A polar vector field u is a 1-field

$$u = \sum_{[ij]} u_{ij}(i, j) \tag{2.1}$$

where the coefficients are antisymmetric $u_{ji} = -u_{ij}$. An axial vector field v is a 2-field

$$v = \sum_{[ijk]} v_{ijk}(i, j, k) \tag{2.2}$$

again with antisymmetric coefficients. The summations are over distinct p-simplices. Thus, to each graph vertex i (each point in discrete space) there corresponds a set of tangent spaces generated by all the p-simplices that contain i. These simplices serve as a geometric basis. The finite-dimensional vector space generated by this set is analogous to the local cotangent space of grade p in the calculus of differential forms. The space of 0-fields (scalar fields) at i is generated by the single basis object (i), while the space of 1-fields is the real or complex vector space generated by the union over all points i of the star of edges radiating from i. Each of these edges is of the form (i, j) with j adjacent to i, which we denote by $j \,@\, i$. A p-field, then, is a vector in the space generated by all p-simplices of the graph.

Let $\mathcal{C}_p$ represent the space of p-fields. The boundary ∂_p maps $\mathcal{C}_p$ into $\mathcal{C}_{p-1}$, while the coboundary $\partial_p^\dagger$ maps $\mathcal{C}_p$ into $\mathcal{C}_{p+1}$. The map subscript indicates the domain in each case. Sometimes it can be omitted without causing confusion, but for the most part it will be retained here for clarity. ∂ is defined to be the linear map such that

$$\partial_0(i) = 0 \tag{2.3a}$$

$$\partial_1(i, j) = (j) - (i) \tag{2.3b}$$

$$\partial_2(i, j, k) = (j, k) - (i, k) + (i, j) \tag{2.3c}$$

$$\partial_3(i, j, k, l) = (j, k, l) - (i, k, l) + (i, j, l) - (i, j, k) \tag{2.3d}$$

the rule being to delete each vertex in turn with alternating sign. Thus in each case ∂ takes a simplex onto its oriented boundary.

An inner product between p-fields $\langle \ldots, \ldots \rangle$, the analogue of integration in standard calculus, is defined for each p by

$$\langle (i, j, \ldots), (k, l, \ldots) \rangle = \det \begin{bmatrix} \delta_{ik} & \delta_{il} & \cdots \\ \delta_{jk} & \delta_{jl} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \tag{2.4}$$

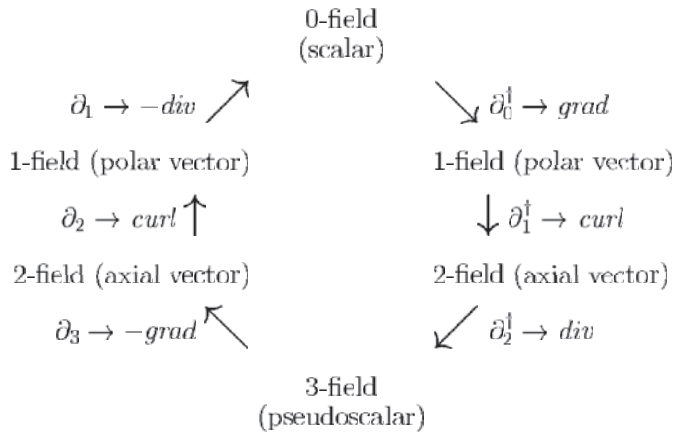

Figure 2. Relation between $\partial^\dagger$ and ∂ and div, grad and curl.

where $(i, j, \ldots)$ and $(k, l, \ldots)$ are oriented simplex basis elements of $\mathcal{C}_p$. As in the standard calculus, the inner product is defined for two p-fields only if the corresponding summation converges (perhaps to infinity). The coboundary of a basis simplex in $\mathcal{C}_p$ is a sum of simplices in $\mathcal{C}_{p+1}$, the boundary of each of which contains the basis simplex with coefficient +1. With respect to the inner product, the coboundary map $\partial_p^\dagger$ is simply the dual of the boundary map ∂_{p+1} defined by the identity

$$\langle \partial_p^\dagger \psi, \phi \rangle = \langle \psi, \partial_{p+1} \phi \rangle \tag{2.5}$$

where ϕ is a $(p+1)$-field and ψ is a p-field, provided these fields satisfy some physically reasonable conditions [1].

In the analogy to vector calculus, ∂ and $\partial^\dagger$ take on the role of ∇ in forming gradient, divergence and curl. The duality between ∂_{p+1} and $\partial_p^\dagger$ gives rise to Stokes-type integral theorems. For example, let c be a 1-field with zero coefficients except for coefficients +1 on a directed polygonal path from vertex i to vertex f. This is the discrete version of an oriented contour. The contour integral of vector field u along c is then $\langle u, c \rangle$. If ψ is a scalar field, the fundamental theorem of calculus is just the identity

$$\int_c \nabla \psi \cdot \mathrm{d}\vec{r} = \langle \partial_0^\dagger \psi, c \rangle = \langle \psi, \partial_1 c \rangle = \psi_f - \psi_i. \tag{2.6}$$

This shows that $\partial_0^\dagger$ acts as the gradient. Discrete analogues of vector integral theorems, including Green's, Gauss' and Stokes' theorems, developed in this way, guide the identification of the actions of ∂ and $\partial^\dagger$ with standard vector operations. The correspondence is worked out in [2] and is shown in figure 2. The essential property of the boundary map is $\partial^2 = 0$, meaning that $\partial_{p-1} \partial_p \phi = 0$ for any arbitrary p-field. Hence also $(\partial^\dagger)^2 = 0$. This is necessary so that the composite operations div $\circ$ curl and curl $\circ$ grad give zero.

One can now transcribe physical models from the continuum to the lattice in a natural way. For example, a vacuum electromagnetic theory can be built from discrete Maxwell equations. We assume a three-dimensional lattice, and, in order to concentrate on the physical idea rather than the subscripts, use the generic notations ∂ and $\partial^\dagger$. From figure 2,

$$\partial E = -\rho \tag{2.7a}$$

$$\partial B - \frac{\mathrm{d}E}{\mathrm{d}t} = J \tag{2.7b}$$

$$\partial^\dagger E + \frac{\mathrm{d}B}{\mathrm{d}t} = 0 \tag{2.7c}$$

$$\partial^\dagger B = 0. \tag{2.7d}$$

Polarization response of an elastic medium with displacement from equilibrium given by the 1-field u can also be included. We adopt a Navier equation of motion for u,

$$m\frac{\mathrm{d}^2 u}{\mathrm{d}t^2} = qE - ku - a\partial\partial^\dagger u - b\partial^\dagger\partial u \tag{2.8}$$

where m and q reflect mass and charge per unit volume, a and b are combinations of Lamé elastic constants and the local spring constant k pins the medium to prevent uniform translation. Next, couple the 1-fields u and E via

$$J = q\frac{\mathrm{d}u}{\mathrm{d}t} \tag{2.9}$$

so that the medium is non-dissipative. Thus one can assume

$$\rho = \rho_0 + \rho_1 \tag{2.10a}$$

$$\rho_1 = \partial(q\,u) \tag{2.10b}$$

so that

$$\partial J = \frac{\mathrm{d}\rho_1}{\mathrm{d}t}. \tag{2.11}$$

One arrives at coupled equations of motion for u and E, which decouple in the frequency domain to give

$$[((\omega_0^2 - \omega^2) + \alpha^2\partial\partial^\dagger + \beta^2\partial^\dagger\partial)(\partial\partial^\dagger - \omega^2) - \omega_1^2\omega^2]E = F \tag{2.12}$$

where $\omega_0 = \sqrt{k/m}$, $\omega_1 = q/\sqrt{m}$, $\alpha = \sqrt{a/m}$ and $\beta = \sqrt{b/m}$, and an external driving term $F(\omega)$ (a 1-field) has been added. This example, though mostly germane to three-dimensional space, shows the form of a fairly typical lattice operator.

3. Fundamental operators

From the correspondence between ∂_p and $\partial_p^\dagger$ and divergence, gradient and curl, it follows that the combinations $\partial_{p+1}\,\partial_p^\dagger$ and $\partial_{p-1}^\dagger\,\partial_p$ act as the differential operators div $\circ$ grad, grad $\circ$ div or curl $\circ$ curl depending on the value of p. From these fundamental operators it follows that the Laplacian has the same form for each p,

$$\nabla_p^2 = -(\partial_{p-1}^\dagger\,\partial_p + \partial_{p+1}\,\partial_p^\dagger). \tag{3.1}$$

For p-fields u and v,

$$\langle\partial_{p+1}\,\partial_p^\dagger u, v\rangle = \langle\partial_p^\dagger u, \partial_p^\dagger v\rangle = \langle u, \partial_{p+1}\,\partial_p^\dagger v\rangle \tag{3.2a}$$

$$\langle\partial_{p-1}^\dagger\,\partial_p u, v\rangle = \langle\partial_p u, \partial_p v\rangle = \langle u, \partial_{p-1}^\dagger\,\partial_p v\rangle \tag{3.2b}$$

so that $\partial_{p+1}\,\partial_p^\dagger$ and $\partial_{p-1}^\dagger\,\partial_p$ are Hermitian. Their eigenvalues are apparently non-negative so that the eigenvalues of the discrete Laplacian are non-positive. $\partial_{p+1}\,\partial_p^\dagger$ and $\partial_{p-1}^\dagger\,\partial_p$ are orthogonal and hence commute since $(\partial_{p+1}\,\partial_p^\dagger)(\partial_{p-1}^\dagger\,\partial_p) = 0 = (\partial_{p-1}^\dagger\,\partial_p)(\partial_{p+1}\,\partial_p^\dagger)$. In the current paper one is not concerned with the numerical weights required to make equation (2.6), for example, reduce to the continuum limit. These weights are tabulated for the case of the triangle lattice in [2]. The difference operators presented above have correct topological or combinatorial properties. The GFs derived below are thus to be scaled according to the application one wishes to make of the corresponding difference operators.

Of interest at present is the relation between the fundamental operators and certain graph adjacency matrices. In general, $\partial_1\,\partial_0^\dagger$ relates simply to the adjacency matrix H of the graph defined such that $H_{ij} = 1$ when i @ j and $H_{ij} = 0$ otherwise. This comes about because $\partial_0^\dagger$ is an incidence matrix for edges incident to a given vertex and ∂_1 is the Hermitian adjoint of the matrix $\partial_0^\dagger$. (This relation may appear notationally awkward, but recall that the map suffix specifies the domain.) Therefore vertices are adjacent because they are incident to the same bond. Thus,

$$\partial_1\,\partial_0^\dagger = -H + P \tag{3.3}$$

where P is the diagonal matrix with entries equal to the coordination numbers of the vertices of the graph so that $P_{ij} = \delta_{ij}\sum_k H_{jk}$. Since ∂_p (or $\partial_p^\dagger$) for each p is a generalized incidence matrix, the other fundamental Hermitian operators for a two-dimensional lattice, namely $\partial_0^\dagger\,\partial_1$, $\partial_2\,\partial_1^\dagger$ and $\partial_1^\dagger\,\partial_2$, correspond to edge adjacency matrices or to face (triangular cell) adjacency matrices. The correspondences give rise to various types of lattice duality.

Laplace or Fourier transforming a linear inhomogeneous system of differential-difference equations of the general form

$$f(\partial_{p+1}\,\partial_p^\dagger, \partial_{p-1}^\dagger\,\partial_p, \mathrm{d}/\mathrm{d}t)u = F \tag{3.4}$$

where F is a source term, leads one to consider an operator of the form $G(z) = f(\partial_{p+1}\,\partial_p^\dagger, \partial_{p-1}^\dagger\,\partial_p, z)^{-1}$. Then, the fact that $\partial^2 = 0$ and $(\partial^\dagger)^2 = 0$ reduces $G(z)$ to

$$G(z) = f(\partial_{p+1}\,\partial_p^\dagger, 0, z)^{-1} + f(0, \partial_{p-1}^\dagger\,\partial_p, z)^{-1} - f(0, 0, z)^{-1}. \tag{3.5}$$

For a rational function $f(x, y, z)$, equation (3.5) may be expressed using the extension theory for lattice GFs [11] (see also appendix B) in terms of matrix elements of the resolvents

$$G(\partial\partial^\dagger; z) = (z - \partial_{p+1}\,\partial_p^\dagger)^{-1} \tag{3.6a}$$

$$G(\partial^\dagger\partial; z) = (z - \partial_{p-1}^\dagger\,\partial_p)^{-1}. \tag{3.6b}$$

Thus very general linear problems defined on a given lattice are solved in terms of only the GFs of the fundamental operators. To illustrate this point, consider the electromagnetic example of the previous section. In view of equation (3.5) there are two pertinent GFs, namely

$$G_a(\omega) = [\alpha^2(\partial\partial^\dagger)^2 - [(1+\alpha^2)\omega^2 - \omega_0^2]\partial\partial^\dagger + \omega^2(\omega^2 - \Omega^2)]^{-1} \tag{3.7a}$$

$$G_b(\omega) = \frac{1}{\omega^2}[(\omega^2 - \Omega^2) - \beta^2\partial^\dagger\partial]^{-1}. \tag{3.7b}$$

With these, the general solution is

$$E(\omega) = G_a(\omega)F(\omega) + G_b(\omega)F(\omega) - \frac{1}{\omega^2(\omega^2 - \Omega^2)}F(\omega) + E_0(\omega) \tag{3.8}$$

where $E_0(\omega)$ is any homogeneous solution and we have used the notation $\Omega = \sqrt{\omega_0^2 + \omega_1^2}$. Using the residue methods of [11],

$$G_a(\omega) = \frac{1}{\sqrt{R(\omega)}}\left[G\left(\partial\partial^\dagger; \frac{(1+\alpha^2)\omega^2 - \omega_0^2 - \sqrt{R(\omega)}}{2\alpha^2}\right)\right.$$
$$\left. -G\left(\partial\partial^\dagger; \frac{(1+\alpha^2)\omega^2 - \omega_0^2 + \sqrt{R(\omega)}}{2\alpha^2}\right)\right] \tag{3.9}$$

where

$$R(\omega) = [(1-\alpha^2)\omega^2 - \omega_0^2]^2 + 4\alpha^2\omega_1^2\omega^2 \tag{3.10}$$

and

$$G_b(\omega) = \frac{1}{\beta^2\omega^2} G\left(\partial^\dagger\partial;\, \frac{\omega^2 - \Omega^2}{\beta^2}\right). \tag{3.11}$$

One sees $G_a(\omega)$ is the propagator for transverse or polariton modes, while the GF $G_b(\omega)$ characterizes longitudinal or plasmon excitations. In a like manner the GFs for a wide range of physical models represented by equation (3.4) can be reduced to closed formulae, provided the lattice GFs for the fundamental operators are known.

4. Lattice Green functions

Of primary interest are elements of the resolvent matrix obtained from equation (1.1) with each of the fundamental linear operators in turn substituted for the generic H. We specialize to planar lattices of the triangle family, so there are no 3-fields, and 2-fields behave as pseudoscalars rather than as axial vectors. To simplify notation, let

$$A_0 = -\partial_1\,\partial_0^\dagger \tag{4.1a}$$

$$A_1 = \partial_2\,\partial_1^\dagger \tag{4.1b}$$

$$B_1 = -\partial_0^\dagger\,\partial_1 \tag{4.1c}$$

$$B_2 = \partial_1^\dagger\,\partial_2. \tag{4.1d}$$

The index set of each of these matrices is that of the set of basis simplices for the p-fields on which they operate; thus it is the set of vertices for A_0, edges for A_1 and B_1 or faces of the lattice in the case of B_2. Signs in equations (4.1a)–(4.1d) are chosen to make the operators A_0, A_1, B_1 and B_2 correspond to div ∘ grad and curl ∘ curl for 1-fields, and grad ∘ div and curl ∘ curl for 2-fields, respectively.

Figure 3(a) shows the triangle lattice with lattice spacing taken as 1 and vertex coordinates (m, n) with respect to a Bravais lattice with translation bases $\vec{a}_1 = \hat{x}$ and $\vec{a}_2 = \hat{x}/2 + \sqrt{3}\hat{y}/2$. It is convenient to use a special notation for the simplex basis. The particular choice defined in figure 3 is useful for fluid dynamics, since a 1-field with all positive components is a net flow to the right. As we shall see presently it will sometimes be useful to choose $\hat{e}^2_{m,n}$ to point the opposite way, which can be effected by sign changes. Figure 3(b) shows the rhombic unit cell associated with (m, n). The cell edges are indexed 1, 2 or 3 and the faces 1 or 2 so that $\hat{e}^\alpha_{m,n}$ stands for an edge or face with index α in a cell with coordinates (m, n) (the distinction between edges and faces should be clear from the context of the equations). In this notation, entries of the matrix $G(H; z)$ are

$$\langle \hat{e}^\alpha_{p,q}, G(H; z)\hat{e}^\beta_{m,n}\rangle = G^{\alpha\beta}_{m-p,n-q}(H; z) \tag{4.2}$$

where H can be A_1, B_1 or B_2. The case of $H = A_0$ is simple since there is only one vertex per cell.

Due to translation symmetry, the defining relation

$$(z\,I - H)G(H; z) = I$$

implies

$$\sum_{p,q,\mu} [z\,\delta_{p\,0}\,\delta_{q\,0}\,\delta_{\alpha\mu} - H^{\alpha\mu}_{(p,q)(0,0)}]G^{\mu\beta}_{m-p,n-q}(H; z) = \delta_{m\,0}\,\delta_{n\,0}\,\delta_{\alpha\beta}. \tag{4.3}$$

It is convenient to introduce generating functions for each operator H and for each of the GFs:

$$g^{\alpha\beta}(H; x, y; z) = \sum_{m,n} G^{\alpha\beta}_{m,n}(H; z)\,x^m\,y^n \tag{4.4}$$

$$h^{\alpha\beta}(x, y) = \sum_{m,n} H^{\alpha\beta}_{(m,n)(0,0)}\,x^m\,y^n. \tag{4.5}$$

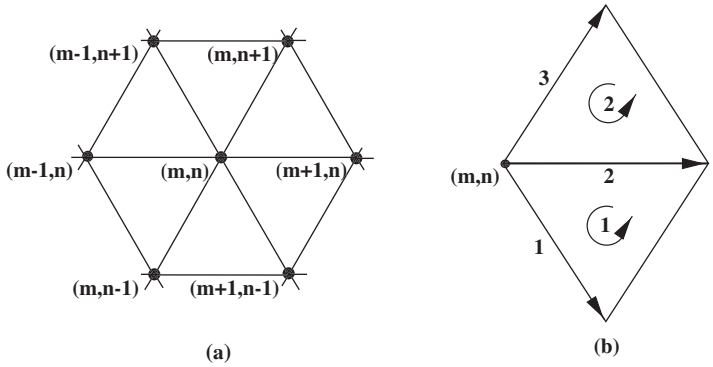

Figure 3. The triangle lattice (*a*) with vertex labels and (*b*) cell (m, n).

With matrix notations $g(H; x, y; z)$ and $h(x, y)$ equation (4.3) becomes

$$(z\,I - h(x, y))g(H; x, y; z) = I \tag{4.6}$$

where I is the identity of appropriate rank.

The matrix forms A_0, A_1 and B_2 of the fundamental linear operators of the triangle lattice are related to the graph adjacency matrices of several standard lattices:

$$A_0 = H_{\text{triangle}} - 6\,I \tag{4.7a}$$

$$\sigma A_1 \sigma = H_{\text{Kagomé}} + 2\,I \tag{4.7b}$$

$$\tau B_2 \tau = H_{\text{honeycomb}} + 3\,I \tag{4.7c}$$

since $H_{\text{Kagomé}}$ and $H_{\text{honeycomb}}$ correspond to edge and face duals of the original lattice, which is the graph of H_{triangle} (hereafter abbreviated to H_{Kag}, H_{hon} and H_{tri}). The matrix σ only changes the sign of the $\alpha = 2$ component of 1-fields. This unitary transformation adjusts signs to make the entries of the adjacency matrix H_{Kag} either 0 or +1. Similarly, τ makes a sign change in the $\alpha = 1$ component of 2-fields to bring H_{hon} into standard form.

Starting with A_0, the generator $A_0(x, y)$ is a single function (i.e. it is one dimensional) such that

$$\begin{aligned} g(A_0; x, y; z) &= (z - A_0(x, y))^{-1} = (z + 6 - H_{\text{tri}}(x, y))^{-1} \\ &= \left(z + 6 - \frac{1}{x} - x - \frac{1}{y} - y - \frac{x}{y} - \frac{y}{x}\right)^{-1}. \end{aligned} \tag{4.8}$$

For A_1,

$$g(A_1; x, y; z) = \begin{bmatrix} z-2 & 1+y & -(1+1/x)y \\ 1+1/y & z-2 & 1+y/x \\ -(1+x)/y & 1+x/y & z-2 \end{bmatrix}^{-1}. \tag{4.9}$$

Taking the inverse,

$$g(A_1; x, y; z) = \frac{1}{z}\,\Delta(x, y; z)\,g(A_0; x, y; z(z-6)) \tag{4.10}$$

where the factor $\Delta(x, y; z)$ is a 3×3 matrix of Laurent polynomials in x, y and z. Likewise,

$$g(B_2; x, y; z) = \begin{bmatrix} z-3 & 1+(1+1/x)y \\ 1+(1+x)/y & z-3 \end{bmatrix}^{-1} \tag{4.11}$$

so that

$$g(B_2; x, y; z) = \Lambda(x, y; z)\, g(A_0; x, y; z(z-6)) \tag{4.12}$$

where $\Lambda(x, y; z)$ is a 2×2 matrix of Laurent polynomial factors.

Expanding equation (4.8) in x and y, the GFs $G_{m,n}(A_0; z)$ are obtained as coefficients. Comparing with [9], one finds that

$$G_{m,n}(A_0; z) = \frac{1}{2}\,\Gamma\left(\frac{(z+6)}{2}, 2m+n, n\right) \tag{4.13}$$

where $\Gamma(t, m, n)$ is the triangle lattice GF for scalar fields computed by Horiguchi. Comparing to the GFs obtained from

$$G(H_{\text{tri}}; z) = (zI - H_{\text{tri}})^{-1} \tag{4.14}$$

one sees that

$$G(H_{\text{tri}}; z) = G(A_0; z-6). \tag{4.15}$$

As a notational convenience, let

$$\mathcal{G}(z) = G(A_0; z). \tag{4.16}$$

Expanding equation (4.10) in x and y leads to GFs of the Kagomé lattice, obtained from the resolvent

$$G(H_{\text{Kag}}; z) = (zI - H_{\text{Kag}})^{-1} \tag{4.17}$$

via

$$G(H_{\text{Kag}}; z) = \sigma\, G(A_1; z+2)\, \sigma. \tag{4.18}$$

The Kagomé GFs are thus expressed in terms of those for the triangle lattice. Similarly, the honeycomb lattice GFs are obtained by expanding equation (4.12) in x and y and making use of the relation

$$G(H_{\text{hon}}; z) = \tau\, G(B_2; z+3)\, \tau. \tag{4.19}$$

By means of this type of expansion and equation (4.18) with (4.13) or (4.15), the GFs for the Kagomé lattice are written alternatively in terms of either the GFs defined above from $G(H_{\text{tri}}; z)$ or else formulae of [9] involving complete elliptic integrals of the first and second kinds. The GFs for A_1, B_1 and B_2 as well as for the Kagomé lattice adjacency matrix are tabulated in the appendix. For completeness, the GFs for the honeycomb lattice adjacency matrix (in agreement with [9]) are also tabulated. All the GFs in appendix A are expressed via $\mathcal{G}(z)$ for the A_0 operator, which in turn relates to Horiguchi's study by way of equation (4.13).

5. Diagonal Green functions

Here we give the diagonal GFs for each lattice type. These give densities of states or projected eigenvalue densities. They also provide spectral functions used for the GF extension formalism of [11]. For any α,

$$G^{\alpha\alpha}_{0,0}(A_1; z) = \frac{1}{3z} + \frac{2}{3z}(z^2 - 3z + 3)\, \mathcal{G}_{0,0}(z(z-6)) \tag{5.1}$$

$$G^{\alpha\alpha}_{0,0}(B_1; z) = \frac{2}{3z} + \frac{1}{3z}(z+12)\, \mathcal{G}_{0,0}(z) \tag{5.2}$$

$$G^{\alpha\alpha}_{0,0}(B_2; z) = (z-3)\, \mathcal{G}_{0,0}(z(z-6)). \tag{5.3}$$

The honeycomb and Kagomé scalar GFs are therefore as follows.

$$G^{\alpha\alpha}_{0,0}(H_{\mathrm{Kag}};z) = \frac{1}{3(z+2)} + \frac{2}{3(z+2)}(z^2+z+1)\,\mathcal{G}_{0,0}((z-4)(z+2)) \tag{5.4}$$

$$G^{\alpha\alpha}_{0,0}(H_{\mathrm{hon}};z) = z\,\mathcal{G}_{0,0}((z-3)(z+3)). \tag{5.5}$$

The GF for A_0 relates to [9] through equation (4.13). Thus $\mathcal{G}_{0,0}(z)$ is evaluated as follows. Let

$$r = \sqrt{z+9} \tag{5.6a}$$

$$q = (r-1)^{-3/2}(r+3)^{-1/2} \tag{5.6b}$$

$$k = \sqrt{r}\,q \tag{5.6c}$$

then

$$\mathcal{G}_{0,0}(z) = \frac{2}{\pi} q\,\tilde{K}(k) \tag{5.7}$$

where $\tilde{K}(k)$ is the analytic continuation described in [9] of the complete elliptic integral

$$K(k) = \int_0^{\pi/2} \frac{\mathrm{d}\theta}{\sqrt{1-k^2\sin^2\theta}}. \tag{5.8}$$

The integral is analytic in k except for a cut from 1 to ∞ on the positive real axis, and another from -1 to $-\infty$ along the negative real axis. Start with k just above the cut on the positive real k axis where the phase is near 0. Sheet I of k is the region of analyticity on which $\tilde{K}(k) = K(k)$. The part of the Riemann surface reached by moving upward across the cut on the negative k axis into the second quadrant is sheet II. The part reached by crossing the same cut downward into the third quadrant is sheet III. The analytic continuation onto sheet II is $\tilde{K}(k) = K^{\mathrm{II}}(k) = K(k)+2\mathrm{i}K(k')$ and that onto sheet III is $\tilde{K}(k) = K^{\mathrm{III}}(k) = K(k)-2\mathrm{i}K(k')$, with $k' = \sqrt{1-k}\sqrt{1+k}$. Useful formulae for computing $\mathcal{G}_{m,n}(z)$ are also given by Kleinert [12].

Finally, the van Hove singularities in each case are as follows. Both A_0 and B_1 have singularities in z at -9, -8 and 0, while both A_1 and B_2 have singularities at 2, 3, 4 and 6. Kagomé lattice van Hove singularities are at -2, 0, 1, 2 and 4, and the honeycomb lattice van Hove singularities are at 0, ±1 and ±3.

6. Conclusion

The lattice GFs for the fundamental second-order linear difference operators $\partial_{p+1}\partial_p^\dagger$ and $\partial_{p-1}^\dagger\partial_p$ appearing in a development of vector difference calculus on a triangular lattice are related to the scalar GFs computed by Horiguchi [9]. In particular, the main results are the explicit GFs for the polar vector operators A_1 and B_1 corresponding to curl $\circ$ curl and grad $\circ$ div, respectively. Formulae for all the GFs are tabulated in appendix A. With them, GFs for the general linear system, equation (3.4), for problems involving scalar or vector fields on a triangular lattice can be obtained in closed form in terms of complete elliptic integrals. The scalar GFs on the honeycomb and Kagomé lattices were found in determining the GFs on a triangle lattice.

For each case tabulated in appendix A, the boundary condition $|\langle\hat{e}^\alpha_{p,q}, G(z)\hat{e}^\beta_{m,n}\rangle| \leqslant M$ for some M has been assumed as $(m-p)^2+(n-q)^2 \to \infty$. GFs for operator A with more general boundary conditions are constructed using the kernel or null space of A, i.e. the subspace of $\mathcal{C}_p$ annihilated by A. For example, the kernel of the discrete Laplacian $\nabla_p^2 = -(\partial_{p-1}^\dagger\partial_p + \partial_{p+1}\partial_p^\dagger)$ contains for $p = 1$ the two 1-fields with constant components, namely $\hat{w}_1 = (1, 2, 1)$, $\hat{w}_2 = (1, 0, -1)$, independent of the site or position index (m, n). But

to match boundary requirements in compact regions we relax the constraint that the solution w of $\nabla^2 w = 0$ remain bounded at ∞. Because the difference equation is linear with constant coefficients, we assume $w^{\alpha}_{m,n} = c_\alpha x^m y^n$ and relate x to y so that the equation $\nabla^2 w = 0$ is satisfied. This requires $p(x, y) = 0$, where

$$p(x, y) = 6 - x - \frac{1}{x} - y - \frac{1}{y} - \frac{x}{y} - \frac{y}{x}. \tag{6.1}$$

Solving simultaneously $p = 0$ and $\mathrm{d}p = 0$ shows a critical point at $(x, y) = (1, 1)$, from which we obtain the parametric family of roots

$$x(t) = -\frac{(t+1)(t+2)}{t\,(t-1)} \tag{6.2a}$$

$$y(t) = \frac{(t+1)(2t+1)}{t-1} \tag{6.2b}$$

and so the general solution for $\nabla^2 w = 0$ is

$$w_{m,n} = \int \Phi(t)\, x(t)^m\, y(t)^n ((t+1)(2t+1), 2t+1, t+2)\, \mathrm{d}t \tag{6.3}$$

where $\Phi(t)$ is arbitrary. In general, t is complex and the integral is over a two-dimensional region in $\mathrm{Re}\,(t)$ and $\mathrm{Im}\,(t)$. In generic terms, the more general GF is of the form $G'(z) = G(z) + w$, with $G(z)$ as tabulated in the appendix and w to correct the boundary conditions.

It is interesting to consider the algebraic origin of the relationships among the GFs for the operators of equations (4.1*a*)–(4.1*d*). First, if $A_p u = \lambda u$, then $B_{p+1}\partial_p^\dagger u = \partial_p^\dagger A_p u = \lambda \partial_p^\dagger u$. Thus

$$\begin{aligned} G(B_{p+1}; z) = (z - \partial_p^\dagger\, \partial_{p+1})^{-1} &= \frac{1}{z}\left(1 - \frac{1}{z}\,\partial_p^\dagger\,\partial_{p+1}\right)^{-1} \\ &= \frac{1}{z}\left(1 + \frac{1}{z}\,\partial_p^\dagger\,\partial_{p+1} + \frac{1}{z^2}\,\partial_p^\dagger\,\partial_{p+1}\,\partial_p^\dagger\,\partial_{p+1} + \frac{1}{z^3}\,\partial_p^\dagger\,\partial_{p+1}\,\partial_p^\dagger\,\partial_{p+1}\,\partial_p^\dagger\,\partial_{p+1} + \cdots\right) \\ &= \frac{1}{z}(1 + \partial_p^\dagger\,(z - \partial_{p+1}\,\partial_p^\dagger)^{-1}\,\partial_{p+1}) \\ &= \frac{1}{z}(1 + \partial_p^\dagger G(A_p; z)\partial_{p+1}). \end{aligned} \tag{6.4}$$

This accounts for the relationship between the GFs of A_0 and B_1 and between A_1 and B_2. The origin of the relationship between GFs for A_0 and B_2 is also algebraic, which can be seen as follows.

First, it is easy to see by induction that if H is the adjacency matrix for some graph, then the number of walks of length n from vertex j to vertex i is $(H^n)_{ij}$. The honeycomb lattice is a bipartite graph, meaning that it divides into two sublattices a and b with a sites adjacent only to b sites and vice versa. Thus H^2_{hon} is the direct sum of two identical adjacency matrices, one for the a and one for the b sublattice. The non-zero entries $(H^2_{\mathrm{hon}})_{ij}$ are for pairs (i, j) connected by a two-step walk, hence either $i = j$ or else i and j are neighbours on the same sublattice. Therefore the aa and bb sub-blocks of (H^2_{hon}) are each $H_{\mathrm{tri}} + 3I$. This shows there is an algebraic relationship between H_{tri} and H_{hon}. To obtain equation (4.12) from it one must use the graph duality between triangle faces and honeycomb sites and take sign changes due to antisymmetry of the 1-simplex basis into account.

Finally, we have seen that the GFs for a rather general linear model come from the GFs of the fundamental operators. To make use of this it is convenient to know some of the spectral properties of the operator algebra generated by the orthogonal pair $A_p = -(-1)^p \partial_{p+1}\partial_p^\dagger$ and $B_p = (-1)^p \partial_{p-1}^\dagger \partial_p$, particularly for $p = 1$. The diagonal GFs for each operator discussed

above are expressed in terms of $\mathcal{G}_{0,0}(z)$, which in turn is given explicitly in terms of an elliptic integral. The density of eigenvalues for a generic operator A, as expressed by equation (3.4), is

$$D_A(E) = -\frac{1}{\pi} \lim_{\eta \to 0^+} \mathrm{Im}\,(\mathrm{Tr}[G(A; E + \mathrm{i}\eta)]) \tag{6.5}$$

where the trace is over cell index α. The van Hove singularities are branch points of the analytic continuation of $G(A; z)$. These singularities correspond to the possible continuum limits at which the difference equations can lead to partial differential equations that do not depend on the lattice spacing a as $a \to 0$.

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Appendix A. Green functions for fundamental operators on the triangle lattice

The following is a brief summary of GFs for the complete set of fundamental operators for vector fields on the triangle lattice. Also tabulated are the scalar GFs for the Kagomé and honeycomb lattices. GFs for $A_1 = \partial_2 \partial_1^\dagger$ or curl $\circ$ curl for 1-fields or polar vector fields are as follows. Let $\varepsilon = z(z-6)$, then

$$G^{11}_{m,n}(A_1; z) = \frac{1}{z}[(z^2 - 4z + 2)\,\mathcal{G}_{m,n}(\varepsilon) - \mathcal{G}_{(m-1),(n+1)}(\varepsilon) - \mathcal{G}_{(m+1)(n-1)}(\varepsilon)]$$

$$G^{12}_{m,n}(A_1; z) = -\frac{1}{z}[\mathcal{G}_{(m-1),n}(\varepsilon) + (z-1)\,\mathcal{G}_{m,(n-1)}(\varepsilon) + (z-1)\,\mathcal{G}_{m,n}(\varepsilon) + \mathcal{G}_{(m+1),(n-1)}(\varepsilon)]$$

$$G^{13}_{m,n}(A_1; z) = \frac{1}{z}[(z-1)\,\mathcal{G}_{m,(n-1)}(\varepsilon) + \mathcal{G}_{m,n}(\varepsilon) + \mathcal{G}_{(m+1),(n-2)}(\varepsilon) + (z-1)\,\mathcal{G}_{(m+1),(n-1)}(\varepsilon)]$$

$$G^{21}_{m,n}(A_1; z) = -\frac{1}{z}[\mathcal{G}_{(m-1),(n+1)}(\varepsilon) + (z-1)\,\mathcal{G}_{m,n}(\varepsilon) + (z-1)\,\mathcal{G}_{m,(n+1)}(\varepsilon) + \mathcal{G}_{(m+1),n}(\varepsilon)]$$

$$G^{22}_{m,n}(A_1; z) = \frac{1}{z}[(z^2 - 4z + 2)\,\mathcal{G}_{m,n}(\varepsilon) - \mathcal{G}_{(m-1),n}(\varepsilon) - \mathcal{G}_{(m+1),n}(\varepsilon)]$$

$$G^{23}_{m,n}(A_1; z) = -\frac{1}{z}[\mathcal{G}_{m,(n-1)}(\varepsilon) + (z-1)\,\mathcal{G}_{m,n}(\varepsilon) + (z-1)\,\mathcal{G}_{(m+1),(n-1)}(\varepsilon) + \mathcal{G}_{(m+1),n}(\varepsilon)]$$

$$G^{31}_{m,n}(A_1; z) = \frac{1}{z}[(z-1)\,\mathcal{G}_{(m-1),(n+1)}(\varepsilon) + \mathcal{G}_{(m-1),(n+2)}(\varepsilon) + \mathcal{G}_{m,n}(\varepsilon) + (z-1)\,\mathcal{G}_{m,(n+1)}(\varepsilon)]$$

$$G^{32}_{m,n}(A_1; z) = -\frac{1}{z}[\mathcal{G}_{(m-1),n}(\varepsilon) + (z-1)\,\mathcal{G}_{(m-1),(n+1)}(\varepsilon) + (z-1)\,\mathcal{G}_{m,n}(\varepsilon) + \mathcal{G}_{m,(n+1)}(\varepsilon)]$$

$$G^{33}_{m,n}(A_1; z) = \frac{1}{z}[(z^2 - 4z + 2)\,\mathcal{G}_{m,n}(\varepsilon) - \mathcal{G}_{m,(n-1)}(\varepsilon) - \mathcal{G}_{m,(n+1)}(\varepsilon)].$$

The following are GFs for $B_1 = -\partial_0^\dagger \partial_1$ or grad $\circ$ div for 1-fields, or polar vector fields.

$$G^{11}_{m,n}(B_1; z) = \frac{1}{z}[(z+4)\,\mathcal{G}_{m,n}(z) - \mathcal{G}_{(m-1),n}(z) - \mathcal{G}_{m,(n-1)}(z) - \mathcal{G}_{m,(n+1)}(z) - \mathcal{G}_{(m+1),n}(z)]$$

$$G^{12}_{m,n}(B_1; z) = \frac{1}{z}[\mathcal{G}_{(m-1),n}(z) - \mathcal{G}_{m,(n-1)}(z) - \mathcal{G}_{m,n}(z) + \mathcal{G}_{(m+1),(n-1)}(z)]$$

$$
\begin{aligned}
G^{13}_{m,n}(B_1;z) &= \frac{1}{z}[\mathcal{G}_{m,(n-1)}(z) - \mathcal{G}_{m,n}(z) - \mathcal{G}_{(m+1),(n-2)}(z) + \mathcal{G}_{(m+1),(n-1)}(z)]\\
G^{21}_{m,n}(B_1;z) &= \frac{1}{z}[\mathcal{G}_{(m-1),(n+1)}(z) - \mathcal{G}_{m,n}(z) - \mathcal{G}_{m,(n+1)}(z) + \mathcal{G}_{(m+1),n}(z)]\\
G^{22}_{m,n}(B_1;z) &= \frac{1}{z}[(z+4)\,\mathcal{G}_{m,n}(z) - \mathcal{G}_{(m-1),(n+1)}(z) - \mathcal{G}_{m,(n-1)}(z) - \mathcal{G}_{m,(n+1)}(z)\\
&\quad -\mathcal{G}_{(m+1),(n-1)}(z)]\\
G^{23}_{m,n}(B_1;z) &= \frac{1}{z}[\mathcal{G}_{m,(n-1)}(z) - \mathcal{G}_{m,n}(z) - \mathcal{G}_{(m+1),(n-1)}(z) + \mathcal{G}_{(m+1),n}(z)]\\
G^{31}_{m,n}(B_1;z) &= \frac{1}{z}[\mathcal{G}_{(m-1),(n+1)}(z) - \mathcal{G}_{(m-1),(n+2)}(z) - \mathcal{G}_{m,n}(z) + \mathcal{G}_{m,(n+1)}(z)]\\
G^{32}_{m,n}(B_1;z) &= \frac{1}{z}[\mathcal{G}_{(m-1),n}(z) - \mathcal{G}_{(m-1),(n+1)}(z) - \mathcal{G}_{m,n}(z) + \mathcal{G}_{m,(n+1)}(z)]\\
G^{33}_{m,n}(B_1;z) &= \frac{1}{z}[(z+4)\,\mathcal{G}_{m,n}(z) - \mathcal{G}_{(m-1),n}(z) - \mathcal{G}_{(m-1),(n+1)}(z) - \mathcal{G}_{(m+1),(n-1)}(z)\\
&\quad -\mathcal{G}_{(m+1),n}(z)].
\end{aligned}
$$

The following are lattice GFs for $B_2 = \partial_1^\dagger \partial_2$ or curl $\circ$ curl for 2-fields, which on the triangle lattice are pseudoscalar. Let $\varepsilon = z(z-6)$, then

$$
\begin{aligned}
G^{11}_{m,n}(B_2;z) &= (z-3)\,\mathcal{G}_{m,n}(\varepsilon)\\
G^{12}_{m,n}(B_2;z) &= -[\mathcal{G}_{m,(n-1)}(\varepsilon) + \mathcal{G}_{m,n}(\varepsilon) + \mathcal{G}_{(m+1),(n-1)}(\varepsilon)]\\
G^{21}_{m,n}(B_2;z) &= -[\mathcal{G}_{(m-1),(n+1)}(\varepsilon) + \mathcal{G}_{m,n}(\varepsilon) + \mathcal{G}_{m,(n+1)}(\varepsilon)]\\
G^{22}_{m,n}(B_2;z) &= (z-3)\,\mathcal{G}_{m,n}(\varepsilon).
\end{aligned}
$$

Here are the Kagomé lattice scalar GFs in terms of the scalar triangle GFs. Let $\varepsilon = (z-4)(z+2)$, then

$$
\begin{aligned}
G^{11}_{m,n}(H_{\mathrm{Kag}};z) &= \frac{1}{z+2}[(z^2-2)\,\mathcal{G}_{m,n}(\varepsilon) - \mathcal{G}_{(m-1),(n+1)}(\varepsilon) - \mathcal{G}_{(m+1),(n-1)}(\varepsilon)]\\
G^{12}_{m,n}(H_{\mathrm{Kag}};z) &= \frac{1}{z+2}[\mathcal{G}_{(m-1),n}(\varepsilon) + (z+1)\,\mathcal{G}_{m,(n-1)}(\varepsilon) + (z+1)\,\mathcal{G}_{m,n}(\varepsilon) + \mathcal{G}_{(m+1),(n-1)}(\varepsilon)]\\
G^{13}_{m,n}(H_{\mathrm{Kag}};z) &= \frac{1}{z+2}[(z+1)\,\mathcal{G}_{m,(n-1)}(\varepsilon) + \mathcal{G}_{m,n}(\varepsilon) + \mathcal{G}_{(m+1),(n-2)}(\varepsilon)\\
&\quad +(z+1)\,\mathcal{G}_{(m+1),(n-1)}(\varepsilon)]\\
G^{21}_{m,n}(H_{\mathrm{Kag}};z) &= \frac{1}{z+2}[\mathcal{G}_{(m-1),(n+1)}(\varepsilon) + (z+1)\,\mathcal{G}_{m,n}(\varepsilon) + (z+1)\,\mathcal{G}_{m,(n+1)}(\varepsilon) + \mathcal{G}_{(m+1),n}(\varepsilon)]\\
G^{22}_{m,n}(H_{\mathrm{Kag}};z) &= \frac{1}{z+2}[(z^2-2)\,\mathcal{G}_{m,n}(\varepsilon) - \mathcal{G}_{(m-1),n}(\varepsilon) - \mathcal{G}_{(m+1),n}(\varepsilon)]\\
G^{23}_{m,n}(H_{\mathrm{Kag}};z) &= \frac{1}{z+2}[\mathcal{G}_{m,(n-1)}(\varepsilon) + (z+1)\,\mathcal{G}_{m,n}(\varepsilon) + (z+1)\,\mathcal{G}_{(m+1),(n-1)}(\varepsilon) + \mathcal{G}_{(m+1),n}(\varepsilon)]\\
G^{31}_{m,n}(H_{\mathrm{Kag}};z) &= \frac{1}{z+2}[(z+1)\,\mathcal{G}_{(m-1),(n+1)}(\varepsilon) + \mathcal{G}_{(m-1),(n+2)}(\varepsilon) + \mathcal{G}_{m,n}(\varepsilon) + (z+1)\,\mathcal{G}_{m,(n+1)}(\varepsilon)]\\
G^{32}_{m,n}(H_{\mathrm{Kag}};z) &= \frac{1}{z+2}[\mathcal{G}_{(m-1),n}(\varepsilon) + (z+1)\,\mathcal{G}_{(m-1),(n+1)}(\varepsilon) + (z+1)\,\mathcal{G}_{m,n}(\varepsilon) + \mathcal{G}_{m,(n+1)}(\varepsilon)]\\
G^{33}_{m,n}(H_{\mathrm{Kag}};z) &= \frac{1}{z+2}[(z^2-2)\,\mathcal{G}_{m,n}(\varepsilon) - \mathcal{G}_{m,(n-1)}(\varepsilon) - \mathcal{G}_{m,(n+1)}(\varepsilon)].
\end{aligned}
$$

For completeness we present the honeycomb lattice scalar GFs derived also in [9]. Let $\varepsilon = (z-3)(z+3)$, so

$$G^{11}_{m,n}(H_{\rm hon};z) = z\,\mathcal{G}_{m,n}(\varepsilon)$$
$$G^{12}_{m,n}(H_{\rm hon};z) = \mathcal{G}_{m,(n-1)}(\varepsilon) + \mathcal{G}_{m,n}(\varepsilon) + \mathcal{G}_{(m+1),(n-1)}(\varepsilon)$$
$$G^{21}_{m,n}(H_{\rm hon};z) = \mathcal{G}_{(m-1),(n+1)}(\varepsilon) + \mathcal{G}_{m,n}(\varepsilon) + \mathcal{G}_{m,(n+1)}(\varepsilon)$$
$$G^{22}_{m,n}(H_{\rm hon};z) = z\,\mathcal{G}_{m,n}(\varepsilon).$$

Appendix B. Green function extension theory

Let H be a Hermitian matrix representing a difference operator on any lattice, and suppose the GFs for H, which are entries of the resolvent matrix

$$g(z) = (z-H)^{-1} \tag{B.1}$$

defined for complex z outside the spectrum of H, are known in closed form. Now suppose one needs the GFs defined by

$$G(z) = (z - f(H))^{-1}. \tag{B.2}$$

For simplicity, assume $f(x)$ is a rational function such that the rational expression

$$R(z,x) = \frac{1}{z-f(x)} \tag{B.3}$$

is regular at infinity and has only simple poles $\{x_k(z)\}$ with residues $\{R_k(z)\}$ for $k = 1, 2, 3, \ldots, N$. Using the spectral representation for H in the Cauchy integral formula for $G(z)$ gives

$$G(z) = \frac{1}{2\pi \mathrm{i}} \oint_{\mathcal{C}_1} \sum_{\mu} |\mu\rangle \frac{R(z,x)\,\mathrm{d}x}{x-\lambda_\mu} \langle\mu| = -\frac{1}{2\pi \mathrm{i}} \oint_{\mathcal{C}_2} g(x)\,R(z,x)\,\mathrm{d}x \tag{B.4}$$

where $\mathcal{C}_1$ encloses only the singularity $x = z$, and $\mathcal{C}_2$ contains only the other singularities $x = x_k(z)$ coming from $R(z,x)$. Since H is a large matrix the sum over μ contains a large number of terms, each one difficult to compute; the expansion is only of use formally. However one takes advantage of the fact that $R(z,x)$ is rational. Thus from the residue theorem,

$$G(z) = -\sum_{k=1}^{N} R_k(z)\,g(x_k(z)). \tag{B.5}$$

The sum now is over the N poles in x of $R(z,x)$, of which there are typically only a few. Therefore the latter is an explicit formula for the desired GFs $G(z)$.

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