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Laplacians on Lattices

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Abstract

We consider some lattices and look at discrete Laplacians on these lattices. In particular we look at solutions of the equation

$$\triangle(1)\phi = \triangle(2)Z,$$

where $\triangle(1)$ and $\triangle(2)$ denote two such Laplacians on the same lattice. We show that, in one dimension, when $\triangle(i)$, $i = 1, 2$, denote

$$\triangle(1)\phi = \phi(i+1) + \phi(i-1) - 2\phi(i)$$

and

$$\triangle(2)Z = Z(i+2) + Z(i-2) - 2Z(i),$$

this equation has a simple solution

$$\phi(i) = Z(i+1) + Z(i-1) + 2Z(i).$$

We show that in two dimensions, when the system is considered on a hexagonal (honeycomb) lattice, we have a similar relation. This is also true in three dimensions when we have a very special lattice (tetrahedral with points inside). We also briefly discuss how this relation generalizes when we consider other lattices.

1 Introduction

Recently a Fröhlich Hamiltonian was studied on two-dimensional, discrete, quadratic [1, 2, 3] and hexagonal lattices [5]. The resultant equations were rather complicated to solve but, when one restricted oneself to looking at stationary fields, the equations simplified somewhat and, in the case of hexagonal lattice, one could decouple them and reduce them to the localized discrete nonlinear Schrödinger equation.

The reason for this decoupling lies in the observation that on an hexagonal lattice the equation

$$\triangle(1)\phi = \lambda \triangle(2)Z \tag{1.1}$$

has a simple localized solution for Z as function of ϕ. Here $\triangle(i)$, $i = 1, 2$, refer to the two simplest discrete Laplacians on an hexagonal lattice, i.e. those involving 4 and 7 lattice points (more details are given later). A similar situation holds in one dimension and in fact was used by Davydov [4] in his observation that the interaction of an appropriate Schrödinger field, such as a field describing amide I-vibration in biopolymers with the distortions of the underlying lattice, results in the creation of a localized state which has, since then, been called Davydov's soliton [6].

In this paper we look in detail at equation (1.1) in the case of various lattices. We find that a regular lattice in one dimension, a hexagonal lattice in two dimensions and a tetrahedral lattice (with points inside) in three dimensions are somewhat special as it only in their cases the system possesses simple localized solutions. We discuss the modifications that are required to have localized solutions for other (more complicated) lattices.

2 One dimension

Consider a regular lattice as shown in Fig. 1.

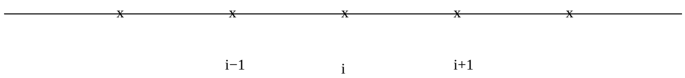

Figure 1. One dimensional lattice.

For simplicity we take the lattice spacing to be given by $a = 1$. Then define $\triangle(1)P(i)$ as

$$\triangle(1)P(i) \;=\; P(i+1) + P(i-1) - 2P(i) \tag{2.1}$$

and

$$\triangle(2)P(i) \;=\; P(i+2) + P(i-2) - 2P(i), \tag{2.2}$$

i.e. the same expression as above but with the displacement by two lattice units.

Then consider the equation:

$$\triangle(1)\phi(i) = \triangle(2)Z(i), \tag{2.3}$$

which we want to solve for $\phi(i)$ in terms of $Z(k)$.

2.1 Continuum limit

Note that in the continuum limit our equation (2.3) reduces to

$$\frac{d^2\phi}{dx^2} \;=\; 4\frac{d^2 Z}{dx^2}, \tag{2.4}$$

which clearly has a solution

$$\phi(x) \;=\; 4Z(x) \tag{2.5}$$

plus of course a linear and a constant piece.

2.2 Discrete case

In this case it is easy to see that a solution is given by

$$\phi(i) \;=\; Z(i+1) + Z(i-1) + 2Z(i). \tag{2.6}$$

Of course to this we can also add $Ai + b$, which are the lattice equivalents of the linear and constant pieces of the continuum case.

Note that our solution (2.6) has the correct continuum limit. Note also that its structure is very similar to the structure of $\triangle\phi(i)$ except that this time all terms carry the positive sign.

3 Two dimensional Cases

3.1 Square lattice

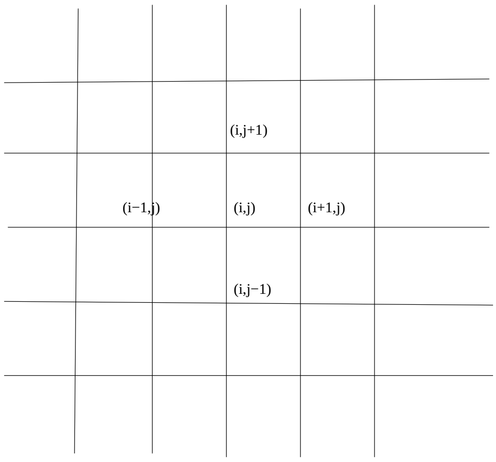

Figure 2. Two-dimensional square lattice.

When we have a square lattice (see Fig. 2) we can consider various Laplacians. One of them, which we call $\triangle(1)$, involves the nearest lattice points and is defined as

$$\triangle(1)\phi(i,j) \;=\; \phi(i+1,j) + \phi(i-1,j) + \phi(i,j+1) + \phi(i,j-1) - 4\phi(i,j). \tag{3.1}$$

The second 'obvious' Laplacian can be defined as the one above with shifts by two lattice points, ie

$$\triangle(2)\phi(i,j) \;=\; \phi(i+2,j) + \phi(i-2,j) + \phi(i,j+2) + \phi(i,j-2) - 4\phi(i,j) \tag{3.2}$$

or we could also 'involve' the corners, ie terms corresponding to $i \pm 1,\ j \pm 1$.

Thus we could define $\triangle(2')\phi(i,j)$ as

$$\begin{aligned}\triangle(2')\phi(i,j) \;=\; &\phi(i+2,j) + \phi(i-2,j) + \phi(i,j+2) + \phi(i,j-2)+\\ &+\alpha\left(\phi(i-1,j-1) + \phi(i+1,j-1) + \phi(i-1,j+1) +\right.\\ &\left.+\phi(i-1,j-1)\right) - 4(1+\alpha)\phi(i,j)\end{aligned} \tag{3.3}$$

for any value of α.

The work mentioned in [1, 2, 3] required a solution of

$$\triangle(1)P(ij) \;=\; \mu\,\triangle(2)Z(ij), \tag{3.4}$$

where $\triangle(2)$ is given by an expression as in (13).

Unfortunately, this equation has no simple local solution. The problem is with the 'corners'; the second Laplacian should involve expressions at $i \pm 1, j \pm 1$.

Thus it is possible to solve

$$\triangle(1)P(ij) \;=\; \mu\,\triangle(2')Z(ij) \tag{3.5}$$

for an appropriate choice of α. To see this, in analogy with (2.6), take

$$P(ij) \;=\; \lambda(Z(i-1,j) + Z(i+1,j) + Z(i,j-1) + Z(i,j+1) + 4Z(i,j)). \tag{3.6}$$

Then

$$\begin{aligned}\triangle(1)P(i,j) \;=\; & \lambda\,(Z(i+1,j) + Z(i-2,j) + Z(i,j-2) + Z(i,j+2) + \\ & +2Z(i+1,j+1) + 2Z(i-1,j+1, +2Z(i+1,j-1) + 2Z(i-1,j-1))\,,\end{aligned} \tag{3.7}$$

which is clearly a solution when $\alpha = 2$ in (3.1).

3.2 Hexagonal (honeycomb) lattice

Next consider a hexagonal lattice as shown in Fig. 3.

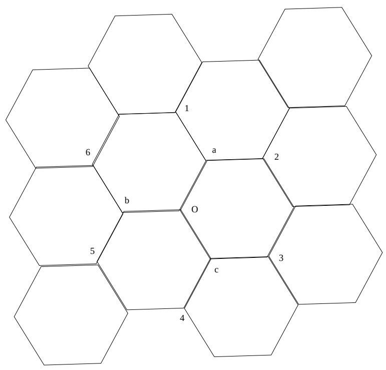

Figure 3. Hexagonal (honeycomb) lattice.

For $\triangle(1)$ take the 4-point Laplacian (involving 0 and 3 'nearest' points), ie take

$$\triangle(1)P(0) \;=\; P(a) + P(b) + P(c) - 3P(0) \tag{3.8}$$

For $\triangle(2)$ take the Laplacian involving the 'next to the nearest' points, ie the 7-point Laplacian defined by

$$\triangle(2)Z(0) \;=\; Z(1) + Z(2) + Z(3) + Z(4) + Z(5) + Z(6) - 6Z(0). \tag{3.9}$$

Then consider

$$\triangle(1)P(0) \;=\; \mu\,\triangle(2)Z(0). \tag{3.10}$$

In fact this is the equation which arose in the study reported in [5]. There it was shown that this equation has a simple local solution and that solution is given by

$$P(0) \;=\; \mu(Z(a)+Z(b)+Z(c)+3Z(0)). \tag{3.11}$$

Thus in this sense the hexagonal lattice mostly resembles the one dimensional case; the double lattice spacing in the one-dimensional case is replaced by the double the angle between the directions on the lattice.

3.3 Triangular lattice

Next we consider a triangular lattice as shown in Fig. 4.

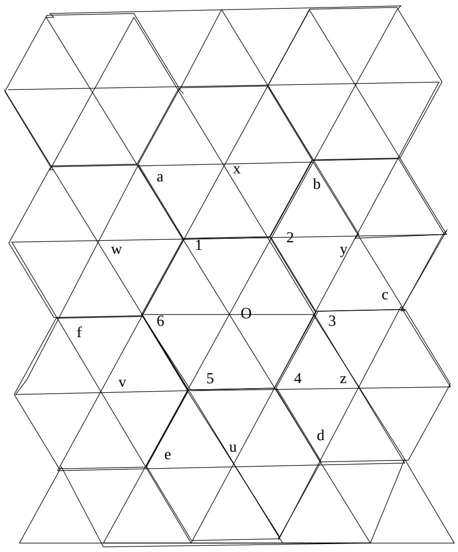

Figure 4. The triangular lattice

This time the obvious $\triangle(1)$ involves taking the 7-point Laplacian

$$\triangle(1)P(0) \;=\; P(1)+P(2)+P(3)+P(4)+P(5)+P(6)-6P(0). \tag{3.12}$$

For the 'second' Laplacian we have more choice. We can take

$$\triangle(2)Z(0) \;=\; Z(a)+Z(b)+Z(c)+Z(d)+Z(e)+Z(f)-6Z(0) \tag{3.13}$$

or we could add to it

$$+\,A(\,Z(u)+Z(v)+Z(w)+Z(x)+Z(y)+Z(z)-6Z(0)). \tag{3.14}$$

However, in general, it is difficult to solve the equation

$$\triangle(1)P(0) = \triangle(2)Z(0). \tag{3.15}$$

Only when $A = 2$, i.e. for $\triangle(2')$ given by (24) and (25) with $A = 2$, have we succeeded in finding a local solution.

This solution is given by

$$P(0) = Z(1) + Z(2) + Z(3) + Z(4) + Z(5) + Z(6) + 4Z(0). \tag{3.16}$$

If guided by the experience gained from the previous cases we take

$$P(0) = Z(1) + Z(2) + Z(3) + Z(4) + Z(5) + Z(6) + 6Z(0), \tag{3.17}$$

we find that the Z field satisfies

$$\begin{aligned} &Z(a) + Z(b) + Z(c) + Z(d) + Z(e) + Z(f) + 2\,[Z(1) + Z(2) + Z(3) + Z(4) + \\ &+Z(5) + Z(6) + Z(u) + Z(v) + Z(w) + Z(x) + Z(y) + Z(z)] - 36Z(0) = 0. \end{aligned} \tag{3.18}$$

We see that in this case we have 19-point Laplacian, ie a Laplacian which involves both the new and the original lattice points.

One can consider other, more complicated cases, but it is clear that the hexagonal lattice is very special as only for it, as in the one-dimensional case for a regular lattice, have we a simple local solution of the problem (3.10) with Laplacians involving the 'nearest' and 'next-to-the-nearest' lattice points only.

4 Three Dimensions

The discussion of the previous sections generalizes very easily to three dimensions. Firstly for a regular cube-like lattice for which in two dimensions we had problems with 'corner' terms, the situation is similar except that now we have more such problems.

Thus, if we take

$$\begin{aligned} \triangle(1)P(i,j,k) = {} & P(i+1,j,k) + P(i-1,j,k) + P(i,j-1,k) + P(i,j+1,k) + \\ & + P(i,j,k-1) + P(i,j,k+1) - 6P(i,j.k) \end{aligned} \tag{4.1}$$

and then consider

$$\begin{aligned} P(i,j,k) = {} & Z(i+1,j,k) + Z(i-1,j,k) + Z(i,j-1,k) + Z(i,j+1,k) + \\ & + Z(i,j,k-1) + Z(i,j,k+1) + 6Z(i,j.k), \end{aligned} \tag{4.2}$$

we find that $Z(i,j,k)$ satisfies a rather complicated expression involving the fields at all points (i,j,k) which correspond to the shift of only one of these indices by ± 2. There are six such terms and they all come with the coefficient $= +1$. In addition we also have to add all terms which involve the shift of two of the indices (i,j,k) by ± 1. There are twelve such terms and we have to add them all with the coefficient $= 2$. Then finally we subtract $-24Z(0,0,0)$. A little thought shows that this is the obvious generalization of the square lattice which we discussed in the previous section.

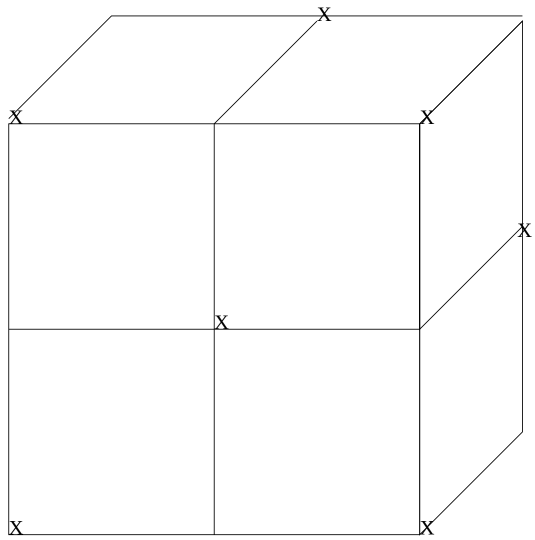

Figure 5. The three-dimensional lattice. Points A shown. In the center of each other cube there is a point B. Points B together form another lattice like the one shown but displaced by $\frac{1}{2}$ lattice spacing in all directions.

However, we have a regular lattice which is a 'natural' three-dimensional generalization of the hexagonal lattice in two dimensions. Such lattice can be constructed in the following way:

Take a regular cube lattice and delete every other lattice point as indicated in Fig. 5. Then place a similar lattice at the points which are the centers of the cubes of the previous lattice. This way we have a body centered lattice with many points missing.

Consider then the points of the original cube lattice as points of type A and those of the additional lattice as points of type B. Then the nearest neighbors of each point A are four lattice points of type B and vice-versa. The next to nearest neighbors (ntn), however, come from the original lattice, ie for a point type A they are points of type A and for the point B they are points of type B. Each point A has four nearest neighbors and 12 ntn points. By construction this is the case for both types of lattice points.

Clearly we have two obvious Laplacians that we can consider - those involving the nearest neighbors and those involving only the ntns.

Consider for simplicity the point B located at (0,0,0) inside a cube of size $2a$ with points of type A located at (1,-1,1), (-1,-1, -1) and (1,1,-1) and (-1,1,1,) (we are using the convention of x horizontally to the right, z vertically up and y away from the observer). Then we can define

$$\begin{aligned}\triangle(1)P(0,0,0) \;&=\; P(1,-1,1)+P(-1,-1,-1)+P(1,1,-1)+\\ &+P(-1,1,1)-4P(0,0,0).\end{aligned} \tag{4.3}$$

In the continuum limit this expression clearly reduces to the Laplacian of P, ie to $(\partial_x^2 + \partial_y^2 + \partial_z^2)P$.

For the second Laplacian we take ntn points. Note that they correspond to points ± 2 and 0 such that one of the coordinates of x, y and z is zero while the others take values ± 2. Thus we define

$$\begin{aligned} \triangle(2)P(0,0,0) \;=\; & P(-2,-2,0) + P(2,-2,0) + P(-2,2,0) + P(2,2,0)+ \\ & + P(-2,0,-2) + P(-2,0,2) + P(2,0,-2) + P(2,0,2)+ \\ & + P(-2,-2,0) + P(-2,2,0) + P(2,-2,0) + P(2,2,0). \end{aligned} \tag{4.4}$$

Now we consider our equation:

$$\triangle(1)P \;=\; \alpha \triangle(2)Z, \tag{4.5}$$

where P and Z are taken at the same lattice point, say $(0,0,0)$.

Guided by our experience from the lower-dimensional cases we take

$$\begin{aligned} P(0,0,0) = \beta(& Z(1,-1,1) + Z(-1,-1,-1) + Z(1,1,-1)+ \\ & + Z(-1,1,1) + 4Z(0,0,0)). \end{aligned} \tag{4.6}$$

Then it is a matter of simple algebra to check that P does indeed satisfy (4.5) when $\beta = \alpha$. A little thought shows that our lattice is really tetrahedral in nature (with points inside it). Hence it is a natural generalization of the hexagonal lattice in two dimensions.

5 Conclusions

In this short note we have discussed various lattices and Laplacians defined on these lattices. Our main interest was the relation between various Laplacians and the existence or not of fully localized solutions of the equation

$$\triangle(1)P(0) = \triangle(2)Z(0) \tag{5.1}$$

involving these Laplacians.

We have found that in one dimension this equation has a localized solution when the lattice is regular and $\triangle(1)$ and $\triangle(2)$ involve the Laplacians constructed with the 'nearest' and 'next-to-the-nearest' lattice points. Moreover the points in each Laplacian are equidistant from the central point.

These conditions are also required in higher-dimensional lattices where they are much more stringent. Thus in two dimensions they require that the lattice be hexagonal (honeycomb) and then $\triangle(1)$ and $\triangle(2)$ involve 1+3 point and 1+6 point Laplacians. For other lattices the Laplacians mix points of different distance from the central point and we have not succeeded in finding a localized solution of (15).

In three dimensions the relevant lattice is the 'body centered tetrahedral lattice'. In this case $\triangle(1)$ involves 1+4 lattice points and $\triangle(2)$ 1+12 points.

Note that in one dimension our Laplacians involve doubling of distance, in two dimensions - doubling the angle and in three dimensions doubling the spherical angles.

Noting the pattern of our results we expect that our results generalize to higher dimensions, where in D dimensions we expect $\triangle(1)$ to involve $1 + (D + 1)$ points and $\triangle(2)$ $1 + D(D + 1)$ points, but lattices with such Laplacians do not appear to be physical and so we have not attempted to construct them.

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