Connecting boundary and interior — “Gauss’s law” for graphs

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The Gauss’s law, in an abstract sense, is a theorem that relates quantities on the boundary (flux) to the interior (charge) of a surface. An identity for soap froths were proved with the same boundary–interior relation. In this article, we try to construct a definition of flux for other graphs, such that a similar boundary–interior relation can be satisfied.

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I. INTRODUCTION

The introduction of random lattice for the description of space-time continuum has provided a new perspective to the foundation of physics [1–3]. The random lattice consists of points distributed at random, with nearby sites connected so as to form the edges of non-overlapping simplices which fill the entire system. Lorentz invariance can be maintained by proper averaging over these random lattices.

Rather than investigating the consequence of this radical approach to physics, we like to look at the random lattice more closely in the perspective of networks. If one consider the simplices formed by nodes and links in the random lattice as a complex network, we can ask about its general properties, such as degree distribution, clustering coefficients, etc of the random lattice and see if these properties of the network have important relation to the field theories that are build on such discretization of space-time.

For now, we still want to narrow down the investigation to a more mundane question, which concerns the relevance of the random lattice in the discretization of classical electrodynamics. As Gauss’s law is fundamental to classical electrodynamics, we like to see if a generalization of this law can be formulated for networks, and if so, what kind of networks will obey Gauss’s law. One immediate example is the trivalent cellular network formed by soap froth. This cellular network has a simple property relating the boundary to the interior, through a quantity called topological charge. We like to generalize this observation in soap froth to complex networks.

II. THEORY

A. Inspiration

Bubbles in 2D soap froth carry a property known as topological charge [4], 6 minus the number of sides of the bubble. With a simple cluster of bubbles, it was shown that the total charge of the cluster is related to the vertices on the cluster’s edge [5], which is a simple application of Euler’s formula \( V - E + F = 2 \). The soap froth is in fact an infinite trivalent graph, with the bubbles as nodes, and contacting faces as edges. In this dual-graph representation, we define the charge \( q_v \) of a node \( v \) as \( 6 - \deg v \), and the flux \( \Phi(S) \) of a connected cluster of nodes \( S \) as the number of triangles with exactly 1 node outside \( S \), minus the number of triangles with exactly 1 node inside \( S \), plus 6. Then we find that (Figure 1a)

\[
\Phi(S) = \sum_{v \in S} q_v.
\]

This can be considered as a topological analog of Gauss’s law \( \Phi(S) = \oint_S E \cdot dS = Q/\epsilon_0 \) as the \( \Phi \) term only related to quantities on the boundary — objects that span across the interior and exterior of \( S \) — and the \( Q \) term is an accumulation of quantities inside \( S \).

The boundary–interior relation can be found on undirected trees (i.e. acyclic graphs) as well. If we define the charge of a tree vertex \( v \) as \( q_v = 2 - \deg v \), and the flux \( \Phi \) of a cluster as 2 minus the number of edges crossing the boundary, then Equation 1 will also be satisfied (Figure 1b).

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From these examples, we conjecture that with a suitable definition of \( q_v \) and \( \Phi(S) \), a corresponding Equation 1 can apply to some classes of graphs. We would like to formulate an expression for \( \Phi \) and \( q_v \), and find out some examples and counter-examples.

### B. Flux

In the following, we suppose \( G = (V, E) \) is a simple undirected graph and is connected.

In both the trivalent graph and tree cases, the flux is defined in terms of count of objects that crosses the boundary. Therefore, we can define the flux of a set of nodes \( S \) inducing a connected subgraph as a count of arbitrary subgraphs across the boundary:

\[
\Phi''(S) = A_0(S) + \sum_{\substack{H \subseteq G \\mid H \cap S \neq \emptyset \\mid H \cap (V \setminus S) \neq \emptyset}} A_{H, |H \cap S|},
\]

where \( A_0(S) \) is an arbitrary real function, and \( A_{H, |H \cap S|} \) is a real constant depending on \( H \) and \( |H \cap S| \). We call \( \Phi'' \) the partial flux of \( S \). Like a physical system, this artificial flux defined here should also satisfy some preconditions. The most important one is the additivity of flux:

\[
\Phi''(S_1 \cup S_2) = \Phi''(S_1) + \Phi''(S_2)
\]

when \( S_1 \cap S_2 = \emptyset \) and \( S_1 \cup S_2 \) induces a connected subgraph. This gives the definition of partial charge in terms of partial flux when we enforce Equation 1:

\[
q''_v = \Phi''(\{v\})
\]

because

\[
\Phi''(S) = \Phi'' \left( \bigcup_{v \in S} \{v\} \right) = \sum_{v \in S} \Phi''(\{v\}) = \sum_{v \in S} q''_v.
\]

Looking at the definition of fluxes of soap froths and trees, we find that there is already a constant term “6” and “2”, so for simplicity we assume \( A_0(S) \) is just a constant. The subgraphs \( H \) are usually chosen with special properties,
such as cliques or cycles. For example, if we choose $H$ to be all complete subgraphs, then, applying distributive law, the partial flux can be rewritten as

$$
\Phi''(S) = A_0 + \sum_{n=3}^{\infty} \sum_{l=1}^{\lceil n/2 \rceil - 1} A_{nl} F_{nl}(S),
$$

where $F_{nl}(S)$ is the count of complete $n$-subgraphs having $l$ nodes inside $S$, and $A_{nl}$ are coefficients derived from the graph’s property. Since for a graph $G$ with $N$ nodes, the highest clique number is $N$, so the infinite sum will stop when $n = N$. Thus, there will be at most $\sum_{n=3}^{N} (\lceil n/2 \rceil - 1) \sim N^2/4$ coefficients.

In the above we assumed both $S$ have exactly 1 connected component. When $S$ is composed of many connected components $S_i$, we impose Equation 2 and define the partial flux for disconnected subgraphs

$$
\Phi'(S) = \sum_i \Phi''(S_i).
$$

Now consider the flux of the whole graph. This set has no boundary, so $\Phi'(V) = A_0$. In particular, $\Phi'(V)$ has no contribution from $A_{H,|H\cap S|}$. Suppose we split $V$ into two subset of nodes $S$ and $V \setminus S$ inducing two subgraphs. Many subgraphs $H$ in the interior of $V$ will now reside on the boundary of $S$ and $V \setminus S$. Enforcing the additivity of flux, these contributions should cancel each other. We could antisymmetrize the partial flux to give the complete flux that expresses this:

$$
\Phi(S) = A_0 + \Phi'(S) - \Phi'(V \setminus S).
$$

The extra $A_0$ is needed to maintain the invariance of $\Phi(V)$ for whatever partition $\{S, V \setminus S\}$ we choose. The complete charge is thus similarly defined

$$
q_v = \Phi(\{v\})
$$

A flux that is not identically zero may not be sensibly definable for every graph.

### III. EXAMPLES

#### A. Undirected Trees

Trees has partial flux

$$
\Phi''_{\text{tree}}(S) = 1.
$$

This is equivalent to the charge defined in Section II A. When a node $v$ has degree $k$, the subgraph $V \setminus \{v\}$ will have $k$ connected components. Therefore,

$$
\Phi(\{v\}) = 1 + \Phi'(\{v\}) - \Phi'(V \setminus \{v\})
= 1 + 1 - \sum_{i=1}^{k} 1
= 2 - k.
$$

The tree is the simplest family of graphs that have a well-defined flux, which the partial flux is just a constant.

This is equivalent to the property that every connected subgraph of a tree is still a tree, and a tree with $N$ nodes has exactly $N - 1$ edges. Suppose we pick any connected set of nodes $S$ of the tree $G$, then the induced subtree it has $|S|$ nodes and $|S| - 1$ edges. Using the handshaking lemma, i.e. the total degree of a graph $G'$ is twice the number of edges $\sum_{v \in G'} k_v = 2 (\#\text{edges of } G')$, we have

$$
\sum_{v \in S} k_v = 2 (\#\text{edges within } S) + (\#\text{edges out of } S)
= 2 |S| - 2 + (\#\text{edges out of } S)
= \sum_{v \in S} \frac{(2 - k_v)}{\Phi((v))} = 2 - \frac{(\#\text{edges out of } S)}{\Phi(S)}.
$$

This proves our definition of flux is correct.
There is no well-defined flux when a defect appears on the boundary. As shown above, the heptagonal node is part of 8 different triangles $K_3$ and 1 tetrahedron $K_4$ ($F_{31} = 8, F_{41} = 1$) in the dual graph, which has an overcount of triangle connecting the three heptagonal nodes. However, the triangular node is part of 3 different triangles $K_3$ and 1 tetrahedron $K_4$ ($F_{31} = 3, F_{41} = 1$) which does not have any overcount.

### TABLE I: Some small graphs that have well-defined fluxes.

| Graph                          | Partial flux $\Phi''(S)$ |
|-------------------------------|---------------------------|
| All of $\mathbb{H}_n$         | $3 - F_{31}$              |
| Hamiltonian graphs with 4 nodes | $4 - 2 F_{41}^c$         |
| Hamiltonian graphs with 5 nodes | $5 - 3 F_{31}^c - F_{52}^c$ |
| Hamiltonian graphs with 6 nodes | $6 - 4 F_{31}^c - 2 F_{52}^c$ |
| Tetrahedron, Octahedron, Icosahedron | $6 - F_{31}$             |
| Cube and $I_4$                | $4 - F_{41}^c$            |
| Dodecahedron                  | $10 - 3 F_{31}^c - F_{52}^c$ |
| $D_5$                         | $30 - 9 F_{51}^c - 3 F_{52}^c - 10 F_{61}^c - 5 F_{62}^c$ |

#### B. Triangular Graphs

Triangular graphs are graphs which the only faces are triangles. The 2D soap froth is of this kind. The partial flux could be defined as

$$\Phi''_{\text{triangular}}(S) = 6 - F_{31}(S),$$

where $F_{31}(S)$ is the same as the definition in Equation 3. Considering the dual graph of triangular graph, $F_{31}(S)$ is the same as $V^+(S)$ in Reference 3, so this definition of partial flux also makes sense — as long as $S$ does not contain a $K_4$ (4-clique, a.k.a. tetrahedron) on its boundary, i.e. a defect (triangular bubble) in the soap froth.

The error when including a defect is due to overcounting of triangles — there should be only 3 triangles in $K_4$ in the planar graph, but when the embedded space is not considered, 4 triangles would be counted. When the defect causes an overcount, this leads to an extra term

$$\Phi''_{\text{triangular}}(S) = 6 - F_{31}(S) + F_{41}(S),$$

but in general defect doesn’t always overcount, e.g. the charge of a defect (Figure 2). Therefore, the triangular graph’s flux is well-defined as long as the defect does not appear on the boundary.

Since the flux of triangular graph is essentially derived from Euler’s formula, it should be generalizable to higher-dimensional simplicial graphs (soap froths).
IV. DISCUSSION

We see that there isn’t a general rule on which types of subgraphs $H$ should be chosen, so it is hard to deny the existence of a definition of nonzero partial flux for a particular graph $G = (V, E)$. However, we could still experimentally prove or reject some possibilities of flux, based on the equality of flux and total charge (Equation 1).

Assume the partial flux is defined with Equation 3, where $A_0$ and $A_{nl}$ are assumed to be unknown. Given an arbitrary induced subgraph $S$, we could compute $F_{nl}(S)$, and thus $\Phi(S)$ and $Q(S) = \sum_{v \in S} q_v$. Both expressions are linear combinations $A_0$ and $A_{nl}$. If the flux is well-defined, $\Phi(S)$ and $Q(S)$ must be equal, i.e.

$$\Phi(S) - Q(S) = 0,$$

and this yields one linear equation involving $A_0$ and $A_{nl}$. There are $2|V|$ possible subgraphs (thus equations), while the number of coefficients $A_{nl}$ is at most $|V|^2/4$. If this overspecified problem can be solved with a nontrivial solution, i.e. the matrix defined by this homogeneous system of linear equations have nonzero nullity, then the solution gives the definition of partial flux. In practice, $2|V|$ is too big even for a relatively small graph, so we may randomly pick $X \gg |V|^2/4$ subgraphs to check. We could also use linear regression to find a best fit, but this may not report the expected result.

Using the above method, we could find that highly symmetrical graphs such as the cube graph and dodecahedron also have well-defined fluxes

$$\Phi'_{\text{cube}}(S) = 4 - F_{41}^c(S),$$

$$\Phi'_{\text{dodecahedron}}(S) = 10 - 3F_{51}^c(S) - F_{52}^c(S)$$

where $F_{nl}^c(S)$ is similar to $F_{nl}(S)$, except that cycles are counted instead of cliques. Table I shows other linear regression results. However, many other graphs do not have a well-defined flux either when counting cliques or simple cycles. A simple counter-example is shown in Figure 3, where Equation 3 is not well-defined. We have seen a number of positive and negative examples already, so we question, what kind of graphs will have a well-defined flux? In particular, do physical graphs defined spatially like the soap froth all have a mostly well-defined flux? If true, this would place an strong restriction on what graphs would be allowed.

Another food for thought is what family of graphs can be generated given a definition of partial flux, e.g. would only trees satisfy $\Phi'(S) = 1$? The partial flux could give an interesting classification of graphs.
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