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A user's guide: Dynamics and fluctuations of cellular cycles on CW complexes

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3. Story of the development

The ideas studied in [**CCK**] are a culmination of my work as a PhD student at Wayne State University with my two advisors and co-authors, Vladimir Chernyak and John Klein. I began the project as soon as I entered the PhD program in January 2012 and finished with my graduation in March 2016. The work was split into three main pieces: the higher Kirchhoff theorem [**CCK15a**], the higher Boltzmann distribution [**CCK15b**], and coalescing them into a result on stochastic dynamics [**CCK**].

The background work began the year before I started working with John and Vladimir. In the summer of 2011, they visited Los Alamos National Laboratory, and together with Nik Sinitsyn, wrote both statistical mechanics and topology papers, in which they defined stochastic current for random walks on graphs. This work was interesting for a variety of reasons, but at least superficially, it mixed algebraic topology with statistical mechanics in a completely novel way. Their main result was to relate stochastic dynamics to two classical results in physics, the Kirchhoff network problem and Boltzmann distribution, to obtain an *integral* homology class, instead of a real homology class as was expected. Interestingly, the integral homology class had been observed in a variety of experiments on molecular motors, ratchets, and in other settings well before they formulated and proved their result. The fact that this result had experimental evidence before it was made precise is something which can't be said for many theorems in topology. Furthermore, their papers included various conjectures about points moving in higher-dimensional CW complexes, but not about the motion of higher-dimensional subcomplexes. This formed the starting point of my contributions.

When I started in January 2012, we began by attempting to generalize Kirchhoff's network theorem to CW complexes. This required the notion of spanning tree for a CW complex of arbitrary dimension. While similar objects had been defined by combinatorialists prior to our work, we were unable to find a definition suitable for our context. So, we defined a higher spanning tree based on what we needed to solve the higher Kirchhoff problem. In March 2012, we discovered a purely algebro-topological proof of the classical theorem had been given in 1961 [**NS61**]. This was of tremendous help, since we could follow their ideas and proofs of the classical Kirchhoff theorem in an attempt to prove the higher Kirchhoff theorem, with the exception of a few key lemmas. It turned out that the one-dimensional formulas of [**NS61**] generalized correctly only when the CW complex X had no torsion in its homology, e.g., a graph. We discovered through trial and error that by appropriately introducing the torsion factors θ_T of Section 2 and modifying the standard inner products on $B_*(X)$ and $C_*(X)$, we obtained a formula that worked in general, and importantly, reduced to the classical result. In May 2012, I travelled to LANL as a summer student, working on a different but related project. There we finished the main proofs and the final form of [**CCK15a**] took shape.

From the first week of speaking with him, Vladimir had been asking me to work out a higher dimensional Boltzmann distribution. It was very unclear at first what properties such an operator should satisfy. We tried to define it using peculiar orthogonality conditions on $C_*(X)$ and $B_*(X)$, with various inner products similar to the Kirchhoff problem. We attempted to solve the problem using spanning trees, but this quickly failed. We next tried to solve the problem algorithmically, writing equations for every codimension one cell of the complex and then solving these equations in the low-temperature limit. This led to trivial (and incorrect) solutions for spaces with torsion in their homology such as Moore spaces. I distinctly recall Vladimir expressing his concern that maybe such a closed form could only be written in the low-temperature limit, and did not exist in general. Given how amazing his intuition about the project (and in general) was up to that point, this was worrisome.

Finally, in January 2014 I was able to write down a simple statement of the Boltzmann problem. The solution to the problem took shape in March 2014 by thinking back to the classical Boltzmann distribution, which is written as a sum over vertices in a graph. Based on our definition of a spanning tree, we asked how one classifies a vertex of a graph homologically. This consideration led us to define a spanning co-tree for a CW complex, so named because they are dual to spanning trees[1]. Our homological approach may seem strange given the enormous discrepancy between graphs and generic CW complexes (e.g., the complexity of general attaching maps as compared to those of graphs), but it provided the solution. We knew they would need to be appropriately weighted and summed for the desired formula to work out correctly.

When we wrote down the Boltzmann distribution, we were unaware of how strong the duality was between it and the Kirchhoff problem. This came to light in April 2014 while we were attempting to prove that our proposed distribution was in fact correct. After several manipulations, we transformed the problem into

[1] It has been only recently pointed out that our spanning co-trees have been defined in other contexts.

a statement of linear algebra, for which we were sure the answer was known. We eventually came across the theory of pseudo-inverses. Pseudo-inverses provide one-sided inverses for maps which fail to be either injective or surjective (or both). It turns out that pseudo-inverses have an explicit expression as a sum, and this sum aligned perfectly with our proposed sum over spanning co-trees. Even more, by applying the pseudo-inverse construction to the boundary map ∂ on $C_*(X)$, we reproduced our prior solution to the Kirchhoff problem. It was both amazing and extremely satisfying that the two main components needed for average current were really different manifestations of the same thing.

By the fall of 2014, the individual pieces for what we thought would give rise to the formula for current were in place. All that remained was to rigorously define the stochastic process that our current described. This turned out to require substantial effort; even rigorously defining what the state space should be took several months worth of discussions and tweaking. In the earlier work of [**CKS13**], the graph on which the dynamics were evolving was the natural and correct choice. The higher dimensional case was dramatically different, in that the CW complex was not adequate. We discovered this fact quickly, since the Fokker-Planck operator (see Eqn. 2 in Topic 1) on a CW complex does not conserve probability. That is, it does not govern the evolution of a probability distribution. By 'enlarging' the state space to an infinite graph, the operator worked just as it should.

Once all the pieces were in place, it did not take very long to prove the main quantization result. This is often how these things work: put a lot of effort into the supporting ideas and the main result might just 'fall out'. The paper [**CCK**] was written in the first few months of 2016 in conjunction with my thesis. All three of us were happy with how the pieces of the project fit together so nicely to describe a new approach to stochastic dynamics.

References

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