Interview with Stuart Whittington
Toufik Mansour

Stuart Whittington was educated at Queens’ College Cambridge and has spent most of his working life at the University of Toronto. He spent a post-doctoral year at the University of California San Diego as a Fulbright fellow, working with Fred Wall on self-avoiding walks, and a second post-doctoral year at the University of Toronto, working with John Valleau, mainly estimating the numbers of embeddings of some classes of graphs in lattices. His primary areas of study are statistical mechanics, especially problems with a combinatorial or topological flavour, self-avoiding walks and related objects like lattice trees and lattice animals, self-averaging in quenched random systems, and random knotting and linking. Most of his research interests are in the statistical mechanics of lattice models, especially those related to the configurational and statistical properties of polymers, as well as phase transitions and critical phenomena. He is also interested in the theory and application of Markov chain Monte Carlo methods.

Mansour: Professor Whittington, first of all, we would like to thank you for accepting this interview. Would you tell us broadly what combinatorics is?

Whittington: I would like to start by thanking you for this opportunity. I think of combinatorics as the mathematical treatment of discrete systems. Of course, that’s too broad since the integers are discrete but clearly form part of number theory. But there are always overlaps between fields. The theory of partitions seems to fit equally well in combinatorics and in number theory. Combinatorial geometry is the interface between combinatorics and geometry but is a big subject in its own right. Going back to combinatorics, there are several types of questions that typically arise. One can ask questions about the existence of a combinatorial object. Does there exist a finite projective plane of a certain order? Or one can ask counting questions. How many Dyck paths are there with \( n \) edges? This is enumerative combinatorics and is where my interests lie.

Mansour: What is statistical physics? What are the main paradigms, questions, and goals of the field?

Whittington: Statistical physics, or statistical mechanics\(^1\), attempts to provide a microscopic description of macroscopic objects and phenomena, such as the structure of liquids, phase transitions (like boiling or freezing of liquids), and critical phenomena (like the Curie point in magnetism). Thermodynamics\(^2\) is a very powerful approach to these macroscopic phenomena but it pays no attention to the behavior at the molecular level. Statistical physics builds a bridge between the description of microscopic objects (atoms and molecules)
by quantum mechanics (or sometimes by classical mechanics) and the description of the macroscopic world by thermodynamics.

**Mansour**: What do you think about the development of the relations between statistical physics and mathematics, in particular combinatorics?

**Whittington**: Physicists are more concerned with finding a theoretical description of the world that we live in than in justifying every step of their treatment with full mathematical rigor. Cyril Domb\(^3\) once said that being trained as a mathematician and then working as a theoretical physicist enabled him to decide when rigor was essential in physics, and when it was not. Having said that, I think that providing rigorous proof has a role in theoretical physics. Sometimes this is seen as the distinction between theoretical physics and mathematical physics. Combinatorics connects to statistical mechanics as the mathematical subject that allows us to count using rigorous arguments, and at a fundamental level statistical mechanics is all about counting. Sometimes the travel is in the opposite direction. Some path problems\(^4\), like Dyck paths and Motzkin paths, which have been traditionally part of combinatorics, have migrated as models of polymers and are now being studied, with some embellishments and additions, by people in statistical mechanics. Another problem that began its life as a combinatorics question, is the number of self-avoiding walks in the square lattice that cross a square to which they are confined, from one vertex to the opposite vertex. This has become something of a cottage industry in statistical mechanics.

**Mansour**: What have been some of the main goals of your research?

**Whittington**: I had been fascinated by statistical mechanics as a student and I decided quite quickly that I wanted to do research in that area, without having a clear idea about a particular problem or sub-field. One of the problems that I started to look at was a model of the arrangement of lipid molecules in membranes and this led me to think about self-avoiding walks. Generally speaking, statistical mechanics aims to understand thermodynamics at a microscopic level and I have spent much of my working life trying to understand the physics of polymers using statistical mechanics.

**Mansour**: We would like to ask you about your formative years. What were your early experiences with mathematics? Did that happen under the influence of your family or some other people?

**Whittington**: I was educated at Chesterfield Grammar School and I was lucky that it was an excellent school with excellent mathematics teachers. When I was fifteen or so I had to choose between doing Classics or Science. I enjoyed Latin and English but eventually chose the Science Sixth Form, where I studied chemistry, physics, and pure and applied mathematics. I especially enjoyed chemistry and pure maths and had some trouble deciding between them when I went to university. I had an excellent grounding in calculus and, more generally, in elementary analysis, and coordinate geometry, though we also touched on other subjects like the theory of equations. My family was supportive though I was the first person in my family to go to university. Probably the person who had the biggest effect on me was my pure maths teacher.

**Mansour**: Were there specific problems that made you first interested in combinatorics?

**Whittington**: At school, I picked up the rudiments of permutations and combinations but it was not until I encountered statistical mechanics at university that I really developed a taste for problems involving counting combinatorial objects. The problems there were of the balls in boxes type and I liked learning and inventing tricks for solving that kind of problem. Later, I discovered various problems with counting different kinds of walks on lattices, such as self-avoiding walks, and I think it was then that I really became interested in using combinatorics as a tool.

**Mansour**: What was the problem you worked on in your thesis?

**Whittington**: I did not work on a single problem but this period gave me the opportunity to publish papers about several different topics. I started by looking at a phase transition, called

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rotational premelting, that occurs in crystals of lipid molecules. One of the approaches that I used was a Monte Carlo calculation and this was my introduction to that technique. I then looked at a model of how lipids behave in biomolecular layers that model biological membranes, again using Monte Carlo methods, and finally, I worked on an approximate treatment of self-avoiding walks. I spent a year at UCSD (University of California San Diego) as a postdoc working with Fred Wall on a self-avoiding walk problem.

Mansour: What would guide you in your research? A general theoretical question or a specific problem?

Whittington: I like problems that have a basis in physics or chemistry or molecular biology where the essence of the problem can be boiled down to something that can be attacked using mathematics with the hope of eventually obtaining a rigorous result. This often means simplifying the original problem and trimming away many details that a biologist, say, might feel are essential parts of the problem. The trick is not to do this to excess. Often these specific questions grow into quite a wide area of research.

Mansour: When you are working on a problem, do you feel that something is true even before you have the proof?

Whittington: Yes. I spend a lot of time trying to develop intuition about a problem and often try simpler versions that might be solvable, or attack the problem numerically before settling down to formulate a theorem or construct a proof.

Mansour: What three results do you consider the most influential at the interplay of statistical physics and combinatorics during the last thirty years?

Whittington: I am going to pick problems that fit into the area that most interests me. When you encounter a problem that is interesting but where it is difficult to make progress it is natural to look for a simpler model that will provide insight into the solution to the original problem. Self-avoiding walks have been used as models of several polymer problems, such as the adsorption of polymers at surfaces, the response of polymers to a force, or the collapse of a polymer in a poor solvent. Of course, the model has to be decorated in various ways to suit the details of the physical problem. Since self-avoiding walks are so intractable, simpler models have been used. Dyck paths, with vertices in the distinguished line being weighted, have proved to be a useful model of polymer adsorption. The model is exactly solvable at the level of generating functions and the asymptotics can be extracted, and this has given some insight into the original physical issue. In a similar way, partially directed walks with a weight for nearest neighbor pairs of vertices, not connected by an edge of the walk, have proved to be a useful model of polymer collapse. This is tougher to solve but considerable progress has been made, using methods from both combinatorics and probability theory.

Mansour: What are the top three open questions in your list?

Whittington: It is hard to pick the top three! For self-avoiding walks, the ultimate question is to find an expression for the number of self-avoiding walks with n edges, cₙ. At the moment this seems completely out of reach. Coming down a level, find the rate of exponential growth of the number of self-avoiding walks on, say, the square lattice. That is, determine the value of the connective constant, κ = limₙ→∞ n⁻¹ log cₙ. With that solved or not, determine the rate of approach to the limit. Proving that

\[ c_n = \exp\{\kappa n + O(\log n)\} \]

would be a major advance. Of course, there are similar questions about the behavior of related objects such as lattice trees and lattice animals. In a somewhat different area of statistical physics, the 3-dimensional Ising problem is a major open problem.

Mansour: What kind of research directions...
would you like to see in the next ten-to-twenty years as the continuation of your work?

**Whittington:** In the general area of self-avoiding walks, I think that the two outstanding questions are (i) the value of the connective constant for several different lattices (other than the hexagonal lattice⁹, where its value is now known), and (ii) the existence of critical exponents such as that characterizing the rate at which the limit defining the connective constant is approached. More generally, I would like to see progress with understanding some phase transitions associated with self-avoiding walks, such as the collapse and adsorption transitions, and progress with our understanding of random knotting of lattice polygons¹⁰.

**Mansour:** What do you think about the distinction between pure and applied mathematics that some people focus on? Is it meaningful at all in your case? How do you see the relationship between so-called “pure” and “applied” mathematics?

**Whittington:** I think it is more a question of what motivates you to attack a problem. I like problems that have their genesis in a scientific problem and in that sense, I do applied mathematics. The techniques used in pure and applied mathematics are often the same.

**Mansour:** What advice would you give young people thinking about pursuing a research career in mathematics or science?

**Whittington:** If you want a research career in theoretical physics or theoretical chemistry, take as many mathematics courses as possible. After that, do not be afraid to learn and use other areas of mathematics. The standard sorts of courses that people in chemistry and physics take at university are real and complex analysis, linear algebra, group theory, ordinary and partial differential equations, probability, and perhaps some elementary statistics. But topology, geometry, number theory, and combinatorics, to mention just a few areas, all have applications in the sciences. If you are tackling a problem that seems to require an area of mathematics that you do not know, read a book!

**Mansour:** Would you tell us about your interests besides mathematics?

**Whittington:** Since I was a small child I have always been interested in natural history. I enjoy bird watching and bird identification but I also enjoy widening my knowledge of plants and animals. I spent a year trying to learn ferns and another trying to learn horsetails! I have to admit that this is not very useful knowledge!

**Mansour:** Polyominoes are interesting combinatorial objects widely used to model distinct physical and chemical phenomena. Mathematicians, unfortunately, have not achieved a complete understanding of their enumerative aspects yet. Do you think we will be able to see the solutions to the most challenging ones soon? For instance, their enumeration in the most general case?

**Whittington:** Let me start by saying something about polyominoes. If we look at the dual to a polyomino (by putting a vertex at the center of each square and joining pairs of vertices by an edge if the two squares share a common edge) we have a (connected) section graph of the lattice. In the physics literature, these are sometimes called strong embeddings or site animals¹¹. If instead of considering section graphs we consider subgraphs then these are sometimes called weak embeddings or bond animals. Let us write \(a_n\) for the number of bond animals with \(n\) vertices. Then we know that \(a_n = \lambda^{n+o(n)}\) but we do not know the value of \(\lambda\) rigorously, though we do have good numerical estimates. It is probably true that \(a_n = \lambda^{n+O(\log n)}\) but we do not have proof of this. There are similar results and conjectures for site animals (polyominoes) and I think that we are much more likely to find the values of \(\lambda\), etc., and establish the conjecture about the sub-dominant asymptotics, than to find an expression for the number of polyominoes.

**Mansour:** With E.J. Janse van Rensburg, you have several interesting publications on self-avoiding walks. Would you tell us about this topic more by emphasizing the combinatorial

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side? What are the most important open questions in this research area?

**Whittington:** The basic question about self-avoiding walks is how many walks are there with $n$ edges? The dream is to find an expression that gives this number, $c_n$, as a function of $n$. We do know that $c_n = e^{\kappa n + o(n)} = \mu^n + o(n)$ but we do not know the value of $\kappa$ for any lattice except the hexagonal lattice, and we do not know much about the $o(n)$ term. John Hammersley and Dominic Welsh\(^{12}\) showed that $\mu^n \leq c_n \leq \mu^{n+O(\sqrt{n})}$ and there have been some improvements since then, notably by Harry Kesten\(^{13}\). It is believed, from a mixture of numerical work and physical arguments, that

$$c_n = An^{-1} \mu^n (1 + o(1))$$

where $\gamma$ is a critical exponent that depends on the dimension but not on the particular lattice. Proving this form is a major challenge. Oddly enough, in two dimensions it is believed that $\gamma = 43/32$ but we do not know that the exponent exists! Self-avoiding walks can be embellished in various ways to model physical situations. Polymers can adsorb at surfaces and there is a well-known self-avoiding walk model of this. Take the square lattice, for instance, with the obvious $(x,y)$-coordinate system. Think of self-avoiding walks that start at the origin and are confined to the half-plane $y \geq 0$, so these are positive walks. Ask for the number, $c_n(m)$ of these walks with $n$ edges and with $m + 1$ vertices in the line $y = 0$. We say that the walk visits the line $m$ times. Weight the walk according to the number of visits by writing $C_n(x) = \sum_m c_n(m) x^m$, so that for large $x$ the walk will visit the distinguished line frequently. This corresponds to adsorption. We know that the limit $\kappa(x) = \lim_{n \to \infty} n^{-1} \log C_n(x)$ exists and $\kappa(x)$ is the free energy. We can prove that there is a critical value of $x$, $x_0$ say, such that $\kappa(x) = \log \mu$ for $x < x_0$ and $\kappa(x) > \log \mu$ for $x > x_0$\(^{14}\) with $x_0$ being the point where adsorption occurs. The value of $x_0$ is not known except for the hexagonal lattice\(^{15}\). Recently, Buks van Rensburg and I\(^{16,17}\) have been looking at the situation when the adsorbed walk is pulled off the line by an applied force. Suppose that the $y$ coordinate of the last vertex is $h$. Then we want to count by the number of visits and by the height, that is, we want the number $c_n(m, h)$ of walks with $n$ edges, $m$ visits, and height $h$. Now, the appropriate quantity to examine is $C_n(x, t) = \sum_m c_n(m, h)x^m t^h$ and we need the behavior of this quantity when $n$ is large.

**Mansour:** Polymer models are widely studied by mathematicians, physicists, and chemists. They play an essential role in understanding physical phenomena such as phase transitions and biological structures such as DNA, RNA, and protein folding. Would you tell us about the main ideas behind these models and the role of combinatorial methods in their study?

**Whittington:** It is true that polymer models have become a popular area of research, especially in probability theory\(^{18}\). They originated as mathematical models of linear polymer molecules in dilute solution (where polymer molecules essentially never encounter another polymer molecule). The original question was about the dimensions of these molecules. People asked how the radius of gyration, or perhaps the mean end-to-end length, depended on the number of monomers in the molecule. The radius of gyration can be measured by light scattering so experimental results were available. The simplest model that you can think of is a random walk, either on a lattice or in the continuum, and then the mean square end-to-end length is given by $\langle \Delta \rangle = A n$ where $A$ depends on the details of the random walk. The problem with a random walk model is that it can self-intersect and this corresponds to two monomers occupying the same space. But monomers do occupy space and exclude


other monomers. This is called the excluded volume effect\textsuperscript{19} and leads to a change in the $n$-dependence. In 1949, Paul Flory\textsuperscript{19} developed an approximate physical treatment that predicted that, in three dimensions, $\langle R_n^2 \rangle = An^{2\nu}$ with $\nu = 3/5$. This roughly agreed with the experiment and with Monte Carlo results. In about 1965, Sam Edwards\textsuperscript{20} developed a beautiful self-consistent field treatment that gave the same result for the exponent $\nu$. Self-avoiding walks respect this excluded volume effect and they have become the standard model.

Of course, there are lots of other questions in the polymer business. Polymers undergo a collapse transition as the temperature or the solvent changes. They can adsorb at a surface. Molecules like circular DNA can knot and link.

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The concept of universality plays an important role in statistical physics. Would you tell us about this concept and how it helps us to understand nature?

Whittington: Universality\textsuperscript{25} is a very useful concept in statistical physics, even though the term is a bit vague. The basic idea is that in some circumstances (when a fluid or a magnet is close to its critical point, or when a polymer is near its critical temperature) different systems can show the same critical behavior. This is called universality. It means that the critical exponents for different systems are the same, and it allows for the prediction of properties that can be checked experimentally or numerically.

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is very large) some properties do not depend strongly on the particular system being studied. For instance, if we take various polymers like polyethylene or polypropylene, and measure their radius of gyration (say by light scattering) in dilute solution in certain solvents, the radius of gyration will behave like $An^\nu$, where $n$ is the number of monomers in the polymer. The amplitude $A$ will depend on the polymer but the critical exponent $\nu$ will be the same for many polymers. The fact that $\nu$ does not depend on the chemical details is an example of universality. In a similar way, if we measure how the magnetic susceptibility diverges near the Curie point for different magnetic materials, the exponent characterizing this divergence will be the same for many different materials. When the exponent changes we say that we have moved into a different universality class.

Mansour: When we read papers on statistical physics, we usually encounter the terms phase transition, critical exponents, scaling limits. What are they? Why are they important?

Whittington: A phase transition is when a system changes from one phase to another. When a solid melts to form a liquid, it is undergoing a phase transition. The transition happens at a particular temperature at fixed pressure and this is the transition temperature. The pressure dependence of the transition temperature is a curve in the (pressure, temperature)-plane and describes a phase boundary. In thermodynamics, a phase transition corresponds to a singularity in the free energy of the system. Staying with 1-component systems where we have melting, boiling, and sublimation, the phase boundary between the liquid and vapor phases stops at some pressure and temperature. This point is the critical point. Critical exponents characterize how various properties behave near the critical point. Scaling limits are a bit different. Sometimes phenomena can be described by lattice models and by continuum models, where the ambient space is $R^2$ or $R^3$. Roughly speaking, if the lattice model maps to the continuum model as the lattice size is decreased, then the continuum model is the scaling limit.

Mansour: You use Monte Carlo methods in some of your works. Simulations are essential to understand some theoretically intractable models. Are there also some interesting combinatorial questions motivated by these methods?

Whittington: If I can slightly expand combinatorics to include discrete probability, then the answer is yes. One family of Monte Carlo methods involves sampling along a realization of a Markov chain, defined on the space of interest. To take self-avoiding walks as an example, the space might be the set of self-avoiding walks of length $n$, or perhaps the set of all self-avoiding walks of all lengths. We are interested in making sure that the Markov chain has a unique limit distribution so that the sample won’t depend too seriously on the initial state in the realization of the Markov chain. Proving that the Markov chain has a unique limit distribution or characterizing its ergodic classes usually requires arguments from combinatorics or discrete probability. There are lots of Markov chains that are in popular use where we don’t have this information at a rigorous level.

Mansour: Journal of Physics A: Mathematical and Theoretical is an important journal for interdisciplinary research, and you have been on the editorial board for many years. What do you think about the role of journals in scientific development? What factors make a journal prestigious, influential, and long-lasting?

Whittington: I think that journals are still the primary means of communicating research results, although preprint servers like arXiv are becoming more important. For a journal to be prestigious and influential, it has to attract high-quality papers. Eventually, this becomes a self-fulfilling prophecy – the more prestigious a journal is, the more likely that it will attract high-quality papers. I think that good refereeing is essential. The journal has to find referees who are competent and fair and who will put in the time to make the right decisions about a submission.

Mansour: Mathematicians usually classify the results in mathematical physics as mathematically rigorous or not. Do you think that mathematical standards are essential for the validity of a claim about how nature works?

Whittington: While I do not think that rigor...
is essential for progress in theoretical physics, I do think that it is desirable. I can think of problems in statistical physics that seemed to be "solved" by non-rigorous arguments but, when a rigorous treatment was developed, the solution proved to be somewhat different. The other side of the coin is that there are lots of places in theoretical physics where we "know" the answer, by a combination of numerical work and physical reasoning, but where we do not have proof.

**Mansour:** In your work, you have extensively used combinatorial reasoning to address important problems. How do enumerative techniques engage in your research?

**Whittington:** Self-avoiding walks are a sufficiently tricky problem that standard enumeration methods don’t work. One has to use very robust and general techniques, like subadditivity to prove the existence of limits and bounds to get useful information about the general behavior and the existence of phase transitions. One often looks at simpler models when progress can’t be made on the self-avoiding walk version. These simpler models have some additional features like directedness or convexity. Examples are Dyck paths, ballot paths, Motzkin paths, partially directed walks, row-convex polygons, etc. For these problems, there are combinatorial techniques that work well. Generating functions are often useful tools and one can often find equations determining the generating function by using ideas like wasp-waist factorizations.

**Mansour:** Would you tell us about your thought process for the proof of one of your favorite results? How did you become interested in that problem? How long did it take you to figure out a proof? Did you have a “eureka moment”?

**Whittington:** My favorite result is about self-avoiding walks confined to a wedge geometry\textsuperscript{27}, though I have written other papers that have attracted more attention! Consider the square lattice and ask for the number of self-avoiding walks such that the walk starts at the origin and the \((x, y)\)-coordinates of every vertex satisfy \(x \geq 0\) and \(0 \leq y \leq ax\) for some positive value of \(a\). Write \(c_n(a)\) for the number of these walks. What can we say about \(c_n(a)\)? How does this compare with \(c_n\)? I first thought about this problem when I was working on a self-avoiding walks model of polymer adsorption. I wanted to know something about the behavior of the number of walks starting at the origin and confined to the half-space \(y \geq 0\). These are now called positive walks and the number is often written as \(c_n^+\). I showed that the exponential growth rate of \(c_n^+\) is the same as that of \(c_n\). This raised the question of how severe the geometrical constraint has to be to change the exponential growth rate. After quite a lot of effort I constructed a proof that walks in a quarter space have the same exponential growth rate but otherwise, the problem defeated me and I put it aside. A few years later I was on sabbatical at Trinity College, Oxford, collaborating with John Hammersley. I talked to him about this problem and we decided to work on it. We solved it and proved a stronger result. Suppose that the walk starts at the origin and the coordinates of the vertices satisfy \(x \geq 0\), \(0 \leq y \leq f(x)\) where \(f(x) \geq 1\) and \(\lim_{x \to \infty} f(x) = +\infty\). Call the number of these walks \(c_n(f)\). Then the exponential growth rate of \(c_n(f)\) is equal to that of \(c_n\). This struck us as a very pretty result. Returning to the question of how strong the constraint has to be to change this behavior, confining the walk between two parallel lines is sufficient.

**Mansour:** Is there a specific problem you have been working on for many years? What progress have you made?

**Whittington:** I will pick two different problems but both are tales of failure! In the early 1970’s I started working on the self-avoiding walk model of polymer adsorption, attacking it mainly by Monte Carlo methods and by exact enumeration (for small \(n\)) and series analysis. This gave lots of information but not many rigorous results. Around 1980, John Hammersley visited Toronto and we discussed the problem. Over the next couple of years, in collaboration with Glenn Torrie\textsuperscript{14}, we made a lot of progress at the rigorous level and developed a complete qualitative understanding but with lots of quantitative questions outstanding. We have not made much progress since then on the original problem though Buks van Rensburg and I\textsuperscript{16,17} have recently made progress on the extension where a force is applied to pro-

mote desorption.

The other problem that I will mention is random knotting. In around 1986, I was at a conference and listened to a talk by De Witt Sumners about a conjecture in random knotting. I thought that I saw a way to approach a proof, introduced myself, and we started working on it. It took a year or so but we finally published a paper proving that all except exponentially few polygons on the simple cubic lattice $\mathbb{Z}^3$ are knotted. So unknotted polygons are exponentially rare. A few years later, in a collaboration with Chris Soteros, we extended this result in various ways and showed that polygons were typically badly knotted. But we could not prove much about the probability that a polygon would have a particular knot type. We turned our attention to the knotting of $p$-spheres in the $(p+2)$-dimensional hypercubic lattice but could only prove anything useful if the 2-sphere was confined in a “tube” where we could use transfer matrix methods. More recently we extended this to look at the entanglement complexity of 2-manifolds without boundary. We have continued to work on both the 3-dimensional and $d$-dimensional cases but without much success.

Mansour: Professor Stuart Whittington, I would like to thank you for this very interesting interview on behalf of the journal Enumerative Combinatorics and Applications.