trips also decrease the provisioning rate of the chicks, because adults cannot bring back more food in their stomachs to their brood just because they have been away longer.

Despite some promise in computerenhanced automatic recognition systems based on individual markings<sup>8</sup>, researchers clearly must continue tagging animals for various reasons. Like non-tag marking methods, such as branding<sup>9</sup> or clipping toes<sup>10</sup>, tags inevitably affect some aspect of an animal. The aspiration is that the nature of the beast is not changed by the process. However, given that selection can act on minute differences between individuals, this seems naive.

Instead, we should acknowledge that tags will impair animals. We can then strive to minimize the effects, quantifying them where possible so that we can put the resulting data into perspective. With such an informed background, proposed tagging programmes can consider whether the gain in (imperfect) knowledge from a scientific viewpoint ethically justifies the harm inflicted.

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#### PARTICLE PHYSICS

## **Beyond Feynman's** diagrams

Generations of physicists have spent much of their lives using Richard Feynman's famous diagrams to calculate how particles interact. New mathematical tools are simplifying the results and suggesting improved underlying principles.

### **NEIL TUROK**

The world works in mathematical ways that we are occasionally privileged to discover. The laws of particle physics, for example, allow us to describe the basic constituents of the Universe, and their interactions, mathematically with astonishing precision and power. However, many important physical processes are so complicated that to perform the required calculations in traditional ways was, until recently, simply unfeasible. In near-simultaneous and complementary papers, Alday et al.1 and Arkani-Hamed et al.2 have introduced mathematical concepts that bring the calculations under control and provide insights of both immediate practical and deep theoretical importance.

The mathematical framework that we use to describe elementary particles such as electrons and photons, and their interactions, is known as quantum field theory. It was born from the synthesis of quantum mechanics with Maxwell's classical theory of electromagnetic fields and light. Unlike classical fields, quantum fields can be excited only in certain pre-specified, quantized packets of energy called particles. A photon, for example, is the elementary

particle of the quantized electromagnetic field. In the very simplest quantum field theories, the particles do not interact with each other; they merely travel singly through space at a fixed speed. But in more realistic quantum field theories, the particles collide, scatter off each other, and emit or absorb additional particles at rates that are governed by an overall parameter called the interaction coupling.

The physicist Richard Feynman developed a beautiful pictorial shorthand, called Feynman diagrams, for describing all of these processes. The diagrams show a number of initially widely separated particles moving towards each other, interacting, and flying apart again. To calculate the probability of any particular particle-interaction outcome, one draws all the contributing Feynman diagrams at each order of the interaction coupling, translates them into mathematical expressions using Feynman's rules, and adds all of the possible contributions together. This is a well-defined procedure, but at successive orders of the interaction coupling, the number of contributing diagrams grows rapidly and calculations quickly become arduous. Generations of physicists have spent large parts of their lives working out Feynman's formulae for many kinds of scattering processes, and then testing those formulae in detailed experiments.

The work of Arkani-Hamed et al.<sup>2</sup> originates in a heroic, if mundane, computation undertaken in 1985 by two particle physicists at Fermilab in Batavia, Illinois. Parke and Taylor<sup>3</sup> decided to compute all of the Feynman contributions to one of the simplest processes involving the strong nuclear force, whose elementary particle — the gluon — binds quarks together into protons and neutrons. They considered two incoming gluons colliding and producing four outgoing gluons. This is one of the most common processes: for example, in the Large Hadron Collider (LHC), located at CERN, near Geneva, Switzerland, it takes place 100,000 times per second and generates an enormous 'background' signal, which particle physicists must accurately predict and subtract as they search for signals indicating new physics.

The leading contribution to this six-gluon process involves no less than 220 Feynman diagrams, encoding tens of thousands of mathematical integrals. Yet Parke and Taylor found that they could express the final result in just three simple terms. This was the first indication that Feynman diagrams were somehow complicating the story, and that there might be a simpler and more efficient description of these scattering processes.

Further insight into this simplicity was gained by Bern, Dixon and Kosower<sup>4</sup>, and by Britto, Cachazo, Feng and Witten<sup>5,6</sup>, who developed powerful new techniques - not involving Feynman diagrams - to infer higher-order scattering processes from lower-order ones. Their methods are not only of interest for experiments such as the LHC, but also for testing the mathematical consistency of theories such as supergravity, which is a candidate quantum field theory of gravity.

Work done over the past year has shown why these new methods are simpler than Feynman's. The formulation of quantum field theory used in Feynman's rules emphasizes locality, the principle that particle interactions occur at specific points in space-time; and unitarity, the principle that quantum-mechanical probabilities must sum to unity. However, the price of making these features explicit is that a huge amount of redundancy (technically known as gauge freedom) is introduced at intermediate steps, only to eventually cancel out in the final, physical result.

The calculations of Alday et al.1 and Arkani-Hamed et al.<sup>2</sup> work differently. They assert relations between quantities in a new way, so that the relations are free of these redundancies and they turn out to be sufficient to define the theory. The first big surprise is that such relations exist, and the second is that they are expressed in quantities that are explicitly nonlocal — that is, quantities that are spread out over space and time.

Both sets of authors perform calculations within a particularly simple family of four-dimensional quantum field theories,



with interactions, known as N = 4 supersymmetric theories. These theories are not realistic descriptions of real-world particle physics, but they do have elementary particles such as gluons and quarks (and even Higgs bosons), and they provide a valuable testing ground for new calculational techniques.

Arkani-Hamed and colleagues<sup>2</sup> exploit a combination of twistor theory — a non-local description of space-time developed by Roger Penrose in the 1970s - and algebraic geometry to obtain a complete description of the scattering of all the elementary particles in these theories, in ascending powers of the interaction coupling. In doing so, the authors provide an excellent characterization of the scattering process when the interaction coupling is small. By contrast, Alday and colleagues<sup>1</sup> derive relations between non-local quantities known as Wilson loops, named after their inventor, the Nobel prizewinner Kenneth G. Wilson. The loops represent the flux of the strong nuclearforce fields through various geometrical areas. Using the powerful mathematical machinery of quantum integrability, Alday et al. are able to determine the behaviour of these fluxes in the limit at which the interaction coupling is large. The two sets of authors have therefore described the theory in its two opposite extreme limits small and large coupling - and the hunt is now on for a complete description, one that is valid for any value of the interaction coupling.

Quantum field theory is the most powerful mathematical formalism known to physics, successfully predicting, for example, the magnetic moment of the electron to one part in a trillion. The recent discovery of mathematical structures that are now seen to control quantum field theory is likely to be of enormous significance, allowing us not only to calculate complex physical processes relevant to real experiments, but also to tackle fundamental questions such as the quantum structure of space-time itself. The fact that the new formulations of the theory<sup>1,2</sup> jettison much of the traditional language of quantum field theory, and yet are both simpler and more effective, suggests that an improved set of founding principles may also be at hand.

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# Finding the wet spots

The functions of proteins are critically coupled to their interplay with water, but determining the dynamics of most water molecules at protein surfaces hasn't been possible. A new spectroscopic method promises to change that.

#### VINCENT J. HILSER

roteins in cells are responsible for the vast majority of biological functions. Because life evolved in water, protein molecules are uniquely adapted to use their aqueous environments to facilitate their functions<sup>1</sup>. Yet remarkably little is known about the interactions between solvent water and protein molecules, or how those interactions affect (or are affected by) the conformational changes at the heart of protein function. In Nature Structural and Molecular Biology, Nucci et al.<sup>2</sup> now report that nuclear magnetic resonance (NMR) spectroscopy of proteins encapsulated in reverse micelles<sup>3</sup> — cell-like compartments in which nanometre-scale pools of water are surrounded by a membrane — can provide a comprehensive picture of how water molecules bind to proteins. This picture not only challenges current dogma about protein hydration, but also promises to illuminate key aspects of the relationship between protein and water dynamics, and of how proteins use water to perform their functions.

Early studies<sup>4,5</sup> of protein-water interactions - the exchange of water molecules between a protein's surface and the surrounding bulk water - were performed in bulk solution using NMR. But because of ambiguities resulting from the timescale of the exchange process, as well as the inability to distinguish between that process and another in which labile hydrogens in the protein exchange with those in water<sup>6</sup>, direct experimental analysis of protein-water dynamics (hydration dynamics) was restricted to only the most long-lived of interactions. Attempts to rectify this have relied mostly on X-ray crystal structures of proteins to identify the locations of resolvable water molecules in the structure, which, in spite of welldocumented reservations<sup>7</sup>, have generally been presumed to represent the 'hydration shell' of water molecules around the protein<sup>8</sup> (Fig. 1a). Nucci and colleagues' new NMR approach<sup>2</sup> overcomes the previous experimental limitations, thus providing a comprehensive picture of the whole hydration shell around a test protein, ubiquitin.

The reverse-micelle technology used by Nucci *et al.*<sup>2</sup> was previously developed<sup>3</sup> to overcome the protein-size limitation inherent to NMR studies — large proteins can't be studied by NMR because they tumble too slowly in solution. Encapsulation of large proteins in



Figure 1 | Crystallographic versus NMR views of protein hydration. a, Certain sites at which water molecules associate with protein surfaces can be identified in X-ray crystal structures, as shown schematically here for ubiquitin. The sites are assumed to be those where water molecules reside for longest (that is, where the dynamics of water movement are slowest). b, This cartoon depicts the NMR view of hydration obtained by Nucci et al.<sup>2</sup>, wherein a complete picture of the locations and dynamics of water molecules bound to ubiquitin was ascertained. They observed that water molecules cluster into regions corresponding to slow, intermediate and rapid average dynamics. Little correlation was found between the crystallographic and NMR views of hydration dynamics. Arrows indicate that the rates of watermolecule exchange between the protein's surface and the solvent are directly measured by NMR. By contrast, the X-ray picture is static, and exchange rates must be inferred or calculated. Images were created using PyMOL<sup>15</sup>.

reverse micelles dissolved in a low-viscosity fluid, however, allows them to tumble at rates similar to those of much smaller proteins. What's more, such encapsulation dramatically slows both the hydration dynamics and the hydrogen-exchange kinetics of proteins compared with the same quantities in bulk solvent. This is the cornerstone of Nucci and colleagues' advance<sup>2</sup>, because it enables