# Enthralled by symmetries

Nanophysicist **Professor Jan von Delft** shares details of his career in quantum nanoscience, and the computational cost-saving approaches he has helped devise in this important area

PROFESSOR JAN VON DELFT

**What sparked your curiosity in quantum mechanics?**

As a high school student, I read somewhere that Heisenberg's uncertainty principle implies that the notion of causality has to be revised. The quantum mechanical uncertainty principle states that it is not possible to simultaneously know the position and momentum of a particle with certainty, implying that its future trajectory cannot be predicted with certainty either. This intrigued me to such an extent that I decided to study physics, and in these studies I continued to find myself attracted to phenomena involving quantum mechanics.

**Could you briefly outline your project on the exploitation of non-abelian symmetries for the numerical treatment of two-dimensional (2D) quantum lattice models using tensor networks?**

Many quantum lattice models have some kind of symmetry, meaning that the energy of the system does not change under certain symmetry operations. Examples would be rotating the spin on every lattice site by the same angle – a so-called SU(2) symmetry – or, for models with *N* bands, mixing particles from different bands in the same way on every lattice site – a so-called SU(*N*) symmetry.

If a quantum system has a symmetry, the allowed quantum states can be organised into sets that all have the same energy – each set is called a

# Science through symmetry

A partnership of researchers based at **Ludwig Maximilian University of Munich**, Germany, is combining computational physics and nontrivial mathematics to solve some of quantum physics' most challenging models

**QUANTUM MECHANICS IS** the field of physics that deals with interactions on the smallest scale known to man – which is very small indeed. For example, the action of lifting a 1 kg weight one metre off the ground would cost around 10 joules of energy; quantum mechanics works in terms of Planck's constant, the smallest measurable unit of action, which is roughly $6.626 \times 10^{-34}$ $Js^{-1}$. Because of this incomprehensible difference in scale, the laws of physics also differ; uncertainty plays a significant role in quantum interactions, and the distinction between matter and waves is no longer clear. When scientists attempt to study quantum mechanics, therefore, calculations of vast complexity are required.

In fact, some of these interactions are so complex as to be functionally incalculable. A system of particles of the sort commonly occurring in nature may contain $10^{20}$ particles, which all behave in a way influenced by the behavior of all the others; this is too much information to process. In order to effectively study such systems, limited models often operating in one or two dimensions are necessary, and even here shortcuts are needed to save calculation time. Quantum lattice models represent interactions on a lattice or grid. Each site on the grid can be occupied by a particle such as an electron. In order to facilitate calculations solving these models, scientists exploit symmetries – many lattice models have symmetries that can be utilised to speed up calculations and reduce memory requirements.

## THE 2D CHALLENGE

Interacting quantum lattice models attract a lot of interest from scientists, but solving them reliably is extremely difficult.

In fact, the successful numerical treatment of two dimensional (2D) lattice models is considered to be a 'Holy Grail' of computational physics. One of the most sophisticated approaches proposed to date involves tensor networks; these have great potential but their numerical cost increases exponentially with size in 2D systems. This is a significant problem, because if a system is too small then it will be unreliable for the prediction of bulk properties. It is possible, however, that sufficient shortcuts could be made to dramatically increase the efficiency of tensor network methods to the extent that reliable predictions for low-temperature properties could become possible for significantly larger systems.

degenerate symmetry multiplet. This offers the enthralling possibility of making numerical calculations vastly more efficient, by only keeping track of entire multiplets instead of individual states. My co-worker, Dr Andreas Weichselbaum, got this to work for 1D chain models with non-abelian symmetry groups, and the efficiency gains were amazing. Thus, our next goal is to implement this strategy for 2D quantum lattice models, treated using tensor product methods.

**How could your research be translated for application to models of general interest?**

For many years, Andreas and I have worked on quantum impurity models, which describe a discrete quantum system coupled to a continuum of excitations. While these models have numerous applications in our research field of nanophysics, the numerical *methods* that have been developed to treat them have potentially even greater applicability. One possibility is via 2D tensor network treatments of 2D lattice models; another is within the context of dynamical mean field theory (DMFT), which describes a correlated lattice system in terms of an effective quantum impurity model that has to be solved self-consistently. I believe that DMFT-related work, too, will greatly benefit from the symmetry gold mine.

**What have been the biggest obstacles you have faced to date? How have you sought to overcome them?**

On a conceptual level, getting to grips with SU(*N*) and its mathematical representation theory certainly was a challenge to me, but the skill and dedication of student Arne Alex and patient guidance from our mathematics colleagues, Professors Alan Huckleberry from Ruhr University Bochum and Peter Littelmann from the University of Cologne, got us over that hump. The biggest challenge was certainly finding an efficient, user-friendly scheme for implementing symmetries in the numerical codes of the numerical renormalisation group and the density matrix renormalisation group. Andreas conquered this all by himself, by devising a unifying tensor representation for quantum symmetry spaces, which he dubbed QSpace. It hides most of the complications that arise when implementing symmetries in a cleverly designed tensor library of subroutines, so that end users of the code hardly need to worry about them. This works so well that once Andreas had his code up and running for SU(3), he was able to get it to work for a problem involving a different non-abelian symmetry, called Sp(6), in just a matter of days – which I found truly amazing.

**Will you be presenting your findings at any upcoming events or conferences? Is dissemination something you regard as important?**

Dissemination is essential. Our work on Clebsch-Gordan coefficients was published a few years ago, and so was Andreas' QSpace approach. Moreover, I am delighted that Andreas has recently accepted an invitation to write a *Springer Brief* about his work on tensor networks and symmetries. I myself advertise the benefits of the symmetry gold mine whenever I report on a physics project conducted in our group using Andreas' new code. However, I mostly treat the code as a 'black box', inviting the audience to ask about it afterwards, if interested. The technical details are better suited for one-on-one discussions between consenting adults behind closed doors. They would certainly also be a very suitable topic for an extended series of lectures in a summer school.

This is exactly the possibility being explored by a group of physicists at the Arnold Sommerfeld Center for Theoretical Physics in the Ludwig Maximilian University of Munich (LMU), Germany. The researchers are in the process of exploiting symmetries in the treatment of quantum lattice models with general non-abelian symmetry groups, a process that may dramatically reduce calculation times in 2D models. In the last three years, they have succeeded in developing shortcuts in the solution of 1D quantum chain models involving *N* equivalent types of particles and hence having an *N*-fold symmetry, called SU(*N*). This generalises existing approaches which utilise the much simpler structure of SU(2) only. Results have shown that for $N = 3$ the gain in efficiency from doing so is enormous. Calculations that previously took weeks can now be completed in a matter of hours, and new calculations that would previously have been impossible are now accessible. Professor Jan von Delft, one of the project's three principle investigators, adds: "Symmetry is a gold mine for enhancing efficiency". Thus, the idea arose to similarly exploit symmetries in studies of 2D lattice models.

## MERGING METHODS

To this end, von Delft initiated a collaboration with two Munich colleagues, Dr Andreas Weichselbaum and Professor Ulrich Schollwöck. Their methods originate in the numerical treatment of 1D quantum chain models using matrix product states, or tensor trains. von Delft and Weichselbaum have specialised in one numerical approach within this category, using the numerical renormalisation group (NRG) to treat a certain type of 1D quantum chain associated with quantum impurity models. Schollwöck also studies 1D chain models, but specialises in using the density matrix renormalisation group (DMRG) for this purpose.

In 2005, the Munich researchers realised that NRG and DMRG share the same mathematical structure – both are based on matrix product states, which represent quantum states in terms of products of matrices. This important discovery uncovered numerous opportunities for merging advantages of both methods and formed the basis for a powerful NRG-DMRG hybrid code developed by Weichselbaum. In particular, he recently devised a way to implement SU(*N*) symmetries for general *N* explicitly in his code. Meanwhile, Schollwöck had branched out to study 2D models, using both SU(2)-based DMRG and more general 2D tensor networks, which are the natural generalisations of 1D matrix product states to two dimensions. Since all these methods have a related mathematical structure, von Delft suggested a collaboration aiming to apply Weichselbaum's treatment of symmetries in 1D chains to 2D tensor networks.

## INTELLIGENCE

### NON-ABELIAN SYMMETRIES IN TENSOR NETWORKS

### OBJECTIVES

To exploit non-abelian symmetries for the numerical treatment of strongly interacting quantum lattice models in two dimensions using tensor networks.

### KEY TEAM MEMBERS

**Dr Andreas Weichselbaum**, Arnold-Sommerfeld Zentrum and Center for NanoScience, Ludwig-Maximilians-Universität, Munich, Germany

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**Professor Peter Littelmann**, Mathematisches Institut, Universität zu Köln, Germany

**Professor Alan Huckleberry**, Institut für Mathematik, Ruhr-Universität Bochum, Germany

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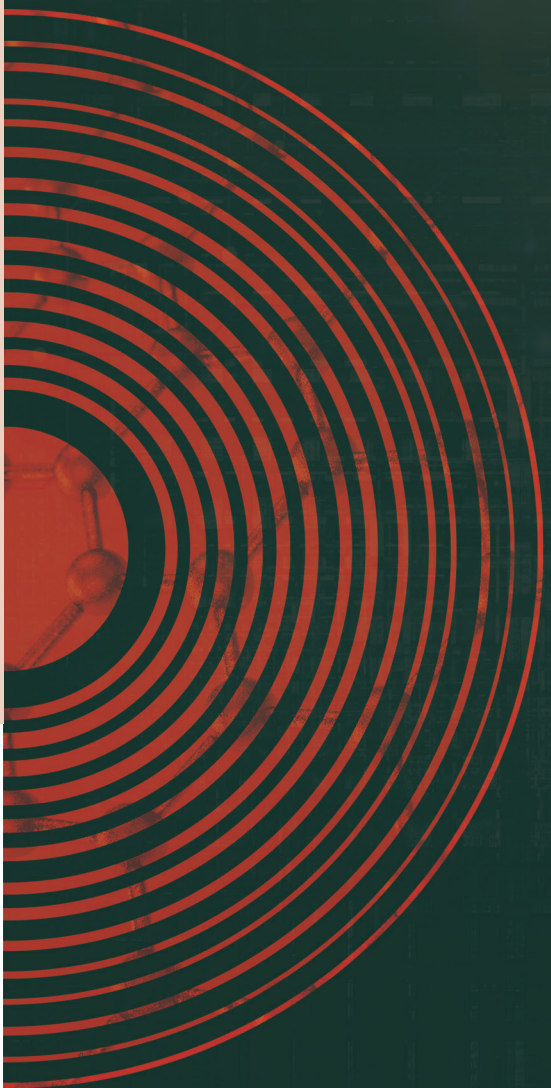
**PROFESSOR JAN VON DELFT** received his PhD in Physics from Cornell University, USA, in 1995. He then earned his Habilitation from the University of Karlsruhe in 2000. In the same year, he briefly joined the ranks of the Physikalisches Institut at the University of Bonn, before moving to the Arnold Sommerfeld Center for Theoretical Physics in the Ludwig Maximilian University of Munich, where he remains today.

### BEAUTIFUL BOTTLENECKS

Several years into the project, the researchers are now finding that their successes in exploiting symmetries are uncovering further challenges. By tracking symmetry multiplets rather than individual states, Weichselbaum circumvented the formerly most severe computational bottleneck, which stemmed from limits on the size of the matrices comprising the matrix product states that could be dealt with. This advance led to the emergence of a different, mathematically very interesting bottleneck, involving the treatment of Clebsch-Gordan coefficients (CGCs).

von Delft describes CGCs as the 'glue' of symmetry-based approaches, and indeed they are essential to the process of obtaining symmetry multiplets for larger systems. CGCs are determined by purely mathematical considerations, and an essential first step for the Munich researchers, performed in collaboration with mathematicians from Bochum and Cologne, was to develop a numerical algorithm computing general tables of CGCs. However, the time required to calculate CGCs, and to combine them in the ways needed for NRG-DMRG algorithms, increases exponentially with the complexity of the symmetry. At present, this constitutes the computational bottleneck for large $N$ – with beautiful opportunities for making further progress via pure mathematics. It turns out that one actually needs only particular sums of products of CGCs, so-called 6-$j$ symbols, which have well-defined mathematical properties of their own. The Munich researchers have ambitious plans to refine their algorithm to directly calculate and tabulate only the required 6-$j$ symbols rather than the individual CGCs, which promises further huge savings in calculation time.

As time advances, quantum modelling becomes less abstract and more relevant to our daily lives. Successive generations of computers shrink motherboard components including processing units to ever smaller sizes, calling for a closer understanding of physics on a smaller scale which, in turn, involves more complex computations and more powerful algorithms and computers. The Munich team, therefore, not only contributes to quantum physics through computational research, but also to the future of computation – and by developing systems that reduce computational bottlenecks, they help scientists to stay one step ahead in the continuous cycle of increasing knowledge and innovation.



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