Theory of Condensed Matter

TCM and CDT graduate admission web pages

http://www.tcm.phy.cam.ac.uk/vacancies/postgrad.html

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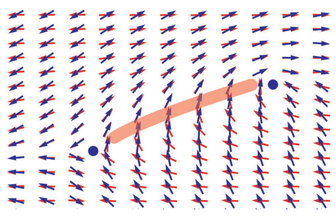
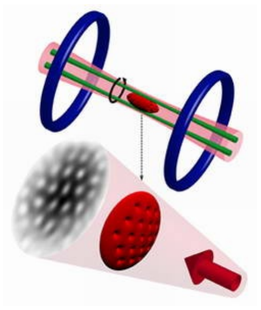
Ultracold atomic gases



Matter doesn't have to be dense to condense. One of the frontiers of modern condensed matter physics is the study of gases of atoms a million times thinner than air. At sufficiently low temperatures (microkelvin!), the wavelength of the atoms exceeds the interparticle separation and the properties of the gas are determined by quantum mechanics. This radical departure from classical behaviour is typified by a BoseEinstein condensate, which existed only as a textbook example for more than seventy years before its experimental discovery launched this field in 1995.

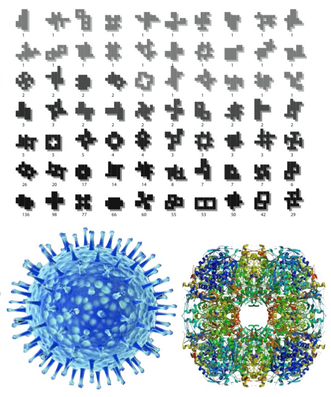
Since then the list of phenomena observed some familiar from the solid state and the relatively balmy world of low temperature physics, and others completely new has grown with the ingenuity of experimentalists. Changing scale by six orders of magnitude is easier for theorists, of course. Researchers in TCM are studying novel magnets, artificial gauge fields, and atomic analogues of Mott insulators and superconductors. There are close links to the experimental groups in ultracold physics at the Cavendish and elsewhere in the world.



Benjamin Beri, Gareth Conduit, Nigel Cooper, Austen Lamacraft, Richard Needs, Andreas Nunnenkamp, and Ben Simons

Self assembly and physical complexity in biology

The interface between statistical physics and biology is a rapidly growing area of research. An area of particular interest is self assembly, which is an ubiquitous phenomenon in biology. In this context we study deterministic and non deterministic self assembly of structures on a lattice (top figure), the relationship between assembly and structural complexity, as well as the assembly and evolution of self assembling structures in biology, such as protein complexes and viruses (lower figures).



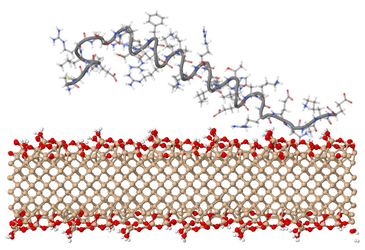
Self assembled lattice structures (top) and examples of self assembly in biology: a virus (bottom left) and a protein complex (bottom right).

Sebastian Ahnert and Mike Payne

Biologically-inspired computer modelling

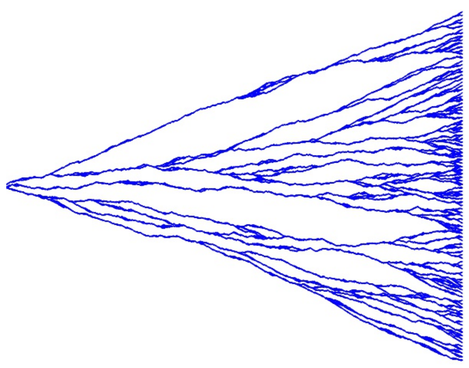
Molecular Dynamics (MD) simulations are computational experiments that are used to investigate the relationship between molecular structure, movement and function. In classical MD, interactions between atoms are approximations based on experimental data or more accurate, but also more time-consuming, quantum mechanical simulations. These simplifications mean that we can model the behaviour of systems of many thousands of atoms, such as biomolecules, on nanosecond timescales.

One such example is the investigation of protein assembly on solid surfaces, which is of great importance for the design of materials for implantable biosensors. The adsorption behaviour of the protein, collagen, on silicon devices is found to depend strongly on the hydrophobicity of the solid surface.



Mike Payne

Nonequilibrium Physics



The notion of thermal equilibrium plays a crucial role in any attempt to understand the macroscopic properties of matter in terms of its microscopic constituents. The fundamental reason that matter can be characterised by certain variables (temperature, pressure, magnetisation, etc.) independent of its past history is that the equilibrium macrostate occurs with overwhelming probability in a large system. Despite this, nonequilibrium states are an important feature of the macroscopic world. This may be because a system has not had time to forget its initial state: think of the growth of a crystal from a supersaturated solution, or the evolution of the universe after the Big Bang. Alternatively, a system may be sustained out of equilibrium by an external source of energy (as in a turbulent fluid) or low entropy (life on Earth!). Such behaviour is technologically important — a computer's memory must not come to thermal equilibrium — and can occur in any system of many entities where collective behaviour can emerge — as in a traffic jam.

Researchers in TCM are exploring the nonequilibrium dynamics of defects in novel magnetic systems (Castelnovo), quantum systems of molecules, ultracold atoms and light (Cooper, Nunnenkamp), and classical stochastic models that can mapped to quantum many body systems (Lamacraft).

Benjamin Beri, Claudio Castelnovo, Nigel Cooper, Austen Lamacraft, and Andreas Nunnenkamp

Overview

Theoretical condensed matter physics is about building models of physical processes, often driven by experimental data, generalising the solutions of those models to make experimental predictions, and transferring the concepts gained into other areas of research. Starting at the first principles microscopic level – with the Schrödinger equation – many properties of materials can now be calculated with a high degree of accuracy. We work on refining and developing new calculational tools and applying them to problems in physics, chemistry, materials science, and biology.

Solids also often show unusual collective behaviour which results from cooperative quantum or classical phenomena. For this type of physics a more model based approach is appropriate, and we are using such methods to attack problems in magnetism, superconductivity, nonlinear optics, atomic gases, polymers, and colloids.

Collective behaviour comes even more to the fore in systems on a larger scale. As examples, we work with statistical mechanics on self organising structures in 'soft' condensed matter systems, nonlinear dynamics of interacting systems, and models of biophysical processes, from the molecular scale up to neural systems.

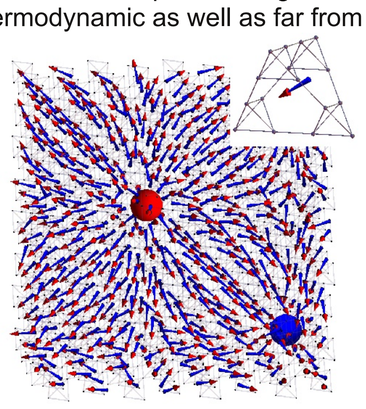
Professor Ben Simons

Frustrated magnetism

One of the most fascinating phenomena in condensed matter is the ability of strong correlations to give rise to phases that behave as vacua for new types of degrees of freedom not directly present in the microscopic constituents of the system. These quasiparticles are not bound by the same laws of nature that constrain the `real' elementary constituents. Examples include fractional electric charge in acetylene, spin-charge separation in $SrCuO_2$, emergent magnetic monopoles in spin ice (figure), and anyons with fractional statistics in topologically ordered phases of matter.

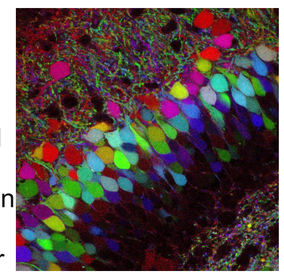
Frustration in magnetic systems has been fertile ground for these phenomena. The term "frustration" indicates the inability of a system to reach its lowest energy state where all interaction terms are simultaneously minimised (e.g., ferromagnetic order). The variety of new phenomena that emerge in frustrated magnets, combined with the many experimental probes that have been developed for magnetic systems, continue to produce new and exciting physics both concerning thermodynamic as well as far from equilibrium behaviours.

Spin ice materials are a notable recent example of this area of research, where frustration leads to an emergent gauge symmetry and magnetic monopole excitations at low temperatures. Several open questions remain to be addressed -- for instance, understanding how emergent quasiparticles behave out of equilibrium is key to investigate the intriguing possibility of manipulating these exotic degrees of freedom into new kinds of currents and circuits for technological applications.



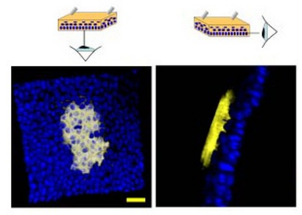
Claudio Castelnovo

The life of cells



In adult organisms, many tissues are maintained and repaired by stem cells, which divide and differentiate to generate more specialised progeny. The mechanisms that control the balance between self-renewal and differentiation of stem cells promise fundamental insights into the origin and design of multi-cellular organisms. However, stem cells are often difficult to distinguish from their more differentiated progeny, and resolving these mechanisms has proved controversial and challenging.

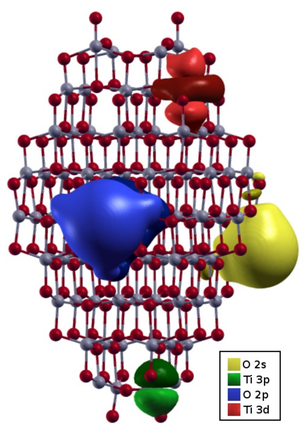
The development of inducible genetic labelling methodologies has provided indirect access to cell fate characteristics of stem cells and their progeny *in vivo*. Drawing on a wide range of data, researchers in the condensed matter theory group have employed methods of non-equilibrium statistical mechanics to address clonal evolution. These investigations demonstrated how scaling behaviour and spontaneous patterning reveal stochastic stem and progenitor cell fate. The results provide insight into the molecular regulatory mechanisms controlling the maintenance and repair of adult tissues, and point at common organisational principles.



Ben Simons

Computational Simulation of Nanomaterials

Nanomaterials offer us exciting new ways to control material properties, by varying material attributes which are not available in bulk systems. For example, in nanocrystals, growth conditions can be tuned to vary particle size, shape, surface terminations, composition and defect structure, and in an aggregate of nanocrystals, alignment, mutual interactions and interations with a solvent come into play. Nanomaterials are thus the key to making a success of many emerging technologies, in particular Photovoltaics and Photocatalysis, means of turning light from the sun into other useful forms of energy. However, these many variable factors result in a vast phase space to explore in order to design optimal materials for a given purpose. First principles computational simulation can be used to explore this space, enabling computational "experiments" to disaggregate competing factors influencing a property, in a way which is impossible in real world tests. For example, by modelling TiO2 nanocrystals, an important component in many photoactive devices, we can understand how to expose specific surfaces to maximise their potential for photocatalysis. Possible projects include developing new simulation tools for theoretical spectroscopy, which will greatly augment experimental methods, eg Electron Energy Loss Spectroscopy, by elucidating the origin of spectral features.



A TiO_2 nanocrystal, showing local orbitals optimised using the ONETEP code. Use of local orbitals enables calculations on very large systems (1000s of atoms)

Similarly, nanoscale thin films of ferroelectric and multiferroic materials are very promising for nanodevices of different sorts, which can offer much more efficient and energy efficient solutions to future electronics and spintronics. These materials can be simulated and new materials can be proposed from theory. Nanoconfined liquid water is also simulated with analogous techniques. It is of great importance for understanding the behaviour of water between hydrated objects in close proximity, as encountered between organelles and macromolecules in a living cell.

Emilio Artacho and Mike Payne