

Physics Department

Colloquia Speakers 2023/24

Prof Nigel Hussey (University of Bristol, UK and Radboud University, Netherlands)

The allure of linearity: Exploring the link between strange metallicity and high-temperature superconductivity

Friday 9 February 2024

In typical metals, the electrical resistivity ρ tends to vanish at the extremes of temperature T and magnetic field strength H , albeit for different reasons. At intermediate temperatures, however, $\rho(T)$ is invariably linear due to the scattering of electrons off phonons – the quantized vibrations of the lattice. Electron-phonon coupling is also responsible for superconductivity in many of these metals. Indeed, a robust correlation exists between the coefficient of the T -linear resistivity α and the superconducting transition temperature T_c ; a link enshrined in the old adage “bad metals make good superconductors”.

Despite being discovered almost four decades ago, the high- T_c cuprates still boast the highest ambient-pressure T_c values of all known materials. Intriguingly, a similar correlation between α and T_c exists in cuprates too, prompting many in the field to argue that whatever is the cause of this (T -linear) scattering is also the pairing mechanism for high-temperature superconductivity. Despite a prolonged and intense search, however, the origin of this scattering has not been identified. Crucially, the linearity in ρ in cuprates extends over an anomalously broad temperature and field range, implying an unconventional electronic state. Moreover, the magnetoresistance has a linear-in-field slope that also correlates with T_c . In this colloquium, I will discuss the profound implications of these correlations, along with a number of other simple observations linking the (magneto)transport properties of cuprates with their corresponding superconducting properties. Collectively, these observations motivate the search for an entirely new paradigm for high-temperature superconductivity, one in which these T - and H -linearities play a central role.

Dr Alessandro Principi (University of Manchester)

Viscous fluids in solid state systems: a tale of interacting electrons

Friday 23 February 2024

Strong interactions are at the origin of emergent phenomena like magnetism and superconductivity which already impact our everyday life, or could change it forever opening a whole new era. While the physics of these equilibrium phases has been studied for quite some time, the impact of interactions (in particular electron-electron interactions) on non-equilibrium properties is much less understood. Notwithstanding the importance of new transport regimes such as many-body localisation, in this colloquium I will focus on the impact of interactions on

normal Fermi liquids. These conventional conducting materials typically exhibit either diffusive or ballistic charge transport. However, when electron-electron interactions dominate, a “hydrodynamic” regime emerges. Under these conditions, electrons can behave as a viscous liquid and exhibit hydrodynamic phenomena similar to classical liquids. In this colloquium I will review the history of this field, old and modern theories of hydrodynamic transport in clean materials, and more recent experiments.

Prof Jascha Repp (Universität Regensburg)

Accessing non-equilibrium at the intrinsic scales of molecules

Thursday 7 March 2024

While scanning probe microscopy (SPM) has revolutionized our understanding of the atomistic world it is usually too slow to capture non-equilibrium excitation processes. Two complementary approaches that allow accessing non-equilibrium phenomena with SPM will be presented.

Accessing ultra-fast phenomena is enabled by combining lightwave electronics with scanning tunneling microscopy (STM), allowing for combined femtosecond and sub-angstrom resolution in observing matter (1). Lightwave STM also provides access in the control of matter by utilizing localized electric fields to exert atom-scale femtosecond forces (2). Further, we show how lightwave STM can be extended to its ultrafast spectroscopy variant (3). The corresponding ultrafast and atomically resolved tunnelling spectra reveal transient energy shifts of a single selenium vacancy in a WSe₂ monolayer on gold. Another approach gives us access to intermediate timescales that are relevant for spin precession and relaxations. We exploit the high sensitivity of atomic force microscopy (AFM) to perform STM and spectroscopy on molecules in absence of any conductance of the underlying substrate. Thereby, we gain access to out-of-equilibrium charge states (4) that are out of reach for conventional STM. Extending this technique by electronic pump-probe spectroscopy, we measured the triplet lifetime of individual molecules and its quenching by nearby oxygen molecules (5). Combined with radio-frequency magnetic-field driving we introduce AFM-based electron spin resonance and spin manipulation showing long spin coherence in single molecules (6).

References:

- T. Cocker et al., Nature 539, 263 (2016).
- D. Peller et al., Nature 585, 58 (2020).
- C. Roelcke et al., in press (2023).
- L. L. Patera et al., Nature 566, 245 (2019).
- J. Peng et al., Science 373, 452 (2021).
- L. Sellies et al., Nature 624, 64 (2023).

Prof Amalia Patanè (University of Nottingham)

Emergent atomically-thin semiconductors

Friday 8 March 2024

Atomically-thin semiconductors present an opportunity to revolutionize modern science and technologies. However, transforming the semiconductor landscape requires new scalable materials. In particular, the design of advanced functionalities for future electronic components relies on high-quality heterostructures, which are still difficult to create and characterize. Here, I will present my research on atomically-thin semiconductors, also referred to as two-dimensional semiconductors (2SEM), and a bespoke facility (EPI2SEM) for the EPitaxial growth and In situ analysis of 2SEM in ultra-high vacuum (UHV). By integration of growth, scanning probe microscopy and electron spectroscopy in UHV, we can create atomically-thin semiconductors and heterostructures with engineered electronic properties beyond the current state-of-the-art.

Dr Oleksandr Kyriienko (University of Exeter)

Quantum computing and quantum machine learning: from theory to practice

Friday 15 March 2024

Quantum computing represents a powerful concept, which suggest performing computing using inherently quantum mechanical objects, and solving problems that are classically intractable. Quantum computers draw strength from increasing a number of qubits – quantum objects storing superpositions of two quantum levels – and extending coherence of the entire system. Rapid advances of quantum hardware have recently led to the appearance of intermediate size computers made of dozens or even hundreds of noisy qubits. This has shifted the focus from theoretical to practical quantum computing. The capabilities of contemporary quantum computers largely depend on quantum software that they can run. Giving the current coherence limitations, new ways to design protocols are much needed.

In the talk I will introduce the basics of quantum computing. Next, I will discuss areas of applications and how QC can be pushed closer to practical use cases. I will explain how quantum computers can be trained to perform various tasks in an efficient way. Describing the basics of quantum machine learning, I will show how to master near-term devices and solve problems ranging from solving differential equations to phase recognition and fraud detection.

Prof Mete Atatüre (University of Cambridge)

Shedding Light on Nuclear Spins: Through the looking-glass

Friday 22 March 2024

Optically active spins in solids are strong candidates for scalable devices towards quantum networks. Semiconductor quantum dots set the state-of-the-art as single-photon sources with high level tuneability, brightness, and indistinguishability. In parallel, their inherently mesoscopic nature leads to a unique realisation of a tripartite interface between light as information carrier, an electron spin as a proxy qubit, and an isolated nuclear spin ensemble. The ability to control

these constituents and their mutual interactions create opportunities to realize an optically controllable ensemble of ~50,000 spins. In this talk, I will present a journey from treating the quantum dot nuclei as an uncontrolled noise source limiting spin coherence to the observation of their collective magnon modes and eventually to their capacity as quantum registers, all witnessed via a single electron spin driven by light.

Dr Sergei Tretiak (Los Alamos National Laboratory)

Machine learning in chemistry: reactive force fields and beyond

Friday 28 March 2024

Machine learning (ML) became a premier tool for modeling chemical processes and materials properties. ML interatomic potentials have become an efficient alternative to computationally expensive quantum chemistry simulations. In the case of reactive chemistry designing high-quality training data sets is crucial to overall model accuracy. To address this challenge, we develop a general reactive ML interatomic potential through unbiased active learning with an atomic configuration sampler inspired by nanoreactor molecular dynamics. The resulting model is then applied to study five distinct condensed-phase reactive chemistry systems: carbon solid-phase nucleation, graphene ring formation from acetylene, biofuel additives, combustion of methane and the spontaneous formation of glycine from early-earth small molecules. In all cases, the results closely match experiment and/or previous studies using traditional model chemistry methods. Importantly, the model does not need to be refit for each application, enabling high throughput in silico reactive chemistry experimentation. Active learning can be further boosted with uncertainty driven dynamics that can rapidly discover configurations to meaningfully augment the training data set. This approach modifies the potential energy surface used in molecular dynamics simulations to favor regions of configuration space for which there is large model uncertainty. Finally, a training procedure based on Iterative Boltzmann Inversion suggests a practical framework of incorporating experimental data into ML models to improve accuracy of molecular dynamics simulations. Altogether, explosive growth of user-friendly ML frameworks, designed for chemistry, demonstrates that the field is evolving towards physics-based models augmented by data science.

References:

- N. Fedik, R. Zubatyuk, N. Lubbers, J. S. Smith, B. Nebgen, R. Messerly, Y. W. Li, M. Kulichenko, A. I. Boldyrev, K. Barros, O. Isayev, and S. Tretiak, *Nature Rev. Chem.* 6, 653 (2022).
- S. Zhang, M. Z. Makos, R. B. Jadrich, E. Kraka, B. T. Nebgen, S. Tretiak, O. Isayev, N. Lubbers, R. A. Messerly, and J. S. Smith, "Exploring the frontiers of chemistry with a general reactive machine learning potential," *Nature Chem.* (2024, in press)
<https://chemrxiv.org/engage/chemrxiv/article-details/6362d132ca86b84c77ce166c>
- M. Kulichenko, K. Barros, N. Lubbers, Y. W. Li, R. Messerly, S. Tretiak, J. S. Smith, and B. Nebgen, *Nature Comp. Sci.*, 3, 230 (2023).

S. Matin, A. Allen, J. S. Smith, N. Lubbers, R. B. Jadrach, R. A. Messerly, B. T. Nebgen, Y. W. Li, S. Tretiak, K. Barros, "Machine learning potentials with iterative Boltzmann Inversion: training to experiment," (2024, submitted) <https://doi.org/10.48550/arXiv.2307.04712>.

Prof Stephen Smartt (University of Oxford)

Searching the sky for explosive transients, stellar mergers and kilonovae

Friday 19 April 2024

For the first time in history, we can survey the whole visible sky multiple times every 24hrs and process the data in real time to find everything that moves, explodes or varies. With an extended group, I exploit the NASA funded surveys ATLAS and Pan-STARRS for extragalactic explosive transients. We search for supernovae and luminous transients from compact object mergers which may be accompanied by high energy triggers (gamma ray bursts) or gravitational wave sources. There is only confirmed electromagnetic counterpart to a gravitational wave source - the kilonova and gamma ray burst associated with the neutron star merger GW170817. Perhaps surprisingly, no kilonova candidates have been discovered in independent wide-field optical surveys since 2017. However two kilonovae have been found associated with long duration gamma ray bursts. I will review these discoveries, what we can learn about heavy element production from the spectra of these sources and the promise of the Rubin Observatory when it begins operations in 2025.

Prof Monica Craciun (University of Exeter)

Integration of 2D materials with textiles for applications in wearable electronics

Friday 10 May 2024

2D materials, with exceptional electrical conductivity and mechanical flexibility, are emerging systems for wearable electronics and smart textiles, offering opportunities for the seamless incorporation of electronic devices in textiles. I will give an overview of our progress in integrating 2D materials with textile substrates, encompassing fibres and fabrics, for a range of textile electronics applications. We demonstrated a versatile technique for coating common insulating textile fibres with monolayer and few-layer graphene produced through Chemical Vapor Deposition (CVD). Various fibre materials, including polypropylene, polylactic acid, polyethylene, and nylon, exhibited sheet resistance values as low as 600 Ohm sq⁻¹, highlighting that the exceptional conductivity of graphene remains intact when applied to textile fibres. These graphene conductive fibres served as a foundation for integrating electronic devices directly within textiles. For instance, we demonstrated touch-sensitive and light-emitting functionalities in graphene electronic textile fibres. Additionally, the weaving of these fibres into fabrics facilitated the creation of display pixels and position-sensitive features. Finally, we showcased the use of graphene-coated polypropylene fibres as temperature sensors within a low-voltage carbon-graphene e-textile system. In the area of fabric-based wearable devices, a pivotal obstacle lies in seamlessly integrating electronics into fabrics while preserving their softness and comfort. A crucial aspect involves achieving electrically conductive coatings on textiles that adapt to the irregular and coarse structures of fabrics without compromising their properties. We introduced a straightforward, cost-effective, and highly scalable method, the ultrasonic spray

coating. This technique was effectively used to coat various types of textile fabrics such as meta-aramid, polyester, and nylon using water-based suspension of graphene and create fabric electrodes displaying good conductivity, and resilience to bending, compression and tension. We further demonstrated the application of these graphene conductive fabric electrodes in self-powered sensing technologies embedded in textiles. The steppingstone for these advances is a new class of triboelectric energy harvesters able to convert presently unused sources from our living environment such as sounds and vibrations into electrical energy. Due to the conformation ability of the triboelectric sensors, they were implemented on key moving parts of the human body and used to monitor biomechanical motion through electrical signals. The self-powered sensors demonstrate their potential for wearable bioelectronics, intelligent robotics, prostheses, and rehabilitation purposes. Finally, we also demonstrated the use of CVD multilayer graphene on fabrics for a novel textile-integrated triboelectric nanogenerator capable of sensing and harvesting low-frequency acoustic energy.

Dr Dimitra Georgiadou (University of Southampton)

Nanoscale Materials and Devices for Greener Emerging Technologies

Friday 24 May 2024

Nanotechnology is widely used in electronics to further miniaturise electronic components. Nanomaterials have played a major role in this, as they possess many attractive inherent properties derived from their low dimensionality. However, nanoparticles and self-assembled monolayers are usually processed from solution and they are difficult to be implemented with high yield in large area electronics. On the other hand, two-terminal electronic devices commonly comprise a generic metal/semiconductor/metal structure in a vertical (sandwich) configuration. This poses restrictions in the device fabrication when nanomaterials are involved, as the quality of the film is often compromised due to the small scale of the nanomaterials that do not guarantee uniform, continuous and pinhole-free film formation. A solution to this is offered by lateral devices, where the two metals are placed on the same plane and separated by a gap, which is filled by the semiconductor. If this gap is small enough, comparable to the dimensions of the materials used, the nanomaterials can effectively bridge this gap and connect the two electrodes electrically without causing a short-circuit.

Adhesion lithography (a-lith) is a nanopatterning technique with reduced manufacturing energy cost, as compared, for example, with e-beam lithography, that allows the fabrication of asymmetric nanogap metal electrodes at a low cost and with high throughput on a variety of rigid and flexible substrates of arbitrary size. We have so far demonstrated ultra-high speed (GHz) Schottky diodes (1) and fast photodetectors (2) as well as multi-bit and ferroelectric memories (3) based on different solution-processed semiconductors and a-lith patterned electrodes separated by a <10 nm gap.

In this talk I will present an overview of the work performed currently in my group at the University of Southampton, where we study different classes of materials, from metal oxides and polyoxometalates to organic materials and hybrid Pb-free perovskites, as well as layered 2D materials that are successfully implemented in nanoscale optoelectronic and memory applications. I will show that the combination of coplanar nanogap electrodes with functional materials holds great promise for achieving low power consumption and fast switching speeds in

electronic devices, while their planar geometry facilitates a light-controlled operation, enabling optoelectronically controlled neuromorphic systems.

This work paves the way to the development of a new form of greener devices and systems that merge photonic, electronic and ionic effects, bringing new prospects for in-memory computing and artificial visual memory applications.

References:

- (1) Georgiadou, D.G., et al, Nature Electronics, 2020. 3(11): p. 718
- (2) Georgiadou, D.G., et al, Advanced Functional Materials, 2019. 0(0): p. 1901371
- (3) Kumar, M., D.G. Georgiadou, et al, Advanced Electronic Materials, 2020. 6(2): p. 1901091

Prof Anna Baldycheva (University of Oxford)

In search of universality: towards a statistical mechanics of collisionless plasma

Friday 31 May 2024

Much of existing plasma (astro)physics is done hovering in the vicinity of a Maxwellian equilibrium, which is the maximum point of the standard Gibbs entropy and is achieved dynamically by means of two-particle collisions. In this colloquium, I would like to discuss what I believe to be the next frontier for (astro-)plasma theoreticians — and, to an extent, generally for theoretical physicists concerned with complex many-body systems — and attempt to grapple with the fact that many natural plasmas are too collisionless to be Maxwellian (in the sense that their dynamics occur on shorter timescales than interparticle collisions). The central question is then whether there exist universal collisionless equilibria, or classes thereof, and what they are. What is the meaning of entropy in a collisionless plasma? (Similar questions are asked in galactic dynamics, where the collisionless particles are stars.) I will discuss some simple ideas, going back to the work of Lynden-Bell in the 1960s, about the statistical mechanics of collisionless systems, leading to a class of universal collisionless equilibria — these are reminiscent of the equilibria of Fermi gases, with phase-volume conservation imposing (an infinite set of) Casimir invariants, whose effect is analogous to that of the Pauli exclusion principle. The generalised Lynden-Bell equilibria obtained in this way cover quite a wide variety of distributions — most intriguing perhaps is that they will generically feature “nonthermal” power-law tails [1] — a matter of some interest, e.g., for the theory of cosmic rays and of the nonthermal particle distributions routinely measured in the solar wind, as well as in statistical mechanics of various soft-matter systems. I will then outline a programme for how one might do to this statistical mechanics what Boltzmann did to Gibbs: derive a “collisionless collision integral” that describes the dynamical relaxation of a plasma towards the Lynden-Bell equilibria. It turns out that in order to make progress in this task, one must understand the structure of chaotic fluctuations in phase space. Lynden-Bell-like equilibria are recoverable under some very restrictive assumptions — roughly speaking, when these fluctuations are treated as structurally similar to a thermal noise [2]. In fact, they are more likely to behave like fully-fledged turbulence — with phase mixing (“Landau damping”) and stochastic echoes conspiring to process a constant flux of energy [3]. What universal equilibria (if any) exist against such a background is a topic of ongoing research.

References:

- [1] R. J. Ewart, M. L. Nastac, and A. A. Schekochihin, J. Plasma Phys. 89, 905890516 (2023) [e-print arXiv:2304.03715]
- [2] R. J. Ewart, A. Brown, T. Adkins, and A. A. Schekochihin, J. Plasma Phys. 88, 925880501 (2022) [e-print arXiv:2201.03376]
- [3] M. L. Nastac, R. J. Ewart, W. Sengupta, A. A. Schekochihin, M. Barnes, and W. D. Dorland, PRE, in press [e-print arXiv:2310.18211]

Prof Alexander Schekochihin (University of Oxford)

In search of universality: towards a statistical mechanics of collisionless plasma

Friday 7 June 2024

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Dr Jessica Wade (Imperial College London)

Harnessing the functional properties of chiral materials for next-generation technologies

Friday 21 June 2024

The use of organic semiconductors as low-cost, lightweight, easy-to-process active layers in optoelectronic devices has attracted considerable research and technological interest for over thirty years. The functional properties of chiral organic semiconductors, including the absorption and emission of circularly polarised light or the transport of spin-polarised electrons, are highly anisotropic. As a result, the orientation of chiral molecules impacts the functionality and efficiency of chiral devices. We have developed a strategy to control the orientation of helicenes, prototypical chiral small molecules. Our approach forces the helicenes to adopt a face-on orientation and self-assemble into upright supramolecular columns oriented with their helical axis perpendicular to the substrate, or an edge-on orientation with parallel-lying supramolecular columns, which can independently switch on and switch off low- and high-energy chiroptical responses. Our templating methodologies provide a simple way to engineer orientational control and, by association, anisotropic functional properties of chiral molecular systems for a range of emerging technologies. In this talk I will speak about our efforts to control and characterise the orientation, order and supramolecular assembly of chiral small molecules and polymers, and the impact that has on the functional properties of chiral thin films and devices.

Dr Alexander Gumennik (Indiana University Bloomington)

Engineering of Functional Monofilament Fibers

Friday 28 June 2024

Fiber looming, weaving, and knitting into a textile to create garments that warm and protect us from scratches have been known to humans for thousands of years. With the emergence of the Internet of Things (IoT), textiles are increasingly seen as real estate for sensing and stimulation functionalities in addition to traditional passive ones. How cool it would be if your t-shirt could sense stress and give a relaxing massage, or your pants could embed a rechargeable battery, powering the smartphone in your pocket! Smart fibers and textiles have recently been a booming interdisciplinary area of research that is transformative to multiple technologies, from biomedical devices through apparel and fashion to composites for aerospace, automotive, and construction. Applications of smart fibers and textiles span but are not limited to energy

harvesting and management, physiological monitoring and stimulation, brain-computer interfacing, active camouflaging, and data harvesting, processing, and communication.

The realization of high-performance systems in fibers necessitates embedding various materials and structures, including electronic and photonic, into fiber cladding in an ordered, addressable, and scalable manner. The figure of merit for any active device is defined primarily by the architectural precision of its structure. However, whether glass- or polymer-based, monofilament fibers and the materials they encapsulate are shaped from a melt and thus prone to fluid dynamics phenomena, such as capillary instability – non-linear and even chaotic – challenging the architectural control.

To solve this problem, we invented the Very Large-Scale Integration for Fibers (VLSI-Fi). VLSI-Fi combines molten-phase material processing techniques that piggyback on, rather than circumvent, the fluidic phenomena to attain the desired outcome. We prove, both analytically and experimentally, the existence of material processing parameter's range in which capillary instability predictably drives the self-assembly of functional devices in fibers with tight architectural control.

Developing VLSI-Fi into a full-scale technology can deliver impactful products. Recently, we demonstrated an electroceutical fiber that prevents the proliferation of bacteria, including antibiotic-resistant strains. Used as sutures and incorporated into gauzes and sponges, this fiber could assist antibiotics in point-of-care wound treatment, such as on the battlefield. Additionally, we have recently developed a sub-THz fiber antenna acting as a stress and temperature gradiometer that, incorporated into a catheter or wire guide, provides physiological monitoring to prevent hemorrhage, thrombosis, and inflammation in minimally invasive surgical procedures. In the long run, VLSI-Fi is expected to deliver fiber photonics that will intimately and efficiently interface the emerging high-performance computing platforms, such as quantum, to enable their incorporation into the larger Internet.