

Talks

10:30 Spin Alignment in Supermassive Black Hole Binaries - Joanna Piotrowska, Astrophysics

Supermassive Black Hole (SMBH) binaries naturally occur as a consequence of galaxy mergers and are thought to approach each other at approximately 1 parsec separations through interaction with a gaseous circumbinary disk. The merger event can result in an arbitrary orientation of the SMBH spins, which evolve in time and influence the recoil velocities associated with the final merger. In extreme cases, these recoil kicks can exceed the SMBH host escape velocities, potentially ejecting the merger remnant and affecting the fraction of SMBH residing in galactic centres. During my Master's Project, I performed two hydrodynamic simulations with the AREPO framework in order to investigate this potential influence in a 1:1 and a 3:1 mass ratio binary surrounded by a gaseous circumbinary disk. I found the shortest timescales associated with the binary inspiral to be 2110 Myr and 4080 Myr in the two systems and estimated their maximum spin alignment times, which amounted to 881 Myr and 801 Myr respectively. In this brief talk I would like to introduce the physical mechanism driving spin alignment in SMBH binaries, its implementation within the code and the results we arrived at after evolving the system for a total of 500 binary orbits.

10:42 Constrained Bayesian Optimisation for Automatic Chemical Design - Ryan-Rhys Griffiths, Theory of Condensed Matter

Automatic Chemical Design provides a framework for generating novel molecules with optimized molecular properties. The current model suffers from the pathology that it tends to produce invalid molecular structures. By reformulating the search procedure as a constrained Bayesian optimisation problem, we showcase improvements in both the validity and quality of the generated molecules. We demonstrate that the model consistently produces novel molecules ranking above the 90th percentile of the distribution over training set scores across a range of objective functions. Importantly, our method suffers no degradation in the complexity or the diversity of the generated molecules.

10:54 A quasicrystalline potential for ultracold atoms - Matteo Sbroscia, Atomic, Mesoscopic and Optical Physics

Quasicrystals are long-range ordered and yet non-periodic. This interplay results in a wealth of intriguing physical phenomena, such as the inheritance of topological properties from higher dimensions, and the presence of non-trivial structure on all length scales. Here we report on the first experimental demonstration of an eightfold symmetric optical lattice, realising a two-dimensional quasicrystalline potential for ultracold atoms, which we probe via matter-wave diffraction. The diffraction dynamics on short timescales constitutes a continuous-time quantum walk on a homogeneous four-dimensional tight-binding lattice. On longer timescales, the atoms are adiabatically loaded into the lattice and the equilibrium properties of the quasicrystal can be investigated.

11:06 Understanding dissipative behaviour in Kinetic Inductance Detectors - Tess Skyrme, Quantum Sensors

Kinetic inductance detectors (KIDs) have applications in both astronomy and quantum computing. KIDs are low noise, high quality factor superconducting microresonators, potentially capable of

detecting single photons. It is widely understood that there are different dissipative loss mechanisms which can degrade the performance of KIDs, reducing their quality factor and increasing noise equivalent power by multiple orders of magnitude. Understanding sources of loss in KIDs, and their relationship with applied readout power, is essential. We present a method to solve for multiple dissipative losses; beginning with two level systems noise and quasiparticle heating, simultaneously over a wide range of readout powers. Our method attributes quality factors to different loss mechanisms, and considers the steady state values of quasiparticle population and energy in a resonator. This new technique allows the large signal behaviour of KIDs to be simulated, with the results verified with multiple sets of experimental data. We show that the relationship between quality factor and readout power ultimately determines the best operating point of the system, and warn against the consequences of ignoring the effects of dissipative loss in resonators used for high sensitivity applications such as qubit readout, or red shift measurement.

11:40 Bayesian non-parametric density estimation - Vidhi Lalchand, Scientific Computing

Density estimation is a fundamental particle discovery tool in modern day HEP. One of the problems in the HEP domain is that of non-parametric density estimation of the invariant mass spectrum. The mass spectrum is a reconstructed quantity computed using equations of the standard model of physics. Its estimated probability density is used to carefully characterize the bumps in this mass spectrum. Known particles would show up as bumps at known mass levels however a protuberance at mass levels with no known particles could point to the existence of exotic particles. It is difficult to capture this protuberance mainly because the signal is embedded within a very large background and traditional density estimation techniques with known kernels are limited in capacity to learn these complex overlapping densities. Non-parametric Bayesian techniques which yield distributions over densities rather than a single estimated density are a powerful method to model the invariant mass.

11:52 Contact and Patterning of Topological Surface States - Ankita Anirban, Semiconductor Physics

Topological insulators (TIs) are a novel class of material which host helical surface states with exciting and unique electronic properties. They can provide insights into new physics and also pave the way for potential spintronic applications. Much work has been done to identify and characterise these surface states, but in order to utilise them towards multifunctional devices, we need a way to control the exchange gap opening in a tailored way and pattern them accordingly. We present results from devices which allow selective contact and patterning of topological surface states. We interface a TI with a ferromagnetic insulator to open up a gap in the Dirac cone, in an effort to have independent contact to the top and bottom surface states of a single TI film, enabling the characterisation and utilisation of the two surface states separately. We also study heterostructures with two TI layers separated by a trivially insulating tunnel barrier, allowing for a way of probing the dispersion relation of TIs using spin and momentum resolved tunnelling.

12:04 Quantum Monte Carlo method for Vibrational Frequencies - Fredrik Liu, Theory of Condensed Matter

Quantum Monte Carlo methods have become a leading contender for high accuracy calculations for the electronic structure. Calculating energy derivatives such as atomic forces and the matrix of force constants is important in relaxing structures, calculating vibrational properties, and performing

molecular dynamics simulations. We develop a quantum mechanical expectation value to evaluate the matrix of force constants directly in Quantum Monte Carlo. The approach allows the full modeling of correlation effects such as Van der Waals force, opening new applications to molecules and solids in condensed matter.

12:16 Realising a high efficiency perovskite-silicon tandem solar cell - Kyle Frohna, Optoelectronics

Metal-halide perovskite solar cells are an exciting class of materials for use in photovoltaic applications. Perovskites can be deposited at low cost and can obtain efficiencies comparable to established solar technologies. However, the vast industrial scale that the incumbent silicon solar cells are produced at make commercialising perovskite solar cells challenging. Perovskite-silicon tandem solar cells represent a promising avenue to improve the efficiency of already commercialised silicon solar cells at low additional cost. Tandem solar cells can attain efficiencies higher than the fundamental limits set for single junction solar cells and represent the most likely first step in commercialisation of perovskite technologies.

In this talk, I will discuss some recent work on the compositional engineering of wide bandgap perovskites to improve stability and efficiency for tandems. I will also discuss the device engineering and light management techniques we have employed to achieve a 25% efficient, perovskite-silicon tandem solar cell.

12:28 Topological Terms and Central Extensions - Joseph Stanley Smith, High Energy Physics

From the Landau problem to the motion of a rigid body, topological terms are of great prevalence in quantum physics. The issue is that often such problems don't lend themselves to study by harmonic analysis (Fourier transform). By looking at the symmetry group involved it may be possible to take what is called a "central extension" of a group and recast the problem in a form that can be studied by harmonic analysis. Due to the heavy use of topology, differential geometry and group theory in this area, it is not surprising that it is jargon filled. This talk will give a non-technical description of the area of research.