Theoretical and Mathematical Physics in Cergy Paris, Singapore, and Warwick – 9th -10th July 2020

Organisers

Rudolf Römer is professor in the Physics Department of the University of Warwick, UK, and associated with Warwick's Centre for Scientific Computing (CSC) which he led 2005-10. He is currently fellow-in-residence at CY|AS, invited by laboratory LPTM.

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Background and Purpose

Theoretical and mathematical physicists at Cergy, Singapore and Warwick have many common research interests, for example mathematical and computational methods, artificial intelligence, quantum physics in all its manifestations, etc., and potential for future projects for collaboration. In order to communicate these better to each other, we want to meet virtually for a 2-half-day workshop with selected presentations.

Researchers are free to present in-progress projects, talk about completed papers or give overview talks of their research interest. Similarly, PhD and MSc level students are encouraged to present their work, either as a talk or as a virtual poster.

Abstracts

Arpit Arora - Nanyang Technological University

Cooperative orbital moments and edge magnetoresistance in monolayer WTe2

Quantum Spin Hall (QSH) edge states exhibit dissipationless transport that is insensitive to the crystal structure and disorder of the sample device as long as time-reversal symmetry is preserved. Here we argue that when a magnetic field is applied, the edge states of QSH insulators become highly sensitive to bulk crystalline symmetries. In particular, we find that the QSH insulator 1T'- WTe2 displays an anisotropic edge magnetoresistance that depends on edge termination, and can be controlled by the breaking of (bulk) in-plane and out-of-plane inversion symmetry. Strikingly, maximum edge magnetoresistance occurs when magnetic field is applied at a canted angle θ oblique to the plane, which can be tuned by the strength of inversion symmetry breaking. This behavior is in stark contrast to that found in HgCdTe QSH insulators (where magnetoresistance is maximum for out-of-plane magnetic fields) or ideal QSH insulators (where maximum magnetoresistance is expected to arise for in-plane magnetic fields). We find this behavior proceeds from an unconventional orbital contribution to the edge magnetic moment that arises from "cooperative orbital moments" due to the unique low-symmetry crystal structure of 1T'-WTe2. This surprising high sensitivity to bulk symmetry breaking demonstrates that the edge states of QSH insulators are not completely independent of the bulk.

Djenabou Bayo – CY Cergy Paris Université

Machine Learning the Anderson and the Percolation Transitions

D. Bayo, A. Honecker, and R. Römer

The percolation problem is one of the simplest models in statistical physics displaying a phase transition. A classical lattice occupied randomly with a given probability at each site (or bond). A phase transition from a non-percolating to a percolating state appears around a probability pc, the so-called percolation threshold. The Anderson metal-insulator transition (MIT) [1] is characterized by a transition from a delocalized to a localized quantum state in the presence of strong disorder. This phenomenon has been investigated for many years and numerical studies have given valuable insight through the determination of the critical properties of the localization length. Machine Learning (ML) and Deep Learning (DL) techniques are still relatively new methods when applied to physics. Recent work shows that ML/DL techniques allow to detect phase transitions directly from images of computed quantum states[2,3] . The 3D Anderson model and the 2D percolation model are good candidates for an ML/Dl-based kind of analysis because of a good knowledge of the states around the phase transitions. Here, we implement ML/DL techniques to identify the percolation threshold and the MIT and to characterize their universal properties. We employ a standard image classification strategy with a multi-layered convolutional neural network. In addition, we also work directly with the numerical "raw data". Common ML/DL libraries such as Keras, TensorFlow, FastAI and PyTorch are employed as backbones in our implementation.

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Leonardo Benini - University of Warwick

Loschmidt echo singularities as dynamical signatures of strongly localized phases

Localization (being it Anderson or many-body) comes with the emergence of localized conserved quantities - whose conservation is precisely at the heart of the absence of transport through the system.

In the case of fermionic systems and S=1/2 spin models, such conserved quantities take the form of effective two-level systems, called l-bits. Their existence is suggested by several theoretical observations, yet their experimental observation remains elusive. Here we show that strongly localized l-bits bear a dramatic universal signature, accessible to state-of-the-art quantum simulators, in the form of periodic cusp singularities in the Loschmidt echo following a quantum quench from a charge-density-wave/Néel state. Such singularities are perfectly captured by a simple model of Rabi oscillations of an ensemble of independent two-level systems, which also reproduces the shorttime behavior of the entanglement entropy and of the imbalance dynamics.

Dhiman Bhowmick - Nanyang Technological University

Topological magnon bands in the flux state of Shastry-Sutherland lattice model

We investigate low-energy magnon excitations above the noncollinear flux state and noncoplanar canted flux state in a Heisenberg antiferromagnet with Dzyaloshinskii-Moriya interaction (DMI) on a Sashtry-Sutherland lattice. While previous studies have shown the presence of topological magnetic excitation in the dimer and ferromagnetic phases on the Shastry-Sutherland lattice, our results establish the nontrivial topology of magnons in the antiferromagnetic flux and canted flux states. Our results uncover the existence of a multitude of band topology transitions in the magnon sector—evidenced by the changing Chern numbers of the single magnon bands—as the Hamiltonian parameters are varied, even when the ground state remains unchanged. The thermal Hall conductivity is calculated and its derivative is shown to exhibit a logarithmic divergence at the boundaries of band topology transitions, independent of the type of band touching involved. A simple analytical form of the temperature dependence of a logarithmic peak is derived for a generic spin model. This may provide a useful means to identify the energy at which the band topological transition of magnon bands occurs. We also propose the way to realize the studied model in a practical material.

Yidong Chong - Nanyang Technological University

Band Topology in Non-Hermitian Systems

The topological classification of non-Hermitian band structures is currently an unsettled subject. I present some recent theoretical and experimental studies showing how concepts such as topological edge states carry over into the non-Hermitian regime. One example is a novel class of non-Hermitian systems hosting Dirac points rather than exceptional points, which can exhibit phenomena such as non- Hermitian topological phase transitions and gain/loss induced Landau levels.

Burak Civitcioglu - CY Cergy Paris Université

Machine Learning and Phases of the Ising model using transfer learning methods

We study Convolutional Neural Networks (CNN) prediction success on recognising the temperature by having the image of the configuration as an input for the Ising Model in 2D. In the Ising Model case, we train a CNN on a square lattice and test it on a triangular lattice and vice versa; in order to conclude if the transfer learning methods work for the Ising model. Several studies have been done on transfer learning in various physical problems with promising results. We explore the limitations of the transfer learning problem. We conclude that the transfer learning works in a limited way; the problem benefits from the transfer learning, yet it is undoubtedly not enough to confidently state that one can only use transfer learning to make valid predictions. There are patterns observed with the misplaced predictions that need future exploration and predictions about the conditions required to have better scoring transfer learning in Ising Model in 2D.

Andrea de Luca - CY Cergy Paris Université

Quantum chaos in extended many-body systems

I will briefly review recent advances in the understanding and the definition of quantum chaos in the context of systems with local interactions and an extensive number of degrees of freedom. I will emphasise the connection between the Butterfly effect and the growth in time of the complexity of local operators (out-of-time order correlator). Moreover, I will discuss the repulsion between energy eigenstates as a well-known fingerprint of quantum chaos. By introducing a class of solvable models, I will explain how random matrix behavior and level repulsion generally emerge and I will discuss universality beyond random matrices.

Yérali Gandica - CY Cergy Paris Université

Bali ancient rice terraces: A Hamiltonian approach

In this communication, I will present a Hamiltonian approach inspired by the Subak irrigation system. In a previous work, Lansing et al. [1] found out that the cluster-size distribution of the rice patches in Bali-Subak fields is a powerlaw function with an exponent (approx. 1.9) similar to the one found on the Potts model. I will show how the beautiful mosaics characterising several rice-growing regions in Bali-Indonesia, which are the consequence of the self-organising process ruled by the Subak since the 11th century in that tropical island, can be explained by two main mechanisms behind Subak farmers' decisions. Pest stress is the local mechanism promoting order, namely, using the same schedule within neighbouring patches. On the other hand, an antiferromagnetic interaction controlled by water stress is set by a global mechanism, fixing a limit in the total number of cells in the same state. Our Subak Hamiltonian presents a rich behaviour, showing several phase transitions, studied by the regular tools of Statistical Mechanics. I will present our last results and main conclusions obtained from this scientific collaboration.

Laura Hernandez - CY Cergy Paris Université

Collective effects of the cost of opinion change

Hendrik Schawe and Laura Hernandez

We study the dynamics of opinion formation in the situation where changing opinion involves a cost for the agents. To doso we couple the dynamics of a heterogeneous bounded confidence Hegselmann-Krause model with that of the resourcesthat the agents invest on each opinion change. The outcomes of the dynamics are non-trivial and strongly depend on thedifferent regions of the confidence parameter space. In particular, a second order phase transition, for which we determine thecorresponding critical exponents, is found in the region where a re-entrant consensus phase is observed in the heterogeneousHegselmann-Krause model. For regions where consensus always exist in the heterogeneous Hegselmann-Krause model,the introduction of cost does not lead to a phase transition but just to a continuous decrease of the size of the largest opinioncluster. Finally in the region where fragmentation is expected in the heterogeneous HK model, the introduction of a very smallcost surprisingly increases the size of the largest opinion cluster.

Nicholas Hine - University of Warwick

Layered Material Heterostructures: A new twist on 2D materials

A 2D material that is incorporated into any kind of device automatically becomes in effect part of a heterostructure, since the atomic-scale widths of these novel materials also mean their `bulk' regions are never really independent of their surroundings. Furthermore, novel physics often emerges from the hybridisation of the bandstructure that results when materials are combined. Controlling the properties of layered material heterostructures is therefore crucial to the success of devices based on the novel capabilities of 2D materials.

However, while monolayer 2D materials are very well-studied, theoretical insight into heterostructures has been limited by the large system sizes required to study the interfaces between pairs of materials, which in general will be incommensurate and may be rotated with respect to one another. My group develops and uses a code called ONETEP which can to perform linear-scaling DFT calculations with non-local vdW functionals, and exploit bandstructure unfolding for insight into electronic properties. We have used it to explore large-scale models of heterostructures of interest for device applications.

I will present results for heterostructures including MoS_2/$MoSe_2$, $MoSe_2$/WSe_2, hBN/Phosphorene and InSe/graphene. Band-structure changes caused by stacking and rotation of the layers are obtained by unfolding the supercell spectral function into the primitive cells, incorporating spin-orbit coupling. Changes in spectral weight and band-structure between the monolayers and heterostructured interfaces show how lattice mismatch (MoS2/MoSe2) or spacer layers (Phosphorene/hBN/Phosphorene) can allow the component monolayers to retain more independence in heterostructures than in homo-stacks. Applying electric fields allows the behaviour of gated structures to be predicted and explained. Finally, we find that in the case of InSe, the choice of substrate can be used to dramatically tune the nature of the bandgap, potentially driving transitions from indirect to direct gap in the monolayer.

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Xiao Lin - Nanyang Technological University

Actively controlling the near-field directionality with graphene plasmons

Here we study the near-field directionality of complex dipoles such as circularly polarized dipole, Huygens dipole and Janus dipole in 2D materials and van der Waals heterostructures, and we reveal some new phenomena. First, an inverse Doppler frequency shift of light, i.e., superlight inverse Doppler effect, is shown possible even in homogeneous media with positive-refractive index, contrary to the status quo ante. We show an example with graphene plasmons and find the superlight inverse Doppler effect can introduce some new exotic features of near-field directionality. Second, we propose a strategy to actively control the near-field directionality by using the hybrid graphene-metasurface waveguide. Third, we find the near-field directionality can also be efficiently manipulated via twisted van der Waals heterostructures, such as twisted α-MoO_3 slabs and twisted bilayer graphene.

Jie Liu - Xiangtan University

Localization, phases and transitions in the three-dimensional extended Lieb lattices

Jie Liu, Xiaoyu Mao, Jianxin Zhong, and Rudolf A. Römer

We study the localization properties and the Anderson transition in the 3D Lieb lattice $\mathcal{L}3(1)$ and its extensions $\mathcal{L}3(n)$ in the presence of disorder. We compute the positions of the flat bands, the disorder-broadened density of states and the energy-disorder phase diagrams for up to 4 different such Lieb lattices. Via finite-size scaling, we obtain the critical properties such as critical disorders and energies as well as the universal localization lengths exponent. We find that the critical disorder Wc decreases from 16.5 for the cubic lattice, to 8.6 for $\mathcal{L}3(1)$, 5.9 for $\mathcal{L}3(2)$ and 4.8 for $\mathcal{L}3(3)$. Nevertheless, the value of the critical exponent for all Lieb lattices studied here and across disorder and energy transitions agrees within error bars with the generally accepted universal value= 1.590(1.579, 1.602).
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Critical properties of the Anderson transition through the looking-glass of the CBS and CFS peaks

In disordered media, the absence of diffusion arising from the spatial localization of single-particle states is known as Anderson localization (AL). In three dimensions, AL manifests itself as a phase transition which occurs at a critical energy or at a critical disorder strength (the mobility edge) separating a metallic phase where states are spatially extended, from an insulating one where states are localized. Theoretically, much efforts have been devoted to the study of the critical properties of the Anderson transition (AT), such as wave-function multifractality or critical exponents. In practice however, only a handful of experiments have found evidence for the 3D Anderson transition, among them cold atoms, and even fewer have investigated its critical features (mostly in the context of quantum-chaotic dynamical localization). In addition to the intrinsic difficulty of achieving wave localization in three dimensions, one reason for the rareness of experimental characterizations of the Anderson transition is the lack of easily measurable observables displaying criticality. In this talk, I will show that the critical properties of the AT are encoded in two emblematic interference effects observed in momentum space: the coherent backscattering (CBS) and the coherent forward scattering (CFS) peaks, the latter being a critical quantity of the transition. By a finite-time scaling analysis of the CBS width and of the CFS contrast temporal dynamics, one

can extract accurate values of the mobility edge and critical exponents of the transition in agreement with their best-known values to this date.
Furthermore, exactly at the mobility edge, the CFS peak contrast is directly related to the so-called information dimension and reflects multi-fractal properties of the wave functions.

Ahmed Missaoui - CY Cergy Paris Université

Electronic properties in bilayer graphene monitored by selective functionalization

We study numerically the electronic properties of bilayer graphene functionalized by adatoms, such as hydrogen, using a tight binding model and DFT calculations. We focus first on the effects of a selective distribution of adsorbates on specific sublattices in Bernal bilayer [1], and study the electronic structure and the microscopic conductivity within Kubo formalism [2]. In some particular cases, depending on Fermi energy value and the adsorbate distribution, a mobility gap appears; whereas and in other cases, the conductivity is abnormal: conductivity increases when the concentrations of defect increases.
Other than the selectivity of the adsorbate in simple Bernal bilayer, we can also control the electronic properties of the bilayer graphene by a rotation of one of the two layers with respect to the other. In this system, called twisted bilayer graphene, we analyze the dependence of the conductivity with the rotation angle in presence of functionalization by adatoms [3].

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Dario Poletti - Nanyang Technological University

Tensor network based machine learning of non-Markovian quantum processes

We show how to learn structures of generic, non-Markovian, quantum stochastic processes using a tensor network based machine learning algorithm. We do this by representing the process as a matrix product operator (MPO) and train it with a database of local input states at different times and the corresponding time-nonlocal output state. In particular, we analyze a qubit coupled to an environment and predict output state of the system at different time, as well as reconstruct the full system process. We show how the bond dimension of the MPO, a measure of non-Markovianity, depends on the properties of the system, of the environment and of their interaction. Hence, this study opens the way to a possible experimental investigation into the process tensor and its properties.

Hendrik Schawe - CY Cergy Paris Université

When open mindedness hinders consensus

We perform a detailed study of the Hegselmann-Krause bounded confidence opinion dynamics model with heterogeneous confidence ε_i drawn from uniform distributions in different intervals $[\varepsilon_l, \varepsilon_u]$. The phase diagram reveals a highly complex and non monotonous behaviour, with a re-entrant consensus phase in the region where fragmentation into multiple distinct opinions is expected for the homogeneous case. A careful exploration of the phase diagram, along with an extensive finite-size analysis, allows us to identify the mechanism leading to this counter-intuitive behaviour.

Pinaki Sengupta - Nanyang Technological University

Strange correlations in symmetry protected topological phases

In the absence of long-range entanglement, emergent fractional charge/fractional statistics for finite-energy excitations, or emergent gauge theory (due to its short-range entanglement), the detection and characterization of Symmetry Protected Topological (SPT) phases is challenging, especially for interacting many body systems. On top of that, the key identifying feature, viz., gapless surface states, are only symmetry protected (as opposed to topologically protected) and is robust only against local perturbations that do not break the protecting symmetry, making the use of entanglement spectrum to detect SPT phases conditional on the way the system is partitioned. The “strange correlator” that was proposed as a direct probe for gapless surface states in SPT phases, overcomes all the difficulties mentioned above. Furthermore, the approach does not rely on properties of band structure, and is hence valid for interacting systems as well. Using projective quantum Monte Carlo, we are able to directly access the strange correlator in a variety of phases, and examine its critical behavior at the quantum phase transition between trivial and non-trivial symmetry protected topological phases. After finding the expected long-range behavior in these two symmetry conserving phases, we go on to verify the trivial (non-trivial) topological nature of even- (odd-) leg spin-1 Heisenberg antiferromagnetic ladders and finally identify the topological character of a 2-D system od weakly coupled chains.

Vedran Sohinger - University of Warwick

Gibbs measures of nonlinear Schrödinger equations as limits of many-body quantum states

Gibbs measures of nonlinear Schrödinger equations are a fundamental object used to study low regularity solutions with random initial data. In the dispersive PDE community, this point of view was pioneered by Bourgain in the 1990s. We are interested in the problem of the

derivation of Gibbs measures as mean-field limits of Gibbs states in many-body quantum mechanics.
Our proof is based on a functional integral representation of the quantum Gibbs state. In this framework, the limit is formally deduced by using a infinite-dimensional stationary phase argument. In order to make this rigorous, we introduce an auxiliary white-noise-type field, through which the functional integral is represented in terms of propagators of heat equations with time-dependent periodic random potentials, and subsequently as a gas of interacting Brownian paths. This is joint work with J. Fröhlich, Knowles, and B. Schlein.

Nyayabanta Swain - Nanyang Technological University

Complex magnetic ordering and associated topological Hall effect in two-dimensional metallic chiral magnets

Motivated by recent experiments on the observation of room temperature skyrmions in a layered heterostructure and subsequent demonstration of topological Hall effect in the same system, we have studied a minimal model of itinerant electrons coupled to local moments with competing interactions in an external magnetic field. Working in the limit of strong magneto-electric coupling where the fast dynamics of the electrons can be decoupled from the slow dynamics of the local moments (treated as classical spins), we analyze the multiple field induced magnetic phases and the associated electronic transport properties in these regimes. Our results help understand the microscopic origin of the observed phenomena and further provide crucial insight into unconventional magneto-transport in twodimensional metallic chiral magnets.

Bobby Tan - Nanyang Technological University

Negativity of quasiprobability distributions as a measure of nonclassicality

I discuss some recent progress in the use of quasiprobability distributions to identify and quantify the nonclassicality of light systems. Quasiprobability distributions are representations of state that fully describes a given quantum state, similar to the density matrix. They share some similarities with standard probability distributions but may permit negative values in general, and it is traditionally argued that the existence of such negativities imply nonclassical behaviour in light. I will discuss how such negativities are physically meaningful by discussing possible physical interpretations for the extent of the negativity, and show how such negativities fit into the modern resource theoretical approach of quantifying quantum nonclassicality.

Daniel Ueltschi - University of Warwick

Spin nematic phase in quantum spin 1 system

I will describe a quantum spin system with S=1 and general SU(2)-invariant pair interactions. Its low temperature phase diagramme includes a "planar nematic" phase with long-range order in dimensions d=3 and higher. This model can be studied with the help of a d+1 dimensional loop model.

Javad Vahediaghmashhadi - Technische Universität Braunschweig

Magnetism of magic-angle twisted bilayer graphene

Recently, correlated insulators and superconductivity have been discovered experimentally in twisted bilayer graphene (TBG) [1]. The Moiré pattern of the bilayers at so-called “magic angles” leads to localization of the low-energy electrons in the AA-stacking regions, reflected by very flat regions in the band structure [2]. This reduction of the kinetic energy enhances the relative importance of interactions and thus renders the bilayer systems much more susceptible to correlation effects than a single layer.
We investigate the magnetic instabilities at half filling in TBG using a real-space Hartree-Fock and RPA analysis. We find that at charge neutrality an antiferromagnetic state localized in the AA region emerges for values of the Coulomb interaction U that are an order of magnitude smaller than what would be required to render an antiferromagnetic state in a single graphene sheet. Furthermore, doping of a few electrons per Moiré unit cell pushes the system into a ferromagnetic phase.

Somepalli Venkateswarlu - CY Cergy Paris Université

Electronic localization in twisted bilayer MoS2 with small rotation angle

Somepalli Venkateswarlu, Andreas Honecker & Guy Trambly de Laissardière

Vertically stacked transition metal dichalcogenides of multilayer structures have gained increasing attention because of their fascinating features in electronics and optical properties. Moiré patterns are known to confine electronic states in Transition Metal Dichalcogenide bilayers, thus generalizing the notion of magic angles discovered in twisted bilayer graphene to semiconductors. We computed structural and electronic properties of nontwisted and twisted MoS2 bilayers using first-principles calculations and the tight-binding method. In particular, we obtained a new Slater-Koster tight-binding model that allows the first reliable and systematic studies of electronically confined states in twisted bilayer MoS2 for the whole range of rotation angles . We show that isolated bands appear at low energy for $\theta \lesssim 5-6^\circ$. Moreover, these bands become “flat bands", characterized by a vanishing average velocity, for the smallestangles $\theta \lesssim 2^\circ$.

Contribution based on arXiv:2005.13054.

Ying Xiong - Nanyang Technological University

Multistable excitonic Stark effect

Excitonic optical Stark effect arises from strong light-matter interaction whereby irradiation of an excitonic system with frequency below the exciton resonance continuously shifts the exciton transitions to higher energies as the light intensity increases. Here we demonstrate that when an excitonic system is coupled to a nanophotonic cavity, the optical Stark effect gives rise to strong nonlinear effects due to the mutual tuning between the exciton and the photon mode. When the excitons and the cavity are driven, such mutual tuning leads to multi-stable stationary states and hysteresis. We illustrate that sizable discontinuous Stark shift jumps of a few meV can be readily realized in 2D transition metal dichalcogenides with moderate driving intensities. The Stark-induced multi-stability provides a highly tunable way for the manipulation of quantum matter.

Huawen Xu - Nanyang Technological University

Universal self-correcting with disordered exciton polariton neural networks

Huawen Xu, Sanjib Ghosh, Michal Matuszewski, Timothy C. H. Liew

We show theoretically that neural networks based on disordered exciton-polariton systems allow the realization of Toffoli gates. A Toffoli gate is a binary logic gate with three inputs and three outputs, which flips the third input if and only if the first two inputs are 1. One of the most remarkable features of neural networks is their ability to operate with noisy data. Noise in input signals is self-corrected for by the networks, such that the obtained Toffoli gates are in principle cascadable, where their universality would allow for arbitrary circuits without the need of additional error correcting codes. We further find that the networks can directly simulate composite circuits, such that they are a highly efficient platform allowing circuits to operate in a single step, minimizing the delay of signal transport between elements and error correction overhead. As an example, we consider the full adder circuit. The architecture is generic, with potential applications in ultracold atomtronic systems and nonlinear optical cavities. These findings suggest that small scale neural networks based on disordered exciton-polariton systems can be used as building blocks (e.g., Toffoli gates and composite modules like full adders) for efficient universal self-correcting computing.

References

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Oleg Zaboronski - University of Warwick

Dualities and representations of Hecke algebras for interacting particle systems

Markov dualities are vital for the exact solvability of a large class or interacting particle systems in one dimension, such as exclusion processes, reaction-diffusion systems and the voter model. The search for such dualities is often an adhoc process. We show that all models listed above have a hidden Hecke algebra structure and that the duality functions appear as spanning vectors of the algebra's representation spaces.