Mathematical aspects of Quantum Science and Technology
(Org: **Jonas Fransson** (Uppsala University) and/et **Artur Sowa** (University of Saskatchewan))

MAHTA ABDOLLAHZADEHZARE, University of Saskatchewan
High-performance spectrum calculation of 3d transition metals in oxide compounds

In the early 20th century, the principles of quantum mechanics revolutionized the study of materials, leading to the invention of the transistor, the key component of modern day technologies. To sustain advancements in technology, innovations in the discovery of new materials are needed. One family of elements with immense potential in creating new functional materials is the 3d transition elements, especially in the form of oxide compounds. A common method in the study of the electronic structure of such compounds is X-ray Absorption Spectroscopy (XAS). This method yields spectra of the energy-dependent absorption which, for energies near atomic resonances, contains detailed electronic and magnetic information about the materials. However, interpreting experimental spectra can be challenging due to complicated lineshapes arising from quantum many-body interactions. Therefore, theoretical methods are often necessary to extract information and analyze the spectra. This study focuses on quantum double cluster models to simulate spectra, in particular constructing real, symmetric Hamiltonian matrices for oxide compounds containing 3d transition elements with atomic numbers 21 to 29. We employ the SLEPc library to determine the ground state eigenvalues of specific Hamiltonians, and utilize the Lanczos iterative method to calculate the XAS spectra. Our results reveal the range of necessity of this double cluster model over the series of 3d elements via the extracted covalency from the ground state wavefunction and the differences of XAS spectra compared to simpler single cluster models.

MAHMUD AZAM, University of Saskatchewan
TQFTs and Quantum Computing

Quantum computing is captured in the formalism of the monoidal subcategory of $\mathbf{Vect}_{\mathbb{C}}$ generated by $\mathbb{C}^2$ – in particular, quantum circuits are diagrams in $\mathbf{Vect}_{\mathbb{C}}$ – while topological quantum field theories, in the sense of Atiyah, are diagrams in $\mathbf{Vect}_{\mathbb{C}}$ indexed by cobordisms. We outline a program to formalize this connection. In doing so, we first equip cobordisms with machinery for producing linear maps by parallel transport along curves under a connection and then assemble these structures into a higher category. Finite dimensional complex vector spaces and linear maps between them are given a suitable higher categorical structure which we call $\mathbb{F}\mathbf{Vect}_{\mathbb{C}}$. Finally, we realize quantum circuits as images of cobordisms under higher monoidal functors from these modified cobordisms to $\mathbb{F}\mathbf{Vect}_{\mathbb{C}}$, which are computed by taking parallel transports of vectors and then combining the results in a pattern encoded in the domain category. This talk reports on joint work with Steven Rayan.

MADELINE BEREZOWSKI, University of Saskatchewan
How Boson Dimers Reproduce Spin Projection Operators

The Bose-Hubbard Hamiltonian can be simplified to have only two lattice sites, in which case the system being described is referred to as a dimer. Due to its structure, the hopping term of the dimer Hamiltonian enjoys invariance in a family of subspaces indexed by a whole number k, each subspace corresponding to a system of only k particles. We have invented an inductive argument using the bosonic canonical commutation relations to find the eigenvalues and eigenvectors of the dimer hopping Hamiltonian in its k-particle subspaces. In particular, this Hamiltonian, when restricted to one of the k-particle subspaces, is exactly the spin projection operator along the x-axis, where the number of particles k in the dimer system yields the projection matrix for spin quantum number $s = k/2$. Thus, a new method for computing the eigenvalues and eigenvectors of the x-axis spin projector has been unearthed. In this talk, I will outline the mathematical framework used and discuss our argument and results. This talk represents work done in collaboration with Artur Sowa (University of Saskatchewan) and Jonas Fransson (Uppsala University).

MANDANA BIDARVAND, University of Saskatchewan
Analyzing arrays of qubits via a multi-scale approach

A quantum metamaterial is an engineered structure whose modes of interaction with the environment depend on its quantum state. A prototypical example of such a material is a structure consisting of an array of qubits interacting with the electromagnetic field. Motivated by the challenges of analyzing such structures, we have developed a custom scale-based approach. It furnishes an alternative albeit formally equivalent model of quantum information. Its framework is naturally analytic, rather than linear-algebraic. It is especially well-suited for the study of the physics of finite as well as infinite arrays of qubits. Foundational to our approach are the Borel isomorphism and the multiresolution analysis in the Haar basis, both of which appear in classical mathematical literature in non-quantum contexts. We use them as devices that enable an identification between $L_2(0,1]$ and the Hilbert space of an infinite array of qubits. In the resulting framework, quantum operations and observables are represented through geometric integral operators. Prior studies demonstrated that in some cases the dynamics of qubit arrays is solvable in the sense that the spectra of crucial operators can be given explicitly. We extend those results and show a path to further systematic explorations. As an unexpected upshot, we observe that the fundamental concept of calculus is inherent in an infinite array of qubits; indeed, the antiderivative arises as a natural and indispensable operator in this context. In other words, if a mathematical structure encompasses a full theory of the infinite array of qubits, then it can support calculus.

HUBERT DE GUISE, Lakehead University

The regular representation of S_n in interference of fermions and bosons

Using tools from group representation theory, I will discuss the coincidence rate of partially-distinguishable particles in an interferometry experiment. In an experiment with n particles (fermions or bosons) the expressions contain blocks of terms for each partition of n; Gamas's theorem is used to determine which of these terms are automatically zero based on the pairwise level of distinguishability between particles. The computational complexity of the associated group function is introduced to show that, if the known algorithms are used, the problem of evaluating fermionic coincidence rates will contains, with probably close to 1, some functions with cost exponential in n.

This work was done in collaboration with:

- Dylan Spivak, Department of Mathematical Sciences, Lakehead University,
- Murphy Yuezhen Niu, Department of Physics, MIT
- Barry C. Sanders, Institute for Quantum Science and Technology, University of Calgary

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RAINER DICK, University of Saskatchewan

Where are the photons?

The question for a probability measure for photon location is an old and still controversial topic of quantum theory. However, progress in photonics and quantum technology does not care about this debate. Single-photon sources and detectors have been around for decades, and single-photon diffraction has been observed since 2013. In the talk, I intend to provide a summary of the relevant technologies, a description of the problem of photon location, and an overview of different proposals for probability measures for photon location.

JONAS FRANSSON, Uppsala university

Current Induced Spin-Polarization in Chiral Molecules

The inverse spin-galvanic effect, or, current induced spin-polarization is mainly associated with interfaces between different layers in semiconducting heterostructures, surfaces of metals, and bulk semiconducting materials. Here, we theoretically predict that the inverse galvanic effect should also be present in chiral molecules, as a result of the chiral induced spin selectivity effect. As proof-of-principle, we calculate the non-equilibrium properties of a model system which previously has been successfully used to explain a multitude of aspects related to the chiral induced spin selectivity effect. Here we show that current driven spin-polarization in a chiral molecule gives rise to a magnetic moment which is sensitive to external magnet field. The chiral molecule then behaves like a soft ferromagnet. This, in turn, suggests that magnetic permeability measurement in otherwise non-magnetic systems may be used non-invasively to detect the presence of spin-polarized currents.

ELIAS HASSANI, University of Saskatchewan
A post-quantum, post-AI data encryption method

We discuss a new symmetric-key cipher for digital data encryption. Its implementations are fast, memory efficient, and resilient against classical, AI-assisted, and quantum attacks. Let x, k, and c be elements of a finite abelian group G with operation $+$ and the neutral element 0. Suppose one is given ciphertext $c = x + k$. Retrieving the plaintext $x = c - k$ from the ciphertext c is trivial when one knows the key k. However, not knowing the key, the task is a blind search. To recover x, we would require an efficient criterion for distinguishing x by its characteristic features, if such were known, from all other group elements. Furthermore, even if one were availed of such a tool, the average number of trials is prohibitively difficult when the group is sufficiently large. The challenge to achieve a real-life implementation of the said schema is to find a very large G, and to construct algorithms enabling an immersion of *real digital data* in G and efficient operations $\pm$. In real life, even more security considerations need to be addressed. We outline a solution for this challenge, characterized by additional desirable features. This is joint work with Artur Sowa, Francis Bui, Grant Harris, and Jonathan Norton (all based at USASK).

MASAHIRO HORI, University of Saskatchewan and quanTA, Tokyo University of Science
Multifractal and hyperuniform analysis of quasicrystalline patterns in bosonic systems with and without disorder

The multifractal and hyperuniform analyses are two of the methods to quantify the properties of a nonuniform spatial pattern. Most of nonuniform spatial patterns are either multifractal or hyperuniform. The vertices of random systems are multifractal, while those of all crystals and most quasicrystals are hyperuniform. A quasicrystal can be obtained as projection of a periodic lattice in higher dimensions called a hypercubic lattice onto lower dimensions. The Ammann-Beenker quasicrystal is an example of a two-dimensional quasicrystal, which is projection of a hypercubic lattice in four dimensions. We investigate the effects of quasiperiodicity on physical quantities by using the multifractal and hyperuniform analyses.

In this study, we consider the physical quantities in the Bose-Hubbard model on the Ammann-Beenker tilings. The system shows Mott insulating phase and superfluid phase. In both of these phases, the distribution of the physical quantities is found to be hyperuniform. Moreover, analyzing the order metric that quantifies the complexity of nonuniform spatial patterns, we find that the Ammann-Beenker tilings show a significantly large order metric at a phase boundary, in stark contrast to periodic square lattices. Our results suggest that hyperuniformity is a useful method to differentiate crystalline and quasicrystalline systems.

Next, we introduce on-site random potentials in our model, leading to a Bose glass phase. Contrary to the Mott insulating and superfluid phases, we find that the Bose glass phase is multifractal. To the best of our knowledge, this is the first report of a phase transition between hyperuniform and multifractal phases.

VICKY HOWSE, University of Saskatchewan
Vortex 'molecules', a hydrodynamic analog for hadrons

Hydrodynamic analogs constitute a rich field with ties to every area of physics – including quantum foundations, via the walking droplet pilot-wave system and the nascent field of hydrodynamic quantum analogs. Vortex 'molecules', theoretical bound states of fractionally-quantized vortices in multi-component Bose-Einstein condensates (BECs), provide a hydrodynamic analog for hadrons in a theory of SU(2) quantum chromodynamics in 2+1 space-time dimensions. Similarly to the walking droplet system, an oscillatory driving field leads to the unique dynamics: when each component of a BEC is a different hyperfine state of the same atom, one can introduce a Rabi (Josephson) coupling between them, allowing for these states with hadron-like properties. In a two-component BEC, a vortex will be attached by a sine-Gordon soliton to either an antivortex in the same component or to a vortex in the other component, creating a 'meson' or 'baryon', respectively, by analogy. When the connecting soliton is stretched to a critical length, it breaks creating a vortex-antivortex pair, demonstrating confinement of the fractionally-quantized vortices similarly to quark confinement in QCD. One can identify topological quantities with quantum numbers, i.e. the total circulation or winding with the baryon number, and the winding of the relative phase between the two components with the color charge. The low-energy effective theory of two-component BECs is an extension of Polyakov's dual photon model in 2+1 dimensions, a model which can be obtained as a low-energy effective theory of an SU(2) gauge field

similar to QCD.

CHRISTOPHER MAHADEO, University of Illinois at Chicago
Quantization in hyperbolic band theory

Recent work by the quanTA center has pioneered the idea of hyperbolic band theory, the mathematical formulation of a new class of quantum materials. In this talk, I will discuss how techniques borrowed from random matrix theory have the potential to produce fascinating results about these materials.

GORDON SARTY, University of Saskatchewan
A Concept for Direct MRI using Diamonds with Nitrogen Vacancies

Magnetic Resonance Imaging (MRI) is currently achieved by preparing a distribution of phases into the magnetization of the object you want to image. An MRI signal point is then the integration of the magnetization from the object. Many of these spatially encoded signal points are required which are then subsequently Fourier transformed into an image. The many measurements required for this process makes the MRI imaging process slow. However, an object with unencoded magnetization produces a magnetization field in the space surrounding it. Using small sensitive magnetometers, made with Diamonds with Nitrogen Vacancies, we could measure that field and infer the distribution of the magnetization in the object we want to image by solving the inverse problem. The inverse problem is generally ill-posed but the severity of that ill-posed-ness might be reduced with an appropriate distribution of the magnetometers. With that design and an appropriate inverse problem based image reconstruction, instantaneous MRI with only one measurement becomes conceivable and we'd have an MRI version of fluoroscopy.

CARLO MARIA SCANDOLO, University of Calgary
Choi-Defined Resource Theories

The resource theories of separable entanglement, non-positive partial transpose entanglement, magic, and imaginarity share an interesting property: an operation is free if and only if its renormalized Choi matrix is a free state. In this talk, I refer to resource theories exhibiting this property as Choi-defined resource theories. I demonstrate how and under what conditions one can construct a Choi-defined resource theory, and I prove that when such a construction is possible, the free operations are all and only the completely resource non-generating operations.

ARTUR SOWA, University of Saskatchewan
Wielding the Dirichlet series to analyse the physics of bosons

I will discuss a new mathematical approach to the physics of an infinite array of boson sites. It crucially relies on the Dirichlet series and harmonic analysis on the group of positive rationals. This framework yields nonlocal coherent states (NCS) for the bosonic Fock space. The NCS enable rigorous calculations for a quantum system with infinitely many degrees of freedom. The research has been conducted in collaboration with Jonas Fransson (Department of Physics and Astronomy, Uppsala University).

KAORI TANAKA, University of Saskatchewan
Gapless topological superconductivity identified by the spectral localiser

Ever since the first discovery of a topological insulator in the integer quantum Hall effect in 1980, topological band theory has played a pivotal role in the discovery and classification of topological insulators, semimetals, and superconductors. Furthermore, recent advances in real-space topological theory has enabled one to calculate local topological markers and identify topological phases in disordered or aperiodic systems such as quasicrystals. However, in metals or other gapless systems, any topological energy eigenstate would be a member of highly degenerate zero-energy eigenstates and thus be mixed strongly with bulk states,

making it impossible to identify topological edge states. In this work, we demonstrate the occurrence of gapless topological superconductivity in Ammann-Beenker quasicrystals. Utilising a recently developed, general theory of gapless topological materials, we show that topological states can be characterised by a local Chern number derived from the system's spectral localiser. We explore topological phase diagrams in terms of the local Chern number and possible interplay of topological edge states and confined states in the bulk.

ALEX ZAGOSKIN, Loughborough Universityy
Pechukas-Yukawa approach to quantum systems with discrete energy spectra

The success of a perturbation theory expansion is determined by the appropriate choice of the zero-order approximation. The Pechukas-Yukawa formalism provides a promising alternative approach to the description of perturbed quantum systems with discrete energy spectra. It implicitly uses the matrix elements of the Hamiltonian in the basis of exact instantaneous eigenstates rather than the eigenstates of the unperturbed Hamiltonian. In this formalism, the evolution of the energy spectrum due to the perturbation is reduced to the classical dynamics of a 1D gas with cubic repulsion (a modified Calogero-Sutherland model). We develop the kinetic theory of this gas (BBGKY chain of equations for the probability distribution functions), which serves at the basis for the equations for the density matrix of the underlying quantum system.