Quantum Optimal Transport and Applications

Palazzone di Cortona, September 1-6, 2024

Schedule

	Monday	Tuesday	Wednesday	Thursday	Friday
9:00-10:30	Giacomo De Palma 1	Manuela Girotti 1	Simone Rademacher 2	Giacomo De Palma 2	Manuela Girotti 3
coffee break					
11:00-12:30	Simone Rademacher 1	Alice Cortinovis	Manuela Girotti 2	Simone Rademacher 3	Giacomo De Palma 3
		Melchior Wirth			
lunch break					
14:00-16:00	Tamás Titkos	Anna Kausamo	Free afternoon	Emanuela Sasso	
	Dániel Virosztek	Julia Liebert		Lorenzo Portinale	
	Chiara Boccato	Paul Ayers		Sonia Mazzucchi	
coffee break					
16:30-18:30	Short talks	Niels Benedikter Open discussion		Damiano Aliverti Open discussion	

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Mini-courses

Mon 2, 9:00-10:30
Thu 5, 9:00-10:30
Fri 6, 11:00-12:30

The quantum Wasserstein distance of order 1
Giacomo De Palma (University of Bologna)

Quantum optimal transport is a rapidly growing field at the intersection of quantum mechanics and optimal transport theory. Optimal transport theory searches for the most efficient way to transport resources from one location to another, and non-commutativity makes the quantum version of the problem extremely challenging. We will focus on the generalisation of the Wasserstein distance of order 1 to qudits and quantum spin systems of [De Palma et al., IEEE Trans. Inf. Theory 67,6627 (2021)], which recovers the Hamming distance for the states of the canonical basis. We will prove the basic properties of the distance and hint at some of its applications in quantum computing and quantum statistical mechanics.

Mon 2, 11:00-12:30
Wed 4, 9:00-10:30
Thu 5, 11:00-12:30

Many-body quantum dynamics
Simone Rademacher (University of Munich)

This mini-course is dedicated to the mathematical analysis of the time evolution of many-body quantum systems given by the solution of the many-body Schrödinger equation. The goal is the mathematical rigorous derivation of effective equations for the N-body time-evolution in the large particle limit. In this course we study one specific physical model: the N-particle mean-field Bose gas, modelling weakly interacting bosons.

Bose gases undergo a peculiar phase transition at extremely low temperatures: a large fraction of the bosons condense into the same quantum state (called Bose-Einstein condensate) and behave like one big quantum wave when performing measurements of observables. This phenomenon was first predicted by Bose and Einstein in 1924, and later observed in experiments by the groups of Cornell, Ketterle and Wieman for which they were awarded with the Nobel prize in 2001.

We study this phenomenon mathematically using probabilistic language: A physical measurement of one-particle operators on the time-evolved N-particle Bose gas can be mathematically described by a random variable with law given by the solution of the corresponding N-particle Schrödinger equation. These random variables are identically distributed, due to the bosons symmetry, and furthermore

correlated, due to the particle's mean-field interactions .
We show that in average these correlated random variables satisfy a weak law of large numbers with limit described by the condensate's behaviour, that is the Hartree dynamics. Furthermore, we discuss the mathematical description of quantum fluctuations around the condensate through Bogoliubov theory. We will show that the fluctuations of the random variables around the condensate's behaviour satisfy a central limit theorem, where the variance of the limiting Gaussian is determined through Bogoliubov theory. Moreover, Bogoliubov theory leads to large deviation estimates.
Furthermore, it was recently shown that Bogoliubov theory can also be applied beyond the mean-field regime in the Gross-Pitaevski regime leading to a central limit theorem for singular interacting bosons.

Tue 3, 9:00-11:30
Wed 4, 11:00-12:30
Fri 6, 9:00-10:30

Determinantal Point Processes and Random Matrices in a nutshell
Manuela Girotti (Emory University)

In this course we will be talking about the following two classical models arising from Physics.

- Determinantal point processes: DPP are elegant probabilistic models of repulsion that originally appeared in Quantum Physics, but have been extensively applied also in other branches of Mathematics and Physics, as combinatorics, random matrices, growth models, representation theory, and in the "outside world" (machine learning, finance, wireless networks…). The name is due to the fact that their probability distribution is characterized as a determinant of some given function.

- Random Matrices: Random Matrices are one of those transversal theories which appear in different fields of Mathematics and Physics, providing unexpected links between for example Probability, Number Theory and Integrable Systems. As the name suggests, a random matrix is a matrix M whose entries M_ij are random, according to a given probability measure. Alternatively, we can consider a given set of matrices equipped with a probability distribution, thus the matrix itself is a random variable. We will focus on the following questions:
1. What can we say about the eigenvalues/singular values of a random matrix M? If we have a probability distribution dμ(M) for the matrix, the distribution of its spectrum may depend in a highly nontrivial way on it;
2. How do these (random) eigenvalues/singular values look like if we let the dimension of the matrix M grow to infinity? Surprisingly, for a large collection of matrix models the limiting distribution is deterministic and it doesn't depend on the specific finite-dimension probability measure dμ(M). This aspect is called universality.

Classical results will be presented in details, but part of the lectures will also be dedicated to discussing recent developments and research directions.
Most of the material can be found here: https://mathemanu.github.io/talks.html
Possible supplemental material will be mentioned and distributed in due time.

This series of lectures is supposed to be widely accessible, requiring basic background knowledge on analysis and probability.

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Talks Schedule
Monday, September 2

14:15-14:45

Quantum Wasserstein isometries on the qubit state space
Tamás Titkos (Corvinus University & Renyi Institute)

We describe Wasserstein isometries of the quantum bit state space with respect to distinguished cost operators. We derive a Wigner-type result for the cost operator involving all the Pauli matrices: in this case, the isometry group consists of unitary or anti-unitary conjugations. In the Bloch sphere model, this means that the isometry group coincides with the classical symmetry group O(3). On the other hand, for the cost generated by the qubit "clock" and "shift" operators, we discovered non-surjective and non-injective isometries as well, beyond the regular ones. This phenomenon mirrors certain surprising properties of the quantum Wasserstein distance.
Joint work with Gy.P. Gehér, J. Pitrik, and D. Virosztek

14:50-15:20

On the metric property of quantum 2-Wasserstein divergences
Dániel Virosztek (HUN-REN Alfréd Rényi Institute of Mathematics)

Although the theory of classical optimal transport has been playing an important role in mathematical physics (especially in fluid dynamics) and probability since the late 80s, concepts of optimal transportation in quantum mechanics have emerged only very recently.
Quantum Wasserstein divergences are modified versions of quantum Wasserstein distances defined by channels, and they are conjectured to be genuine metrics on quantum state spaces by De Palma and Trevisan.
I will present some aspects of our recent results [*] regarding this conjecture. In particular, I will outline the analytical proof of the triangle inequality for quantum Wasserstein divergences for every quantum system described by a separable Hilbert space and any quadratic cost operator under the assumption that a particular state involved is pure and all the states have finite energy. Joint work with Gergely Bunth, József Pitrik, and Tamás Titkos.

[*] G. Bunth, J. Pitrik, T. Titkos, D. Virosztek. On the metric property of quantum Wasserstein divergences. Physical Review A (2024), in press, arXiv:2402.13150.

15:25-15:55

Correlation energy in many-body bosonic systems.
Chiara Boccato (Università di Pisa)

We consider quantum systems composed of a very large number of particles with totally symmetric wavefunction. Below a critical temperature, a phase transition to a Bose-Einstein condensate is expected to occur, and collective behavior emerges from the underlying many-body theory.

At zero temperature we have precise information on the spectrum of the many-body Hamilton operator (at least in certain scaling limits). However, much less is known close to the transition temperature. In this talk I will discuss how thermal excitations can be described beyond Bogoliubov theory, to obtain an estimate of the free energy of the Bose gas in the Gross-Pitaevskii regime.

Workshop Quantum Optimal Transport and Applications

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Short talks Schedule
Monday 16:30-18:30

16:30-16:39
Gaussian Quantum Markov Semigroups
Damiano Poletti (Università di Genova)

16:40-16:49
Mixed states on quantum devices
Stijn De Baerdemacker (UNB, Canada)

16:50-16:59
On quantum Wasserstein distance based on an optimization over separable couplings
József Pitrik (Budapest University of Technology)

17:00-17:09 - Short break I

17:10-17:19
Quantum Optimal Transport with general convex regularization
Nataliia Monina (University of Ottawa)

17:20-17:29
TBA
Andrea Basteri (INRIA)

17:30-17:39
Rate of convergence of a quantum neural network towards its Gaussian limit
Anderson Melchor Hernandez (Università di Bologna)

17:40-17:49 - Short break II

17:50-17:59
Mathematical aspects of 1-electron Reduced Density Matrix Functional Theory
Pavlo Pelikh (University of Ottawa)

18:00-18:09
1-electron Reduced Density Matrix Theory: An Optimal Transport Approach
Rik Chuiko (McMaster University)

18:00-18:09
Quantum Optimal Transport for Gaussian states
Fanch Coudreuse (Université Claude Bernard Lyon 1)

Quantum Optimal Transport and Applications

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Talks Schedule
Tuesday, September 3

11:15-11:45

On the approximation of the trace of matrix functions
Alice Cortinovis (Stanford University)

In this talk, we consider the problem of numerically computing the trace of a matrix function f(A), such as the logarithm, the entropy, or the exponential. We describe the Hutchinson trace estimator, which is a randomized algorithm that computes an approximation based on quadratic forms involving f(A) and random vectors. We provide concentration bounds for this estimator and discuss variance reduction techniques. We also show how quadratic forms involving f(A) can be approximated using Krylov subspace methods.

11:50-12:20

Gradient Flow Approach to Logarithmic Sobolev Inequalities for Quantum Markov Semigroups
Melchior Wirth (IST, Austria)

For the heat flow on Riemannian manifolds, there are several formulations of the logarithmic Sobolev inequality, which are equivalent as a consequence of the chain rule. If one considers the heat flow on discrete graphs or more generally quantum Markov semigroups (QMS), this equivalence breaks down and one gets the stronger logarithmic Sobolev inequality (LSI) and the weak modified logarithmic Sobolev inequality (MLSI).

Carlen and Maas developed a gradient flow approach using a noncommutative transport metric on the space of density matrices so that MLSI can be deduced from geodesic convexity properties. A key property of the MLSI for this approach is that the right side is the negative derivative of the left side along the QMS. In this talk I will show that the right side of the LSI can similarly be written as minus the derivative of the left side along a non-linear flow and that this non-linear flow can also be written as a gradient flow of the relative entropy for a modified noncommutative transport distance. Moreover, I will present a gradient estimate formulation of the corresponding geodesic convexity property that implies the LSI.

14:15-14:45

The optimality of cyclically monotone plans in optimal L_infty transport
Anna Kausamo (University of Florence)

c-cyclical monotonicity is the most important optimality condition of a transport plan. In this talk I will present a Gamma-convergence-based strategy, developed by myself and Luigi De Pascale, to prove the sufficiency of cyclical monotonicity for optimality in the multi-marginal L^infty-optimal transport case that had previously been elusive.

14:50-15:20

Ensemble density matrix functional theory for excited states
Julia Liebert (LMU Munich)

Reduced density matrix theories offer a promising tool to circumvent the exponential scaling of the N-fermion Hilbert space with the system size. Moreover, the treatment of quantum systems with strong correlations is a central challenge in modern quantum chemistry and condensed matter physics. In this talk, we therefore focus on one-particle reduced density matrix functional theory (RDMFT) as it is conceptually well-suited to describe strongly correlated many-particle systems. To go beyond ground state calculations, we first introduce a so-called w-ensemble RDMFT that allows to target ensembles of low-lying excited states with fixed spectrum w variationally. Various obstacles which historically have doomed such an approach to be unfeasible are circumvented. In particular, we employ elegant tools from convex analysis to solve the underlying N-representability problem. Remarkably, this reveals that crucial information about the excitation structure of molecular systems is contained in the functional's domain. Moreover, a generalization of Pauli's famous exclusion principle for mixed states follows.

To initiate the common process of developing more and more accurate and sophisticated functionals, we provide the theoretical foundations for an ensemble Hartree-Fock theory for excited states by extending Lieb's variational principle to w-ensembles. To introduce a systematic approach, we propose and work out a list of three essential properties any underlying Hartree-Fock functional has to satisfy. By exploiting the one-to-one correspondence between free states and one-particle reduced density matrices through an extension to classical mixtures of free states, we finally succeed in systematically deriving a functional satisfying all three properties.

15:25-15:55

Quantum Optimal Transport for Reduced Density Matrices
Paul Ayers (McMaster University)

We demonstrate how the exact reduced density matrix functional can be expressed as a (regularized) quantum optimal transport problem. This provides a mathematical framework and computational platform for exploration of the exact functional and its derivative. Our approach is practical even for strongly-correlated electrons (where density-matrix functional theory may be expected to surpass density functional theory) and can be applied to molecules larger than those considered by analogous density-functional problems.

16:30-17:00

Bosonization of Large Systems of Interacting Fermions
Niels Benedikter (Università degli Studi di Milano)

The behavior of electrons in a metal presents a wide variety of emergent behavior including a number of phase transitions. The mean-field scaling limit acts as a simplified model capturing part of this complexity. In this limit, results going beyond the precision of Hartree-Fock theory have recently been obtained by bosonization methods. I will review the expansion of the ground state energy and present results extending to the dynamics and momentum distribution of excitations

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Talks Schedule
Thursday, September 5

14:15-14:45

The role of the decoherence-free subalgebra in the study of Quantum Markov Semigroups
Emanuela Sasso (Università di Genova)

In this talk we want to explain the role of the structure of the Decoherence free-subalgebra N(T) for a uniformly continuous Quantum Markov Semigroup (QMS). We introduce the particular and "rich" case in which N(T) is atomic. showing that, for a QMS with a faithful normal invariant state, the atomicity of N(T) and environmental decoherence are equivalent.
Loosely speaking one can say that, for QMSs with a faithful invariant state, the same conclusions can be drawn replacing finite dimensionality of the system Hilbert space by atomicity of the decoherence-free sub algebra. Moreover, the block structure of an atomic N(T) induces the same block structure for many objects related to the QMS, as the invariant states, the reversible states, basins of attraction and set of fixed point. Finally we will say what results are also true whenever N(T) is not atomic.

14:50-15:20

Unbalanced quantum optimal transport with convex regularisations
Lorenzo Portinale (University of Bonn)

We study both the balanced and the unbalanced quantum optimal transport problem in their static, finite dimensional formulations. We discuss duality results, characterisations for optimisers, and limit behaviors for the marginal trade-off parameter going to $+\infty$, i.e. convergence results from unbalanced to balanced. An important tool we define and analyse is a noncommutative version of the classical (c, ε)-transforms associated with a general convex regularization.

15:25-15:55

Mathematical definition of Feynman Path Integrals: new results and open problems.
Sonia Mazzucchi (Università di Trento)

Since their introduction in the early 40s, Feynman path integrals have always been a pow-erful tool for theoretical physics on the one hand and a mathematical challenge on the other. Despite decades of effort, a definitive mathematical theory of Feynman path integration is still missing and, while some steps have been taken in this direction, there are fundamental issues that still deserve further investigation. In this talk I shall give an overview of this topic with a historical perspective, highlighting recent developments and some open problems.

16:30-17:00

What is entanglement among identical particles?
Damiano Aliverti-Piuri (LMU)

Entanglement is one of the most fascinating features of quantum physics, and it represents a key resource for the realization of quantum information processing tasks. While its foundations are well-established in the context of distinguishable particles, the concept of entanglement in identical particle systems is still subject to controversial views. In this talk we propose a possible explanation of this controversy: we prove that the algebra of observables of a single particle cannot be embedded as a subalgebra of the algebra of N identical particles in any meaningful way. This result means that single particles do not define proper quantum subsystems of a system of N identical ones. This suggests that there cannot exist a notion of entanglement or other correlation types among identical particles. We conclude that valid notions of 'electron correlation' can be defined only ad hoc, e.g., by referring to the deviation of a quantum state from the manifold of mean-field states.