Workshop I: Optimal Transport for Density Operators: Theory and Numerics

Monday March 31, 2025

8:00 *Moderator - Tryphon Georgiou*

8:00–8:55 *Check-in/Breakfast (hosted by IPAM)*

8:55–9:00 *Welcome and Opening Remarks*

9:00–9:50 **Shmuel Friedland** (University of Illinois at Chicago)
On Quantum Optimal Transport

10:00–10:15 *Break*

10:15–11:05 **Daniel Stilck Franca** (University of Copenhagen)
Optimal quantum algorithm for Gibbs state preparation

11:15–11:30 *Break*

11:30–12:20 **Lorenzo Portinale** (University of Bonn)
Entropic quantum optimal transport and Pauli exclusion principle

12:30–2:30 *Lunch (on your own)*

2:30 *Moderator - Dario Trevisan*

2:30–3:20 **Nataliia Monina** (University of Ottawa)
Quantum Optimal Transport with Convex Regularization

3:30–4:00 *Break*

4:00–4:50 **Eugene De Prince** (Florida State University)
Lower Bounds in Quantum Chemistry

5:00–6:30 *Reception (Location: IPAM Lobby)*

Tuesday April 1, 2025

8:00 *Moderator - Kasia Pernal*

8:00–8:55 *Check-in/Breakfast (hosted by IPAM)*

9:00–9:50 **Paul Ayers** (McMaster University)
A Quantum Optimal Transport Approach to the (Exact) 1-Electron Density-Matrix Functional

10:00–10:15 *Break*

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10:15–11:05 **Julia Liebert** (Ludwig-Maximilians-Universität München)
Ensemble density matrix functional theory for excited states

11:15–11:30 *Break*

11:30–12:20 **Sarina Sutter** (Vrije Universiteit)
Reduced Density Matrix Functional Theory for the Canonical Ensemble in Finite Basis Set

12:30–2:30 *Lunch (on your own)*

2:30 *Moderator - Eugene De Prince*

2:30–3:20 **Michele Pavanello** (Rutgers University-Newark)
Learning functional theories of the 1- and 2-electron reduced density matrices

3:30–4:00 *Break*

4:00–4:50 **Nick Rubin** (Google Inc.)
The sum-of-squares hierarchy and faster quantum simulation by spectrum amplification

Wednesday April 2, 2025

8:00 *Moderator - Lorenzo Portinale*

8:00–8:55 *Check-in/Breakfast (hosted by IPAM)*

9:00–9:50 **Tryphon Georgiou** (University of California, Irvine (UCI))
Sub-Riemannian geometry of Optimal Transport: mostly classical and a bit of quantum

10:00–10:15 *Break*

10:15–11:05 **Emily Beatty** (École Normale Supérieure de Lyon)
Order p quantum Wasserstein distances from couplings

11:15–11:30 *Break*

11:30–12:20 **Marvin Randig** (Leipzig University)
Dual Block Gradient Ascent for Entropically Regularised Quantum Optimal Transport

12:20–12:30 *Group Photo*

12:30–2:30 *Lunch (on your own)*

2:30 *Moderator - Stijn De Baerdemacker*

2:30–3:20 **Bobak Toussi Kiani** (Harvard University)
Slow Mixing of Quantum Gibbs Samplers

3:30–4:00 *Break*

4:00–4:50 *Lightning Talks - Valerii Chuiko, Peixue Wu and Jannis Erhard*

Thursday April 3, 2025

8:00	*Moderator - Shmuel Friedland*
8:00–8:55	*Check-in/Breakfast (hosted by IPAM)*
9:00–9:50	**Rafael Oliveira** (University of Waterloo) *Scaling problems and entropic optimal transport*
10:00–10:15	*Break*
10:15–11:05	**Stijn De Baerdemacker** (University of New Brunswick) *Real-space quantum chemistry on quantum devices*
11:15–11:30	*Break*
11:30–12:20	**Alice Cortinovis** (Stanford University) *Numerical approximation of traces of matrix functions*
12:30–2:30	*Lunch (on your own)*
2:30	*Moderator - Julia Liebert*
2:30–3:20	**Andreas Deuchert** (Virginia Polytechnic Institute and State University) *The Gibbs state of the mean-field Bose gas*
3:30–4:00	*Break*
4:00–4:50	**Simone Rademacher** (Ludwig-Maximilians-Universität München) *Large deviations for Bose-Einstein condensates*

Friday April 4, 2025

8:00	*Moderator - Paul Ayers*
8:00–8:55	*Check-in/Breakfast (hosted by IPAM)*
9:00–9:50	**Peter Knowles** (Cardiff University) *How far can we go with single-configuration quantum chemistry?*
10:00–10:15	*Break*
10:15–11:05	**Eberhard Gross** (The Hebrew University of Jerusalem) *Exact factorization of the many-particle wave function*
11:15–11:30	*Break*
11:30–12:20	**Milad Marvian** (University of New Mexico) *The Quantum Wasserstein Distance of Order 1 and Its Applications*

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