

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

