Numerical Analysis for Quantum Optimal Transport

Scientific Context: The *static* (Kantorovich) formulation is a semidefinite program for a cost operator C on $\mathcal{H} \otimes \mathcal{H}$,

$$T^C(\rho, \sigma) = \inf\big\{\mathrm{Tr}[C\pi] \ : \ \pi \in \mathcal{D}(\mathcal{H} \otimes \mathcal{H}),\ \mathrm{Tr}_2\, \pi = \rho,\ \mathrm{Tr}_1\, \pi = \sigma\big\},$$

while the *dynamic* (Benamou–Brenier) formulation is built on a Lindbladian $\mathcal{L}$ with detailed balance and derivations $\partial_j A = [V_j, A]$,

$$W_2^{\mathcal{L}}(\rho, \sigma)^2 = \inf \int_0^1 \sum_j \big\langle \partial_j U_t, [\rho_t]_{\omega_j} \partial_j U_t \big\rangle \, dt \quad \text{s.t.} \quad \dot\rho_t + \mathrm{div}\big([\rho_t]_\omega \nabla U_t\big) = 0,$$

with $\rho_0 = \rho$, $\rho_1 = \sigma$. Each formulation sacrifices a classical property (triangle inequality, faithfulness, or flexibility of the underlying geometry), and no two-sided bounds $c\, W_a \le W_b \le C\, W_a$ between them are known. Existing algorithms were mainly designed as proofs of concept. To push QOT towards physical applications, one must understand how discretization, perturbation and choice of basis affect its solutions. A rigorous numerical analysis is largely lacking.

Objective: The project aims at a rigorous understanding of the approximation properties of existing QOT formulations and at their systematic comparison. Possible tasks include:

- **Numerical framework** For competitive experiments, validated on cases with known answers: commuting states (classical W_p), Gaussian states, and qubits.
- **Basis truncation.** For a Galerkin space $V_n \subset \mathcal{H}$ with projector P_n and $\rho_n = P_n \rho P_n / \mathrm{Tr}[P_n \rho]$, derive a priori bounds $|W(\rho_n, \sigma_n) - W(\rho, \sigma)| \le C\, \eta_n(\rho, \sigma)$ in terms of best-approximation errors, including consistency of the truncated cost $C_n = (P_n \otimes P_n)\, C\, (P_n \otimes P_n)$.
- **Stability.** Establish moduli of continuity $|W(\rho + \delta\rho, \sigma) - W(\rho, \sigma)| \le \omega(\|\delta\rho\|_1)$, and analyze rank-deficient states through $\rho_\delta = (1 - \delta)\rho + \delta\, \mathbb{1}/d$ as $\delta \to 0$.
- **Algorithms.** Prove convergence of time-discretized dynamical schemes (K time steps, $K \to \infty$) and quantify the bias of entropic regularization $T_\varepsilon = \inf_\pi \mathrm{Tr}[C\pi] - \varepsilon S(\pi)$, which satisfies $T - 2\varepsilon \log d \le T_\varepsilon \le T$ and hence couples ε to the basis size $d = \dim V_n$.
- **Quantum chemistry.** Transport one-body reduced density matrices γ ($0 \le \gamma \le 1$, $\mathrm{Tr}\,\gamma = N$) between ground states at nuclear geometries R_0, R_1, and assess the interpolant γ_t by the energy error $E_{R_t}(\gamma_t) - E_0(R_t)$ across Hartree–Fock, Kohn–Sham and FCI models in Gaussian or plane-wave bases.

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Candidate Profile: Applied mathematics. Expertise in Optimal Transport and spectral theory would be preferable.

References.

1. E. Beatty, *Wasserstein distances on quantum structures: an overview*, Rev. Math. Phys. (2026), 2630003.

2. G. Dusson, V. Ehrlacher, E. Obermeyer, *An algorithm for dynamical quantum optimal transport with applications to quantum chemistry*, arXiv:2606.10075 (2026).

3. J. Maas et al. (eds.), *Optimal Transport on Quantum Structures*, Springer, 2024.