PhD subject: Quantum Optimal Transport for Quantum Chemistry Calculations

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Quantum chemistry simulations aim at predicting physical properties of molecular and materials systems such as the potential energy, spatial conformation, response properties. They are numerically very demanding and represent a large part of the use of supercomputers (around 35% [8]). Indeed, due to the small size of the considered systems, quantum models (e.g. Density Functional Theory, Hartree-Fock, arising as simplified models of the Schrödinger equation) modelling the electronic structure of the systems must be used to obtain accurate predictions of such physical quantities. Mathematically speaking, these models are nonlinear and eigenvalue partial differential equations. Reducing the computational cost of such simulations is therefore key to reduce the footprint of such calculations, and/or increase the size of the simulated quantum systems.

Recently, optimal transport [4], which allows to compare probability densities, has gained a lot of attention, and has been used in many applications, such as color transfer or texture synthesis in vision [3], financial products valuation, as well as rapid calculation of approximate solutions of partial differential equations [2]. Unfortunately, methods based on optimal transport cannot directly be used in the context of quantum chemistry, as the solutions to the corresponding equations are not probability distributions but density matrices (self-adjoint, trace-class operators).

In this PhD, the goal will be to focus on a recent extension of optimal transport called Quantum Optimal Transport [1] (QOT), and which aims at generalizing optimal transport for density matrices. Interestingly, density matrices also appear in the context of quantum computing as e.g. qbits are density matrices. Potential applications of QOT also include using QOT for solving combinatorial optimization problem in a quantum way (quantum annealing [6]), quantum channels and distances on multiqbits systems [5].

The first objective will be to develop and study, from a mathematical and numerical point of view, quantum Wasserstein barycenters, in the sense of QOT, e.g. extending the traditional notion of Wasserstein barycenters in the context of optimal transport between probability measures as introduced in the seminal paper [9]. Indeed, such barycenters should be used in principle to interpolate self-adjoint trace-class operators in a Wasserstein sense, such as qbits or multiqbits systems (in the finite-dimensional case) or density matrices as appearing in quantum chemistry (infinite-dimensional case).

The second objective of this PhD is to propose novel numerical methods for constructing new reduced-order models in order to accelerate parametrized electronic structure calculations. In particular, we would like to focus on reduced-order modeling techniques in order to efficiently compute approximations of the density matrix in parameter-dependent electronic structure calculations.

To summarize, the objectives of this PhD will be to

- study from a mathematical point of view the properties of quantum Wasserstein barycenters;
- design efficient numerical methods in order to compute them;
- use these objects to build efficient reduced-order models for the computation of the density matrix of parameter-dependent electronic structure calculation problems in quantum chemistry, in the spirit of the method proposed in [10] for the computation of the electronic density.

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