M2 subject "Neural networks for the approximation of the Lieb functional in quantum chemistry"

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The aim of this M2 internship will be to develop new numerical methods in order to approximate the so-called Lieb functional, which is a key quantity in Density Functional Theory for electronic structure calculations for molecules. The Lieb functional was actually shown by Lieb to be a convexification of the so-called Lévy-Lieb functional. Given an electronic density for a system of N electrons, which may be seen as a probability density on $\mathbb{R}^3$, the value of the Lieb functional for this density is defined as the solution of a quantum multi-marginal optimal transport problem, which reads as a minimization problem defined on the set of trace-class operators acting on the space of electronic wave-functions that are anti-symmetric L^2 functions of $\mathbb{R}^{3N}$, with partial trace equal to the prescribed electronic density. Recently, a relaxation of this quantum optimal transport problem has been introduced in [EN23] where the full partial trace constraint is replaced by a finite number of moment constraints on the partial trace of the set of operators. It is then shown that, under mild assumptions on the electronic density, there exist sparse minimizers to the resulting moment constrained approximation of the Lieb (MCAL) functional that read as operators with rank at most equal to the number of moment constraints. A numerical algorithm has also been recently developed in order to compute the solution of this relaxed problem. However, the algorithm currently requires the resolution of many-body Schrödinger problems, which read as high-dimensional eigenvalue problems when the number of electrons in the system is large. As a consequence, the approach is currently impossible to carry out for the moment for realistic systems. The aim of the M2 internship is to propose new numerical approaches in order to alleviate this difficulty and we propose to use Physically Informed Neural Networks (PINNs) [PSMF20] to circumvent the curse of dimensionality and efficiently solve the underlying high-dimensional eigenvalue problems. More precisely, we aim at studying the following questions:

- analyze from a mathematical point of view some PINN method for the resolution of eigenvalue problems. One first possible track in this direction could be to analyze the Wasserstein gradient flow in the space of probability measures on the set of neural network parameters to understand PINN approaches with infinite width two-layer neural networks. That is, given a solution to the eigenvalue problem we would like to understand how good is the approximation with the PINN method.
- use an appropriate PINN method for the resolution of high-dimensional eigenvalue problems in order to compute approximations of multi-marginal quantum optimal problem.

The M2 intern will be based at LMO (Laboratoire de mathématiques d'Orsay), Paris-Saclay university and will be supervised by V. Ehrlacher (Cermics, ENPC) and L. Nenna (LMO). Moreover, he/she will benefit of the high quality scientific environment of LMO and interact with the members of the PaRma Inria team, devoted to Optimal Transport, based at LMO as well as the Matherials at Inria Paris and the members of the ANR GOTA project members.
Please send a CV and transcripts.

References

[EN23] Virginie Ehrlacher and Luca Nenna. A sparse approximation of the Lieb functional with moment constraints. *arXiv preprint arXiv:2306.00806*, 2023.

[PSMF20] David Pfau, James S Spencer, Alexander GDG Matthews, and W Matthew C Foulkes. Ab initio solution of the many-electron Schrödinger equation with deep neural networks. *Physical Review Research*, 2(3):033429, 2020.