Optimal Transport Methods in Density Functional Theory

Mathieu Lewin (CNRS and Université Paris Dauphine) ,
Paola Gori-Giorgi (Vrije Universiteit Amsterdam),
Brendan Pass (University of Alberta)

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1 What is Density Functional Theory?

1.1 An approximation of Schrödinger's first eigenvalue

Quantum mechanics is a very impressive theory, developed in the beginning of the XX century to describe the microscopic world. One of its most important achievements is the Schrödinger equation, which allows, in principle, to predict properties of materials and chemical compounds, including the outcome of chemical reactions. Central to computational chemistry, solid state physics and materials science is the lowest eigenvalue E_0 (a.k.a. ground-state energy) of the N-electron hamiltonian H_{el} for given positions X_i of the M nuclei with charges Z_i (Born-Oppenheimer approximation),

$$H_{el} = \underbrace{-\frac{\hbar^2}{2}\sum_{i=1}^{N}\Delta_{x_i}}_{=\hbar^2\, T} + \underbrace{\sum_{1\leq i<j\leq N}\frac{1}{|x_i-x_j|}}_{=V_{ee}} + \sum_{i=1}^{N} v(x_i), \qquad v(x) = -\sum_{\alpha=1}^{M}\frac{Z_\alpha}{|x-X_\alpha|}, \tag{1}$$

with $x_i, X_i \in \mathbb{R}^3$ and

$$E_0 = \inf_{\Psi\in\mathcal{A}_N}\langle\Psi, H_{el}\Psi\rangle, \qquad \mathcal{A}_N = \left\{\Psi\in H^1((\mathbb{R}^3\times\{\uparrow,\downarrow\})^N;\mathbb{C}) \;:\; \Psi \text{ antisymmetric},\; ||\Psi||_{L^2}=1\right\}. \tag{2}$$

Unfortunately, the apparent simplicity of Eq. (1) is an illusion. Even if this one-line operator is believed to describe the richness of the microscopic world, it has no known analytical eigenvalue for more than one electron and one nucleus, and the numerical cost involved to compute approximate solutions for realistic materials and chemical compounds grows extremely fast with the number of particles in the system. Physicists and chemists are obliged to turn to approximations, relying partly on empirical considerations.

Density functional theory (DFT), by virtue of its excellent compromise between computational efficiency and accuracy, is the method of choice for the electronic structure calculations in computational chemistry and solid-state physics. Invented in the early days of quantum mechanics, DFT uses the one-electron density $\rho(x)$ (marginal) as key variable,

$$\rho(x) = N\sum_{s_1,\cdots,s_N\in\{\uparrow,\downarrow\}}\int_{\mathbb{R}^{3(N-1)}}|\Psi(x,s_1,x_2,s_2,\cdots,x_N,s_N)|^2 dx_2\cdots dx_N, \tag{3}$$

to rewrite the infimum in Eq. (2) as

$$E_0 = \inf_{\rho \in \mathcal{R}_N} \left\{ F_\hbar^{\mathrm{LL}}[\rho] + \int_{\mathbb{R}^3} v(x)\rho(x)dx \right\}, \tag{4}$$

with the set of N-representable densities

$$\mathcal{R}_N = \left\{ \rho \geq 0,\ \int_{\mathbb{R}^3} \rho = N,\ \sqrt{\rho} \in H^1(\mathbb{R}^3) \right\},$$

and where the (universal) Levy-Lieb universal functional $F_\hbar^{\mathrm{LL}}[\rho]$ is defined as

$$F_\hbar^{\mathrm{LL}}[\rho] = \inf_{\substack{\Psi \in \mathcal{A}_N \\ \rho_\Psi = \rho}} \left\langle \Psi, (\hbar^2\, T + V_{ee})\Psi \right\rangle. \tag{5}$$

DFT only became popular in the 70's in solid-state physics thanks to the Kohn-Sham (KS) formalism, in which the functional $F_\hbar^{\mathrm{LL}}[\rho]$ is decomposed as

$$F_\hbar^{\mathrm{LL}}[\rho] = \hbar^2 T_s[\rho] + U[\rho] + E_{xc}[\rho]$$

where

$$U[\rho] = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} dxdy$$

is the classical Coulomb energy of the density ρ and

$$T_s[\rho] = \min \left\{ \frac{1}{2} \sum_{i=1}^N \int_{\mathbb{R}^3} |\nabla \phi_i|^2 \ :\ \sum_{i=1}^N |\phi_i|^2 = \rho,\ \langle \phi_i, \phi_j \rangle = \delta_{ij},\ \phi_i \in H^1(\mathbb{R}^3 \times \{\uparrow, \downarrow\}) \right\},$$

is the lowest kinetic energy that can be achieved with N independent electrons having the prescribed density ρ. Since $T_s[\rho]$ is a somewhat better understood functional, in this form only the exchange-correlation functional $E_{xc}[\rho]$ needs to be approximated. The mother of all models for $E_{xc}[\rho]$ is the so-called Local Density Approximation (LDA) where the exchange-correlation energy is taken to be the average over all $x \in \mathbb{R}^3$ of the lowest energy per unit volume $e_{\mathrm{xc}}^{\mathrm{HEG}}\big(\rho(x)\big)$ of an infinite electron gas having the constant density $\rho(x)$ at this point $x \in \mathbb{R}^3$:

$$E_{xc}[\rho] \simeq \int_{\mathbb{R}^3} e_{\mathrm{xc}}^{\mathrm{HEG}}\big[\rho(x)\big]\, dx. \tag{6}$$

For a general mathematical presentation of DFT, we refer for instance to [34, 5].

Kohn-Sham DFT became very popular in the 90's in chemistry with the introduction of empirical approximations for $E_{xc}[\rho]$ beyond the local-density approximation (6). One central idea is to introduce gradient corrections, taking into account the fact that ρ is indeed not constant locally. But other improvements have played an important role, like for hybrids models using a bit of the exact exchange energy in Hartree-Fock theory.

Despite its enormous success, the predictive power of Kohn-Sham DFT is still hampered by inadequate approximations for near-degenerate and strongly-correlated systems. Crucial examples are transition metal complexes (key for catalysis), stretched chemical bonds (key to predict chemical reactions), technologically advanced functional materials, and man-made nanostructures.

On the other hand, DFT is a source of difficult mathematical problems, whose resolution requires top-level mathematical research. This research, in turn, has the potential to influence real applications in Chemistry and Physics.

1.2 The use of Optimal Transport methods in DFT

The purpose of the BIRS workshop held in January 2019 was to bring together physicists, chemists and applied mathematicians working on the **use of Optimal Transport (OT) methods in DFT**. This very fruitful line of research has emerged very recently and a new community is currently exploring its ability to improve our understanding of correlations in Coulomb systems [41].

Over the last 30 years, the theory of optimal transportation has grown into a fertile mathematical field. It has many applications, both within and beyond Mathematics, in such diverse fields as economics, meteorology, geometry, statistics, fluid mechanics, design problems and engineering. An overview of this theory can be found in the monograph written by the fields medalist Cédric Villani [45].

It was only realized recently by mathematicians [9, 4, 16, 11] that the central problem of finding the lowest Coulomb energy of N-particle probabilities at given first marginal (a.k.a. the charge density) $\rho(x)$, appearing as the $\hbar \to 0$ limit of $F_\hbar^{\rm LL}[\rho]$,

$$F_{\hbar\to 0}^{\rm LL}[\rho] = V_{ee}^{\rm SCE}[\rho] + O(\hbar), \qquad V_{ee}^{\rm SCE}[\rho] = \inf_{\substack{\Psi\in\mathcal{A}_N \\ \rho_\Psi=\rho}} \langle \Psi, V_{ee}\Psi\rangle \tag{7}$$

is a *multi-marginal optimal transport problem*. The infimum on the right side is always attained if the set of anti-symmetric Ψ's is enlarged to N-particle symmetric probability measures, having the prescribed marginal ρ. Methods in the spirit of optimal transport had however been used before in Physics and Chemistry, in particular in the seminal works of Seidl [40] and his collaborators [43, 42, 22, 39] on the *strictly-correlated electrons* (SCE) model, as well as in the older work of Lieb-Oxford [35] who derived a lower bound on this energy.

In order to address the full complexity of this new field and make significant progress, it seems mandatory to use an interdisciplinary approach. From the point of view of Chemistry and Physics, it is important to have a good knowledge of the mathematical properties of the problem, in order to develop new efficient and reliable approximations. DFT is a quantum theory in which a large part of the quantum effects are well captured by the Kohn-Sham formalism. Its semi-classical (strongly correlated) limit provides new information on the effects that are missed by Kohn-Sham DFT. The understanding of this limit is thus essential to develop approximate functionals that can address strongly-correlated systems. From the point of view of mass transportation theory, the Coulomb problem in DFT poses new challenges which have the potential to impact other applications. The fact that there are N prescribed marginals in the Coulomb DFT problem, contrary to the standard OT case $N = 2$, poses new mathematical difficulties, which have not yet been completely understood.

This BIRS workshop allowed for very fruitful interactions between different communities: chemists and physicsts working on DFT and on the quantum many-body problem, mathematicians from optimal transport, mathematical physics, probability theory, and numerical methods.

The first challenge in this kind of interdisciplinary workshops is to set a common language. For this reason, we had scheduled a series of review/introductory talks from experts of the various disciplines. This was extremely helpful, and was very much appreciated by all the participants. At the end of the workshop we have also organized a round table, where several perspectives or general strategies have been discussed. Overall, the workshop was a real success.

2 Some Highlights and Open Problems

In this section we discuss some important points raised during the workshop, as well as open problems.

Monge or not Monge?

An important question, which has been mentioned several times during the workshop, is to understand when there are Monge-type N-particle minimizers of the Kantorovich multi-marginal optimal transport problem (7). Monge states indeed can be parametrized by much less variables, leading to a dramatic decrease of complexity in practical computations. In addition, Monge states have a clearer physical interpretation in terms of "strictly correlated systems". This is because in a Monge state the positions $x_2, ..., x_N$ of $N-1$ electrons are completely determined by the position x_1 of the remaining electron. The corresponding probability measure is therefore typically supported over a space of very low dimension.

The standard method for establishing the existence of Monge solutions for optimal transport problems, which consists of showing that any Kantorovich solution has Monge structure, fails for multi-marginal problems with repulsive costs. One issue is symmetry; for $N = 3$ or more electrons, there is no mapping

$\mathbb{R}^3 \to \mathbb{R}^{3(N-1)}$ other than the diagonal $x \mapsto (x, x, ..., x)$ (which is clearly not optimal) whose graph is symmetric under all permutations, and so the direct Monge ansatz cannot allow for all solutions. Even allowing for symmetrized Monge states does not capture all solutions, however, as competing interactions can lead to solutions degenerating onto higher dimensional submanifolds. Therefore, existence of (symmetrized) Monge solutions remains a challenging open problem.

In his review talk, Luca Nenna has given several numerical examples taken from [2] where minimizers are Monge or not. No clear intuition of what property of ρ implies the existence of Monge minimizers has emerged yet. On the other hand, Gero Friesecke has proposed in his review talk the concept of *quasi-Monge states* [17] which still imply a big decrease of complexity. Those have been proved to be minimizers in a toy model with discrete marginals but more investigation is required for general marginals.

More generally, it seems important to improve our understanding of the structure, regularity and sparsity properties of optimal plans for multi-marginal transport problems. Results in this direction for certain cost functions include [18, 21, 27, 38, 36], but repulsive costs, including the Coulomb cost arising in DFT, are much more challenging. This was explained at length by Liugi De Pascale in his review talk about the theory of multi-marginal optimal transport.

The challenging semi-classical limit $\hbar \to 0$

The second-order asymptotic in $\hbar$ of the limit in (7) has been predicted in [24]. It is only recently that the first order could be fully justified mathematically [9, 3, 31, 10]. It has been mentioned several times in the workshop that establishing the second-order rigorously is an important open problem. This essentially reduces to a semi-classical limit *at fixed density*, a very original setting which has never been considered in the mathematical literature, to our knowledge.

In the same direction, it has been predicted in [23, 24, 25] that the fermionic nature of the electrons should only affect the $\hbar$ expansion by an exponentially small error. Providing a proof of this fact is a very challenging open problem.

Towards a more solid mathematical foundation of DFT

During his review talk, Éric Cancès has summarized our mathematical knowledge about the foundations of Density Functional Theory. Several important questions remain. This includes for instance the understanding of when the Kohn-Sham nonlinear eigenvalues satisfy the aufbau principle (that is, are the N first eigenvalues of the corresponding mean-field operator). This problem has already been mentioned ten years ago in [6] and no real progress has been made in this direction.

The Hohenberg-Kohn theorem is the main mathematical result in DFT. Until recently, it was however plagued with a missing *unique continuation principle* for many-particle Schrödinger operators. This problem has been solved recently by Louis Garrigue in [19, 20] and announced at the conference, but the assumptions on the potentials are not yet optimal. In addition, the magnetic field case and current density functional theories need to be better understood [28], as was largely discussed by Andre Laestadius in his talk.

Finally, Jonas Lampart has discussed in his talk the difficulties of giving a mathematical basis to time-dependent DFT [15]. It was indeed mentioned several times during the conference that extending the OT limit of DFT to time-dependent problems is an interesting problem. In particular one should focus on understanding exact properties of adiabatic kernels. First results in this direction have already appeared in [29, 8].

Local Density Approximation and the Homogeneous Electron Gas

We have mentioned above in (6) the Local Density Approximation which consists in assuming that ρ is essentially constant locally (in boxes of volume dx) and to replace the local energy per unit volume by that of an infinite gas having the constant density $\rho(x)$ in the whole space. Understanding the regime in which the approximation is valid was the object of several discussions during the workshop. Kieron Burke has mentioned in his review talk several possible regimes in which he thinks that the LDA must be right. In the classical case $\hbar = 0$, a result of this kind was recently proved and reported during the conference [33, 13], for densities rescaled in the manner $\rho(x/N^{1/3})$. Extending these results to the quantum case is an important question.

In Physics and Chemistry, the Homogeneous Electron Gas is always identified with another system, sometimes called *Jellium*, where the density is not assumed to be constant over the whole space, but the electrons are instead submitted to an external positively-charged compensating uniform background. The link between Jellium and the Homogeneous Electron Gas is uncertain mathematically, especially after it was recently remarked that the usual proof does not work [32] for the Coulomb potential. In her talk, Codina Cotar has announced the recent theorem [12] that only the Coulomb potential poses some problems. For any potential in the form $|x|^{-s}$ with $s > 1$, Jellium and the Homogeneous Electron Gas have the same ground state energy in infinite volume. During the round table, Kieron Burke has however insisted on the remark that the values of the densities which matter in real systems are all above the solid-fluid phase transition of Jellium, hence are in the regime where Jellium necessarily coincides with the HEG.

A somewhat related question is to better understand the optimal constants in the Lieb-Oxford inequality [35, 32, 44], which provides exact constraints on the functional $F_\hbar^{\mathrm{LL}}[\rho]$. The optimal constant is sometimes believed to be the low-density limit of the uniform electron gas energy. In his talk, Simone Di Marino has reviewed the situation and started to explain a work in preparation about the 1D case, which can be fully understood using optimal transport methods.

Numerical challenges in Kohn-Sham(-SCE)

In his review talk Jianfeng Lu has introduced the Kohn-Sham density functional theory and he has especially focused on the self-consistent iteration in order to find a fixed point of the Kohn-Sham map. He has also presented the state of the art concerning the development of fast numerical solvers to solve these very high-dimensional problems. Concerning some recent developments which have been presented during the workshop we mention the one by Z. Musslimani [7] who numerically solve KS fixed point equation by mean of a spectral renormalization method and the preconditioning approach by A. Levitt [30].

Numerics for multi-marginal optimal transport

In his review talk Luca Nenna has presented the three main approaches to solve optimal transport problems and then he focused on the entropic regularization of Optimal Transport and the Sinkhorn algorithm [1, 37]. However this kind of approach presents some limitations in the case of multi marginal optimal transport with Coulomb cost since the computational cost increases exponentially in the number of marginal. This problem can be partially avoided by a multi-scale approach as the one introduced in [2]. Another kind of promising approaches (which seems to overcome the computational cost of the number of marginals) has been presented during the session on the numerical method for multi-marginal optimal transport: the one by L. Ying [26] and the one based on an approximation of the OT problem via marginals constraints moment by R. Coyaud [14].

3 Outcome of the Meeting

We expect that the cross-fertilization initiated by bringing together researchers in mathematical physics, optimal transport, physics and chemistry will have a significant impact on the field moving forward, contributing in particular to the resolution of many of the open problems described above. Informal discussion with the participants indicate that one important impact of the workshop will be the integration of the cultures of the various communities involved. We expect in particular that mathematicians, through their discussions with physicists and chemists, will consider problems holding increased physical or chemical relevance.

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