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On some contributions to numerics in quantum mechanics, regularization by noise and minimization of quantum entropies

Romain Duboscq

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Institut de Mathématiques de Toulouse
Université Toulouse III - Paul Sabatier

Habilitation à diriger les recherches

Spécialité: Mathématiques Appliquées

On some contributions to numerics in quantum mechanics, regularization by noise and minimization of quantum entropies

Romain Duboscq

Soutenu le 16 février 2024 devant le jury composé de:

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Introduction

This document aims to gather my research work since the completion of my thesis, which I defended at the end of 2013. During this thesis, I was able to address several themes that have remained dear to me thereafter: stochastic partial differential equations, numerical schemes for computing ground states or simulating nonlinear Schrödinger equations, as well as the development of a scientific computing library. Of course, I have since had the opportunity to expand my research areas, but you will find some works that naturally fit into the continuation of my thesis. On the other hand, throughout my research career, some encounters have turned out to be turning points towards new mathematics and the prelude to fruitful collaborations. This notably explains the emergence of two new themes that are now present in my research: the study of noise-induced regularization phenomena and the problem of quantum entropy minimization under constraints. To better understand the current point of my research, it may be virtuous to trace a (approximate) chronology from my memories and the archaeological data available in my email inbox.

I arrived in Toulouse as an associate professor in 2014. Among the people I knew there, Christophe Besse was probably the one I had the most affinity with, and we immediately worked together on issues related to the numerical simulation of Schrödinger equations. This was mainly done through the co-supervision of two postdocs: Vittorio Rispoli (co-supervised with Xavier Antoine, my thesis advisor), with whom we published an article on accelerating the imaginary time method via the introduction of an inertia term (see Section 1.1), and Juan Pablo Alvarez Zúñiga (co-supervised with David Guéry-Odelin), with whom we published on the quantum system's passage through a region of rotating speeds, potentially making the system unstable but revealing stability in the presence of vortices (see Section 1.3). While wandering in the world of nonlinear Schrödinger equations, I met Stefan Le Coz with whom we started investigating, still with Christophe, the computation of excited states in interacting quantum systems. This work took some time to materialize, due to a fairly long break, but resulted in a recent article where we study, in a radial framework, a method based on Nehari manifolds (see Section 1.1). In the course of 2018, Christophe began to take an interest in quantum graphs and enthused Stefan and me. From there, we undertook numerical simulations on graphs to gain a clearer understanding of the behavior of stationary and dynamic solutions, and possibly to establish new numerical methods. Noticing that the graphs in the literature were very diverse, we gradually made our code more flexible to automate the discretization of the Laplacian on arbitrary graphs. This eventually led to the development of a Python library called GraFiDi. In parallel, we examined the convergence of the imaginary time method for computing ground states on graphs, which led us to publish a result (see Section 1.2). During a conference organized by Nicolas Rougerie in 2015, he and I began discussions about certain quantum systems, and in particular, a topic he was starting to delve into: anyons. Later, I was able to meet two of his co-authors, Michele Correggi and Douglas Lundholm, and we embarked on the study of vortices in anyon systems in a mean-field regime (see Section 1.3). In the first half of 2019, David Guéry-Odelin proposed that I participate in a project on curved waveguides with one of his collaborators, François Impens, and we were able to successfully develop a method for calculating a curvature that significantly improves the propagation of particles (or particle systems) in these guides (see Section 1.3).

When I arrived at the INSA Toulouse, I wanted to continue studying stochastic partial differential equations, especially the case of the nonlinear Schrödinger equation perturbed by noise. I was very intrigued by the result of Debussche-Tsutsumi because, contrary to what I was used to reading, the introduction of a noise in the equation improved the results of the Cauchy problem.

So, I wondered if it was possible to achieve similar results with the formulas on the (random) propagator of the linear part the equation that I had obtained and see if other similar phenomena could manifest themselves. However, due to the structure of the bi-characteristics that are used to build the propagator and given how the stochastic process used (in this case, the Brownian motion) was intertwined with them, it was difficult to see clearly what could be expected. I then stumbled, somewhat by chance, upon articles dealing with the regularization by noise phenomenon, and, more specifically, the Itô-Tanaka trick which is obtained through the resolution of a backward stochastic differential equation. The problem was that, in my case, it was not possible to use this strategy because of the random nature of my propagator. While making progress on these issues, I had shared my advances with Anthony Réveillac, who had been recruited at the same time as me at the INSA Toulouse and who also worked on stochastic processes. One day, he proposed discussing it in front of a whiteboard and it turned out to be the perfect interlocutor since he almost had the solution ready for me: to study the backward stochastic differential equation as a stochastic backward differential equation. While exploring this strategy, we realized that this problem was specifically mentioned in the literature of regularization by noise in stochastic differential equations, and we decided to temporarily set aside the connection with the perturbed Schrödinger equation and its random propagator, to immerse our result in the context of SDEs (with random drift here) (see Section 2.1). Subsequently, using this approach, we attempted to improve the result of Debussche-Tsutsumi, based on a conjecture. Unfortunately, the problem turned out to be difficult, but we were nevertheless able to provide a new approach via a stochastic Hardy-Littlewood-Sobolev inequality (see Section 2.2). During the submission process of our first article, the assigned referee pointed out the existence of an article dealing with regularization by noise in stochastic differential equations driven by an additive fractional Brownian motion (*i.e.*, a non-Markovian process) for which there was no direct generalization of our approach. Intrigued by this type of process that was outside our area of expertise, we contacted Laure Coutin, who explained to us the various possibilities to bypass the lack of stochastic calculus for fractional Brownian motion. In the end, we finally implemented a strategy based on a clever discretization that allowed us to prove a generalization of the Itô-Tanaka trick in the case of a fractional Brownian motion and a random function (see Section 2.1). Meanwhile, in the first half of 2016, we organized a conference in Toulouse on regularization by noise and among the guests was Rémi Catellier. From this meeting, we started discussing the possibilities of using a fractional Brownian motion to regularize functions and, a little later, we began a collaboration and were able to prove that the regularization by noise phenomenon also worked in the context of rough differential equations (see Section 2.3).

In the course of the year 2014, I had the opportunity to cross paths with Olivier Pinaud. The following year, he invited me to participate in a mini-symposium he was organizing at the SMAI conference. Under an unassuming appearance, this was going to be the beginning of a very long and highly fruitful collaboration. I had always had a certain fondness for quantum mechanics, but until then, I hadn't had the opportunity to engage in mathematical analysis of quantum systems. Olivier opened for me the door into the world of trace-class operators, and thanks to his knowledge and enthusiasm, I was able to pick up where he had previously left off in his work on quantum entropy minimization. The first question we tackled was to determine if it was possible to prove the existence (and uniqueness) of a minimizer for the Boltzmann quantum entropy when three local constraints are fixed: the density, current, and energy. The main issue here is that the operators that we consider belong in a space that allows to bound the L^1 norm of these three moments but no more than that. In practice, we face a lack of compactness to deduce that the minimizing sequence converges to an operator in the space of constraints, meaning that we can not directly prove that the limiting operator satisfies the local energy constraint (we have sufficient compactness to obtain the first two moments). Nevertheless, it turns out that we do have weak convergence, and therefore, we must essentially demonstrate that the global energy (the integral of the local energy) is indeed

equal to that obtained in the constraint space. If we think of this global energy as the system's temperature, thermodynamics dictates a relation between this temperature and the system's entropy. This physical argument is confirmed, as we can show that there exists a monotonic relationship between the quantum entropy and the global energy. From there, we can prove that the global energy will be different from that of the constraint space if and only if the same holds for the entropy. An argument by contradiction based on inequalities regarding the global energy and the entropy of the limiting operator then allows us to deduce that the global energy is correct (see Section 3.3). This result was subsequently accompanied by a characterization of the minimizer. For this, the main difficulty lies in obtaining an Euler-Lagrange equation corresponding to the first-order optimality condition. To do so, one must differentiate the quantum entropy in the constraint space, meaning one must be able to identify perturbations rich enough to fully identify the minimizer after the differentiation. The idea to find these perturbations is to determine operators that will be multiplied on the right and left of the minimizer (to preserve its self-adjointness) and that will modify its density, current, and energy in a simple but sufficient way for proper differentiation (see Section 3.4). The existence and uniqueness of the minimizer and its characterization were subsequently extended to other cases. Notably, the many body case, where the compactness problem for the existence of a minimizer arises both for density and energy (see Section 3.5).

Publications list

The publications with a \star are not discussed in this document.

- ★[AD1] Xavier Antoine and R. D. : [Robust and Efficient Preconditioned Krylov Spectral Solvers for Computing the Ground States of Fast Rotating and Strongly Interacting Bose-Einstein Condensates](#). In: *Journal of Computational Physics*, 258C:509–523 (2014).
- ★[AD2] Xavier Antoine and R. D. : [GPELab, a Matlab Toolbox to Solve Gross-Pitaevskii Equations I: Computation of Stationary Solutions](#). In: *Computer Physics Communications*, 185 (11) (2014) pp. 2969–2991.
- ★[AD3] Xavier Antoine and R. D. : [GPELab, a Matlab Toolbox to Solve Gross-Pitaevskii Equations II: Dynamics, Stochastic Simulations](#). In: *Computer Physics Communications*, 193 (2015) pp. 95–117.
- ★[PDNK] Bikash Padhi, R. D., Ankita Niranjana and Ravi K. Soni : [Vortex dynamics of rotating Bose-Einstein condensate of microcavity polaritons](#). In: *The European Physical Journal B*, 88.5 (2015).
- ★[D] R. D. : [A construction of the fundamental solution of the Schrödinger equation with a perturbed quadratic Hamiltonian](#). In: *Nonlinearity*, 29.2 (2016).
- ★[MD] R. D. and Renaud Marty : [Analysis of a Time-Splitting Scheme for a Class of Random Nonlinear Partial Differential Equations](#). In: *ESAIM: Probability and Statistics*, 20 (2016) pp. 572–589.
- [DR1] R. D. and Anthony Réveillac : [Stochastic regularization effects of semi-martingales on random functions](#). In: *Journal de Mathématiques Pures et Appliquées* 106.6 (2016), pp. 1141–1173.
- [BBDGZ] Christophe Besse, Juliette Billy, R. D., David Guéry-Odelin and Juan Pablo Alvarez Zúñiga : [Restoring quasireversibility with a single topological charge](#). In: *Computer Physics Communications* 219 (2017), pp. 70–78.
- [ABDV] Xavier Antoine, Christophe Besse, R. D. and Vittorio Rispoli : [Acceleration of the imaginary time method for spectrally computing the stationary states of Gross-Pitaevskii equations](#). In: *Physical Review A* 96.5 (2017), pp. 053618.
- [CDLR] Michele Correggi, R. D., Douglas Lundholm and Nicolas Rougerie : [Vortex patterns in the almost-bosonic anyon gas](#). In: *Europhysics Letters* 126.2 (2019), p. 20005.
- [DP1] R. D. and Olivier Pinaud : [On the minimization of quantum entropies under local constraints](#). In: *Journal de Mathématiques Pures et Appliquées* 128 (2019), pp. 87–118.

- [DP2] R. D. and Olivier Pinaud : [Constrained minimizers of the von Neumann entropy and their characterization](#). In: *Calculus of Variations and Partial Differential Equations* 59.3 (2020), pp. 1–29.
- [IDG] François Impens, R. D. and David Guéry-Odelin : [Quantum control beyond the adiabatic regime in 2D curved matter-wave guides](#). In: *Physical Review Letters*, 124.25, (2020), pp. 250403.
- [DP3] R. D. and Olivier Pinaud : [A constrained optimization problem in quantum statistical physics](#). In: *Journal of Functional Analysis* 281.9 (2021), p. 10916.
- [DP4] R. D. and Olivier Pinaud : [Entropy minimization for many-body quantum systems](#). In: *Journal of Statistical Physics* 185.1 (2021), pp. 1–2.
- [DR2] R. D. and Anthony Réveillac : [On a stochastic Hardy-Littlewood-Sobolev inequality with application to Strichartz estimates for a noisy dispersion](#). In: *Annales Henri Lebesgue* 5 (2022), pp. 263–27.
- [CDR] Laure Coutin, R. D. and Anthony Réveillac : [The Itô-Tanaka Trick: a non-semimartingale approach](#). In: *ALEA. Latin American Journal of Probability & Mathematical Statistics* 19.1 (2022).
- [BDL1] Christophe Besse, R. D. and Stefan Le Coz : [Gradient Flow Approach to the Calculation of Ground States on Nonlinear Quantum Graphs](#). In: *Annales Henri Lebesgue* 5 (2022), pp. 387–428.
- [BDL2] Christophe Besse, R. D. and Stefan Le Coz : [Numerical simulations on nonlinear quantum graphs with the GRAFIDI library](#). In: *The SMAI journal of computational mathematics* 8 (2022), pp. 1–47.
- [DP5] R. D. and Olivier Pinaud : [On local quantum Gibbs states](#). In: *Journal of Mathematical Physics* 63.10 (2022).
- [CD] Rémi Catellier and R. D. : [Regularization by noise for rough differential equations driven by Gaussian rough paths](#), submitted.
- [BDL3] Christophe Besse, R. D. and Stefan Le Coz: [Computation of excited states for the nonlinear Schrödinger equation: numerical and theoretical analysis](#), submitted.



1. Numerics

1.1 Stationary states in quantum mechanics

In quantum mechanics, a Hamiltonian operator is associated to the total energy of a system of quantum particles. This operator is used to describe the evolution of the system *via* the Schrödinger (or Liouville-Von Neumann) equation but also gives information about its so-called stationary states. These states are in fact the eigenfunctions of the Hamiltonian operator and are associated to energies (which are the corresponding eigenvalues). Among these stationary states, the ground state (if it exists) is the one associated with the lowest energy and corresponds to an absolute zero temperature configuration of the system. The other states are called excited states and are associated to higher energies. In this section, we investigate the problem of computing such stationary states (both the ground and excited states) in different situations. As we will see below, in the nonlinear setting, there exist other definition of the ground state (and excited states) depending on the functional that is minimized.

Bose-Einstein condensates are peculiar state of matter that emerges when a gas of bosons is cooled to a temperature near absolute zero. This state opens the possibility of studying quantum physics at a macroscopic scale since a large portion of the particles of the system will be in the same state: the ground state. Hence, this state of this system will give its most important features and, due to the difficulty of measuring precisely a quantum system, the use of numerical methods to simulate it makes its study much simpler. Based on the Gross-Pitaevskii model, the stationary states are solutions of the following (nonlinear) eigenvalue problem

$$\mu\phi(x) - \frac{1}{2}\Delta\phi(x) + V(x)\phi(x) + \beta|\phi(x)|^2\phi(x) = 0 \quad (1.1)$$

where ϕ is the wavefunction associated to the condensate (an eigenfunction), μ is its chemical potential (an eigenvalue), V is an external potential (usually confining), $\beta \in \mathbb{R}$ corresponds to the strength of the interaction between particles and $x \in \mathbb{R}^d$, with $d = 1, 2, 3$. An approach to solve this problem is to recast it as a minimization problem (under constraint). That is, ϕ is a critical point on $\mathbb{S}_{L^2} = \{\psi \in L^2(\mathbb{R}^d) : \|\psi\|_{L^2} = 1\}$ of the following energy

$$E(\psi) = \int_{\mathbb{R}^d} \left(\frac{1}{2}|\nabla\psi(x)|^2 + V(x)|\psi(x)|^2 + \frac{\beta}{2}|\psi(x)|^4 \right) dx$$

We notice that the ground state will be the global minimizer of E and that μ can be recovered through ϕ since $\mu = E(\phi) + \beta\|\phi\|_{L^4}^4/2$. A considerable literature revolves around numerical

methods to solve this minimization problem in different contexts [10, 20, 31, 89]. Among these, the most standard approach is to use gradient methods [6, 9, 32, 61, 71, 92]. A basic gradient method for a minimization problem under constraint is the so-called projected gradient method (also called *imaginary time method* in the physics literature). In our case, it writes as

$$\begin{cases} \partial_t \phi(t, x) = -\nabla_{\phi^*} E(\phi) = \frac{1}{2} \Delta \phi(x) - V(x) \phi(x) - \beta |\phi(x)|^2 \phi(x), \forall (t, x) \in (t_n, t_{n+1}) \times \mathbb{R}^d, \\ \phi(t_{n+1}, x) = \lim_{t \rightarrow t_{n+1}} \frac{\phi(t, x)}{\|\phi(t, x)\|_{L^2}}, \end{cases}$$

with $\phi(0, \cdot) = \phi_0 \in \mathbb{S}_{L^2}$ the initial data. The idea is to follow the steepest descent of the function E (which is the opposite of the gradient) on a small time period then to project the solution on the constraint space \mathbb{S}_{L^2} . In [ABDV], we investigate a new method based on the idea of introducing an inertial term in the projected gradient method then using an semi-implicit time discretization which stems from the so-called *iPiano method* [82]. The algorithm is given by, for any $n \in \mathbb{N}^*$,

$$\begin{cases} \phi_{0,n} = \phi_n + \beta_{\text{iPiano}} (\phi_n - \phi_{n-1}), \\ \phi_{1,n} = \phi_{0,n} + \delta t \left(\frac{1}{2} \Delta - V - \beta |\phi_{0,n}|^2 \right) \phi_{1,n}, \\ \phi_{n+1} = \phi_{1,n} / \|\phi_{1,n}\|_{L^2}, \end{cases}$$

where $\beta_{\text{iPiano}} \in [0, 1)$ is the inertial parameter. Thanks to some numerical studies, we are able to validate the fact that this method accelerates the standard projected method (when $\beta_{\text{iPiano}} = 0$) and can divide the global computational cost by a factor of 4.

Let us now consider the nonlinear eigenvalue problem (1.1) with $\omega = \mu/2$, $V \equiv 0$ and $\beta = -1/2$ which writes as

$$-\Delta \phi + \omega \phi - f(\phi) = 0, \quad (1.2)$$

with $f(z) = |z|^{p-1}z$ and $p = 3$. We notice that the choice $\beta < 0$ leads to a *focusing* nonlinearity which tends to concentrate the solution (in opposition to the effect of the Laplace operator which tends to spread it). This is why this equation may admit solutions that are not trivial (see [15, 16, 17]). Moreover, we do not fix the mass as for Equation (1.1). Among the solutions of (1.2), we can distinguish the ground state from the excited states as the former is the unique global minimizer of the action functional given by

$$S(\psi) = \frac{1}{2} \|\nabla \psi\|_{L^2}^2 + \frac{\omega}{2} \|\psi\|_{L^2}^2 - \frac{1}{p+1} \|\psi\|_{L^{p+1}}^{p+1}.$$

We remark that this definition does not match the one that we used in the beginning of this section where the ground state is the global minimizer of the energy. It is known that the ground state is unique, radial and positive [54, 67]. Our knowledge on excited states is more scarce but we know that they necessarily change sign (or may be complex valued) [70] and need not be radial [7]. A way to approach Equation (1.2) is to consider the associated *Nehari functional*, defined by

$$I(\psi) = \|\nabla \psi\|_{L^2}^2 + \omega \|\psi\|_{L^2}^2 - \|\psi\|_{L^{p+1}}^{p+1},$$

which also leads to the definition of the *Nehari manifold*

$$\mathcal{N} = \{\psi \in H^1(\mathbb{R}^d) : I(\psi) = 0, \psi \neq 0\}.$$

It is rather direct that, if ϕ is a solution of (1.2), then $\phi \in \mathcal{N}$. Furthermore, it is proved that a minimizing sequence in \mathcal{N} of the action S converges (up to a translation) to the ground state [85]. In [BDL3], we extend this procedure to compute excited states. The idea being that, in order to obtain an excited state, one can constraint the state to have its positive (and negative) part in the Nehari manifold. That is, we search for a solution that belongs in the *Nehari nodal set* given by

$$\mathcal{N}_{\text{nod}} = \{\psi \in H^1(\mathbb{R}^d) : I(\psi^+) = 0, I(\psi^-) = 0, \psi^\pm \neq 0\},$$

where $\psi^+ = \max(\psi, 0)$ and $\psi^- = \max(-\psi, 0)$. However, there is an issue here: the minimum of S cannot be achieved in \mathcal{N}_{nod} . This is due to the fact that its positive (resp. negative) part must then be a ground state which needs to be positive (resp. negative) on the whole space. To circumvent this problem, we work on the radial setting and define

$$\mathcal{N}_{\text{nod,rad}} = \{\psi \in H_{\text{rad}}^1(\mathbb{R}^d) : I(\psi^+) = 0, I(\psi^-) = 0, \psi^\pm \neq 0\}.$$

We prove the following result.

Theorem 1.1 Let $\{\phi_n\}_{n \in \mathbb{N}} \subset \mathcal{N}_{\text{nod,rad}}$ be such that

$$\lim_{n \rightarrow +\infty} S(\phi_n) = \inf_{\psi \in \mathcal{N}_{\text{nod,rad}}} S(\psi).$$

Then, there exists $\phi_\infty \in \mathcal{N}_{\text{nod,rad}}$ such that $\phi_n \rightarrow \phi_\infty$ in $H^1(\mathbb{R}^d)$. Moreover, ϕ_∞ is a solution of (1.2) with exactly two nodal domains.

The previous result only yields the excited state with the least amount of nodal domains. Higher order excited states (with a higher number of nodal domains) can be constructed by setting $N_{\text{nodes}} \geq 1$ the number of nodes thanks to the following result [12].

Proposition 1.1 Let $N_{\text{nodes}} \geq 1$. Then, there exists a radial solution $\phi_{N_{\text{nodes}}}$ of (1.2) having exactly N_{nodes} nodes, *i.e.* there exists

$$\rho_0 = 0 < \rho_1 < \dots < \rho_{N_{\text{nodes}}} < \rho_{N_{\text{nodes}}+1} = \infty,$$

such that

$$\phi_{N_{\text{nodes}}}^{-1}(0) = \{x \in \mathbb{R}^d : |x| = \rho_j, \text{ for } 1 \leq j \leq N_{\text{nodes}}\}.$$

The set $\{\rho_j\}_{0 \leq j \leq N_{\text{nodes}}+1}$ is the minimizer of $\sum_{j=0}^{N_{\text{nodes}}} s_{\rho_j, \rho_{j+1}}$ where

$$s_{\rho_j, \rho_{j+1}} = \min \{S(\psi) : \psi \in H_0^1(\mathcal{A}(\rho_j, \rho_{j+1})), I(\psi) = 0\},$$

with $\mathcal{A}(\rho_j, \rho_{j+1})$ the annulus of \mathbb{R}^d of radii ρ_j and ρ_{j+1} . The solution $\phi_{N_{\text{nodes}}}$ is given by

$$\phi_{N_{\text{nodes}}}(x) = (-1)^j v_{\rho_j, \rho_{j+1}}(x), \text{ if } \rho_j \leq |x| < \rho_{j+1},$$

where $v_{\rho_j, \rho_{j+1}} \in \text{argmin} \{S(\psi) : \psi \in H_0^1(\mathcal{A}(\rho_j, \rho_{j+1})), I(\psi) = 0\}$ is positive.

This lead us to introduce a numerical method, called the *Nehari method*, to compute excited states in the radial setting which consist in a projected gradient method in a suitable functional space. For this, we define the nodal Nehari space

$$\mathcal{N}_{N_{\text{nodes}}} = \left\{ \varphi \in \mathcal{H}_{d,\text{rad}}^1 : I(\varphi|_{[\rho_j, \rho_{j+1}]}) = 0 \text{ for } 0 \leq j \leq N_{\text{nodes}} \text{ with } \{\rho_1, \dots, \rho_{N_{\text{nodes}}}\} = \varphi^{-1}(0) \right\},$$

where

$$\mathcal{H}_{d,\text{rad}}^1 = \left\{ \varphi : \mathbb{R}^+ \rightarrow \mathbb{R} : \int_0^\infty (|\varphi'(r)|^2 + |\varphi(r)|^2) r^{d-1} dr < \infty \right\},$$

as well as, for a given set $\{\rho_j\}_{1 \leq j \leq N_{\text{nodes}}}$,

$$\mathcal{H}_{N_{\text{nodes}}} = \left\{ \varphi \in \mathcal{H}_{d,\text{rad}}^1 : \varphi^{-1}(0) = \{\rho_1, \dots, \rho_{N_{\text{nodes}}}\} \right\}.$$

Then, we can define the projection $\Pi_{\mathcal{N}_{N_{\text{nodes}}}} : \mathcal{H}_{N_{\text{nodes}}} \mapsto \mathcal{N}_{N_{\text{nodes}}}$ by

$$\Pi_{\mathcal{N}_{N_{\text{nodes}}}} \varphi = \sum_{j=0}^{N_{\text{nodes}}} \varphi|_{[\rho_j, \rho_{j+1}]} \left(\frac{\|\nabla \varphi|_{[\rho_j, \rho_{j+1}]}\|_{L^2}^2 + \|\varphi|_{[\rho_j, \rho_{j+1}]}\|_{L^2}^2}{\|\varphi|_{[\rho_j, \rho_{j+1}]}\|_{L^{p+1}}^{p+1}} \right)^{1/(p-1)}.$$

With all these definitions at hand, we can numerically solve the problem of finding a solution to the minimization problem

$$\min_{\varphi \in \mathcal{N}_{N_{\text{nodes}}}} S(\varphi),$$

thanks to the following projected gradient descent

$$\begin{cases} \varphi^{(0)} \in \mathcal{N}_{N_{\text{nodes}}}, \\ \varphi^{(n+1)} = \Pi_{\mathcal{N}_{N_{\text{nodes}}}} (\varphi^{(n)} + \tau S'(\varphi^{(n)})), \quad \forall n \geq 0, \end{cases}$$

where $\tau > 0$ is the time-step. This method was implemented by using a second order finite differences method for the space-discretization and compared to the well-known *shooting method* which, incidentally, was used theoretically to prove the existence of radial solutions admitting a certain number of nodes [27]. We observe that each method converges to the same solutions with the Nehari method being numerically more costly but also more robust and accurate. Numerical investigations are also performed on relation between the height of excited states and their number of nodes, the positions of the nodes, the position (and value) of the local maxima and the shape of the oscillations.

1.2 Quantum graphs

Equations (1.1) and (1.2) are usually studied on \mathbb{R}^d , with $d = 1, 2, 3$, where the cases $d = 1, 2$ correspond to models that are derived thanks to a dimension reduction due to the effects of a strong confining potential (see [14] for instance). There exists also instances where the dimension reduction might not lead to a Schrödinger equation on \mathbb{R}^d as in the Y -junctions [86], H -junctions [62] or T -junctions [19] examples. In these cases, the reduction to a one-dimensional model will lead to what is called a *quantum graph* approximating the underlying spatial structure. These mathematical models have become much more popular in recent decades due to the many applications in physics, chemistry and engineering. For instance, one can mention free-electron theory of conjugated molecules, quantum wires, photonic crystals and thin waveguides [59, 66, 73]. On the theoretical level, mathematical investigations can be traced back to the 70's [72] and, more recently, several surveys on the subject are available (see for instance [18]).

Quantum graphs are metric graphs of the form $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, that is a collection of vertices \mathcal{V} and edges \mathcal{E} with lengths $\ell_e \in (0, \infty]$ associated to each edge $e \in \mathcal{E}$, equipped with an Hamiltonian operator \mathcal{H} . We notice that two vertices might be connected by several edges, called a *bridge*, and one edge can link a vertex to itself, called a *loop*. Furthermore, each edges $e \in \mathcal{E}$ can be identified with a segment $I_e = [0, \ell_e]$ if $\ell_e < \infty$ or a half-line $I_e = [0, \infty)$ if $\ell_e = \infty$. Examples of metrics graphs are given in Figure 1.1 where a *compact graph* is depicted (*i.e.* a graph where every edge is of finite length), Figure 1.2 where *non-compact graphs* are illustrated (*i.e.* graphs that contain at least one edge of infinite length) and Figure 1.3 where periodic graphs are given.



Figure 1.1: Example of compact graph: the dumbbell graph

The operator \mathcal{H} will act on functions that are defined on \mathcal{G} . A function $\psi : \mathcal{G} \mapsto \mathbb{C}$ is a collection $\{\psi_e\}_{e \in \mathcal{E}}$ of one dimensional mappings given by $\psi_e : I_e \mapsto \mathbb{C}$, for any $e \in \mathcal{E}$. We can naturally define generalizations of the usual Lebesgue's and Sobolev's space on \mathcal{G} by

$$L^p(\mathcal{G}) = \bigoplus_{e \in \mathcal{E}} L^p(I_e) \quad \text{and} \quad H^k(\mathcal{G}) = \bigoplus_{e \in \mathcal{E}} H^k(I_e),$$

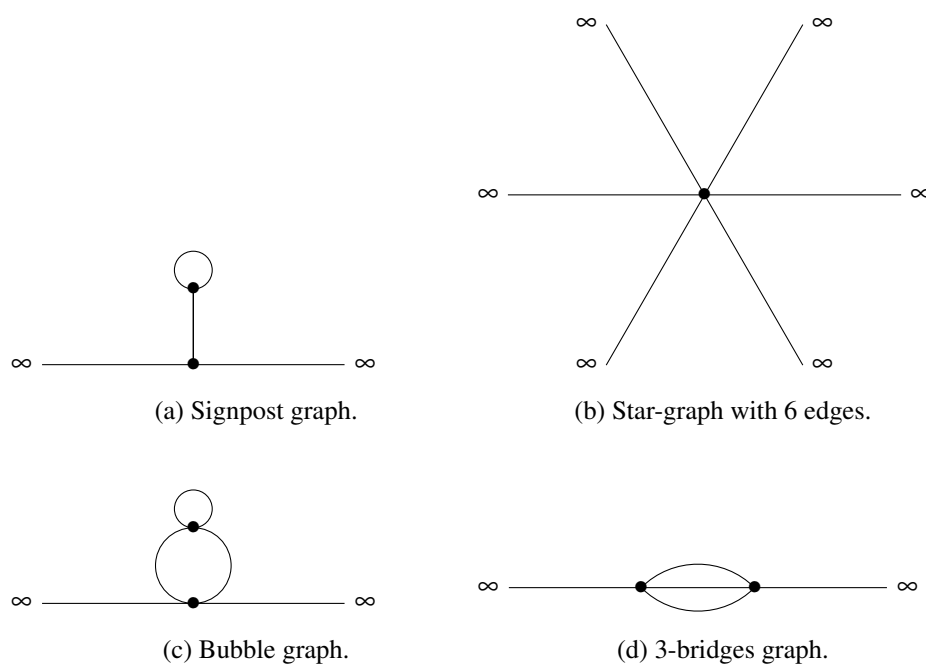


Figure 1.2: Examples of non-compact graphs

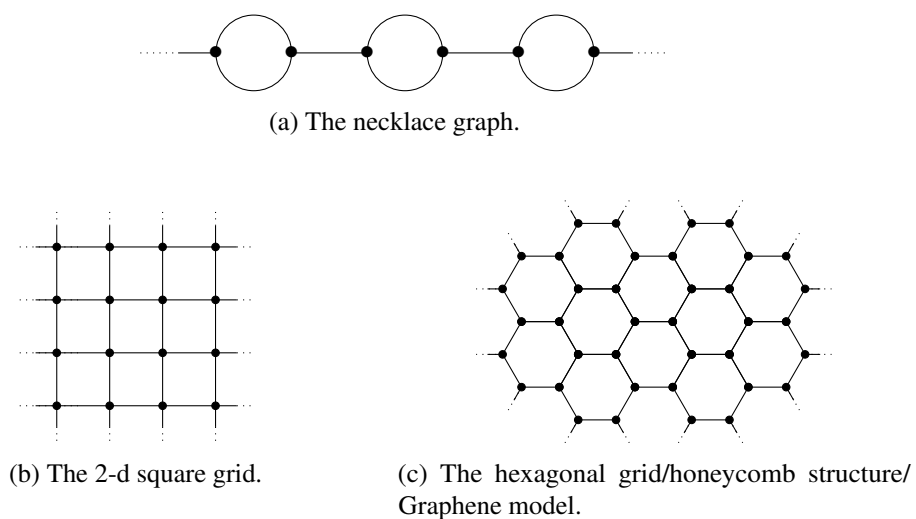


Figure 1.3: Examples of periodic graphs.

for any $p \in [1, \infty]$ and $k \in \mathbb{N}^*$, equipped with the following norms

$$\|\psi\|_{L^p(\mathcal{G})} = \sum_{e \in \mathcal{E}} \|\psi_e\|_{L^p(I_e)} \quad \text{and} \quad \|\psi\|_{H^k(\mathcal{G})} = \sum_{e \in \mathcal{E}} \|\psi_e\|_{H^k(I_e)}.$$

The space $L^2(\mathcal{G})$ can be made a Hilbert space by setting the scalar product, for any $\psi, \phi \in L^2(\mathcal{G})$,

$$\langle \psi, \phi \rangle_{L^2(\mathcal{G})} = \sum_{e \in \mathcal{E}} \Re \int_0^{\ell_e} \psi_e(x) \phi_e^*(x) dx.$$

Of course, at the vertices of the graph, these functions can admit different values depending on the incident edge considered. For any $v \in \mathcal{V}$, we denote \mathcal{E}_v the collection of edges that are incident to v and d_v the *degree* of v (or the cardinal of \mathcal{E}_v). The remaining point to properly define a quantum graph is to set $D(\mathcal{H})$, the domain of \mathcal{H} . This is done by setting boundary conditions at each vertices $v \in \mathcal{V}$. From now on, we consider that \mathcal{H} is a second order differential operator (typically the Laplace operator $-\Delta$) so that $D(\mathcal{H}) \subset H^2(\mathcal{G})$. In this context, the boundary conditions (also called the *compatibility conditions*) are given, for any $\psi \in D(\mathcal{H})$ and for each $v \in \mathcal{V}$, by the relation

$$A_v \psi'(v) + B_v \psi(v) = 0,$$

where A_v, B_v are $d_v \times d_v$ real-valued matrices and with

$$\psi(v) = (\psi_e(v))_{e \in \mathcal{E}_v} \in \mathbb{R}^{d_v} \quad \text{and} \quad \psi'(v) = (\psi'_e(v))_{e \in \mathcal{E}_v} \in \mathbb{R}^{d_v}.$$

In the previous expression, $\psi'_e(v)$ is the outer derivative of ψ_e evaluated at v . Hence, the domain of \mathcal{H} will be given by

$$D(\mathcal{H}) = \{ \psi \in H^2(\mathcal{G}) : A_v \psi'(v) + B_v \psi(v) = 0, \text{ for any } v \in \mathcal{V} \}.$$

The operator \mathcal{H} is self-adjoint if and only if, for every vertex $v \in \mathcal{V}$, the $d_v \times 2d_v$ matrix (A_v, B_v) has the maximal rank and the matrix $A_v B_v^*$ is self-adjoint [18] (and we assume that this condition is satisfied from now on). In that case, for each vertex v there exist three orthogonal and mutually orthogonal operators $P_{D,v}$ (Dirichlet part), $P_{N,v}$ (Neumann part) and $P_{R,v} = Id - P_{D,v} - P_{N,v}$ (Robin part), acting on \mathbb{C}^{d_v} and an invertible self-adjoint operator Λ_v acting on the subspace $P_{R,v} \mathbb{C}^{d_v}$ such that the boundary values of $\psi \in D(H)$ at the vertex v verify

$$P_{D,v} \psi(v) = P_{N,v} \psi'(v) = P_{R,v} \psi'(v) - \Lambda_v P_{R,v} \psi(v) = 0.$$

Using this expression of the boundary conditions, we can express the quadratic form corresponding to \mathcal{H} [18], which we denote by Q and is given by

$$Q(\psi) = \frac{1}{2} \|\psi'\|_{L^2}^2 + \frac{1}{2} \sum_{v \in \mathcal{V}} \langle \Lambda_v P_{R,v} \psi(v), P_{R,v} \psi(v) \rangle_{\mathbb{C}^{d_v}}.$$

The domain of Q is given by

$$H_D^1(\mathcal{G}) = \{ \phi \in H^1(\mathcal{G}) : \forall v \in \mathcal{V}, P_{D,v} \phi = 0 \}.$$

Let us now give some examples of compatibility conditions at a vertices $v \in \mathcal{V}$:

1. the *Kirchhoff-Neumann* condition given by

$$\psi_e(v) = \psi_{\tilde{e}}(v), \text{ for any } e, \tilde{e} \in \mathcal{E}_v, \quad \text{and} \quad \sum_{e \in \mathcal{E}_v} \psi'_e(v) = 0,$$

2. the δ -type condition given by, for some $\alpha_v \in \mathbb{R}$,

$$\psi_e(v) = \psi_{\tilde{e}}(v), \text{ for any } e, \tilde{e} \in \mathcal{E}_v, \quad \text{and} \quad \sum_{e \in \mathcal{E}_v} \psi'_e(v) = \alpha_v \psi(v),$$

3. the δ' -type condition given by, for some $\beta_v \in \mathbb{R}$,

$$\psi'_e(v) = \psi'_{\tilde{e}}(v), \text{ for any } e, \tilde{e} \in \mathcal{E}_v, \quad \text{and} \quad \sum_{e \in \mathcal{E}_v} \psi_e(v) = \beta_v \psi'(v).$$

With a quantum graph \mathcal{G} at hand, we can define a quantum system on \mathcal{G} thanks to wave-functions belonging in $L^2(\mathcal{G})$. It follows that we can model the dynamic of such system by a (nonlinear) Schrödinger equations on \mathcal{G} by

$$i\partial_t \psi = \mathcal{H} \psi + f(\psi), \quad (1.3)$$

with $\psi \in \mathcal{C}(\mathbb{R}; D(\mathcal{H}))$, that can be understood as a collection of PDEs on each edge (in the most straightforward sense). For simplicity, the function $f: \mathbb{C} \mapsto \mathbb{C}$ is assumed to be of the power-type, *i.e.* $\forall z \in \mathbb{C}, f(z) = g(|z|^2)z = \pm |z|^{p-1}z$, for some $p \in (1, 1 + 4/d)$. In the context of quantum graphs, such equation naturally arise when modeling Bose-Einstein condensate (see [55] and references therein). Of course, as explained in the previous section, the computation of stationary states (and, most importantly, the ground state) can provide some of the most important features of a quantum system. The stationary states are understood as critical points of the energy given by

$$E(\psi) = \frac{1}{2} \langle \mathcal{H} \psi, \psi \rangle_{L^2(\mathcal{G})} + \frac{1}{p+1} \int_{\mathcal{G}} |\psi|^{p+1}, \quad (1.4)$$

where we denote, for any $\phi \in L^1(\mathcal{G})$,

$$\int_{\mathcal{G}} \phi = \sum_{e \in \mathcal{E}} \int_0^{\ell_e} \phi(x) dx.$$

The theoretical study of (local or global) minimizers of this energy under a mass constraint was carried out, for instance, in [4, 5] for star-graphs, [81] for the tadpole graph, [76] for the dumbbell graph and [1, 2, 3, 46, 83] for more general graphs. Concerning their numerical study, the literature is less extensive and we mention the implementation of finite differences on graphs for the computation of ground states [76], which was extended by an investigation on bifurcations [57], as well as the dynamical analysis of the interaction between a soliton and a point defect in [58]. We notice that the work from [57, 58] led to the release of a Matlab library that is freely available¹.

In [BDL1], we investigate the convergence of the normalized gradient flow for the computation of ground states. We notice that a similar study was carried out in [47] for the ground states in the real line. At the continuous level, the normalized gradient flow applied to (1.4) writes as

$$\partial_t \psi = -E'(\psi) + \|\psi\|_{L^2(\mathcal{G})}^{-2} \langle E'(\psi), \psi \rangle_{L^2(\mathcal{G})} \psi \quad (1.5)$$

with

$$E'(\psi) = \mathcal{H} \psi + f(\psi).$$

We prove the following result on the behavior of this scheme (but for a more general function f).

Theorem 1.2 Assume that there exists a stationary state ϕ , *i.e.* a solution to

$$\mathcal{H} \phi + \omega \phi + f(\phi) = 0$$

for some $\omega \in \mathbb{R}$, and that there exists $\kappa > 0$ such that, for any $\varphi \in D(\mathcal{H})$ verifying $\langle \phi, \varphi \rangle_{L^2(\mathcal{G})} = 0$, we have

$$\langle (\mathcal{H} + \omega + f'(\phi)) \varphi, \varphi \rangle_{L^2(\mathcal{G})} \geq \kappa \|\varphi\|_{H^1(\mathcal{G})}^2.$$

Then, for every $\mu \in (0, \kappa)$, there exist $\varepsilon > 0$ and $C > 0$ such that, for every $\psi_0 \in H_D^1(\mathcal{G})$

¹<https://github.com/manroygood/Quantum-Graphs>

verifying $\|\psi_0 - \phi\|_{H^1(\mathcal{G})} < \varepsilon$, there exists a unique solution $\psi \in \mathcal{C}([0, \infty); H_D^1(\mathcal{G}))$ to (1.5) which converges exponentially fast to ϕ , that is, for any $t \in [0, \infty)$, we have

$$\|\psi(t) - \phi\|_{H^1(\mathcal{G})} \leq C e^{-\mu t} \|\psi_0 - \phi\|_{H^1(\mathcal{G})}.$$

Furthermore, we prove that the (semi-implicit) imaginary time method is indeed a (time) discretization of (1.5). This scheme reads, for any $n \in \mathbb{N}$, as

$$\begin{cases} \frac{\tilde{\psi}^{n+1} - \psi^n}{\delta t} = (-\mathcal{H} - g(|\psi^n|^2)) \tilde{\psi}^{n+1}, \\ \psi^{n+1} = \sqrt{m} \frac{\tilde{\psi}^{n+1}}{\|\tilde{\psi}^{n+1}\|_{L^2(\mathcal{G})}} \end{cases}$$

where $\delta t > 0$ is the time-step and $m = \|\phi\|_{L^2(\mathcal{G})}$ is the mass of the stationary state. Finally, we provide a numerical study of the imaginary time method thanks to a finite differences space discretization under the assumption that \mathcal{G} is compact. This discretization only concerns the operator \mathcal{H} and its boundary conditions at each vertex $v \in \mathcal{V}$. For each edge $e \in \mathcal{E}$, we consider a uniform discretization $\{x_{e,k}\}_{0 \leq k \leq N_e+1}$, where $N_e \geq 3$ is the number of interior points, of the interval $I_e = [0, \ell_e]$, that is

$$x_{e,0} = 0 < x_{e,1} < \dots < x_{e,N_e} < x_{e,N_e+1} = \ell_e,$$

with $\delta x_e = x_{e,k+1} - x_{e,k} = \ell_e / (N_e + 1)$, for any $0 \leq k \leq N_e$. The discretization of $\mathcal{H} = -\Delta$ on the interior points is straightforward and we use a second order approximation given, for any $2 \leq k \leq N_e - 1$, by

$$\mathcal{H} \psi_e(x_{e,k}) \approx -\frac{\psi_{e,k-1} - 2\psi_{e,k} + \psi_{e,k+1}}{\delta x_e}, \quad (1.6)$$

where we use the notation $\psi_{e,k} = \psi_e(x_{e,k})$ for any $0 \leq k \leq N_e + 1$. From here, we need to be able to evaluate ψ_e at the vertices and, to do so, we use the boundary conditions. We denote $v_1 \in \mathcal{E}$ the vertex at $x_{e,0}$ and $v_2 \in \mathcal{E}$ the vertex at x_{e,N_e+1} . Since the boundary conditions involve the outgoing derivative of ψ_e , we use the second order approximation, for $v \in \{v_1, v_2\}$,

$$\psi'_e(x_{e,v}) \approx \frac{3\psi_{e,v,0} - 4\psi_{e,v,-1} + \psi_{e,v,-2}}{2\delta x_e},$$

where we denote $x_{e,v_1} = x_{e,0}$, $x_{e,v_2} = x_{e,N_e+1}$ as well as, for $-2 \leq j \leq 0$,

$$\psi_{e,v_1,j} = \psi_e(x_{e,|j|}) \quad \text{and} \quad \psi_{e,v_2,j} = \psi_e(x_{e,N_e+1+j}).$$

With this discretization at hand and by assuming, for simplicity, that $\delta x = \delta x_e$ for every $e \in \mathcal{E}$, the boundary conditions at $v \in \{v_1, v_2\}$ are approximated by

$$A_v \psi_{v,0} + B_v \left(\frac{3\psi_{v,0} - 4\psi_{v,-1} + \psi_{v,-2}}{2\delta x} \right) = 0,$$

where we denote $\psi_{v,j} = (\psi_{e,v,j})_{e \in \mathcal{E}_v}$. We notice that the values of ψ at the vertices are contained in the vector $\psi_{v,0}$ and that $\psi_{v,-1}$ and $\psi_{v,-2}$ contain values that are on the interior points of one of the edge belonging in \mathcal{E}_v . Thus, the previous expression can be understood as a linear system whose unknown is the vector $\psi_{v,0}$, *i.e.* we have, by assuming that $2\delta x A_v + 3B_v$ is invertible,

$$\psi_{v,0} = (2\delta x A_v + 3B_v)^{-1} B_v (4\psi_{v,-1} - \psi_{v,-2}).$$

Thanks to the previous relation, we can compute the coefficients $(\alpha_{e,v})_{e \in \mathcal{E}_v} \subset \mathbb{R}$ such that

$$\psi_{e,0} = \sum_{r \in \mathcal{E}_{v_1}} \alpha_{r,v_1} (4\psi_{e,1} - \psi_{e,2}) \quad \text{and} \quad \psi_{e,N_e+1} = \sum_{r \in \mathcal{E}_{v_2}} \alpha_{r,v_2} (4\psi_{e,N_e} - \psi_{e,N_e-1}),$$

which we use to approximate \mathcal{H} at $x_{e,1}$ and x_{e,N_e} , that is

$$\Delta\psi_e(x_{e,1}) \approx \frac{\psi_{e,2} - 2\psi_{e,1} + \sum_{r \in \mathcal{E}_{v_1}} \alpha_{r,v_1} (4\psi_{e,1} - \psi_{e,2})}{\delta x^2} \quad (1.7)$$

and

$$\Delta\psi_e(x_{e,N_e}) \approx \frac{\psi_{e,N_e-1} - 2\psi_{e,N_e} + \sum_{r \in \mathcal{E}_{v_2}} \alpha_{r,v_2} (4\psi_{e,N_e} - \psi_{e,N_e-1})}{\delta x^2}. \quad (1.8)$$

It follows from (1.6), (1.7) and (1.8) that we have the approximation

$$\mathcal{H}\psi \approx [\mathcal{H}]\psi,$$

where $\psi = (\psi_{e,k})_{1 \leq k \leq N_e, e \in \mathcal{E}} \in \mathbb{R}^N$, where $N = \sum_{e \in \mathcal{E}} N_e$, is a vector containing all the value of ψ at the interior points of every edge of the graph and $[\mathcal{H}] \in \mathbb{R}^{N \times N}$ is a matrix that corresponds to a second order finite difference approximation of \mathcal{H} . Thanks to this discretization, we are able to perform numerical experiments and, in particular, to verify that the fully discretized normalized gradient flow converges to the ground state (for graphs where there is an analytical expression of the ground state). Our code was then expanded into a Python library called GraFiDi [BDL2]. GraFiDi is built to simplify the space discretization, by finite differences approximations of second order, of the operator \mathcal{H} as well as the wave-functions. It also includes functions for the computation of observables and the depiction of wave functions on graphs. Thanks to this, it is then rather easy, and convenient, to implement numerical methods for the computations of stationary states (see Figure 1.5 for the ground state on a tree graph) or the dynamic through the (nonlinear) Schrödinger equation (1.3) (see Figure 1.4 for a soliton in a tadpole-type graph) on any compact quantum graph. We also performed some numerical investigations on properties of ground states on the dumbbell graph (and compare our results with the theoretical ones from [76]) as well as periodic graphs.

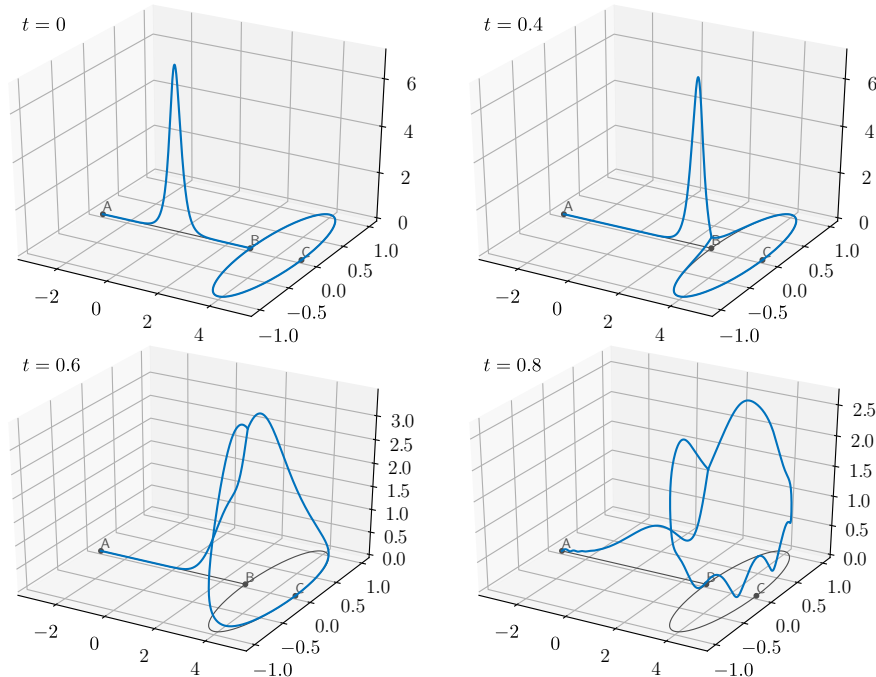


Figure 1.4: Dynamical simulation of (1.3) with $p = 3$ at time $t = 0, 0.4, 0.6, 0.8$ with the relaxation scheme.

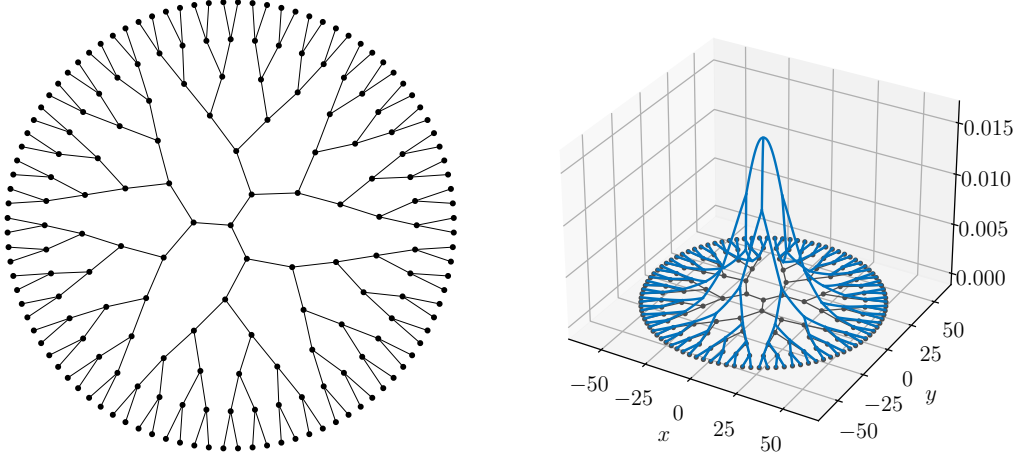


Figure 1.5: Tree graph (left) and ground state with mass constraint $\sqrt{m} = 0.1$ (right) for $f(u) = |u|u$ nonlinearity.

1.3 Computational quantum mechanics

In this section, we present some of the papers that were done with physicists around quantum mechanics. Our contribution is mostly to discuss and elaborate numerical studies to support certain assertions in quantum mechanics.

Quasireversibility restored with a topological defect

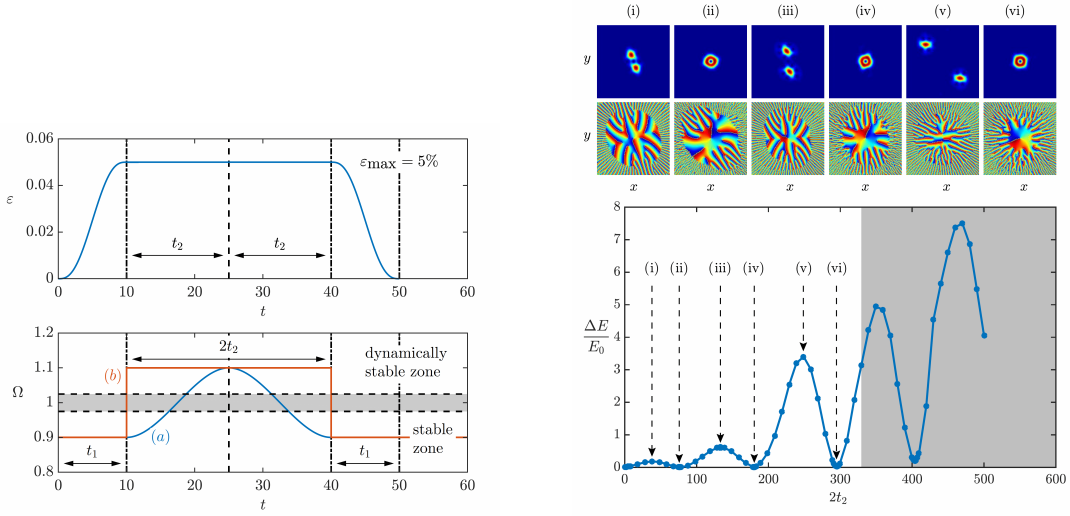
The Bose-Einstein condensate is a particular state of matter that exhibits some strange phenomena. For instance, when rotated, one will see the nucleation of quantum vortices, a type of topological defect in the wave function. This nucleation can be experimentally realized by using a rotating anisotropy that is superimposed to the confining potential, which is usually quadratic. To model this, we rely on the following 2D Gross-Pitaeski equation

$$i\partial_t \psi(t, x, y) = -\frac{1}{2} \Delta \psi(t, x, y) + \frac{1}{2} ([1 + \varepsilon(t)]x^2 + [1 + \varepsilon(t)]y^2) \psi(t, x, y) + \beta |\psi|^2 \psi(t, x, y) - \Omega L_z \psi(t, x, y), \quad (1.9)$$

where ε is the time-dependent anisotropy, $\beta > 0$ the strength of the interactions, Ω the rotation frequency and L_z the rotation operator given by

$$L_z = i(y\partial_x - x\partial_y).$$

The vortices are nucleated due to a dynamical instability in the frequency domain $\Omega \in [0, 1/\sqrt{2}]$. We observe that the regime $\Omega = 1$ is critical since, in this case, the centrifugal force exactly compensates the confining effect of the quadratic potential leading to an instability. Beyond this critical point, it turns out that, for a large enough rotation frequency, the Coriolis force stabilizes the fluid. These regimes have already been partially explored experimentally [75]. In [BBDGZ], we analytically and numerically investigate the effects of crossing the region near the critical rotating frequency where dynamical instability takes place. In the case $\beta = 0$, it is possible to derive the evolution averaged quantity thanks to the Ehrenfest theorem. In the case where $\beta \gg 1$, we can use the Thomas-Fermi approximation (as well as an ansatz for the solution) to derive a finite set of unknown variables that are solutions to nonlinear equations. Outside of these cases, we need completely solve Equation (1.9). To do so, we start with the computation of a ground state corresponding to the minimizer of the energy associated with Equation (1.9) for $\varepsilon = 0$ and $\Omega = 0.9$. For $\beta = 5$, this yields a ground



(a) Evolution of ε and Ω , depending on the length of time t_2 , through the procedure. In the case of Ω , the crossing is either abrupt (scenario (a)) or smoothly (scenario (b)).

(b) Final states of the system (density and phase) and the relative energy between the initial and final state as a function of $2t_2$.

state with a single (central) vortex. Then, we simulate the evolution of the solution of (1.9) by changing (abruptly or smoothly) the value of Ω and ε as depicted in Figure 1.6a. In each case, we observe oscillations after the crossing, for almost all $t_2 > 0$. However, we note that, in the presence of a single topological defect, there exists specific t_2 such that the final state is almost the same as the initial state leading to a quasireversibility of the procedure (see Figure 1.6b).

Almost-bosonic anyon gas in a mean-field regime

In quantum physics, there exists two fundamental classes of subatomic particles: bosons, whose spin quantum number has an integer value, and fermions, whose spin quantum number has an odd half-integer value. This translates into the fact that a system of N bosons is described by a symmetric wave function so that it belongs in $L^2_{\text{sym}}(\mathbb{R}^{Nd})$, that is exchanging two particles do not change the wave function or, for $\psi \in L^2_{\text{sym}}(\mathbb{R}^{Nd})$ and any $j, \ell \in \{1, \dots, N\}$ with $j \neq \ell$,

$$\psi(x_1, x_2, \dots, x_j, \dots, x_\ell, \dots, x_N) = \psi(x_1, x_2, \dots, x_\ell, \dots, x_j, \dots, x_N).$$

In the case of a system of N fermions, it is described by an antisymmetric wave function which belongs in $L^2_{\text{asym}}(\mathbb{R}^{Nd})$, that is, for $\psi \in L^2_{\text{asym}}(\mathbb{R}^{Nd})$ and any $j, \ell \in \{1, \dots, N\}$ with $j \neq \ell$,

$$\psi(x_1, x_2, \dots, x_j, \dots, x_\ell, \dots, x_N) = -\psi(x_1, x_2, \dots, x_\ell, \dots, x_j, \dots, x_N).$$

However, there exists quasi-particles called anyons, which occur in two-dimensional systems, that do not fall under these rules. For these, exchanging two particles in the system causes a change in the phase of the wave function, that is, there exists $\alpha \in [0, 2)$ such that for any $j, \ell \in \{1, \dots, N\}$ with $j \neq \ell$,

$$\psi(x_1, x_2, \dots, x_j, \dots, x_\ell, \dots, x_N) = e^{i\pi\alpha} \psi(x_1, x_2, \dots, x_\ell, \dots, x_j, \dots, x_N).$$

This leads to a fractional statistic as well as new exotic phenomena in the quantum world. These particles were predicted back in the 70's [88] and their experimental realization has only very recently been achieved [11]. In [CDLR], we numerically investigate the ground state of a mean-field type model of anyons in the so-called *almost bosonic limit* [26]. The energy for this model is given by

$$\mathcal{E}_\beta(\psi) = \int_{\mathbb{R}^2} \left(|(-i\nabla + \beta A[|\psi|^2])\psi(x)|^2 + V(x)|\psi(x)|^2 \right) dx$$

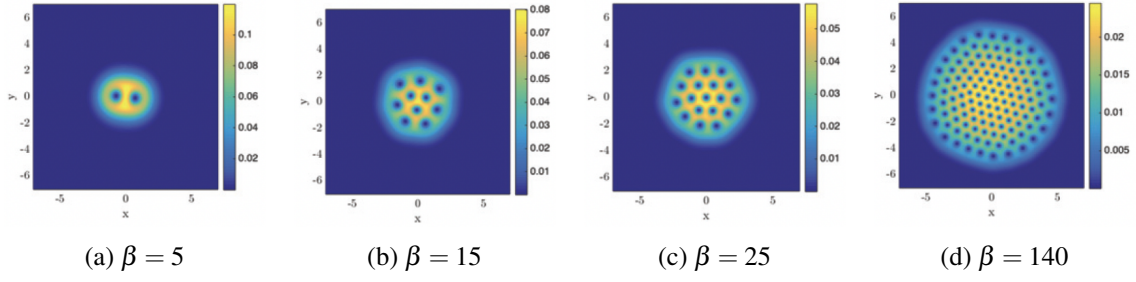


Figure 1.7: Ground states for different values of β and a quadratic trap.

where $\beta = \alpha N$, with N the number of particles, and

$$A[|\psi|^2] = \int_{\mathbb{R}^2} \frac{(x-y)^\perp}{|x-y|^2} |\psi(y)|^2 dy.$$

The potential V is confining and either a quadratic ($V(x) = |x|^2$) or quartic trap ($V(x) = |x|^4$). We notice that the differential operator in the energy is similar to a magnetic Laplacian but with a nonlinear magnetic potential. We observe the presence of topological defects in the computed ground state (see Figure 1.7). Since the mean-field model holds for a large number of particles N , we need to consider large values for β . In particular, we study the Thomas-Fermi limit of the energy and the density of the ground state, that is

$$\mathcal{E}_\beta \underset{\beta \rightarrow \infty}{\sim} \mathcal{E}_\beta^{\text{TF}} \quad \text{and} \quad |\psi_\beta|^2 \underset{\beta \rightarrow \infty}{\sim} \rho_\beta^{\text{TF}},$$

where, for any density $\rho \in L^1(\mathbb{R}^2)$ such that $\rho \geq 0$ and $\|\rho\|_{L^1} = 1$,

$$\mathcal{E}_\beta^{\text{TF}}(\rho) = \int_{\mathbb{R}^2} (\beta e(1,1)\rho(x)^2 + V(x)\rho(x)) dx,$$

with $e(1,1)$ the thermodynamic ground state energy per unit area at density $\rho = 1$ and magnetic flux $\beta = 1$, and ψ_β is the ground state of \mathcal{E}_β under the mass constraint $\|\psi_\beta\|_{L^2} = 1$. The Thomas-Fermi ground state ρ_β^{TF} is in fact explicitly known and given by

$$\rho_\beta^{\text{TF}}(x) = \frac{1}{2\beta e(1,1)} (\lambda_\beta^{\text{TF}} - V(x))_+,$$

where $\lambda_\beta^{\text{TF}}$ is the chemical potential that is set in order to verify the mass constraint $\|\rho_\beta^{\text{TF}}\|_{L^1} = 1$. By scaling arguments, we are able to derive the following expression for $e(1,1)$

$$e(1,1) = \frac{\pi}{2} \left(2 \frac{s+1}{s}\right)^{\frac{s+2}{s}} \left(\frac{s}{s+2}\right)^{2 \frac{s+1}{s}} \frac{\mathcal{E}_\beta^{\text{TF}}(\rho_\beta^{\text{TF}})^{\frac{s+2}{s}}}{\beta},$$

where $s = 2$ for the quadratic trap and $s = 4$ for the quartic trap. Since, for β large enough, $\mathcal{E}_\beta^{\text{TF}}(\rho_\beta^{\text{TF}}) \approx \mathcal{E}_\beta(\psi_\beta)$, we are able to numerically evaluate $e(1,1)$ which is approximately equal to $2\pi \times 1.18 \approx \frac{4}{3}(\pi)^{3/2}$ (see Figure 1.8a). This value turns out to be different from the theoretical guess $e(1,1) \approx 2\pi$ used in the literature. With this value at hand, the Thomas-Fermi profile ρ_β^{TF} turns out to be in good agreement with the experimental density (see Figure 1.8b). We notice that the number of vortices in the ground state can be estimated *via* the Thomas-Fermi model and we also find that the numerical data fits the theoretical values.

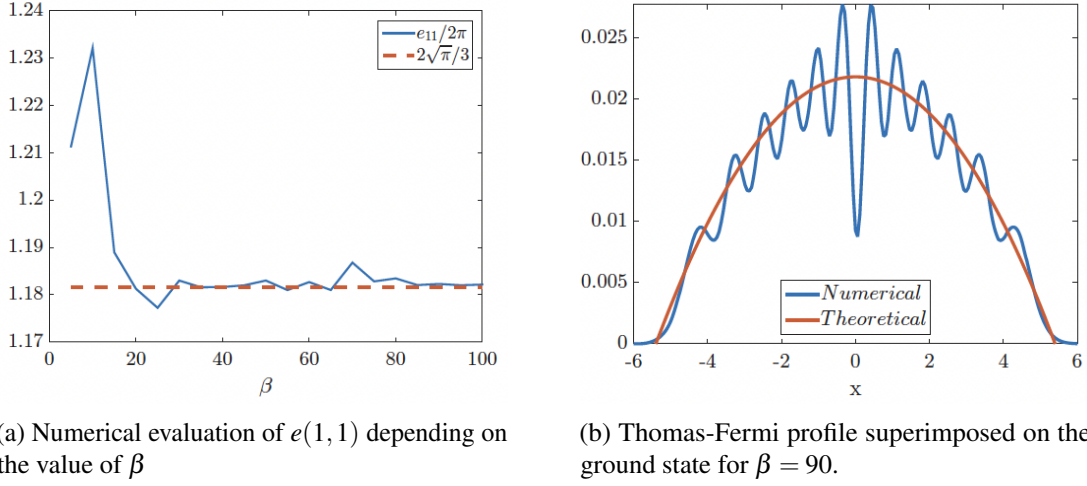


Figure 1.8: Evaluation of $e(1,1)$ and the resulting Thomas-Fermi profile.

Curved matter-wave guides

With the ever miniaturization of circuits, the experiments around atomic waves in guides and the transfer of ions between trap zones, the necessity of developing models for wave propagation in nearly one-dimensional curved geometries has emerged as a crucial concern. Since the pioneering works of Costa [29] as well as Goldstone and Jaffe [56], physicists have predominantly directed their attention towards employing an adiabatic approximation for an efficient one-dimensional approach. The drawback of this approach is that one needs to consider a weak or slow curvature. In [IDG], we investigate the problem of designing reflectionless and robust curved guides that are beyond the adiabatic approximation. The approach does not rely on an effective one-dimensional model but takes into account the real two-dimensional problem.

The coordinates of a material point using curvilinear coordinates is given by

$$x(s, y) = x_c(s) + yn(s),$$

where $x_c : \mathbb{R} \mapsto \mathbb{R}^2$ is the position along the path and $n : \mathbb{R} \mapsto \mathbb{R}^2$ is its local normal. In these coordinates, the Schrödinger equation of a particle (with mass $m \in \mathbb{R}^{+*}$) that is confined around a certain path by a transvers potential V_\perp writes as

$$i\hbar\partial_t\psi(t, s, y) = -\frac{\hbar^2}{2mh(s, y)} \left(\partial_y(h(s, y)\partial_y\psi(t, s, y)) + \partial_s \left(\frac{1}{h(s, y)} \partial_s \psi(t, s, y) \right) \right) + V_\perp(y)\psi(t, s, y), \quad (1.10)$$

where $h(s, y) = 1 - y\kappa(s)$ with $\kappa(s)$ the curvature of the path at s and $V_\perp(y) = \frac{1}{2}m\omega^2y^2$. Our goal is to devise the shape of a guide that connects two straight guides (see Figure 1.9). We can reduce this problem to finding the function κ (that describes the bent guide) that minimizes the amount of oscillations and reflections in the wave function as it goes from the input guide to the output one. This will be achieved by looking for smooth trajectory for the transverse coordinates.

To proceed, the idea is to return to the classical world and recall Newton's law

$$\begin{cases} \ddot{s}(1 - \kappa y) - \dot{s}(\dot{\kappa}y + 2\kappa\dot{y}) = 0, \\ \ddot{y} + \omega^2y + \dot{s}^2\kappa(1 - \kappa y) = 0, \end{cases} \quad (1.11)$$

where $\kappa(t) = \kappa(s(t))$. With these equations, we are able to recover the conservation of energy

$$\dot{y}^2 + \omega^2y^2 + v_\kappa^2 = \frac{2E}{m}, \quad (1.12)$$

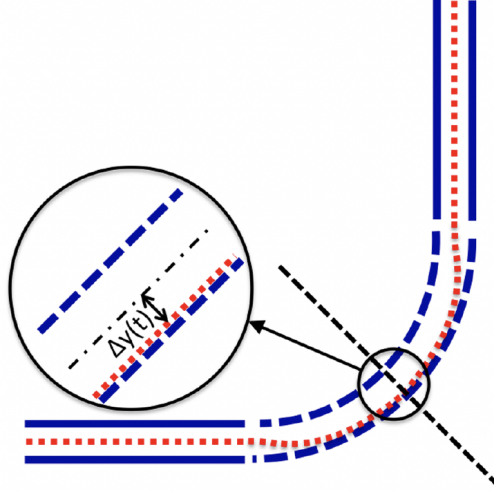


Figure 1.9: Illustration of the problem of tailoring the curvature of the bent waveguide.

where $v_\kappa = s(1 - \kappa y)$. Our approach will be symmetrical in the sense that we only build the trajectory $(s(t), y(t))$ up to a time T (where the particle reaches the middle of the guide) then symmetrize the path. The design of the guide (up to T) is done by finding a smooth function y that satisfies the following boundary conditions

$$y_{\text{sta}}(0) = 0, y_{\text{sta}}(T) = \delta y, \dot{y}_{\text{sta}}(0) = 0, \dot{y}_{\text{sta}}(T) = 0, \ddot{y}_{\text{sta}}(0) = 0 \quad \text{and} \quad \ddot{y}_{\text{sta}}(T) = 0,$$

then use Equation (1.12) to recover the function v_κ which then gives access to s and κ . These boundary conditions are required in order to ensure the continuity of the position and velocity in the middle of the guide as well as enforcing the stability of the trajectory at the end. The parameter δy is fixed later by the choice of the maximum curvature and the time T is determined by the desired angle of the bent (here $\pi/4$). From here, we define

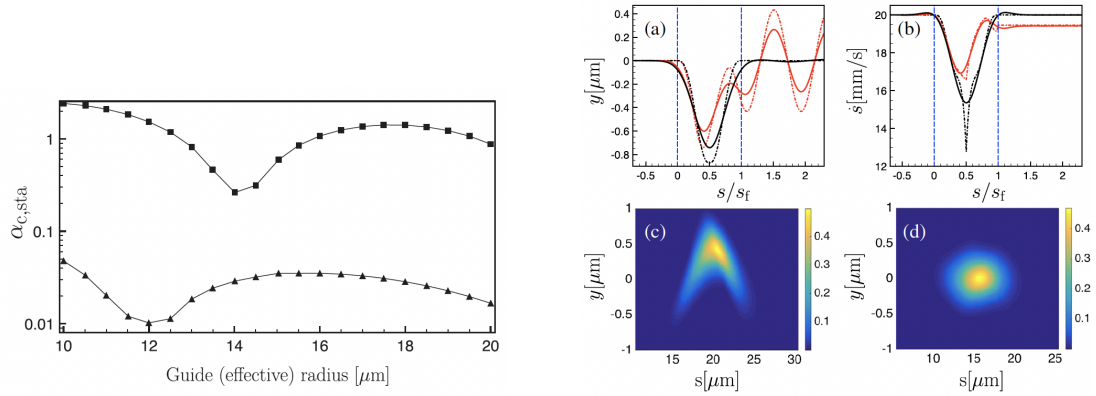
$$P(x) = \delta y(10x^3 - 15x^4 + 6x^5)$$

then set $y_{\text{sta}}(t) = P(t/T)$ for $t \in [0, T]$ then $y_{\text{sta}}(t) = P((1-t)/T)$ for $t \in [T, 2T]$. We notice that other choices are possible but this is the simplest. Let us also remark that, in the case of a simple of a quarter of circle, for a certain initial velocity \dot{s}_0 of a particle, there exists a discrete set of radii for which the transverse oscillations outside of the bend are suppressed. By testing our approach against a quarter of circle for initial velocities v in $[\dot{s}_0(1 - \varepsilon), \dot{s}_0(1 + \varepsilon)]$, with $\varepsilon = 5\%$, we compute the amplitude of the oscillations $a_c(v)$ for the quarter of circle and $a_{\text{stab}}(v)$ for our choice of shape. Then, we evaluate the averaged amplitude by

$$\alpha_{c,\text{sta}} = (2\varepsilon\dot{s}_0\sigma)^{-1} \int_{\dot{s}_0(1-\varepsilon)}^{\dot{s}_0(1+\varepsilon)} a_{c,\text{sta}}(v) dv,$$

where $\sigma = \sqrt{\hbar/m\omega}$ is the width, in the transverse direction, of the particle. The results, depending on the effective radius (which is the radius of the largest quarter circle enclosed within the chosen profile), are depicted in Figure 1.10a. Even in the case where the radius is the most favorable for the quarter of circle, our approach always yields oscillations that are at least 1 order of magnitude smaller.

We also investigated the comparison between the 2D model and the 1D adiabatic model. In the adiabatic limit, the longitudinal motion is independent from the transverse one. The effect of the bend are encapsulated in an effective attractive potential $s \mapsto V_{\text{eff}}(s)$, which is added in (1.11). From here, we use the same y_{sta} as in the 2D case and deduce a curvature for the bend that we



(a) Average oscillations after the turn in the guide for the engineered bend (triangles) and the quarter of circle (squares).

(b) .

Figure 1.10: Comparison with.

denote κ_{1D} (as opposed to the curvature in the 2D case which is denoted κ_{2D}). We simulated the passage of a particle in the guide in 2D by solving either Equations (1.11) or Equation (1.10) with the bend given by either κ_{1D} and κ_{2D} . The results can be found in Figure 1.10b where we see that the adiabatic approach leads to oscillations at the end of the guide as well as a loss of longitudinal velocity whereas our approach yields an excellent conservation of the profile of the particle as well as its velocity. These results also holds when we turn on interactions which can be explained by the quasi-particle behavior of the system.

2. Regularization by noise

2.1 Regularization in SDEs

Even if it does not have a precise definition, we call *regularization by noise* the way a random process improves the well-posedness of an evolution problem (ODE or PDE). This is done through the introduction, in the evolution problem, of a stochastic perturbation driven by a noise corresponding formally to the derivative of a random process. There are mostly two types of improvement one can expect: obtaining the uniqueness of solutions or avoid the emergence of singularities (*i.e.* obtaining the global existence of solutions). Here, we focus solely on achieving uniqueness. To begin with, let us consider a standard ODE in \mathbb{R}^d , for some $d \geq 1$,

$$X_t = \xi + \int_0^t b(s, X_s) ds, \quad (2.1)$$

where $\xi \in \mathbb{R}^d$ and $b : \mathbb{R}^+ \times \mathbb{R}^d \mapsto \mathbb{R}^d$ is a Borel function. Under the assumptions that b is continuous, Peano's theorem states that there exists a local continuous solution to (2.1). We remark that we consider here the classical notion of solution and one could also be interested in weaker forms of solutions as in the DiPerna and Lions approach [43] for instance. From here, we need additional hypothesis on b in order to deduce the uniqueness of the solution. A simple example is to assume the monotonicity of b , that is to assume that, for any $x, y \in \mathbb{R}^d$ and any $t \in \mathbb{R}^+$, $\langle x - y, b(t, x) - b(t, y) \rangle \leq 0$. However, the most common way is to assume that b is Lipschitz with respect to its second variable then use the Cauchy-Lipschitz theorem, *i.e.* we need some additional regularity on b . If this fails to be the case, one might end up with several possible solutions, as in the following example, where $d = 1$,

$$X_t = \int_0^t |X_s|^\alpha ds,$$

for $\alpha \in (0, 1)$, which admits solutions of the form

$$X_t = \begin{cases} 0, & \text{if } t \leq t_0, \\ \left(\frac{t-t_0}{\beta}\right)^\beta, & \text{if } t > t_0, \end{cases}$$

where $t_0 \geq 0$ and $\beta = 1/(1 - \alpha)$.

In the following, $(\Omega, \mathbb{P}, \mathcal{F})$ is a probability space equipped with a filtration $(\mathcal{F}_t)_{t \geq 0}$ that satisfies the usual conditions and W is a d -dimensional \mathcal{F}_t -adapted standard Brownian motion (also called

Wiener process). We consider the following SDE

$$X_t = \xi + \int_0^t b(s, X_s) ds + \int_0^t \sigma(s, X_s) dW_s, \quad \forall t \in \mathbb{R}^+, \quad (2.2)$$

where ξ is a \mathbb{R}^d -value random variable independent of \mathcal{F}_∞ and $b : \mathbb{R}^+ \times \mathbb{R}^d \mapsto \mathbb{R}^d$ and $\sigma : \mathbb{R}^+ \times \mathbb{R}^d \mapsto \mathbb{R}^{d \times d}$ are Borel-measurable functions. The second integral in the rhs of (2.2) is a stochastic integral (in the Itô sense) and Equation (2.2) can be understood as a noisy perturbation of Equation (2.1). As we will see, the assumptions needed for the existence and uniqueness of a solution can be quite different from the ones in the ODE theory. In order to properly define a solution X , we must provide (2.2) with the following requirements

$$\mathbb{P}[X_0 = \xi] = 1 \quad \text{and} \quad \mathbb{P} \left[\sum_{i=1}^d \int_0^t |b_i(s, X_s)| ds + \sum_{j=1}^d \int_0^t |\sigma_{i,j}(s, X_s)|^2 ds < \infty \right] = 1, \quad \forall t \in \mathbb{R}^+. \quad (2.3)$$

Before proceeding with the assumptions on b and σ to solve the Cauchy problem, we notice that there exists two notions of solutions to (2.2): *strong* solutions and *weak* solutions.

- Definition 2.1**
1. (Strong solution) Given a probability space $(\Omega, \mathbb{P}, \mathcal{F})$ equipped with a filtration $(\mathcal{F}_t)_{t \geq 0}$ (satisfying the usual conditions) and a d -dimensional \mathcal{F}_t -adapted standard Brownian motion W , a strong solution X of (2.2) is a continuous \mathcal{F}_t -adapted stochastic process such that (2.2)-(2.3) hold.
 2. (Weak solution) A weak solution is a triple $(X, W), (\Omega, \mathbb{P}, \mathcal{G})$ and $(\mathcal{G}_t)_{t \geq 0}$ where
 - a. $(\Omega, \mathbb{P}, \mathcal{G})$ is a probability space equipped,
 - b. $(\mathcal{G}_t)_{t \geq 0}$ is a filtration satisfying the usual conditions,
 - c. X is a continuous \mathcal{G}_t -adapted process and W is a d -dimensional \mathcal{G}_t -adapted standard Brownian motion such that (2.2)-(2.3) hold.

We immediately notice that a strong solution is a weak solution but the converse is not true in general and, thus, the hypothesis on b and σ to obtain the existence of weak solutions will be weaker than the ones for strong existence. There is one notable example that support this claim: Tanaka's equation, which is given by

$$X_t = \int_0^t \text{sgn}(X_s) dW_s,$$

admits a (non-unique) weak solution where X is a Wiener process. However, X cannot be a strong solution since the trajectory of W doesn't determine that of X . Indeed, it follows from Tanaka's formula that, for any $t \geq 0$,

$$W_t = |X_t| - \lim_{\varepsilon \rightarrow 0} \text{meas}\{s \in [0, t]; |X_s| \leq \varepsilon\},$$

so that, given $(W_s)_{0 \leq s \leq t}$, the sign of X_t is unknown.

It turns out that, under assumptions similar to Peano's theorem, that is $x \mapsto b(t, x)$ and $x \mapsto \sigma(t, x)$ are continuous for any $t \geq 0$, we only obtain the existence of weak solutions. This is due to the fact that, by mimicking the fixed-point arguments from the ODE theory, we do not obtain relative compactness in the space of continuous functions *via* Arzelà-Ascoli's theorem but *tightness* of probability measures which yields, thanks to Prokhorov's theorem, relative compactness in the weak topology of probability measures. From there, we can use Skorohod's representation theorem to construct a weak solution. There are also other strategies to build weak solutions and we briefly mention one of them since it provides another sets of assumptions on b and σ . It is based on Girsanov's theorem: given a probability space and a Wiener process Y started at $y \in \mathbb{R}^d$, we need Z given by

$$Z_t := \exp \left(\sum_{j=1}^d \int_0^t b_j(s, Y_s) dY_s - \frac{1}{2} \int_0^t |b(s, Y_s)|^2 ds \right), \quad \forall t \geq 0,$$

to be a martingale, for any $y \in \mathbb{R}^d$. A common criterion for this is Novikov's condition which holds if $b \in L^q(\mathbb{R}^+; L^p(\mathbb{R}^d))$ where $2/q + d/p < 1$ with $p \geq 2$ and $q > 2$ [65]. Then, after replacing y by ξ , Girsanov's theorem implies that, under a new probability measure, the process

$$W_t := Y_t - \xi - \int_0^t b(s, Y_s) ds,$$

is a Wiener process starting at 0. Then, we can see that Y is a weak solution of (2.2) with $\sigma \equiv 1$. In the end, we have the following result.

Proposition 2.1 Assume one of the following is verified

- $x \mapsto b(t, x)$ and $x \mapsto \sigma(t, x)$ are continuous for any $t \geq 0$,
- $b \in L^q(\mathbb{R}^+; L^p(\mathbb{R}^d))$ where $2/q + d/p < 1$ with $p \geq 2$ and $q > 2$ and $\sigma \equiv 1$.

Then, there exists a weak solution to (2.2).

From here, the remaining questions are: what about the uniqueness of the weak solutions? And the Cauchy problem for strong solutions? The answer for both of these questions lies in the concept of *pathwise uniqueness*.

Definition 2.2 We say that pathwise uniqueness holds if, for two weak solutions

$$\{(X, W), (\Omega, \mathbb{P}, \mathcal{F}), (\mathcal{F}_t)_{t \geq 0}\} \quad \text{and} \quad \{(\tilde{X}, \tilde{W}), (\Omega, \mathbb{P}, \tilde{\mathcal{F}}), (\tilde{\mathcal{F}}_t)_{t \geq 0}\}$$

where W is a Wiener process with respect to $(\mathcal{F}_t)_{t \geq 0}$ and $(\tilde{\mathcal{F}}_t)_{t \geq 0}$, we have

$$\mathbb{P}[X_0 = \tilde{X}_0] = 1 \quad \text{and} \quad \mathbb{P}[X_t = \tilde{X}_t, \forall t \geq 0] = 1. \quad (2.4)$$

Indeed, a result from Yamada and Watanabe [63, 90] states that pathwise uniqueness implies uniqueness in law from which we deduce the existence of strong solutions. Now, the thing is that *strong uniqueness*, that is (2.4) for strong solutions, can be obtained by the same arguments as for pathwise uniqueness. To conclude this section, the strategy that will be used to prove the regularization effect of noise in ODE will be to prove the existence of weak solutions then to prove pathwise uniqueness. This will provide the main arguments to deduce the existence and uniqueness of strong solutions.

The Zvonkin transformation

The first occurrence of the regularization by noise phenomenon is described in [93] where the author transform a SDE with a singular drift into a SDE with a more regular drift. This *Zvonkin transformation* is based on the following strategy. We suppose that

$$|\sigma(t, x) - \sigma(t, y)| \leq C_1 |x - y| \quad \text{and} \quad |b(t, x) - b(t, y)| \leq C_2 \rho(|x - y|), \quad \forall x, y \in \mathbb{R}^d, t \in \mathbb{R}^+,$$

with $\rho : \mathbb{R}^+ \mapsto \mathbb{R}^+$ satisfying $\int_0^\varepsilon \rho(r)/r dr < +\infty$ for any $\varepsilon > 0$. Moreover, we assume the uniform ellipticity of σ , that is there exists $\kappa > 0$ such that, for $a(t, x) := \sigma(x)\sigma(x)^*$, for any $(t, x) \in \mathbb{R}^+ \times \mathbb{R}^d$,

$$\xi \cdot (a(t, x)\xi) \geq \kappa |\xi|^2, \quad \forall \xi \in \mathbb{R}^d.$$

Under these assumptions, there exists weak solutions to (2.2) whose infinitesimal generator is

$$\mathcal{L}_{(t,x)}^X := \frac{1}{2} \sum_{j,k=1}^d a_{j,k}(t,x) \partial_{x_j} \partial_{x_k} + b(t,x) \cdot \nabla, \quad \forall (t,x) \in \mathbb{R}^+ \times \mathbb{R}^d,$$

and, in particular, the solution $F : \mathbb{R}^+ \times \mathbb{R}^d \mapsto \mathbb{R}^d$ to the backward parabolic equation

$$\begin{cases} \partial_t F(t, x) + \mathcal{L}_{(t,x)}^X F(t, x) = 0, \\ F(T, x) = x, \end{cases}$$

where $\mathcal{L}_{(t,x)}^X$ is applied on each components, is such that $F(t, \cdot)$ is a one-to-one mapping from \mathbb{R}^d to itself. Moreover, its second derivatives are bounded and the same holds for its inverse. Setting $Y_t := F(t, X_t)$ (and, thus, $X_t = F^{-1}(t, Y_t)$), one can see, by applying Itô's formula, that

$$\begin{aligned} Y_t &= F(0, x) + \int_0^t \left(\partial_t F(s, X_s) + \mathcal{L}_{(s, X_s)}^X F(s, X_s) \right) ds + \int_0^t \nabla F(s, X_s) \sigma(s, X_s) dW_s \\ &= F(0, x) + \int_0^t \sigma_Y(s, Y_s) dW_s, \end{aligned} \quad (2.5)$$

where $\sigma_Y(t, y) = \nabla F(t, F^{-1}(t, y)) \sigma(t, F^{-1}(t, y))$. In the previous equation, we have transformed the original SDE (2.2) and, somehow, removed the singular drift. We remark that Equation (2.5) is a well-posed SDE since σ_Y has the same regularity properties as σ and, as a consequence, the existence and uniqueness of a strong solution Y leads to the existence and uniqueness of a strong solution X . In [87], this approach was generalized for drifts that are only measurable and bounded. Then, in [65], the authors were able to consider unbounded drifts (but with $\sigma \equiv 1$) belonging in $L^q(\mathbb{R}^+; L^p(\mathbb{R}^d))$ where $2/q + d/p < 1$ with $p \geq 2$ and $q > 2$. This result was then extended in [91] to the case of a multiplicative noise.

In [48], a new technique, called the *Itô-Tanaka* trick, was introduced to transform the singular drift into a more regular drift (without having to introduce a new equation). To be more specific, for a certain $t > 0$, by considering the following backward parabolic equation

$$\begin{cases} \partial_r F(r, x) + \mathcal{L}_{(r,x)}^X F(r, x) = b(r, x), & \forall r \in [0, t], \\ F(t, x) = 0, \end{cases} \quad (2.6)$$

then Itô's formula yields

$$F(r, X_r) = F(0, X_0) + \int_0^r b(s, X_s) ds + \int_0^r \nabla F(s, X_s) dW_s,$$

which leads to

$$\int_0^t b(s, X_s) ds = -F(0, X_0) - \int_0^t \nabla F(s, X_s) dW_s. \quad (2.7)$$

In the previous relation, we can see that we transformed the singular drift into a sum of more regular terms with respect to X . Overall, the idea is to transfer the regularizing properties of the Kolmogorov equation associated to X to the singular drift.

The Young transformation

Another approach, initiated in [34] and extended in [21], consists in approximating the drift in order to benefit from the regularization properties of the Wiener process without relying on the Kolmogorov equation of X (with the drawback of having to set $\sigma \equiv 1$). If we consider the SDE with additive noise

$$X_t = X_0 + \int_0^t b(s, X_s) ds + W_t, \quad \forall t \geq 0, \quad (2.8)$$

then, by setting $Y = X - W$, we can see that Y is a solution of the following ODE with random drift

$$Y_t = X_0 + \int_0^t b(s, Y_s + W_s) ds, \quad \forall t \geq 0.$$

In order to use the regularization properties of W , we need to discretize the integral of the drift. Let $t > 0$ and $\Pi([0, t])$ be the set of subdivisions of $[0, t]$, *i.e.* for $\pi \in \Pi([0, t])$, π is a finite collection of essentially disjoint intervals whose union is $[0, t]$. Then, if $b \in \mathcal{C}(\mathbb{R}^+ \times \mathbb{R}^d; \mathbb{R}^d)$ and $Y \in \mathcal{C}(\mathbb{R}^+; \mathbb{R}^d)$, it turns out that, for any sequence $(\pi_n)_{n \in \mathbb{N}} \subset \Pi([0, t])$ such that $|\pi_n| := \max_{[u,v] \in \pi_n} |v - u| \rightarrow 0$ as $n \rightarrow \infty$, the drift can be approximated as

$$\lim_{n \rightarrow \infty} \sum_{[u,v] \in \pi_n} \int_u^v b(s, Y_u + W_s) ds = \int_0^t b(s, Y_s + W_s) ds.$$

By defining the *averaging operator* T^W such that, for any $[u, v] \in \pi$ and any $x \in \mathbb{R}^d$,

$$T_{u,v}^W b(x) := \int_u^v b(s, x + W_s) ds,$$

the previous ODE is again transformed into a *Young differential equation* (YDE)

$$Y_t = x + \int_0^t T_{ds}^W(Y_s), \quad (2.9)$$

where we consider the following Young integral as the drift

$$\int_0^t T_{ds}^W(Y_s) := \lim_{n \rightarrow \infty} \sum_{[u,v] \in \pi_n} \int_u^v b(s, Y_u + W_s) ds.$$

We remark that if b is continuous and we are able to prove that there exists a unique solution Y to (2.9), this leads to the existence and uniqueness of a solution X of (2.8). The regularization phenomenon will take place in the study of the averaging operator T^W . That is, by standard gaussian computations, we are able to prove that, for any $p \in \mathbb{N}^*$, $x, y \in \mathbb{R}^d$ and $[u, v] \in \mathbb{R}^+$,

$$\mathbb{E} \left[\left\| T_{u,v}^W b \right\|_{\mathcal{C}^{\alpha+\beta}(\mathbb{R}^d; \mathbb{R}^d)}^p \right]^{1/p} \leq C_p \|b\|_{\mathcal{C}(\mathbb{R}^+; \mathcal{C}^\beta(\mathbb{R}^d; \mathbb{R}^d))} |v - u|^{1-\alpha/2},$$

with $\beta \geq 0$ and $\alpha \in (0, 2)$. Then, thanks to the Garsia-Rodemich-Rumsey lemma, we deduce that the following estimate holds almost surely

$$\|T_{u,v}^W b\|_{\mathcal{C}^{\alpha+\beta}(\mathbb{R}^d; \mathbb{R}^d)} \leq \kappa \|b\|_{\mathcal{C}(\mathbb{R}^+; \mathcal{C}^\beta(\mathbb{R}^d; \mathbb{R}^d))} |v - u|^{1-\alpha/2-1/p}, \quad (2.10)$$

for a positive $\kappa \in L^p(\Omega)$. It turns out that, with the help of Young's theory of integration, we are able to prove that (2.9) admits a unique solution under the condition that $\beta > 0$ by taking p large enough. We notice that this approach is easily extended to the case where W is not a Wiener process anymore. In fact, this was the main purpose of using this strategy in [21] where the authors considered a fractional brownian motion. In practice, one essentially needs to be able to deduce an estimate similar to (2.10).

Regularization of random functions

In [DR1], we proved a regularization by noise phenomenon in the case where b is a random function which was left as an open problem in [48]. The main difficulty when dealing with random functions is that there are simple counter-examples to the regularization phenomenon. That is, the Itô-Tanaka trick used in [48] fails to work for instance if we consider $X = W$ a Wiener process and $b(t, x) = f(t, x - W_t)$ where f is a deterministic function. Indeed, this yields in fact

$$\int_0^t b(s, W_s) ds = \int_0^t f(s, 0) ds,$$

so that we do not expect to obtain any regularizing phenomenon due to W . The main issue when trying to derive the Itô-Tanaka trick, if one follows the same arguments as in the deterministic drift case, is that we need the solution F which solve the backward parabolic equation (2.6) where b appears in the operator $\mathcal{L}_{(s,x)}^X$ as well as in the right-hand side. If b is adapted to the filtration of the Wiener process (denoted $(\mathcal{F}_s^W)_{s \geq 0}$), it turns out that F is \mathcal{F}_t^W -measurable so that the stochastic integral in (2.7) will be ill-posed since F needs to be adapted with respect to $(\mathcal{F}_s^W)_{s \geq 0}$.

This problem can be circumvented by replacing (2.6) with the backward stochastic partial differential equation

$$F(r, x) = \int_r^t \left(\mathcal{L}_{(s,x)}^X F(s, x) - b(s, x) \right) ds - \int_r^t Z(s, x) dW_s, \quad \forall r \in [0, t], \quad (2.11)$$

where we need to find the couple (F, Z) that are $(\mathcal{F}_s^W)_{s \geq 0}$ -adapted stochastic fields. Such equations were already studied in the literature but few investigated the regularity properties of F and Z that we need in order to prove the regularization. Incidentally, we proved a new Itô-Tanaka trick as well as a new result on the Cauchy problem of (2.11) under the following assumptions.

■ **Notation 2.1** We denote $W^{m,p}$, $m \in \mathbb{R}^+$ and $p \geq 1$, the Sobolev space defined as

$$W^{m,p} := \left\{ \phi \in L^p(\mathbb{R}^d); \mathfrak{F}^{-1} \left((1 + |\xi|^2)^{m/2} \phi(\xi) \right) \in L^p(\mathbb{R}^d) \right\},$$

where \mathfrak{F} (resp. \mathfrak{F}^{-1}) is the (resp. inverse) Fourier transform, endowed with the norm $\|\phi\|_{W^{m,p}} := \|\mathfrak{F}^{-1}((1 + |\xi|^2)^{m/2} \mathfrak{F}(\phi))\|_{L^p(\mathbb{R}^d)}$, and define, for a certain $T > 0$, $\mathbb{D}^{1,m,p}$ as a Banach space of $(\mathcal{F}_s^W)_{s \in [0, T]}$ -adapted stochastic fields equipped with the norm

$$\|\phi\|_{\mathbb{D}^{1,m,p}}^p := \mathbb{E} [\|\phi\|_{W^{m,p}}^p] + \int_0^T \mathbb{E} [\|D_\theta \phi\|_{W^{m,p}}^p] d\theta,$$

where D is the Malliavin derivative. We also denote $\mathbb{D}_q^{1,m,p} := L^q([0, T]; \mathbb{D}^{1,m,p})$, for any $q > 1$, as well as $\mathbb{W}^{m,p} := L^p(\Omega; W^{m,p})$ and $\mathbb{W}_q^{m,p} = L^q([0, T]; \mathbb{W}^{m,p})$ which are all Banach spaces endowed with their (straightforward) norms.

We can now state the *Itô-Wentzell-Tanaka* trick that we derived.

Theorem 2.1 Let $\gamma \in \{0, 1\}$, $\alpha > \gamma/2$ and $\ell, \bar{\ell} \in [p, \infty]$ such that $1/\ell + 1/\bar{\ell} = 1/p$. We assume that f and b belong to $\mathbb{D}_q^{1,0,p}$ and that:

- i) there exist a function $f' \in L^q([0, T]; L^\ell(\Omega; W^{-\gamma,p}(\mathbb{R}^d)))$, a function $b' \in L^q([0, T]; L^p(\Omega \times \mathbb{R}^d))$ and two mappings $\mathbf{v}_f \in L^{\bar{\ell}}(\Omega; L^\infty([0, T] \times \mathbb{R}^d))$, $\mathbf{v}_b \in L^\infty([0, T] \times \mathbb{R}^d)$ such that

$$D_\theta f(t, x) = f'(t, x) \mathbf{v}_f(\theta, t), \quad \forall \theta \leq t \leq T, \mathbb{P} - a.s.,$$

and $D_\theta b(t, x) = b'(t, x) \mathbf{v}_b(\theta, t), \quad \forall \theta \leq t \leq T, \mathbb{P} - a.s.,$

- ii.a) one of the following statement is in force

- there exist $C_{1,f}, C_{2,f} > 0$ such that, $\forall 0 \leq \theta \leq s \leq t \leq T$,

$$\|\mathbf{v}_f(\theta, t)\|_{L^{\bar{\ell}}(\Omega)} \leq C_{1,f} |\theta - t|^\alpha,$$

$$\|\mathbf{v}_f(\theta, s) - \mathbf{v}_f(t, s)\|_{L^{\bar{\ell}}(\Omega)} \leq C_{2,f} |\theta - t|^\alpha.$$

- $\gamma = 0$ and $\mathbf{v}_f(\theta, t) = \mathbf{1}_{\{\theta \leq \tau_f\}}$ where τ_f is a random variable with values in $[0, t]$,

- ii.b) one of the following statement is in force

- there exist $C_{1,b}, C_{2,b} > 0$ such that, $\forall 0 \leq \theta \leq s \leq t \leq T$,

$$|\mathbf{v}_b(\theta, t)| \leq C_{1,b} |\theta - t|^\alpha,$$

$$|\mathbf{v}_b(\theta, s) - \mathbf{v}_b(t, s)| \leq C_{2,b} |\theta - t|^\alpha,$$

- $\gamma = 0$ and $\mathbf{v}_b(\theta, t) = \mathbf{1}_{\{\theta \leq \tau_b\}}$ where τ_b is a random variable with values in $[0, t]$,

- iii) there exists a function $\tilde{b} \in L^q([0, T])$ such that

$$\|b(t, \cdot)\|_{L^p(\mathbb{R}^d)} + \|b'(t, \cdot)\|_{L^p(\mathbb{R}^d)} \leq \tilde{b}(t), \quad \forall t \in [0, T], \mathbb{P} - a.s..$$

Moreover, if $\gamma = 1$, we also assume that

$$\|\nabla b(t, \cdot)\|_{L^p(\mathbb{R}^d)} \leq \tilde{b}(t), \quad \forall t \in [0, T], \mathbb{P} - a.s..$$

Then, there exists a unique strong (adapted) solution (F, Z) to (2.11) that belongs in $(\mathbb{W}_q^{m,p})^2$

and the following relation holds

$$\begin{aligned} \int_0^T f(s, X_s) ds &= -F(0, X_0) - \int_0^T (\nabla F(s, X_s) + Z(s, X_s)) dW_s \\ &\quad - \int_0^T \nabla \cdot Z(s, X_s) ds, \quad \mathbb{P} - a.s. \end{aligned} \quad (2.12)$$

Thanks to (2.12) and following similar arguments as in [48], we are able to prove pathwise uniqueness of solutions for (2.2) when b is random. Furthermore, in the previous assumptions on f and b , we can see that there is a remarkable relation between the space regularity of f' and b' and the time regularity of v_f and v_b stemming from the chain rule of the Malliavin derivative. Finally, we mention that it should be possible to extend this result for $\sigma \neq 1$ under strict ellipticity assumptions.

The Itô-Wentzell-Tanaka trick was also revisited for non-semimartingales in [CDR] where we considered the case of the fractional brownian motion. The main issue to obtain such a result is that can not rely on Itô calculus anymore. However, we were able to tackle this by using the Clark-Ocone formula which turns out to be related to the Itô-Tanaka trick in the case $X = W$. Indeed, given a probability space endowed with the brownian filtration $\{\mathcal{F}_t\}_{t \in \mathbb{R}}$, the Clark-Ocone formula reads, for $F \in L^2(\Omega)$ that is \mathcal{F}_t -adapted, for some $t \geq 0$, and any $s \in [0, t]$,

$$F = \mathbb{E}[F | \mathcal{F}_s] + \int_s^t \mathbb{E}[D_r F | \mathcal{F}_r] dW_r,$$

which yields, when taking $F = b(t, W_t)$ and for $s = 0$,

$$b(t, W_t) = P_t b(t, W_0) + \int_0^t \nabla P_{t-r} b(t, W_r) dW_r,$$

where $\{P_t\}_{t \geq 0}$ is the heat semigroup. From here, we can integrate with respect to t and deduce

$$\begin{aligned} \int_0^T b(t, W_t) dt &= \int_0^T P_t b(t, W_0) dt + \int_0^T \int_0^t \nabla P_{t-r} b(t, W_r) dW_r dt \\ &= \int_0^T P_t b(t, W_0) dt + \int_0^T \int_t^T \nabla P_{r-t} b(r, W_t) dr dW_t \\ &= -F(0, W_0) - \int_0^T F(t, W_t) dW_t, \end{aligned}$$

which is exactly (2.7) by realizing that $F(t, x) = -\int_t^T P_{s-t} b(s, x) ds$ is the solution of the backward heat equation with b as a source term. We can also apply these steps when W is replaced with a fractional brownian motion W^H with Hurst index $H \in (0, 1)$, which is given, for any $t \geq 0$, by

$$W_t^H = W_0^H + \frac{1}{\Gamma(H + 1/2)} \int_{-\infty}^t \left((t-s)^{H-1/2} - (-s)_+^{H-1/2} \right) dW_s.$$

By apply the same steps as for W , it follows that

$$\int_0^T b(t, W_t^H) dt = \int_0^T P_{t^{2H}} b(t, W_0^H) dt + \int_0^T \int_t^T \nabla P_{(r-t)^{2H}} b(r, W_{t,r}^{2,H}) \frac{(r-t)^{H-1/2}}{\Gamma(H + 1/2)} dr dW_t,$$

where $W_{t,r}^{2,H} = \mathbb{E}[W_r^H | \mathcal{F}_t]$. In the previous relation, it is not possible to identify a solution of a backward heat-like equation since W^H is not Markov but we can still leverage the regularization properties of P and deduce a regularization phenomenon. Let us remark that, when b is random, it is not possible to obtain such result. In order to do so, we rely on a careful discretization of the integral with respect to t and we prove the following result.

Theorem 2.2 Let $b : \Omega \times [0, T] \times \mathbb{R}^d \mapsto \mathbb{R}$ be an adapted random field such that $b \in \mathbb{D}_q^{1, m-\alpha, p}$ with $m, \alpha \in \mathbb{R}$ and $p \geq 2$ verifying

$$1/2 - H\alpha - 1/p > 0.$$

Then, the following relation holds, for any $t \in [0, T]$ and $x \in \mathbb{R}^d$,

$$\begin{aligned} \int_0^t b(s, x + W_s^H) ds &= \int_0^t P_{s^{2H}} b(s, x + W_s^H) ds \\ &+ \int_0^t \int_s^t \nabla P_{r-s^{2H}} b^a(r, s, x + W_{s,r}^{2,H}) \frac{(r-s)^{H-1/2}}{\Gamma(H+1/2)} dr dW_s \\ &+ \int_0^t \int_s^t \operatorname{div}(P_{r-s^{2H}} b^m(r, s, x + W_{s,r}^{2,H})) \frac{(r-s)^{H-1/2}}{\Gamma(H+1/2)} dr ds \\ &+ \int_0^t \int_s^t P_{r-s^{2H}} b^m(r, s, x + W_{s,r}^{2,H}) \frac{(r-s)^{H-1/2}}{\Gamma(H+1/2)} dr dW_s, \end{aligned}$$

where we denoted

$$b^a(r, s, x) = \mathbb{E}[b(s, x) | \mathcal{F}_r] \quad \text{and} \quad b^m(r, s, x) = \mathbb{E}[D_r b(s, x) | \mathcal{F}_r].$$

From here, we can not proceed as in the semi-martingale case since we used the regularization properties of W^H and not the ones from X , the solution of (2.2) with $\sigma \equiv 1$ and W replaced by W^H . Thus, we rely on the Young transformation and the averaging operator

$$T_{u,v}^{W^H} b(x) := \int_u^v b(s, x + W_s^H) ds,$$

and, by using the previous Theorem, we are able to prove the existence and uniqueness of a solution to the associated YDE (2.9).

Proposition 2.2 Let $\ell, q \in (2, +\infty)$, $p \in [2, +\infty)$, $k \in \mathbb{R}$, $\iota \in [0, 1]$ and $\sigma, \bar{\sigma} \in [\ell, +\infty]$ such that

$$\frac{1}{2} - \frac{1}{\ell} - \frac{1}{q} > 0, \quad \frac{1}{H} \left(\frac{1}{2} - \frac{1}{\ell} - \frac{1}{q} \right) + k - 2 - \frac{d}{p} > 0 \quad \text{and} \quad \frac{1}{\sigma} + \frac{1}{\bar{\sigma}} = \frac{1}{\ell}. \quad (2.13)$$

We assume that b is an adapted function which belongs to $L^\ell(\Omega; L^q([0, T]; W^{k,p}(\mathbb{R}^d)))$ and that:

1. there exist a function a function $b' \in L^\sigma(\Omega; L^q([0, T]; L^\infty([0, T]; W^{k-\iota, p}(\mathbb{R}^{d \times d})))$ and a mapping $v \in L^{\bar{\sigma}}(\Omega; L^\infty([0, T] \times \mathbb{R}^{d \times d}))$ such that

$$D_\theta b(t, x) = b'(t, \theta, x) v(\theta, t), \quad \forall \theta \leq t \leq T, \mathbb{P} - a.s.,$$

where, $\forall t \in [0, T]$, $b'(t, \theta, x)$ is \mathcal{F}_t -adapted for any $x \in \mathbb{R}^d$ and $v(\theta, t)$ is a \mathcal{F}_t adapted function for any $0 \leq \theta \leq t$,

2. there exists $C_1 \in L^{\bar{\sigma}}(\Omega; \mathbb{R}^{+*})$ such that one of the following statement is in force
 - for any $0 \leq \theta \leq s \leq t \leq T$,

$$|v(\theta, t)| \leq C_1 |\theta - t|^{H\iota},$$

- $\iota = 0$ and $v(\theta, t) = C_1 \mathbf{1}_{\{\theta \leq \tau_b\}}$ where τ_b is a random variable with values in $[0, t]$,

Then, there exists a unique solution $Y \in \mathcal{C}^\beta([0, T])$, for some $\beta > 1/2$, to (2.9).

2.2 Regularization in randomly modulated PDEs

Until now, we have mostly discussed the regularization phenomenon for ODEs. In the context of PDEs, a large portion of the literature treats the linear equations. Among the nonlinear PDEs that were investigated, let us mention general SPDEs [30], Burger equation [60], scalar conservation laws [23, 52, 53], Hamilton-Jacobi equations [51], p -Laplace equations [13] and fluid mechanics [49, 50]. The class of equations that interest us in this section is the so-called *randomly modulated* PDEs. Example of such equations are: the nonlinear Schrödinger (NLS) equation [25, 35, 36], the Korteweg-de Vries (KdV) equation [24] and the Benjamin-Bona-Mahony equation [22]. The latter equation is a bit particular so we'll focus on the two first ones in dimension $d = 1$. These equations can be written as, for any $t \in \mathbb{R}^+$ and $u_0 \in W^{s,p}(\mathbb{R})$ for some $s \geq 0$ and $p \geq 2$,

$$u_t = u_0 + \int_0^t iP(i\partial_x)u_s \circ dW_s + \int_0^t F(u_s)ds, \quad (2.14)$$

where P is a real polynomial that is either $P(\xi) = |\xi|^2$ or of degree greater than 3, W is a standard brownian motion (and the previous integral is Stratonovich's one) and F is a nonlinearity that is either $F(v) = \partial_x(v^k)$ with $k \in \mathbb{N}$, for the KdV equation, or $F(v) = |v|^{2\sigma}v$ with $\sigma \geq 0$, for the NLS equation. Here, we're interested in proving the Cauchy problem. In [35], the authors were able to solve the Cauchy problem for NLS under the same hypothesis as in the deterministic case (*i.e.* when $W_t \equiv t$). This was then extended in [36] where it is shown that, in the so-called L^2 -critical case, $\sigma = 2$, the solutions are global. This is in contrast to the deterministic case where solutions are known to blow-up in finite time and, thus, suggest a regularization by noise phenomenon. These result were extended in [24, 25] for the NLS and KdV equations where the authors use a Young transformation to deal with the case where W is a fractional brownian motion as well as the periodic setting. For the NLS equation, they solve the Cauchy problem under the same hypothesis as in [36] but with a fractional brownian motion with Hurst index below $1/2$.

A standard way to tackle the Cauchy problem for (2.14) is to consider the *mild* formulation of (2.14) which is

$$u_t = e^{iP(i\partial_x)W_t}u_0 + \int_0^t e^{iP(i\partial_x)(W_t - W_s)}F(u_s)ds, \quad (2.15)$$

then to proceed with a fixed-point argument in a suitable functional space. To do so, we need to use estimates that relies on the dispersive properties of $\{e^{iP(i\partial_x)W_t}\}_{t \geq 0}$, and among them are (local) Strichartz estimates which are well-known in the deterministic setting. The first step to prove these is to notice that, for any $\tau \in \mathbb{R}$ and $v \in L^{p'}(\mathbb{R})$, for some $p \geq 2$,

$$\left\| |i\partial_x|^\alpha e^{iP(i\partial_x)\tau}v \right\|_{L^p(\mathbb{R})} \lesssim |\tau|^{-\beta} \|v\|_{L^{p'}(\mathbb{R})}$$

with $1/p + 1/p' = 1$ and $|i\partial_x|^\alpha u = \mathcal{F}^{-1}(|\xi|^\alpha \hat{u})$, for some $\alpha \geq 0$. In the NLS case, this is obtained with $\alpha = 0$ and $\beta = 1/2 - d/2$ by the Hausdorff-Young inequality and an interpolation. For the KdV case, we refer the reader to [28] where the result is proved with $\alpha = \gamma(1 - 2/p)$ and $\beta = (1 - 2/p)(\gamma + 1)/m$ where $-1 \leq \gamma \leq (m - 2)/2$ and $m \geq 3$ is the degree of P . From here, one usually proceed by integrating with respect to time and deduce the local Strichartz estimates. To handle the potential $|\tau|^{-\beta}$, we need the Hardy-Littlewood-Sobolev inequality. This inequality is well-known in the deterministic case and, in [DR2], we prove a stochastic version of it for the fractional brownian motion.

Theorem 2.3 Let $(W_t^H)_{t \geq 0}$ be a fractional brownian motion of Hurst index $H \in (0, 1)$, $\beta \in (0, 1 - H)$, $p, q \in (1, \infty)$ and $\alpha \in (0, 1)$ such that

$$2 - \alpha = \frac{1}{p} + \frac{1}{q}.$$

Then, there exist $T > 0$ and $C > 0$ such that, \mathbb{P} -a.s., $\forall f \in L^p([0, T])$, $\forall g \in L^q([0, T])$ the following inequality holds

$$\left| \int_0^T \int_0^T f(t) |W_t^H - W_s^H|^{-\alpha} g(s) ds dt \right| \leq CT^{\alpha\beta} \|f\|_{L^p([0, T])} \|g\|_{L^q([0, T])}.$$

The difference between the deterministic and stochastic version (and, thus, the key to the regularization effect) lies in the presence of the term $T^{\alpha\beta}$ on the right-hand-side. This enables us to derive Strichartz estimates for $\left\{ e^{iP(i\partial_x)W_t^H} \right\}_{t \geq 0}$ which have better contraction properties for our fixed-point argument. With this, we can show that the results from [25, 36] extends to the fractional brownian motion for any Hurst index. Even though we solely focused on the NLS equation, this inequality may prove useful for other randomly modulated equations.

2.3 Regularization for rough differential equations

A natural generalization of the Brownian motion is the fractional Brownian motion that we already mentioned in Section 2.1. Thus, one could be interested in knowing if the regularization effect due to the presence of the diffusion term in SDEs still stands when the Brownian motion is replaced by a fractional Brownian motion. In the additive case, the answer was given in [21]. However, the multiplicative case was left open. The difficulty stems mainly from the two facts: the fractional Brownian motion is not markovian as well as its (nonlinear) interplay with the solution in the integral. Furthermore, one has to be careful when handling the latter. If the Hurst parameter H is greater than $1/2$, then we can rely on Young's integration theory, which is quite convenient. However, if H is below $1/2$, the approach is a bit more complicated and we need the help of the *rough path* theory developed by T. Lyons [74].

A first approach to tackle this question, for $H \in (1/3, 1/2]$, was given in [8] where the authors rely on the Lamperti transform in order to fall back to the additive case and use the arguments from [21]. However, the transformation requires that σ , in (2.2), is such that σ^{-1} is a conservative field. Apart from the one dimensional case, this is a stronger assumption that one would expect, *i.e.* some regularity and uniform ellipticity. In [CD], we investigate the problem by using a flow transformation coupled with Malliavin calculus. This enables us to not only obtain results for the fractional Brownian motion with $H \in (1/4, 1/2)$ but also for more general Gaussian rough paths. Let us mention that while the completing the paper, another article with similar results came up [33] where the strategy employed by the authors is completely different from ours. The flow that we consider is the one that is given by the following equation (which essentially corresponds to the 'regularizing' part of (2.2))

$$Y_t = Y_0 + \int_0^t \sigma(Y_s) d\mathbf{W}_s, \quad (2.16)$$

where \mathbf{W} is a gaussian rough path, which we denote ϕ . Then, the solution X of (2.2) (with W replaced by a fractional Brownian motion) writes as

$$X_t = \phi(t, Z_t),$$

where Z is a solution of the ODE

$$Z_t = \xi + \int_0^t (\nabla \phi(s, Z_s))^{-1} b(\phi(s, Z_s)) ds. \quad (2.17)$$

The idea from here is to exploit the regularizing properties of ϕ thanks to a Young transformation

(as in Section 2.1) given by the averaging field

$$\begin{aligned} T_{s,t}b(x) &= \int_s^t (\nabla\phi(r,x))^{-1}b(\phi(r,x))dr \\ &= \int_s^t \mathbb{E} [(\nabla\phi(r,x))^{-1}b(\phi(r,x)) | \mathcal{F}_s] dr \\ &\quad + \int_s^t ((\nabla\phi(r,x))^{-1}b(\phi(r,x)) - \mathbb{E} [(\nabla\phi(r,x))^{-1}b(\phi(r,x)) | \mathcal{F}_s]) dr. \end{aligned}$$

The remaining question is to obtain the regularization effect of ϕ . By using some clever martingale estimates, we essentially have to show the regularization of the operator

$$T_{s,t}^{(1)}b(x) = \int_s^t \mathbb{E} [(\nabla\phi(r,x))^{-1}b(\phi(r,x)) | \mathcal{F}_s] dr.$$

Due to the expression of the averaging field, we are not in position to use any of the tools from [21]. Our approach is based on the integration by parts from Malliavin calculus. Indeed, for some \mathbb{R}^d -valued random variable F which is Malliavin differentiable and $f : \mathbb{R}^d \mapsto \mathbb{R}$ some smooth function, we have

$$D(f(F)) = \sum_{k=1}^d \partial_k f(F) DF_k,$$

which yields the relation, for any $k \in \{1, \dots, d\}$

$$\nabla f(F) = \langle D(f(F)), (\gamma_F)^{-1} DF \rangle_{\mathcal{H}},$$

where \mathcal{H} is the Hilbert space associated to the underlying gaussian process and γ_F is the covariance matrix associated to F . Thanks to this relation and the integration by parts of the Malliavin derivative, we are able to prove that, for any $[s, t] \subset \mathbb{R}^+$, if F is \mathcal{F}_t -measurable,

$$\mathbb{E} [\nabla f(F) | \mathcal{F}_s] = \mathbb{E} [f(F) \delta_{[s,t]}(R(s,t)) | \mathcal{F}_s],$$

for some random variable $R(s,t)$ which depends on γ_F and DF , where $\delta_{[s,t]}$ is the Skorokhod integral. With this relation, we can show that, for $r \leq s$,

$$\mathbb{E} [\nabla b(\phi(s,x)) | \mathcal{F}_r] = \mathbb{E} [H_{r,s}(x)b(\phi(s,x)) | \mathcal{F}_r],$$

where H is a function that satisfies, formally, an estimate of the type

$$\|H_{r,s}(x)\|_{L^p(\Omega)} \lesssim (s-r)^{-H}.$$

With these arguments at hand and under some additional assumptions (notably the ellipticity of σ and the local non-determinism of driving process), we are able to prove the following result.

Theorem 2.4 Let $p \in (2, 4)$ and W be a Gaussian process which can be lifted into a geometric p -rough path whose index of non-determinism is denoted $\alpha > 0$. Assume that σ belongs to $\mathcal{C}_b^\infty(\mathbb{R}^d; \mathbb{R}^{d \times d})$ and is uniformly elliptic and that b belongs in $\mathcal{C}^\kappa(\mathbb{R}^d; \mathbb{R}^d)$ with $\kappa + 1/\alpha > 1/2$. Then, almost surely, there exists a unique solution to Equation (2.2).

3. Quantum entropy minimization

3.1 Quantum hydrodynamics from first principles

Classical hydrodynamic theories

Suppose that you wish to model the evolution of a system of N (classical, interacting and identical) particles, with $N \geq 2$, evolving in \mathbb{R}^d . Thanks to Hamiltonian mechanics, the microscopic evolution of such system is described thanks to its underlying Hamiltonian, denoted $H : \mathbb{R}^{2 \times d \times N} \mapsto \mathbb{R}$, which depends on phase-space coordinates (x, p) where $x \in \mathbb{R}^{d \times N}$ corresponds to the positions of each particles and $p \in \mathbb{R}^{d \times N}$ corresponds to their momenta. For instance, we could consider a classical Hamiltonian of the form

$$H(x, p) = H_0(x, p) + V_{\text{int}}(x), \quad (3.1)$$

where $H_0(x, p) := \frac{1}{2}|p|^2 + V_{\text{ext}}(x)$ (the first term is the kinetic energy and the second term is an external potential, e.g. a quadratic potential $V_{\text{ext}}(x) = \frac{1}{2}|x|^2$) and the last term is an interaction potential given by a two-body interaction

$$V_{\text{int}}(x) = \sum_{j>k \geq 1}^N W_{\text{int}}(x_j - x_k).$$

The function $W_{\text{int}} : \mathbb{R} \mapsto \mathbb{R}$ is an even function which can be, for example, the Coulomb potential

$$W_{\text{E}}(x) = \frac{q}{4\pi\epsilon_0} \frac{1}{|x|},$$

where q is the electric charge of the particles and ϵ_0 is the permittivity of vacuum. The evolution of the system is then given by the function $t \mapsto (x(t), p(t))$ which is a solution of Hamilton's equations

$$\begin{cases} \partial_t x(t) = \nabla_p H(x(t), p(t)), \\ \partial_t p(t) = -\nabla_x H(x(t), p(t)), \end{cases}$$

starting from an initial state $(x(0), p(0)) = (x_0, p_0) \in \mathbb{R}^{2 \times d \times N}$. One can remark that

1. the Hamiltonian is preserved along the trajectories (i.e. $H(x(t), p(t)) = H(x_0, p_0)$ for any $t \geq 0$),
2. Hamilton's equations are reversible: there exists an inversive function $\Phi : (t, x, p) \in \mathbb{R}^+ \times \mathbb{R}^{2 \times d \times N} \mapsto \Phi_t(x, p) \in \mathbb{R}^{2 \times d \times N}$ such that $(x(t), p(t)) = \Phi_t(x_0, p_0)$ which verifies $(x_0, p_0) = \Phi_t^{-1}(x(t), p(t))$.

With the exception of the interaction potential, this microscopic description, through Hamilton's equations, relies on fundamental physical principles and, as such, is the most precise model one could hope for. The price of this precision lies in its extreme complexity when considering a large number of particles which makes it hard to gather useful informations on the system. Furthermore, the numerical simulation of the system through the phase-space coordinates amounts to solve a nonlinear system of $2 \times d \times N$ ODEs which is very costly. It is therefore natural to look for simpler models that describes the evolution of physical (macroscopic) quantities of interest of the system with fewer degrees of freedom. This is the purpose of what is known as kinetic theory.

The idea behind kinetic theory is to model the system by a phase-space distribution function, that is a function $f : (t, x, p) \in \mathbb{R}^+ \times \mathbb{R}^{2 \times d} \mapsto \mathbb{R}^+$ depending on the time $t \geq 0$ and the phase-space coordinates $(x, p) \in \mathbb{R}^{2 \times d}$. By introducing the empirical measure of the particles μ^N then one expect that, under appropriate assumptions on the system, the following weak convergence holds

$$\mu^N(t, x, p) = \frac{1}{N} \sum_{j=1}^N \delta_{(x,p)}(x_j(t), p_j(t)) \xrightarrow{N \rightarrow +\infty} f(t, x, p) dx dp,$$

where $\delta_{(x,p)}$ is the Dirac delta located at (x, p) . This description is based on the following interpretation: when $N \rightarrow +\infty$, there are so many particles in the system that one can see it as a continuum and we can reduce ourselves to a macroscopic (or mean-field) description where we are not really interested in the individual phase-space coordinates of each particles in the system but in the density of particles in the phase-space. One striking point of f is that its moments corresponds to physical quantities. Three of the most famous ones are:

1. the local density n given by

$$n(t, x) = \int_{\mathbb{R}^d} f(t, x, p) dp, \quad (3.2)$$

2. the local current u given by

$$n(t, x)u(t, x) = \int_{\mathbb{R}^d} p f(t, x, p) dp, \quad (3.3)$$

3. the local kinetic energy w given by

$$w(t, x) = \frac{1}{2} \int_{\mathbb{R}^d} |p|^2 f(t, x, p) dp. \quad (3.4)$$

In order to derive the evolution of f (and since there's no interactions), we make a mean-field assumption and consider a system of a single particle. Then, we use Liouville's theorem which states that the phase-space distribution function f is constant along the trajectories of the system. This translates to $\frac{d}{dt}(f(t, \Phi_t(x, p))) = 0$ and gives rise to the transport equation

$$\begin{cases} \partial_t f(t, x, p) + \{H_0(x, p), f(t, x, p)\} = 0, \\ f(0, x, p) = f_0(x, p), \end{cases} \quad (3.5)$$

with the Poisson bracket $\{g(x, p), h(x, p)\} = \nabla_x g(x, p) \cdot \nabla_p h(x, p) - \nabla_p g(x, p) \cdot \nabla_x h(x, p)$. The initial data f_0 is, thus, the initial distribution of the density (in phase-space) of the system. If we wish to add an interaction term, we can either: use a mean-field approach if the interaction potential is sufficiently smooth (leading to a Vlasov mean-field equation) or use a collision operator Q describing (in a macroscopic way) how the particles collide when they are close enough. We remark that, in order to derive a collision operator, we usually use a hard-sphere dynamic to model the contact mechanism between particles. This leads to a nonlinear Boltzmann equation of the form

$$\begin{cases} \partial_t f(t, x, p) + \{H_0(x, p), f(t, x, p)\} = Q(f(t, x, p)), \\ f(0, x, p) = f_0(x, p). \end{cases} \quad (3.6)$$

From here, we immediately remark that we can deduce an evolution equation for n (resp. u and w) by multiplying by 1 (resp. p and $|p|^2$) and integrating Equation (3.6) with respect to p . By assuming that Q satisfies the following conservation properties

$$\int_{\mathbb{R}^d} m(p)Q(f(t,x,p))dp = 0,$$

for $m(p) = 1, p$ or $|p|^2$, we find that the local density is the solution of

$$\begin{cases} \partial_t n(t,x) + \nabla_x \cdot (n(t,x)u(t,x)) = 0, \\ \partial_t (n(t,x)u(t,x)) + \nabla_x \cdot \ell(t,x) + n(t,x)\nabla_x V_{\text{ext}}(x) = 0, \\ \partial_t w(t,x) + \nabla_x \cdot h(t,x) + n(t,x)u(t,x) \cdot \nabla_x V_{\text{ext}}(x) = 0, \end{cases} \quad (3.7)$$

with $\ell(t,x) := \int_{\mathbb{R}^d} p \otimes p f(t,x,p)dp$ and $h(t,x) := 1/2 \int_{\mathbb{R}^d} p|p|^2 f(t,x,p)dp$. Of course, one could be mainly interested in the physical quantities of the system and it would be very desirable to be able to express Equation (3.7) only in terms of n, u and w (*i.e.* to have a closed system), that is to not have to rely on f anymore. This would lead us to a hydrodynamic model for our system of particles. With no extra simplifications on our model, we can not do this. The problem stems from the hierarchy in moments: the equation of each moment depends on moments of high order. In our case, the high orders moments are ℓ and h which cannot be expressed in terms of n, u and w . This compels the need for additional informations on the system *via* the distribution function f .

An idea from Levermore [68] to circumvent this difficulty is the following: the missing information on the system will be given through a statistical ansatz. The choice of this ansatz is motivated by the properties of Equation (3.6). Before proceeding, some additional (yet natural) hypothesis is required on the collision operator: we assume that the following local dissipation relation holds

$$\int_{\mathbb{R}^d} \log(f(t,x,p))Q(f(t,x,p))dp \leq 0.$$

By denoting $s(r) := r \log(r) - r$ (which is such that $s(r)' = \log(r)$) the entropy function, we multiply Equation (3.6) by $\log(f(t,x,p))$ and integrate it in the phase-space to deduce

$$\partial_t S(f) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \log(f(t,x,p))Q(f(t,x,p))dx dp \leq 0,$$

where

$$S(f) := \int_{\mathbb{R}^d \times \mathbb{R}^d} s(f(x,p))dx dp, \quad (3.8)$$

is the total entropy of the system. It follows that the total entropy is non-increasing. Let us remark that, in the definition of the entropy function s , we adopted a sign convention leading to a diminishing entropy. We see that Boltzmann equation becomes time irreversible and its solution relaxes asymptotically to an equilibrium called a Maxwellian distribution that is going to be our ansatz. To be more specific, we want our ansatz to be a Maxwellian distribution with some prescribed moments (which will be n, u and w). This phase-space distribution will then be the solution of the following constrained minimization problem

$$\min \left\{ S(g) \text{ such that } \int_{\mathbb{R}^d} g(x,p)dx = n(x), \int_{\mathbb{R}^d} pg(x,p)dp = n(x)u(x) \right. \\ \left. \text{and } \int_{\mathbb{R}^d} \frac{1}{2}|p|^2 g(x,p)dp = w(x) \right\}. \quad (3.9)$$

The previous minimization problem admits a unique solution given by

$$f_{n,u,w}(x,p) := \frac{n(x)}{(2\pi T(x))^{d/2}} e^{-\frac{|p-u(x)|^2}{2T(x)}}, \quad (3.10)$$

where T is such that $n(x)T(x) := \frac{2}{d}w(x) - \frac{1}{d}n(x)|u(x)|^2$, which is exactly the statistical ansatz that we were looking for. Based on $f_{n,u,w}$, we are now in a position to express the moments ℓ and h as functions of n , u and w :

$$\ell(x) = \int_{\mathbb{R}^d} p_j p f_{n,u,e}(x,p) dx dp = n(x)u(x) \otimes u(x) + n(x)T(x)\text{Id}$$

and $h(x) = \int_{\mathbb{R}^d} \frac{1}{2}p|p|^2 f_{n,u,w}(x,p) dx dp = u(x) (n(x)|u(x)|^2 + 5n(x)T(x)).$

Inserting these expression in (3.7) gives rise to ones the most fundamental equations of fluid mechanics: the compressible Euler equations.

From classical to quantum mechanics

In quantum mechanics, particles are modeled *via* a wave function ψ which is used (in a similar way to the phase-space distribution f) to deduce physical quantities. To be more specific, consider a system of particles whose Hamiltonian is given by H from (3.1), that is

$$H(x,p) = \frac{1}{2}|p|^2 + V_{\text{ext}}(x) + V_{\text{int}}(x). \quad (3.11)$$

The idea behind the Schrödinger equation is to describe a particle as a wave: this is called the first quantization. In order to do so, we use de Broglie's relations to replace the momentums p by a wave number $\hbar k$ and make equal the Hamiltonian of the system H with a time frequency $\hbar\omega$ (where \hbar is Planck's constant). For a plane-wave $\psi = e^{i(x \cdot k - \omega t)}$, we end up with the relation

$$\hbar\omega\psi = H(x, \hbar k)\psi$$

which then translates as the original Schrödinger equation

$$\begin{cases} i\hbar\partial_t\psi(t,x) = H(x, -i\hbar\nabla_x)\psi = \left(-\frac{\hbar^2}{2}\sum_{j=1}^N\Delta_{x_j} + V_{\text{ext}}(x) + V_{\text{int}}(x)\right)\psi(t,x), \\ \psi(t,x) = \psi_0(x). \end{cases} \quad (3.12)$$

We point out some differences between f and ψ : the distribution function f is a real-valued $L^1(\mathbb{R}^d)$ function where the wave function ψ is a complex-valued $L^2(\mathbb{R}^{N \times d})$ function. It is symmetric if the system is composed of bosons particles and anti-symmetric if they are fermions. Furthermore, the L^2 -norm of wave function represents the mass of the system (and is usually set to 1). We also remark that the Hamiltonian $H(x, -i\hbar\nabla_x)$ is now a self-adjoint operator on $L^2(\mathbb{R}^{N \times d})$ and, as such, the L^2 -norm of ψ is preserved along the Schrödinger equation. As for the phase-space distribution, the wave function's interest lies in the physical quantities that can be deduce from it. However, due to the quantum nature of the particles, we can only access the likelihood these quantities. The expectation value of a measurement on a quantum system is done *via* a self-adjoint operator $A : D(A) \mapsto L^2(\mathbb{R}^{N \times d})$ (called an observable) and is written as

$$\langle A \rangle(t) := \langle \psi(t) | A \psi(t) \rangle := \int_{\mathbb{R}^{N \times d}} \psi^*(t,x) A \psi(t,x) dx.$$

An example of such observable is the position of the particle given by $A = x$. These measurement give rise to global quantities. If one wishes to find local quantities, we need to approach things in the sense of (mathematical) distributions: a local quantity z associated to an observable A will be such that, $\forall \phi \in \mathcal{S}(\mathbb{R}^{N \times d})$,

$$\int_{\mathbb{R}^{N \times d}} z(t,x)\phi(x)dx = \langle (\phi A)_s \rangle(t) = \langle \psi(t) | (\phi A)_s \psi(t) \rangle,$$

where $(\phi A)_s = (\phi A + A \phi)/2$ is the symmetrization of ϕA (so that it is indeed an observable). The real-valued function ϕ from the previous equation can be physically understood as a measuring

instrument located on the support of ϕ and the right side as the result of a measurement. Owing to this definition, we can define three physical quantities of interest: the local density with $A = 1$, the local current with $A = -i\hbar\nabla$ and the local kinetic energy with $A = -\hbar^2\Delta/2$. This gives us:

1. the local number density $n(t, x)$ is such that

$$\langle \psi(t) | \phi \psi(t) \rangle = \langle n(t) | \phi \rangle,$$

2. the local mean current $u(t, x)$ is such that

$$-i\hbar \left\langle \psi(t) \left| \left(\phi \nabla + \frac{(\nabla \phi)}{2} \right) \psi(t) \right. \right\rangle = \langle n(t) u(t) | \phi \rangle,$$

3. the local kinetic energy $w(t, x)$ is such that

$$-\frac{\hbar^2}{2} \left\langle \psi(t) \left| \left(\phi \Delta + (\nabla \phi) \cdot \nabla + \frac{1}{2} (\Delta \phi) \right) \psi(t) \right. \right\rangle = \langle w(t) | \phi \rangle.$$

These measurements can be seen through the so-called "Schrödinger picture", which is the one that we just illustrated, or the "Heisenberg picture" where everything is seen in terms of operators, *i.e.* the quantum particle is described by what is called a density operator. Let us now derive formally this point. We can see that the expectation value of an observable A can also be written as

$$\langle A \rangle(t) = \text{Tr}(|\psi(t)\rangle\langle\psi(t)|A),$$

where Tr is the operator trace in $L^2(\mathbb{R}^{N \times d})$ and $|\psi(t)\rangle\langle\psi(t)|$ is the orthogonal projection operator on $\text{Span}\{\psi(t)\}$. By denoting the operator $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$, we can see that, since ψ is a solution of (3.12),

$$\partial_t \rho(t) = |\partial_t \psi(t)\rangle\langle\psi(t)| + |\psi(t)\rangle\langle\partial_t \psi(t)| = -\frac{i}{\hbar} H_0 |\psi(t)\rangle\langle\psi(t)| + |\psi(t)\rangle\langle\psi(t)| \frac{i}{\hbar} H_0,$$

which leads to

$$\begin{cases} i\hbar \partial_t \rho(t) = [H_0, \rho(t)], \\ \rho(0) = \rho_0, \end{cases} \quad (3.13)$$

where $[\cdot, \cdot]$ is the commutator and $\rho_0 = |\psi_0\rangle\langle\psi_0|$. This equation is known as the von Neumann equation (or quantum Liouville equation) and is the equivalent of the Schrödinger equation in the Heisenberg picture. Moreover, the operator ρ is the density operator describing our quantum particle and we have

$$\text{Tr}(\rho(t)) = \|\psi(t)\|_{L^2}^2 = 1.$$

We can see that the expectation value of a measurement of the observable A can now be written as

$$\langle A \rangle(t) = \text{Tr}(\rho(t)A).$$

Hence, we obtain the following dual formulations for the local physical quantities for a given density operator ρ

1. the local number density n is such that

$$\langle n | \phi \rangle = \text{Tr}(\rho \phi), \quad (3.14)$$

2. the local current u is such that

$$\langle nu | \phi \rangle = -i\hbar \text{Tr} \left(\rho \left(\phi \nabla + \frac{(\nabla \phi)}{2} \right) \right), \quad (3.15)$$

3. the local kinetic energy w is such that

$$\langle w|\phi\rangle = -\frac{\hbar^2}{2}\text{Tr}\left(\rho\left(\phi\Delta + (\nabla\phi)\cdot\nabla + \frac{1}{2}(\Delta\phi)\right)\right). \quad (3.16)$$

A density operator that can be written as $|\psi\rangle\langle\psi|$, for some $\psi \in L^2$ with $\|\psi\|_{L^2} = 1$, is called a pure state. A mixed state corresponds to any convex combination of pure state, that is any ρ such that

$$\rho = \sum_{j \in \mathbb{N}} \rho_j |\psi_j\rangle\langle\psi_j|, \quad (3.17)$$

where $(\rho_j)_{j \in \mathbb{N}} \subset \mathbb{R}^+$ with $\sum_{j \in \mathbb{N}} \rho_j = 1$. It is rather direct to check that a mixed state is a density operator. Each ρ_j can be understood as a probability to find the quantum system described by ρ in the state given by the wave function ψ_j . To sum up, density operators are non-negative, trace class (*i.e.* their trace is equal to 1) self-adjoint operator acting on L^2 .

The Levermore method and the problem of quantum entropy minimization

The von Neumann equation (3.13) can be seen as the equivalent of the linear Boltzmann equation (3.5) for a quantum particle. Levermore's method was extended to quantum systems of particles by Degond, Ringhofer and Méhats [37, 38, 41, 42] and, in this section, we follow their arguments. When one wants to deal with a system of interacting quantum particles in a macroscopic fashion and reduce the problem to a single particle, there are two possibilities (just like in the classical case): use a mean-field approach when the interaction potential is smooth (leading to a Hartree equation) or use a collision operator Q . The construction of such collision operator is not straightforward and there exists several possible models (see [40]). One of them is the Bhatnagar-Gross-Krook operator which is simply given by

$$Q(\rho) = -\frac{1}{\tau}(\rho - \rho_{\text{eq}}),$$

where τ is a relaxation time and ρ_{eq} is an (equilibrium) density operator. In the following, we make the hypothesis that, for any density operator ρ (of the form (3.17)),

$$\text{Tr}(\log(\rho)Q(\rho)) \leq 0 \quad \text{and} \quad \text{Tr}((A\phi)_s Q(\rho)) = 0, \quad \forall \phi \in \mathcal{S}(\mathbb{R}^d) \quad (3.18)$$

where $\log(\rho)$ is understood as

$$\log(\rho) = \sum_{j \in \mathbb{N}} \log(\rho_j) |\psi_j\rangle\langle\psi_j|,$$

and $A = 1, -i\hbar\nabla$ or $-\hbar^2\Delta/2$. By introducing the collision operator Q in Equation (3.13), we obtain a nonlinear von Neumann equation

$$\begin{cases} i\hbar\partial_t \rho(t) = [H_0, \rho(t)] + i\hbar Q(\rho(t)), \\ \rho(0) = \rho_0, \end{cases} \quad (3.19)$$

The von Neumann entropy of a density operator is defined as

$$S[\rho] = \text{Tr}(s(\rho)) = \sum_{j \in \mathbb{N}} s(\rho_j) = \sum_{j \in \mathbb{N}} \rho_j \log(\rho_j) - \rho_j. \quad (3.20)$$

For $\rho(t)$ a solution of the von Neumann equation (3.19), we can see that, by assumption (3.18),

$$\begin{aligned} \frac{d}{dt} S[\rho(t)] &= \text{Tr}(\log(\rho(t))\partial_t \rho(t)) = \text{Tr}(-i\hbar^{-1} \log(\rho(t))[H_0, \rho(t)]) + \text{Tr}(\log(\rho(t))Q(\rho(t))) \\ &= \text{Tr}(\log(\rho(t))Q(\rho(t))) \leq 0. \end{aligned}$$

As in the classical case, we can see that the entropy of the system is diminishing and will relax to a Maxwellian, that is a minimum of the entropy function S .

The evolutions of the macroscopic quantities of the quantum system n , u and w are derived by differentiating (3.14), (3.15) and (3.16) with respect to time and using the fact that, on the right-hand-side, ρ is a solution of the von Neumann equation (3.19). For any observable A and $\phi \in \mathcal{S}(\mathbb{R}^d)$, we can see that, thanks to a commutator identity, we have

$$\begin{aligned} [H_0, \rho(t)](\phi A)_s &= [H_0, \rho(t)(\phi A)_s] + \rho(t)[H_0, (\phi A)_s] \\ &= [H_0, \rho(t)(\phi A)_s] + \rho(t)([H_0, \phi]A)_s + \rho(t)([H_0, A]\phi)_s, \end{aligned}$$

and we deduce that

$$\text{Tr}([H_0, \rho(t)](\phi A)_s) = \text{Tr}(\rho(t)([H_0, \phi]A)_s) + \text{Tr}(\rho(t)([H_0, A]\phi)_s).$$

By using the fact that

$$[\Delta, \phi] = 2(\nabla\phi) \cdot \nabla + (\Delta\phi),$$

this yields

$$\begin{aligned} \text{Tr}(\rho(t)[H_0, \phi]) &= -\frac{\hbar^2}{2} \text{Tr}(\rho(t)[\Delta, \phi]) = -\frac{\hbar^2}{2} \text{Tr}(\rho(t)(2\nabla\phi \cdot \nabla + (\Delta\phi))) \\ &= -i\hbar \langle n(t)u(t), \nabla\phi \rangle \\ &= i\hbar \langle \nabla(n(t)u(t)) | \phi \rangle, \\ \text{Tr}(\rho(t)[H_0, (-i\phi\hbar\nabla)_s]) &= i\frac{\hbar^3}{2} \text{Tr}(\rho(t)([\Delta, \phi]\nabla)_s) - i\hbar \text{Tr}(\rho(t)([V_{\text{ext}}, \nabla]\phi)_s) \\ &= i\frac{\hbar^3}{2} \text{Tr}(\rho(t)(2(\nabla\phi) \cdot \nabla \otimes \nabla + (\nabla \cdot \nabla\phi)\nabla)_s) + i\hbar \langle n(t)(\nabla V_{\text{ext}}) | \phi \rangle \end{aligned}$$

and

$$\begin{aligned} \text{Tr}\left(\rho(t)\left[H_0, \left(-\frac{\hbar^2}{2}\phi\Delta\right)_s\right]\right) &= \frac{\hbar^4}{4} \text{Tr}(\rho(t)([\Delta, \phi]\Delta)_s) - \frac{\hbar^2}{2} \text{Tr}(\rho(t)([V_{\text{ext}}, \Delta]\phi)_s) \\ &= \frac{\hbar^4}{4} \text{Tr}(\rho(t)(2(\nabla\phi) \cdot \nabla\Delta + (\nabla \cdot \nabla\phi)\Delta)_s) + i\hbar \langle u(t)n(t) \cdot (\nabla V_{\text{ext}}) | \phi \rangle \end{aligned}$$

It follows from the previous computations, and by using (3.18), that

$$\begin{cases} \partial_t n(t, x) + \nabla \cdot (n(t, x)u(t, x)) = 0, \\ \partial_t (n(t, x)u(t, x)) + \nabla \cdot \ell(t, x) + n(t, x)\nabla V_{\text{ext}}(x) = 0, \\ \partial_t w(t, x) + \nabla \cdot h(t, x) + n(t, x)u(t, x) \cdot \nabla V_{\text{ext}}(x) = 0, \end{cases}$$

where ℓ is such that, $\forall \varphi \in \mathcal{S}(\mathbb{R}^d; \mathbb{R}^d)$,

$$\langle \ell(t) | \varphi \rangle = -\frac{\hbar^2}{2} \text{Tr}(\rho(t)(2\varphi \cdot \nabla \otimes \nabla + (\nabla \cdot \varphi)\nabla)_s),$$

and h is such that

$$\langle h(t) | \varphi \rangle = \frac{i\hbar^3}{2} \text{Tr}(\rho(t)(2\varphi \cdot \nabla\Delta + (\nabla \cdot \varphi)\Delta)_s).$$

This system faces the same issue in classical case: the terms ℓ and h cannot be expressed in terms of n , u and w and, hence, the system cannot be closed. A way of solving this issue is to rely on Levermore's strategy by means of a Maxwellian with prescribed local density, local current

and local kinetic energy. This density operator is the solution of the following quantum entropy minimization problem with local constraints

$$\min \left\{ S(\rho) \text{ such that } \langle n|\phi \rangle = \text{Tr}(\rho\phi), \langle nu|\phi \rangle = \text{Tr} \left(\rho \left(\phi \nabla + \frac{(\nabla\phi)}{2} \right) \right) \right. \\ \left. \langle w(t)|\phi \rangle = \text{Tr} \left(\rho \left(\phi \Delta + (\nabla\phi) \cdot \nabla + \frac{1}{2}(\Delta\phi)\phi \right) \right) \right\}. \quad (3.21)$$

Of course, the Maxwellian we're looking after is a density operator and should resemble somehow the exponential of an operator. Unfortunately, this statement has to be properly restated in order to make sense and one has to be careful when dealing with such problem.

Mathematical preliminaries and notations

Before stating the results that provide a rigorous approach to the minimization of quantum entropy, we need to introduce some new mathematical elements (as well as some notations). For any Banach space X and X^* its dual, we denote $\langle \cdot, \cdot \rangle_{X, X^*}$ the duality bracket. For $X = L^2$, we simply denote $\langle \cdot, \cdot \rangle = \langle \cdot, \cdot \rangle_{L^2, L^2}$. For the free Hamiltonian operator $H_0 = -\Delta$, whose domain is not specified yet, a natural 'energy' space (where the minimizer will be sought) is given by

$$\mathfrak{E} := \{ \rho \in \mathcal{J}_1 : \rho = \rho^* \text{ and } \sqrt{H_0}|\rho|\sqrt{H_0} \in \mathcal{J}_1 \},$$

with \mathcal{J}_1 the space of trace class operators on L^2 and where $|\rho| := \sqrt{\rho^* \rho}$. We also introduce the space \mathcal{J}_2 of operators ρ such that $\rho^* \rho \in \mathcal{J}_1$. We remark that \mathfrak{E} is a Banach space equipped with the norm

$$\|\rho\|_{\mathfrak{E}} := \text{Tr}(|\rho|) + \text{Tr}(\sqrt{H_0}|\rho|\sqrt{H_0}).$$

We'll also use the following closed convex subspace of \mathfrak{E}

$$\mathfrak{E}^+ = \{ \rho \in \mathfrak{E} : \rho \geq 0 \}.$$

For any $\rho \in \mathfrak{E}^+$ and $T > 0$, we define the free energy at temperature T

$$F_T(\rho) := T \text{Tr}(\rho \log(\rho) - \rho) + \text{Tr}(\sqrt{H_0} \rho \sqrt{H_0}) := TS(\rho) + E(\rho), \quad (3.22)$$

and we denote $F := F_1$. For a density operator ρ , we denote $n[\rho]$ its local density (given through (3.14)), $u[\rho]$ its local current (given through (3.15)) and $w[\rho]$ its local kinetic energy (given through (3.16)). We can see that these quantities can be expressed thanks to the eigenelements of ρ , denoted $(\rho_j, \psi_j)_{j \in \mathbb{N}}$, that is

$$n[\rho] = \sum_{j \in \mathbb{N}} \rho_j |\psi_j|^2, \quad n[\rho]u[\rho] = \Im \left(\sum_{j \in \mathbb{N}} \rho_j \psi_j^* \nabla \psi_j \right) \quad \text{and} \quad w[\rho] = \frac{1}{2}e[\rho] - \frac{1}{4}\Delta n[\rho], \quad (3.23)$$

where $e[\rho] := \sum_{j \in \mathbb{N}} \rho_j |\nabla \psi_j|^2 = -\sum_{k=1}^d n[\partial_{x_k} \rho \partial_{x_k}]$. One can easily check that $E(\rho) = \|e[\rho]\|_{L^1}$ and, since

$$\frac{1}{2}\nabla n[\rho] + in[\rho]u[\rho] = \sum_{j \in \mathbb{N}} \rho_j \psi_j^* \nabla \psi_j,$$

the Cauchy-Schwartz inequality yields $|\nabla n[\rho]|^2/4 + n[\rho]^2|u[\rho]|^2 \leq n[\rho]e[\rho]$ which implies the lower bound on the total kinetic energy of ρ

$$\|\sqrt{n[\rho]}\|_{H^1}^2 \leq \|\rho\|_{\mathfrak{E}}. \quad (3.24)$$

The eigenvalues of any density operators are always assumed to be nonincreasing and counted with multiplicity.

For any functions n_0, u_0 and e_0 , we'll denote $\mathfrak{E}^+(n_0)$, $\mathfrak{E}^+(n_0, u_0)$ and $\mathfrak{E}^+(n_0, u_0, e_0)$ the subspaces of \mathfrak{E}^+ given by

$$\begin{aligned}\mathfrak{E}^+(n_0) &:= \{\rho \in \mathfrak{E}^+ : n[\rho] = n_0\}, \\ \mathfrak{E}^+(n_0, u_0) &:= \{\rho \in \mathfrak{E}^+ : n[\rho] = n_0, u[\rho] = u_0\}, \\ \text{and } \mathfrak{E}^+(n_0, u_0, e_0) &:= \{\rho \in \mathfrak{E}^+ : n[\rho] = n_0, u[\rho] = u_0, e[\rho] = e_0\}.\end{aligned}$$

We have the logarithmic Sobolev inequality for orthogonal systems.

Theorem 3.1 (Logarithmic Sobolev inequality [44, 45]) Let $\rho \in \mathfrak{E}^+$. Then, the following inequality holds

$$\text{Tr}(\rho \log(\rho)) + E(\rho) \geq \int_{\Omega} n[\rho](x) \log(n[\rho](x)) dx + \frac{d}{2} \log(4\pi) \text{Tr}(\rho),$$

where $\Omega = \mathbb{R}^d$, with $d \geq 1$, or an interval I .

After an optimization under a scaling preserving the L^2 norm (when $\Omega = \mathbb{R}^d$), the previous inequality writes as

$$\text{Tr}(\rho \log(\rho)) \geq \int_{\Omega} n[\rho](x) \log(n[\rho](x)) dx - \frac{d}{2} \log\left(\frac{e}{2\pi d} \frac{E(\rho)}{\text{Tr}(\rho)}\right). \quad (3.25)$$

3.2 The minimization problem with a density and current constraint

The problem of quantum entropy minimization under local constraints was derived in [39, 41] in the context of quantum hydrodynamics but can be also seen (somehow) in [80] where the so-called *local Gibbs states* are considered. In [41], the authors address the minimization problem by using the Weyl quantization \mathcal{O} which relates a symbol a (depending on the position x and the momentum p) with an operator as, $\forall \phi \in \mathcal{S}(\mathbb{R}^d)$,

$$\mathcal{O}(a)\phi := (2\pi\hbar)^{-d} \int_{\mathbb{R}^d \times \mathbb{R}^d} a\left(\frac{x+y}{2}, p\right) e^{ip \cdot (x-y)/\hbar} \phi(y) dp dy.$$

It is shown that a solution, if it exist, of (3.21) is given by

$$\rho = (s')^{-1}(\mathcal{O}(\hat{H}))$$

where s is a strictly convex twice continuously differentiable function on \mathbb{R}^+ and \hat{H} is of the form

$$\hat{H}(x, p) = \hat{A}(x) + \hat{B}(x) \cdot p + \frac{1}{2} \hat{C}(x) |p|^2,$$

for some functions \hat{A}, \hat{B} and \hat{C} (corresponding to Lagrange multipliers associated to each constraint on the moments). The expression of the minimum is very formal since the question of existence and uniqueness (as well as the space where it has to be sought) is left open.

A first step toward a more rigorous approach is achieved in [77] where the authors prove an existence and uniqueness result in dimension $d = 1$ on the torus $\mathbb{T} = \mathbb{R}/\mathbb{Z}$, as well as the characterization of the minimizer, for the free energy.

Theorem 3.2 ([77, Theorem 2.1]) Let $n_0 \in H_{\text{per}}^1$ such that $n_0 > 0$ on $[0, 1]$. Then, the minimization problem

$$\min_{\rho \in \mathfrak{E}^+(n_0)} F(\rho),$$

is attained for a unique density operator ρ such that

$$\rho = \exp(-(H + A)),$$

where A belongs to the dual space H_{per}^{-1} of H_{per}^1 and the operator $H + A$ is taken in the sense of the associated quadratic form

$$Q_A(\phi, \phi) := \left\| \frac{d\phi}{dx} \right\|_{L^2}^2 + \langle A, |\phi|^2 \rangle_{H_{\text{per}}^{-1}, H_{\text{per}}^1}.$$

In the previous theorem, the domain of the Hamiltonian H_0 is the subspace of $H^2(\mathbb{T})$ (with periodic boundary conditions). The domain of the quadratic form associated to H_0 is denoted H_{per}^1 . The main ingredients that are used to prove the existence of a minimizer are: that F is bounded below as well as lower semicontinuous and that minimizing sequences are compact in \mathfrak{E}_n^+ . The uniqueness follows from the strict convexity of F .

It can be seen that the rank one operator $|n_0\rangle\langle n_0|$ belongs to $\mathfrak{E}^+(n_0)$ so that it is not empty. The free energy F is bounded below on \mathfrak{E}^+ thanks to (3.24) and the logarithmic Sobolev inequality (3.25). From here, we can consider a minimizing sequence in \mathfrak{E}^+ and we can also demonstrate that the minimizing sequence is bounded in \mathfrak{E}^+ with the following lemma.

Lemma 3.1 ([77, Lemma 3.3, (i)]) There exists a constant $C > 0$ such that, $\forall \rho \in \mathfrak{E}^+$, we have

$$\text{Tr}(\rho \log(\rho) - \rho) \geq -CE(\rho)^{1/2}.$$

We can now proceed to deduce some compactness for the minimizing sequence.

Lemma 3.2 ([77, Lemma 3.1]) Let $(\rho_k)_{k \in \mathbb{N}}$ be a bounded sequence of \mathfrak{E}^+ . Then, up to an extraction of a subsequence, there exists $\rho \in \mathfrak{E}^+$ such that

$$\rho_k \xrightarrow[k \rightarrow +\infty]{} \rho, \text{ in } \mathcal{J}_1, \quad \sqrt{\rho_k} \xrightarrow[k \rightarrow +\infty]{} \sqrt{\rho}, \text{ in } \mathcal{J}_2 \quad \text{and} \quad E(\rho) \leq \liminf_{k \rightarrow +\infty} E(\rho_k).$$

Furthermore, if one have $E(\rho) = \liminf_{k \rightarrow +\infty} E(\rho_k)$, then one can conclude in addition that

$$\sqrt{H_0} \sqrt{\rho_k} \xrightarrow[k \rightarrow +\infty]{} \sqrt{H_0} \sqrt{\rho}, \text{ in } \mathcal{J}_2.$$

We are then left with proving that: $n_0 = n[\rho_k] \rightarrow n[\rho] = n_0$ as $k \rightarrow +\infty$, $S(\rho) \leq \liminf_{k \rightarrow +\infty} S(\rho_k)$ and S is strictly convex. The first point is easily proved by using the strong convergence in \mathcal{J}_1 from Lemma 3.2 since it implies the weak convergence: for any bounded operator B on L^2 ,

$$\text{Tr}(\rho_k B) \xrightarrow[k \rightarrow +\infty]{} \text{Tr}(\rho B).$$

Taking $B = \phi$ and using (3.14) yields the result. Concerning the second and third point, it relies on the following lemma.

Lemma 3.3 ([77, Lemma 3.3, (ii) and (iii)])

1. Let $(\rho_k)_{k \in \mathbb{N}}$ be a bounded sequence of \mathfrak{E}^+ such that ρ_k converges to ρ in \mathcal{J}_1 , then $s(\rho_k)$ converges to $s(\rho)$ in \mathcal{J}_1 .
2. The application $\rho \mapsto S(\rho)$ is strictly convex in \mathfrak{E}^+ .

In the end, the authors prove that there exists a unique minimizer of F in $\mathfrak{E}^+(n_0)$. It then remains to give its characterization. A way to find the form of the minimizer would be to write the first order necessary condition of optimality (*i.e.* the Euler-Lagrange equation) that the minimizer should solve. However, one cannot proceed easily since we need to be able to differentiate the free energy properly and this differentiation needs to be done in $\mathfrak{E}^+(n_0)$, that is we need to find perturbations that preserve the local density. In order to get around these difficulties, the authors consider a penalized and regularized version of the minimization problem. That is F is replaced

with $F^{\varepsilon, \eta}$, with $\varepsilon, \eta > 0$, which is such that, $\forall \rho \in \mathfrak{E}^+$,

$$F^{\varepsilon, \eta}(\rho) := F^\eta(\rho) + \frac{1}{2\varepsilon} \|n[\rho] - n\|_{L^2}^2,$$

where $F^\eta(\rho) := \text{Tr}(s_\eta(\rho)) + E(\rho)$, with $s_\eta(r) = (r + \eta) \log(r + \eta) - r - \eta \log(\eta)$, $\forall r \in \mathbb{R}^+$. By following the same arguments as for F , we can prove that the minimization problem

$$\min_{\rho \in \mathfrak{E}^+} F^{\varepsilon, \eta}(\rho),$$

admits a unique solution denoted $\rho_{\varepsilon, \eta}$. Moreover, since s_η is regular, we can show that the application $\rho \in \mathfrak{E}^+ \mapsto \text{Tr}(s_\eta(\rho)) = S_\eta(\rho)$ is Gâteaux differentiable. By considering $\zeta = \sqrt{\rho_{\varepsilon, \eta}} \vartheta \sqrt{\rho_{\varepsilon, \eta}}$, for some bounded Hermitian operator ϑ on L^2 , we have that $\zeta \in \mathfrak{E}^+$ and that the Gâteaux derivative of $F^{\varepsilon, \eta}$ along ζ is

$$DF^{\varepsilon, \eta}(\rho_{\varepsilon, \eta})(\zeta) = \text{Tr}(\sqrt{\rho_{\varepsilon, \eta}}(s'_\eta(\rho_{\varepsilon, \eta}) + H_0 + A_{\varepsilon, \eta})\sqrt{\rho_{\varepsilon, \eta}}\vartheta) = 0,$$

where $A_{\varepsilon, \eta} = \frac{1}{\varepsilon}(n[\rho_{\varepsilon, \eta}] - n)$ (corresponding to the penalization). Letting $\eta \rightarrow 0$ leads to the equation

$$\sqrt{\rho_\varepsilon}(\log(\rho_\varepsilon) + H_0 + A_\varepsilon)\sqrt{\rho_\varepsilon} = 0$$

where $\rho_\varepsilon = \rho_{\varepsilon, 0}$ is the minimizer of the penalized problem with functional $F^{\varepsilon, 0}$ and $A_\varepsilon = A_{\varepsilon, 0}$. One then proves that the kernel of ρ_ε is reduced to $\{0\}$ and, by denoting $(\rho_j^\varepsilon, \psi_j^\varepsilon)_{j \in \mathbb{N}}$ the eigenelements of ρ_ε , that $\text{Span}(\psi_j^\varepsilon)_{j \in \mathbb{N}}$ is dense in H_{per}^1 . The Euler-Lagrange equation can thus be rewritten as

$$Q_{A_\varepsilon}(\psi_j^\varepsilon, \phi) = -\log(\rho_j^\varepsilon) \langle \psi_j^\varepsilon, \phi \rangle, \quad \forall \phi \in H_{\text{per}}^1, \quad (3.26)$$

where, for any $\psi, \phi \in H_{\text{per}}^1$, $Q_{A_\varepsilon}(\psi, \phi) := \langle \sqrt{H_0} \psi, \sqrt{H_0} \phi \rangle + \langle A_\varepsilon \psi, \phi \rangle$.

We conclude that $(-\log(\rho_j^\varepsilon), \psi_j^\varepsilon)$ are the eigenelements of H_{A_ε} , the operator associated to the quadratic form Q_{A_ε} , and, finally, that, in the sense of functional calculus,

$$\rho_\varepsilon = e^{-H_{A_\varepsilon}}.$$

Finally, we need to let $\varepsilon \rightarrow 0$. It turns out that $\rho_\varepsilon \rightarrow \rho$ where ρ is the minimizer of the original problem since $n[\rho^\varepsilon] \rightarrow n$ in H_{per}^1 . Concerning A_ε , Equation (3.26) leads to the identification of the limit $A \in H_{\text{per}}^{-1}$ as a linear form

$$\langle A, \phi \rangle_{H_{\text{per}}^{-1}, H_{\text{per}}^1} = -\text{Tr} \left(\frac{\phi}{n} (\rho \log(\rho)) \right) - \sum_{j \in \mathbb{N}} \left\langle \sqrt{H_0} \sqrt{\rho} \phi_j, \sqrt{H_0} \left(\frac{\phi}{n} \sqrt{\rho} \phi_j \right) \right\rangle. \quad (3.27)$$

We remark that the previous expression is implicit since ρ depends itself on A . In the end, one relies again on (3.26) to prove that $\rho = \exp(-H_A)$ where H_A is associated to the quadratic form Q_A given by

$$Q_A(\phi, \psi) = \langle \sqrt{H_0} \psi, \sqrt{H_0} \phi \rangle + \langle A, \psi^* \phi \rangle_{H_{\text{per}}^{-1}, H_{\text{per}}^1}.$$

This ends the characterization of ρ . It was pushed a little further in [79] where the authors proved the following expression for A (extending (3.27)).

Proposition 3.1 ([79, Proposition 4.1]) Let n_0 be such as in Theorem 3.2. Then, $A \in H_{\text{per}}^{-1}$ admits the following expression

$$A = -\frac{1}{n_0} \left(-\frac{1}{2} \Delta n_0 + \sum_{j \in \mathbb{N}} \rho_j |\nabla \psi_j|^2 + \rho_j \log(\rho_j) |\psi_j|^2 \right),$$

where $(\rho_j, \psi_j)_{j \in \mathbb{N}}$ are the eigenelements of the minimizer ρ from Theorem 3.2.

In [78], the same authors continued the study of the existence and uniqueness of a minimizer for the free energy F on \mathbb{R}^d . They obtain the following result.

Theorem 3.3 ([78, Theorem 2.1]) Let $n_0 \in L^1(\mathbb{R}^d)$ be a positive function such that

$$\|n_0\|_{L^1} = 1, \quad n_0 \log(n_0) \in L^1(\mathbb{R}^d) \quad \text{and} \quad \sqrt{n_0} \in H^1(\mathbb{R}^d).$$

Then, the minimization problem

$$\min_{\rho \in \mathfrak{E}^+(n_0)} F(\rho),$$

is attained for a unique density operator ρ .

The first assumption on the local density n is not crucial but the two other ones are: the first is required to bound the energy thanks to (3.24) and the second one is used to deduce a lower bound on the entropy (deduced by the logarithmic Sobolev inequality (3.25)). The strategy follows the same arguments as in [77] and mainly relies on extensions of Lemma 3.1, Lemma 3.2 and Lemma 3.3 to \mathbb{R}^d . In particular, they use the fact that, for any bounded sequence $(\rho_k)_{k \in \mathbb{N}} \subset \mathfrak{E}^+$, we have, up to a subsequence, for any compact operator K on L^2 ,

$$\text{Tr} \left((1 + H_0)^{1/2} \rho_k (1 + H_0)^{1/2} K \right) \xrightarrow{k \rightarrow +\infty} \text{Tr} \left((1 + H_0)^{1/2} \rho (1 + H_0)^{1/2} K \right), \quad (3.28)$$

for some $\rho \in \mathfrak{E}^+$. Theorem 3.3 is also extended in several directions: the case of the Fermi-Dirac entropy given by $s(r) := r \log(r) + (1 - r) \log(1 - r)$ (or more regular entropies where we do not need the logarithmic Sobolev inequality), the case of bounded domains with Dirichlet or Neumann boundary conditions, adding a potential term in the energy E which may depend in a nonlinear way on ρ (like the Hartree energy or the Hartree-Fock exchange energy) and, finally, taking into account the local current. Concerning this last point, the authors use (3.28) to prove the compactness of the minimizing sequence since by (3.15), for any $\phi \in \mathcal{S}(\mathbb{R}^d)$,

$$\begin{aligned} \langle n[\rho_k] u[\rho_k], \phi \rangle &= -i \text{Tr} \left(\rho_k \left(\phi \nabla + \frac{(\nabla \phi)}{2} \right) \right) = -i \text{Tr} \left((1 + H_0)^{1/2} \rho_k (1 + H_0)^{1/2} K \right) \\ &\xrightarrow{k \rightarrow +\infty} -i \text{Tr} \left((1 + H_0)^{1/2} \rho (1 + H_0)^{1/2} K \right) = \langle n[\rho] u[\rho], \phi \rangle \end{aligned}$$

for some compact operator K which is formally equal to $(1 + H_0)^{-1/2} (\phi \nabla + (\nabla \phi)/2) (1 + H_0)^{-1/2}$. They obtain the following.

Theorem 3.4 ([78, Theorem 4.3]) Let n_0 and u_0 be two functions such that there exists $\rho \in \mathfrak{E}^+$ such that $n[\rho] = n_0$ and $u[\rho] = u_0$. Assume furthermore that $n \log(n) \in L^1(\mathbb{R}^d)$. Then, the minimization problem

$$\min_{\rho \in \mathfrak{E}^+(n_0, u_0)} F(\rho),$$

is attained for a unique density operator ρ .

3.3 The problem of compactness for the energy constraint

As stated in [78], it is not direct to extend Theorem 3.3 to the case of the three local constraints. This is due to the fact that (3.28) is not sufficient to recover the local energy constraint and we lack compactness. Let us consider the following minimization problem, in the same context as in [77],

$$\min_{\rho \in \mathfrak{E}^+(n_0, u_0, e_0)} S(\rho). \quad (3.29)$$

Since $E[\rho] = \|e[\rho]\|_{L^1} = \|e_0\|_{L^1}$, for any $\rho \in \mathfrak{E}^+(n_0, u_0, e_0)$, and thanks to Lemma 3.1, we can consider a minimizing sequence $(\rho_k)_{k \in \mathbb{N}}$ which is bounded in \mathfrak{E}^+ . It follows from Lemma 3.3 that

$$S(\rho) = \lim_{k \rightarrow +\infty} S(\rho_k) = \inf_{\rho \in \mathfrak{E}^+(n_0, u_0, e_0)} S(\rho), \quad (3.30)$$

and we are left with the question: does ρ belongs to $\mathfrak{E}^+(n_0, u_0, e_0)$? Following the same arguments as in [78], we can prove that $\rho \in \mathfrak{E}^+(n_0, u_0)$ and we are only left with the local energy constraint. A key element to recover this constraint lies in the following result.

Lemma 3.4 ([84, Theorem 2.21 and addendum H]) Suppose that $A_k \rightarrow A$ weakly in the sense of operators and that $\|A_k\|_{\mathcal{J}_1} \rightarrow \|A\|_{\mathcal{J}_1}$ as $k \rightarrow +\infty$. Then $\|A_k - A\|_{\mathcal{J}_1} \rightarrow 0$ as $k \rightarrow +\infty$.

Equivalently to (3.28), we can show that

$$\sqrt{H_0} \rho_k \sqrt{H_0} \xrightarrow[k \rightarrow +\infty]{} \sqrt{H_0} \rho \sqrt{H_0}, \text{ weak-* in } \mathcal{J}_1, \quad (3.31)$$

(which implies weak convergence in the sense of operators). Hence, if we are able to prove that

$$\|\sqrt{H_0} \rho_k \sqrt{H_0}\|_{\mathcal{J}_1} \xrightarrow[k \rightarrow +\infty]{} \|\sqrt{H_0} \rho \sqrt{H_0}\|_{\mathcal{J}_1}, \quad (3.32)$$

we can deduce

$$\|e[\rho_k] - e[\rho]\|_{L^1} = \|\sqrt{H_0} \rho_k \sqrt{H_0} - \sqrt{H_0} \rho \sqrt{H_0}\|_{\mathcal{J}_1} \xrightarrow[k \rightarrow +\infty]{} 0,$$

which leads to the fact that $\rho \in \mathfrak{E}^+(n_0, u_0, e_0)$. So we need to show that (3.32) holds or, equivalently, that $\lim_{k \rightarrow +\infty} \|e[\rho_k]\|_{L^1} = \|e_0\|_{L^1}$. It turns out that, thanks to (3.31), we can only prove that

$$\|e[\rho]\|_{L^1} \leq \liminf_{k \rightarrow +\infty} \|e[\rho_k]\|_{L^1} = \|e_0\|_{L^1}.$$

Our approach in [DP1] to demonstrate (3.32) is based on a thermodynamical consideration where we assume, by contradiction, that (3.32) does not hold and that we have, instead

$$\|e[\rho]\|_{L^1} < \|e_0\|_{L^1},$$

which means that the global kinetic energy of ρ is smaller than the global kinetic energy of the density operators from $\mathfrak{E}^+(n_0, u_0, e_0)$. On a thermodynamical level, we know that the kinetic energy should somehow be proportional to the temperature of the system. However, the (mathematical) entropy of ρ would then be strictly larger than the ones from $\mathfrak{E}^+(n_0, u_0, e_0)$ which seems to contradict the equality in (3.30). Of course, this is just an intuition.

To make this argument more rigorous, we need to introduce auxiliary minimization problems and proceed by steps. Let us start with the first one with respect to the free energy F_T , where T corresponds to the temperature of the system, and where we express the minimizer with two local constraint thanks to the minimizer with a single local constraint.

Theorem 3.5 Suppose that $n_0 \in H_{\text{per}}^1$, with $n_0 > 0$, and that $u_0 \in L^2$. Then, for any $T > 0$, the constrained minimization problem

$$\min_{\rho \in \mathfrak{E}^+(n_0, u_0)} F_T(\rho)$$

admits a unique solution that reads

$$\rho_{T, n_0, u_0} = e^{if} \rho_{T, n_0} e^{-if}, \quad f(x) = \int_0^x u_0(y) dy,$$

where ρ_{T,n_0} is the unique solution of the problem

$$\min_{\rho \in \mathfrak{E}^+(n_0)} F_T(\rho).$$

In the previous result, the question of existence and uniqueness for the each minimization problems (for one or two local constraints) follows directly from Theorem 3.3 and an adaptation of Theorem 3.4. We then have to check that $e^{if}\rho_{T,n_0}e^{-if}$ is indeed the minimizer. For any $\rho \in \mathfrak{E}^+$, we can see that the gauge change $\rho \mapsto e^{if}\rho e^{-if} = \sigma$ is such that $\sigma \in \mathfrak{E}^+$ and, by (3.23),

$$n[\sigma] = n[\rho], \quad n[\sigma]u[\sigma] = n[\rho]u[\rho] + n[\rho]u_0 \quad \text{and} \quad F_T(\sigma) = F_T(\rho) + \frac{1}{2} \int_{\mathbb{T}} n_0(x)|u_0(x)|^2 dx. \quad (3.33)$$

Thus, since the eigenfunctions of ρ_{T,n_0} can be chosen to be real-valued, it follows that $u[\rho_{T,n_0}] = 0$ so that ρ_{T,n_0,u_0} belongs to $\mathfrak{E}^+(n_0, u_0)$. One can check that $u[e^{-if}\rho_{T,n_0,u_0}e^{if}] = 0$ so that

$$\begin{aligned} \min_{\rho \in \mathfrak{E}^+(n_0, u_0)} F_T(\rho) &= \min_{\rho \in \mathfrak{E}^+(n_0, 0)} F_T(e^{-if}\rho e^{if}) \geq \min_{\rho \in \mathfrak{E}^+(n_0)} F_T(e^{-if}\rho e^{if}) \\ &\geq \min_{\rho \in \mathfrak{E}^+(n_0)} F_T(\rho) + \frac{1}{2} \int_{\mathbb{T}} n_0(x)|u_0(x)|^2 dx = F_T(\rho_{T,n_0}) + \frac{1}{2} \int_{\mathbb{T}} n_0(x)|u_0(x)|^2 dx \\ &= F_T(\rho_{T,n_0,u_0}). \end{aligned}$$

and we conclude by uniqueness. Let us proceed to the next result which gives a monotonic relation between the temperature of the minimizer and its global kinetic energy as well as its global entropy.

Theorem 3.6 Let $T > 0$, $n_0 \in H_{\text{per}}^2$, with $n_0 > 0$, $u_0 \in L^2$ and ρ_{T,n_0,u_0} given as in Theorem 3.5. Then $T \mapsto E(\rho_{T,n_0,u_0})$ and $T \mapsto -S(\rho_{T,n_0,u_0})$ are strictly increasing continuous functions from \mathbb{R}^{*+} and

$$\lim_{T \rightarrow 0^+} E(\rho_{T,n_0,u_0}) = \frac{1}{2} \left(\int_{\mathbb{T}} |\nabla \sqrt{n_0(x)}|^2 dx + \int_{\mathbb{T}} n_0(x)|u_0(x)|^2 dx \right) =: E_*$$

The proof of this theorem is quite tedious since the relation between the temperature and ρ_{T,n_0,u_0} is implicit. We know that the minimizer can be characterized as $\rho_{T,n_0,u_0} = \exp(-(H_0 + A_T))$ for some potential A_T but the problem is that this potential is a generalized function and it depends itself on ρ_{T,n_0,u_0} in a rather intricate way (see Proposition 3.1). The procedure to prove Theorem 3.6 consists in penalizing the minimization problem to obtain a simpler potential (just like in the proof of Theorem 3.2) and obtain the differentiability of the (penalized) minimizer with respect to T by using an implicit function theorem. This will require down the road some uniform estimates in order to recover the original minimization. From here, it is possible to compute the derivative of the global kinetic energy and the global entropy and deduce the strict monotonicity of $T \mapsto E(\rho_{T,n_0,u_0})$ and $T \mapsto S(\rho_{T,n_0,u_0})$ when letting the penalization parameter go to zero. Concerning the limit, we prove the following inequality, thanks to a gauge change like in Theorem 3.5 and (3.24),

$$\begin{aligned} \lim_{T \rightarrow 0^+} E(\rho_{T,n_0,u_0}) &= \lim_{T \rightarrow 0^+} \min_{\rho \in \mathfrak{E}^+(n_0, u_0)} F_T(\rho) = \min_{\rho \in \mathfrak{E}^+(n_0, u_0)} E(\rho) \\ &= \min_{\rho \in \mathfrak{E}^+(n_0)} E(\rho) + \frac{1}{2} \int_{\mathbb{T}} n_0(x)|u_0(x)|^2 dx = \frac{1}{2} \left(\int_{\mathbb{T}} |\nabla \sqrt{n_0(x)}|^2 dx + \int_{\mathbb{T}} n_0(x)|u_0(x)|^2 dx \right), \end{aligned}$$

where we used the fact that the density operator $|n_0\rangle\langle n_0|$ belongs in $\mathfrak{E}^+(n_0)$.

The previous result states that, for a given minimization problem with two constraints, there exists a specific temperature that enables us to set the global kinetic energy of the minimizer. This leads us to the next result where we consider a minimization problem with two local constraints and a global kinetic energy constraint.

Theorem 3.7 Let $n_0 \in H_{\text{per}}^2$, with $n_0 > 0$, $u_0 \in L^2$ and E_0 given as in Theorem 3.5. Then, for any $E_0 \geq E_*$, the constrained minimization problem

$$\min_{\rho \in \mathfrak{E}^+(n_0, u_0) \cap \mathfrak{E}_g^+(E_0)} S(\rho),$$

admits a unique solution. When $E_0 > E_*$, the solution has the form ρ_{T_0, n_0, u_0} given in Theorem 3.5 for a temperature $T_0 \equiv T_0(n_0, u_0, E_0)$. When $E_0 = E_*$, the set $\mathfrak{E}^+(n_0, u_0) \cap \mathfrak{E}_g^+(E_0)$ is reduced to the operator $e^{if} |\sqrt{n_0}\rangle \langle \sqrt{n_0}| e^{-if}$.

In the previous Theorem, the set $\mathfrak{E}_g^+(E_0)$ corresponds to the global kinetic energy constraint and is given by

$$\mathfrak{E}_g^+(E_0) = \{\rho \in \mathfrak{E}^+ : E(\rho) = E_0\}.$$

This result is essentially due to the following equality

$$\operatorname{argmin}_{\rho \in \mathfrak{E}^+(n_0, u_0) \cap \mathfrak{E}_g^+(E_0)} S(\rho) = \operatorname{argmin}_{\rho \in \mathfrak{E}^+(n_0, u_0) \cap \mathfrak{E}_g^+(E_0)} (E_0 + T_0 S(\rho)) = \operatorname{argmin}_{\rho \in \mathfrak{E}^+(n_0, u_0) \cap \mathfrak{E}_g^+(E_0)} F_{T_0}(\rho) = \rho_{T_0, n_0, u_0}.$$

The case $E_0 = E_*$ is done by seeing that $E(e^{if} |\sqrt{n_0}\rangle \langle \sqrt{n_0}| e^{-if}) = E_*$ and that, for any $\sigma \in \mathfrak{E}^+(n_0, u_0)$ with $E(\sigma) = E_*$, we have

$$E_* = E(\sigma) \geq \min_{\rho \in \mathfrak{E}^+(n_0, u_0)} E(\rho) = \min_{\rho \in \mathfrak{E}^+(n_0)} E(\rho) + \frac{1}{2} \int_{\mathbb{T}} n_0(x) |u_0(x)|^2 dx = E_*,$$

which gives the desired result by uniqueness of the minimizer of E in $\mathfrak{E}^+(n_0)$.

We are now in position to make our thermodynamical argument rigorous. We have a density operator $\rho \in \mathfrak{E}^+(n_0, u_0)$ which is a candidate to the minimization problem (3.29). In order to prove that $\rho \in \mathfrak{E}^+(n_0, u_0, e_0)$, we proceed by contradiction and assume that

$$E^{(1)} := \|e[\rho]\|_{L^1} \leq \|e_0\|_{L^1} =: E^{(0)}.$$

By Theorem 3.7, there exist $\sigma_j \in \mathfrak{E}^+(n_0, u_0) \cap \mathfrak{E}_g^+(E^{(j)})$, $j = 0, 1$, such that

$$E(\sigma_1) = E^{(1)} < E^{(0)} = E(\sigma_0),$$

and, by Theorem 3.6,

$$S(\sigma_1) > S(\sigma_0). \quad (3.34)$$

However, since $\rho \in \mathfrak{E}^+(n_0, u_0) \cap \mathfrak{E}_g^+(E^{(1)})$, we can see that

$$S(\sigma_1) = \min_{\sigma \in \mathfrak{E}^+(n_0, u_0) \cap \mathfrak{E}_g^+(E^{(1)})} S(\sigma) \leq S(\rho) = \min_{\sigma \in \mathfrak{E}^+(n_0, u_0, e_0)} S(\sigma). \quad (3.35)$$

It turns out that the previous inequality cannot hold. To see this, we need the following Lemma.

Lemma 3.5 Let $E_0 > E_*$. Then we have

$$\inf_{\substack{e_0 \in L_+^1 \\ \|e_0\|_{L^1} = E_0}} \inf_{\sigma \in \mathfrak{E}^+(n_0, u_0, e_0)} S(\sigma) = \min_{\sigma \in \mathfrak{E}^+(n_0, u_0) \cap \mathfrak{E}_g^+(E_0)} S(\sigma),$$

where L_+^1 is the set of nonnegative integrable functions on \mathbb{T} .

Taking the minimum over $e_0 \in L_+^1$ in (3.35) yields $S(\sigma_1) \leq S(\sigma_0)$ which contradicts (3.34). Thus, $\|e[\rho]\|_{L^1} = \|e_0\|_{L^1}$ and we deduce the following theorem.

Theorem 3.8 Suppose that $(n_0, u_0, e_0) \in \mathfrak{M}$, with $n_0 > 0$, where

$$\mathfrak{M} := \{(n_0, u_0, e_0) \in H_{\text{per}}^2 \times L^2 \times L_+^1 : n[\rho] = n_0, u[\rho] = u_0, e[\rho] = e_0, \text{ for some } \rho \in \mathfrak{E}^+\}.$$

Then, the constrained minimization problem

$$\min_{\rho \in \mathfrak{E}^+(n_0, u_0, e_0)} S(\rho),$$

admits a unique solution.

This result was then extended in [DP5] to \mathbb{R}^d and for a large class of entropy functions. The approach is a generalization of the strategy from [DP1]. The main trick is to simplify the minimization problem with local constraints thanks to a minimization problem with (corresponding) global constraints *via* an extension of Lemma 3.5. The admissible local constraints are here given by

$$\mathfrak{M} := \left\{ (n_0, u_0, e_0) \in L_+^1 \times (L^1)^d \times L_+^1 : \right. \\ \left. \sqrt{n_0} \in H^1, n[\rho] = n_0, u[\rho] = u_0, e[\rho] = e_0, \text{ for some } \rho \in \mathfrak{E}^+ \right\},$$

and we assume that it is not empty. We fix some $(n_0, u_0, e_0) \in \mathfrak{M}$ and denote $N_0 := \|n_0\|_{L^1}$, $U_0 := \|u_0\|_{L^1}$ and $E_0 := \|e_0\|_{L^1}$. We also denote $S(\rho) := \text{Tr}(\beta(\rho))$, where β is an entropy function which verifies all the assumptions below (which are natural in the context of a minimization problem).

Assumption 3.1 The function β belongs in $\mathcal{C}([0, N_0])$ and such that:

1. it is strictly convex with $\beta(0) = 0$,
2. the function $S : \rho \mapsto S(\rho)$ is well-defined on $\mathfrak{E}^+(n_0, u_0, e_0)$, bounded below and verifies, for any sequence $(\rho_k)_{k \in \mathbb{N}} \subset \mathfrak{E}^+(n_0, u_0, e_0)$ such that $\rho_k \rightarrow \rho$ strongly in \mathcal{J}_1 as $k \rightarrow +\infty$,

$$S(\rho) \leq \liminf_{k \rightarrow +\infty} S(\rho_k).$$

Since we work on the entire space \mathbb{R}^d , we also need some confinement assumption on the density.

Assumption 3.2 There exists a nonnegative potential $V \in L_{\text{loc}}^2$, with $V(x) \rightarrow +\infty$ as $|x| \rightarrow +\infty$, such that $n_0 V \in L^1$.

The potential V enables us to introduce the Hamiltonian self-adjoint operator $H = H_0 + V$ whose spectrum is purely discrete and with a non-degenerate ground state $\{\lambda_0, \psi_0\}$. This operator will be helpful latter to build quasi-explicit minimizers of the free energy. We also consider the associated energy

$$W(\rho) := \text{Tr}(\sqrt{H}\rho\sqrt{H}) = E(\rho) + \|n[\rho]V\|_{L^1},$$

as well as the local energy $w[\rho] := e[\rho] + Vn[\rho]$ and denote $w_0 = e_0 + Vn_0$.

Let us now follow the same arguments as in [DP1]. Thanks to Assumption 3.1, we can consider a bounded minimizing sequence $(\rho_k)_{k \in \mathbb{N}}$ in $\mathfrak{E}^+(n_0, u_0, e_0)$ which converges to a $\rho \in \mathcal{J}_1$. By compactness, we know that $\rho \in \mathfrak{E}^+(n_0, u_0)$ and we only need to prove that $\|e[\rho]\|_{L^1} = \|e_0\|_{L^1}$ or, equivalently, $\|w[\rho]\|_{L^1} = \|w_0\|_{L^1}$. We have $\|w[\rho]\|_{L^1} \leq \liminf_{k \rightarrow +\infty} \|w[\rho_k]\|_{L^1} = \|w_0\|_{L^1}$ and we proceed by contradiction by assuming that

$$W_1 := \|w[\rho]\|_{L^1} < \|w_0\|_{L^1} := W_0. \quad (3.36)$$

We now consider the subspaces of \mathfrak{E}^+ with global constraints given by

$$\begin{aligned}\mathfrak{E}_g^+(N) &:= \{\rho \in \mathfrak{E}^+ : \|n[\rho]\|_{L^1} = N\}, \\ \mathfrak{E}_g^+(N, U) &:= \{\rho \in \mathfrak{E}^+ : \|n[\rho]\|_{L^1} = N, \|u[\rho]\|_{L^1} = U\}, \\ \text{and } \mathfrak{E}_{g,w}^+(N, U, W) &:= \{\rho \in \mathfrak{E}^+ : \|n[\rho]\|_{L^1} = N, \|u[\rho]\|_{L^1} = U, \|w[\rho]\| = W\},\end{aligned}$$

as well as

$$\mathfrak{E}_w^+(n_0, u_0, w_0) := \{\rho \in \mathfrak{E}^+ : n[\rho] = n_0, u[\rho] = u_0, w[\rho] = w_0\}.$$

The density operator ρ belongs in $\mathfrak{E}_{g,w}^+(N_0, U_0, W_1)$ and, thus, we have

$$\inf_{\sigma \in \mathfrak{E}_{g,w}^+(N_0, U_0, W_1)} S(\sigma) \leq S(\rho) \leq \liminf_{k \rightarrow +\infty} S(\rho_k) = \inf_{\sigma \in \mathfrak{E}_w^+(n_0, u_0, w_0)} S(\sigma). \quad (3.37)$$

Thanks to the following result (which is an extension of Lemma 3.5), we reduce our investigation to minimization problems with global constraints.

Lemma 3.6 Let $(N, U, W) \in \mathbb{R}^{*+} \times (\mathbb{R}^*)^d \times \mathbb{R}^{*+}$ such that $\mathfrak{E}_{g,w}^+(N, U, W)$ is not empty, and assume that the minimization problem

$$\min_{\sigma \in \mathfrak{E}_{g,w}^+(N, U, W)} S(\sigma), \quad (3.38)$$

admits a unique solution. Then, the following equality holds

$$\inf_{(n,u,w) \in \mathfrak{M}(N,U,W)} \left(\inf_{\sigma \in \mathfrak{E}_w^+(n,u,w)} S(\sigma) \right) = \min_{\sigma \in \mathfrak{E}_{g,w}^+(N,U,W)} S(\sigma).$$

It follows from the previous result that (3.37) leads to the inequality

$$\inf_{\sigma \in \mathfrak{E}_{g,w}^+(N_0, U_0, W_1)} S(\sigma) \leq \inf_{\sigma \in \mathfrak{E}_{g,w}^+(N_0, U_0, W_0)} S(\sigma), \quad (3.39)$$

and we are left with studying a minimization problem with global constraints. It happens that these problem can further be reduced to a minimization problem with only the global density constraint. In order to do so, we need our last assumption.

Assumption 3.3 There exists $T_* \geq 0$ such that, for each $T \geq T_*$, the free energy $F_T(\rho) = W(\rho) + TS(\rho)$ admits a unique minimizer ρ_T on $\mathfrak{E}_g^+(N_0)$ such that $u[\rho_T] = 0$, $T \mapsto W(\rho_T)$ (resp. $T \mapsto S(\rho_T)$) is continuous strictly increasing (resp. decreasing) with $\lim_{T \rightarrow +\infty} W(\rho_T) = +\infty$ and $\lim_{T \rightarrow T_*} W(\rho_T) = \lambda_0 N_0$, for λ_0 the smallest eigenvalue of H .

To exploit the previous assumption, we consider the problem

$$\inf_{\sigma \in \mathfrak{E}_g^+(N_0, U_0)} F_T(\sigma), \quad (3.40)$$

which can be reduced thanks to a gauge change. Indeed, for any $b \in \mathbb{R}^d$ and $\kappa_b(x) := e^{ix \cdot b}$, we have

$$n[\kappa \sigma \kappa^*] = n[\sigma], \quad u[\kappa \sigma \kappa^*] = u[\sigma] + n[\sigma]b \quad \text{and} \quad w[\kappa \sigma \kappa^*] = w[\sigma] - 2b \cdot u[\sigma] + |b|^2 n[\sigma],$$

as well as $S(\kappa \sigma \kappa^*) = S(\sigma)$. By considering $\rho_T \in \mathfrak{E}_g^+(N_0, 0)$ from Assumption 3.3, we can see that $\kappa_{U_0/N_0} \rho_T \kappa_{U_0/N_0}^* \in \mathfrak{E}_g^+(N_0, U_0)$ and

$$\begin{aligned}\min_{\sigma \in \mathfrak{E}_g^+(N_0, U_0)} F_T(\sigma) &= \min_{\sigma \in \mathfrak{E}_g^+(N_0, 0)} F_T(\kappa_{U_0/N_0} \sigma \kappa_{U_0/N_0}^*) = \min_{\sigma \in \mathfrak{E}_g^+(N_0, 0)} F_T(\sigma) + |U_0|^2 / N_0 \\ &\geq \min_{\sigma \in \mathfrak{E}_g^+(N_0)} F_T(\sigma) + |U_0|^2 / N_0 = F_T(\rho_T) + |U_0|^2 / N_0 = F_T(\kappa_{U_0/N_0} \rho_T \kappa_{U_0/N_0}^*),\end{aligned}$$

which proves that $\kappa_{U_0/N_0} \rho_T \kappa_{U_0/N_0}^*$ is the unique minimizer of (3.40). Since $T \mapsto W(\rho_T)$ is continuous strictly increasing, by hypothesis, and $W(\kappa_{U_0/N_0} \rho_T \kappa_{U_0/N_0}^*) = W(\rho_T) + |U_0|^2/N_0$, we know that, for any $K \in [\lambda_0 N_0 + |U_0|^2/N_0, +\infty)$, there exists a unique $T(N_0, U_0, K)$ such that

$$\rho_{N_0, U_0, K} := \kappa_{U_0/N_0} \rho_{T(N_0, U_0, K)} \kappa_{U_0/N_0}^* \in \mathfrak{E}_{g,w}^+(N_0, U_0, K).$$

From here, it can be shown that $\rho_{N_0, U_0, K}$ is the unique minimizer of

$$\inf_{\sigma \in \mathfrak{E}_{g,w}^+(N_0, U_0, K)} S(\sigma),$$

and the contradiction follows from the fact that (3.39) gives

$$S(\rho_{T(N_0, U_0, W_1)}) = S(\rho_{N_0, U_0, W_1}) \leq S(\rho_{N_0, U_0, W_0}) = S(\rho_{T(N_0, U_0, W_0)}),$$

which contradicts our assumption that $T \mapsto S(\rho_T)$ is continuous strictly decreasing since

$$T(N_0, U_0, W_0) > T(N_0, U_0, W_1).$$

This proves the following Theorem.

Theorem 3.9 Under Assumptions 3.1, 3.2 and 3.3, the entropy S admits a unique minimizer in $\mathfrak{E}^+(n_0, u_0, e_0)$.

To have a more complete picture, we can also prove that Assumptions 3.1 and 3.3 can be simplified (under a small loss of generality).

Theorem 3.10 Let $\beta \in \mathcal{C}^2((0, N_0))$ such that $\beta'' > 0$, $\beta(0) = 0$ and that there exists $y \in (0, N_0)$ and $\gamma \in (d/(d+2), 1)$ such that

$$\sup_{x \in [0, y]} |x|^{1-\gamma} |\beta'(x)| = C_{\gamma, \beta} < +\infty.$$

Suppose that Assumption 3.2 holds and that

1. when $\beta'(0)$ is infinite, that the V from Assumption 3.2 verifies $V^{d/2-\gamma/(1-\gamma)} \in L^1$,
2. when $\beta'(0)$ is finite, that we can take

$$V(x) = 1 + |x|^\theta,$$

with $(\gamma/(1-\gamma) - d/2)\theta > d$ (so that $V^{d/2-\gamma/(1-\gamma)} \in L^1$), and that there exists $z, r > 0$ such that

$$c_- x^r \leq \beta'(x) - \beta'(0) \leq c_+ x^r, \quad \forall x \in [0, z],$$

where c_-, c_+ are positives constants.

Then, Assumptions 3.1 and 3.3 are satisfied.

It can be verified that some entropy frequently encountered in the literature satisfy the assumptions of Theorem 3.10: the von Neumann entropy $\beta(x) = x \log(x) - x$, the Fermi-Dirac entropy $\beta(x) = x \log(x) + (1-x) \log(1-x)$, the Bose-Einstein entropy $\beta(x) = x \log(x) - (1+x) \log(1+x)$ and the Tsallis entropy $\beta(x) = (q-1)^{-1} x^q$ for $q \in (0, 1) \cup (1, +\infty)$. The proof of the previous Theorem is rather technical and, in order to show that Assumption 3.3 is satisfied, it relies on an (quasi)-explicit form of ρ_T which is

$$\rho_T = \xi_T(H + \mu_T) \mathbf{1}_{H + \mu_T \leq -T\beta_-},$$

where $\xi(x) = (\beta')^{-1}(-x/T)$, μ_T is a chemical potential set such that ρ_T verifies the density global constraint and $\beta_- = \lim_{x \rightarrow 0} \beta'(x)$ (which can be finite or not). This expression enables to obtain that $T \mapsto W(\rho_T)$ (resp. $T \mapsto S(\rho_T)$) is continuous strictly increasing (resp. decreasing) by some (careful) differentiations.

3.4 The characterization problem with a density and energy constraint

As we've seen, the characterization of the minimizer was addressed in [77, 79] in the case of a minimization problem on an interval with a local density constraint. In [DP2], we extended this result to the case of the three local constraints (still on an interval, set to be $[0, 1]$). To do so, we first remark that, by the change of gauge $\rho \mapsto e^{if} \rho e^{-if}$ with $f(x) = \int_0^x u_0(y) dy$, the local current constraint can be removed because of (3.33) since the minimizer with (only) the density and kinetic energy constraints can be chosen such that its current is null. Thus, we consider a minimizer of the von Neumann entropy in $\mathfrak{E}_{n_0, 0, k_0}^+$. Furthermore, we make the following assumptions on n_0 and k_0 .

Assumption 3.4 Let

$$a(x) := \left(k_0(x) - \left| \nabla \sqrt{n_0(x)} \right|^2 \right)^{-1},$$

for all $x \in [0, 1]$, and denote

$$n_m = \min_{x \in [0, 1]} n_0(x).$$

We assume that

1. $\sqrt{n_0} \in H^1$, $\Delta n_0 \in L^2$ and $n_m > 0$,
2. $k_0 \in L^\infty$,
3. there exists $a_M > 0$ such that $a(x)^{-1} > a_M^{-1} > 0$, a.e.,
4. there exists $\rho \in \mathfrak{E}^+$ such that $n[\rho] = n_0$ and $k[\rho] = k_0$.

Our approach to obtain the characterization is to derive a Euler-Lagrange equation. However, we have to be cautious since we need to differentiate in the constraints space, that is the space of positive density operators with prescribed local density and local kinetic energy, and in a way that gives rise to a derivative that is sufficiently rich. This can be done by considering the following perturbation of $\rho \in \mathfrak{E}_{n_0, 0, k_0}^+$

$$\rho(t, f) := (\text{Id} + t\rho_1 + f_2 \text{Id} + T_{f_3})(\rho + t\rho_2)(\text{Id} + t\rho_1 + f_2 \text{Id} + T_{f_3})^*,$$

where $t \in [-1, 1]$, $f := (f_2, f_3) \in (L^\infty)^2$, $\rho_1 = \sqrt{\rho_j} |\varphi\rangle \langle \psi_j|$, for a certain $j \in \mathbb{N}$ with $\varphi \in W^{1, \infty}$ and $(\rho_j, \psi_j)_{j \in \mathbb{N}}$ the eigenelements of ρ , $\rho_2 \in \mathfrak{E}^+$ and, for any $g \in L^2$, $T_g : H^1 \mapsto L^\infty$ is a bounded operator defined by

$$T_g \phi(x) := \int_0^x g(y) \nabla \phi(y) dy.$$

The idea in this choice of perturbation is the following: the operators ρ_1, ρ_2 will serve as "test operators" to identify the Euler-Lagrange equation and the operator $f_2 \text{Id}$ (resp. T_{f_3}) will be used to ensure that the local density (resp. kinetic energy) constraint is verified since

$$n[f_2 \rho] = f_2 n[\rho] \quad (\text{resp. } k[T_{f_3} \rho] = f_3 k[\rho]).$$

By using the implicit function theorem, we'll identify $t \mapsto f(t)$ such that

$$n[\rho(t, f(t))] = n_0 \quad \text{and} \quad k[\rho(t, f(t))] = k_0.$$

This is the propose of the following proposition where, for any $(x, y) \in [0, 1]^2$,

$$K_0(x, y) := 2\Re \left(\sum_{j \in \mathbb{N}} \rho_j \psi_j(x) \nabla \psi_j(y) \right), \quad K(x, y) = \frac{K_0(x, y)}{2n_0(x)} + \frac{a(x) \nabla n_0(x)}{4n_0(x)} \nabla_x K_0(x, y),$$

and, for any kernel $N \in L^2 \times L^2$, any $x \in [0, 1]$ and $\varphi \in L^2$,

$$L_N \varphi(x) := \int_0^x N(x, y) \varphi(y) dy.$$

Proposition 3.2 Suppose $\rho_2 = 0$ (resp. $\rho_1 = 0$, $k[\rho_2] \in L^\infty$). Then, there exists $t_0 > 0$ and $f \in \mathcal{C}^1((-t_0, t_0), W^{1,\infty} \times L^\infty)$ (resp. $\mathcal{C}^1([0, t_0), W^{1,\infty} \times L^\infty)$) such that $\rho(t, f(t)) \in \mathfrak{E}^+(n_0, 0, k_0)$ for all $t \in (-t_0, t_0)$ (resp. $t \in [0, t_0)$). Moreover, the derivatives of f_2 and f_3 at $t = 0$ verify

$$\begin{cases} n_1 + n_2 + 2f_2'(0)n_0 + L_{K_0}f_3'(0) = 0, \\ f_3'(0) = L_K f_3'(0) + b, \end{cases}$$

where $n_1 = n[\rho_1 \rho + \rho \rho_1^*] \in L^\infty$, $k_1 = k[\rho_1 \rho + \rho \rho_1^*] \in L^\infty$, $n_2 = n[\rho_2] \in L^\infty$, $k_2 = k[\rho_2] \in L^\infty$ and

$$b := \frac{n_1 + n_2}{2n_0} - \frac{a}{2} \left(k_1 + k_2 - \frac{\nabla \sqrt{n_0}}{\sqrt{n_0}} \nabla(n_1 + n_2) \right).$$

Finally, $t \mapsto \rho(t, f(t)) \in \mathcal{C}^1((-t_0, t_0), \mathcal{I}_1)$ (resp. $\mathcal{C}^1([0, t_0), \mathcal{I}_1)$).

The Euler-Lagrange equation is then deduced by differentiating $t \mapsto S(\rho(t, f(t)))$ (in fact, to be rigorous, we need to regularized the entropy). This yields the desired result which is encapsulated in the next result.

Proposition 3.3 The adjoint problem

$$m_0 = L_K^* m_0 - \gamma,$$

where

$$\gamma(x) := 2\Re \left(\sum_{j \in \mathbb{N}} \rho_j \nabla \psi_j(x) \int_x^1 \psi_j^*(y) \left(\log(\rho_j) - \frac{n[\rho \log(\rho)](y)}{n_0(y)} \right) dy \right),$$

admits a unique solution $m_0 \in L^\infty$. With $m = am_0/2$, we have the Euler-Lagrange equation

$$\text{Tr}(\rho \log(\rho)(\rho_1 + \rho_1^*)) + \langle m, k_1 \rangle + \langle A, n_1 \rangle + \left\langle m \frac{|\nabla \sqrt{n_0}|^2}{n_0}, n_1 \right\rangle - \left\langle m, \frac{\nabla \sqrt{n_0}}{n_0} \nabla n_1 \right\rangle = 0,$$

where

$$A = -\frac{n[\rho \log(\rho)]}{n_0} - \frac{k_0}{n_0} m.$$

In the derivation of the Euler-Lagrange equation, we use the equations that $f_2'(0)$ and $f_3'(0)$ satisfy in Proposition 3.2. In particular, the previous adjoint problem is linked to the equation satisfied by $f_3'(0)$. From the Euler-Lagrange equation, we are able to identify the following quadratic form

$$\mathcal{Q}(\phi, \phi) := \int_0^1 n_0(x) \left(\nabla \left(\frac{\phi^*(x)}{\sqrt{n(x)}} \right) \nabla \left(\frac{\phi(x)}{\sqrt{n(x)}} \right) \right) m(x) dx + \int_0^1 A(x) \phi^*(x) \phi(x) dx,$$

which leads to the main result states below.

Theorem 3.11 Let n_0 and k_0 satisfying Assumption 3.4 and ρ be the unique minimizer of S in $\mathfrak{E}^+(n_0, 0, k_0)$. Then, ρ is full rank and its eigenelements $(\rho_j, \psi_j)_{j \in \mathbb{N}}$ verify the self-consistent nonlinear eigenvalue problem

$$-\log(\rho_j) = \min_{\phi \in \mathcal{K}_j} \mathcal{Q}(\phi, \phi) = \mathcal{Q}(\psi_j, \psi_j), \quad \forall j \in \mathbb{N},$$

where

$$\mathcal{K}_j := \left\{ \phi \in H^1 : \|\phi\|_{L^2} = 1 \text{ and } \phi \in (\text{Span}(\psi_\ell)_{0 \leq \ell \leq j-1})^\perp \right\},$$

with $\mathcal{K}_0 = \{\phi \in H^1 : \|\phi\|_{L^2} = 1\}$.

This result rigorously proves that

$$\rho = e^{-\mathcal{H}},$$

where \mathcal{H} is such that, for any $\phi \in \mathcal{C}_0^\infty$,

$$\mathcal{H}\phi = -\frac{1}{\sqrt{n_0}}\nabla \cdot \left(n_0 m \nabla \left(\frac{\phi}{\sqrt{n_0}} \right) \right) + A\phi. \quad (3.41)$$

We remark that, in the previous result, the minimizer of the quadratic form are directly given thanks to ρ and we are not in a position to construct them from Q itself. This is due to a lack of informations on m (which is only known to be positive and to belong in L^∞) and we are unable to use the min-max principle or to prove if the space

$$H_Q^1 := \left\{ \phi \in L^2 : \int_0^1 (m(x)|\nabla\phi(x)|^2 + |\phi(x)|^2) dx < +\infty \right\},$$

is complete.

The characterization problem was also addressed in [DP3] in the unbounded multi-dimensional case but only with the local density constraint, where we minimize the free energy F_T . To obtain the existence and uniqueness of a minimizer, the assumptions on n_0 are the ones from [78]: $\sqrt{n_0} \in H^1$, $n_0 \log(n_0) \in L^1$ and $\|n_0\|_{L^1} = 1$. In the case where the domain is simply the torus and $n_0(x) \geq n_m > 0$, Theorem 3.2 and Proposition 3.1 provide the necessary characterization. That is, the minimizer ρ is of the form

$$\rho = e^{-\mathcal{H}/T}, \quad (3.42)$$

with $\mathcal{H} = -\Delta + A$, where

$$A := \frac{\Delta n_0}{2n_0} - \frac{Tn[\rho \log(\rho)] + k[\rho]}{n_0}.$$

In particular, the chemical potential A belongs in H_{per}^{-1} . This leads to two difficulties if one would like to mimic the arguments from [77, 79]: $n_0 \in L^1$ cannot be above a certain positive constant and the regularity of A would prevent us from undergoing the identification of the operator *via* a quadratic form. Moreover, additional regularity on n_0 would not necessarily improve the second point. In order to tackle these issues, we rely, just as in [DP2], on the Euler-Lagrange equation associated to the minimization problem and reformulate the characterization as a self-consistent nonlinear eigenvalue problem. We remark that

$$\frac{\Delta n_0}{2n_0} = \frac{\Delta \sqrt{n_0}}{\sqrt{n_0}} + \frac{|\nabla \sqrt{n_0}|^2}{n_0},$$

where the first term on the right-hand-side is the so-called Bohm potential, which can be added in the Laplace operator, and, thus, the operator \mathcal{H} rewrites as

$$\mathcal{H}\phi = -\frac{1}{\sqrt{n_0}}\nabla \cdot \left(n_0 \nabla \left(\frac{\phi}{\sqrt{n_0}} \right) \right) + V\phi - \frac{k[\rho]}{n_0}\phi,$$

where

$$V = \frac{|\nabla \sqrt{n_0}|^2 - n[\rho \log(\rho)]}{n_0}.$$

We note that the term $-n[\rho \log(\rho)]$ is nonnegative since the $\text{Tr}(\rho) = \|n_0\|_{L^1} = 1$ and, thus, $V \geq 0$. However, it is not clear if \mathcal{H} is positive but it is symmetric. This formulation, of course, resembles the one from (3.41) and the potential V is in fact easier to handle than the chemical potential A . As a mean to derive the Euler-Lagrange equation, we need a perturbation that stays in $\mathfrak{E}^+(n_0)$ and which gives enough informations. We choose to consider operators of the form

$$\rho(t) = \sqrt{\frac{n_0}{n(t)}}(\rho + tP)\sqrt{\frac{n_0}{n(t)}},$$

where $n(t) := n[\rho + tP]$, for any $t \in \mathbb{R}$, and P is a projection. With $P = |\phi\rangle\langle\phi|$, for a well chosen ϕ , and $t \geq 0$, we are able to prove that the minimizer is full rank by differentiating $t \mapsto E(\rho(t))$ and $t \mapsto S(\rho(t))$ (by a regularization of the entropy) at 0^+ .

Proposition 3.4 The minimizer is full rank, that is $\rho_j > 0$ for all $j \in \mathbb{N}$.

Then, by doing the same with $P = |\psi_j\rangle\langle\psi_\ell| + |\psi_\ell\rangle\langle\psi_j|$, for some $j, \ell \in \mathbb{N}$, we are able to deduce the next result where Q is a quadratic form given by

$$Q(\phi, \phi) = \int_{\mathbb{R}^d} n_0(x) \nabla \left(\frac{\phi^*(x)}{\sqrt{n_0}} \right) \cdot \nabla \left(\frac{\phi(x)}{\sqrt{n_0}} \right) dx + \int_{\mathbb{R}^d} \left(V(x) - \frac{k[\rho](x)}{n_0(x)} \right) \phi^*(x) \phi(x) dx,$$

and we can see that $Q(\phi, \phi) = \langle \mathcal{H} \phi, \phi \rangle$.

Proposition 3.5 For all $j, \ell \in \mathbb{N}$,

$$Q(\psi_j, \psi_\ell) = -\log(\rho_j) \delta_{j,\ell}.$$

The quadratic form Q is well-defined on the space

$$H_Q^1 := \left\{ \phi \in H^1 : V^{1/2} \phi \in L^2 \right\},$$

which is complete as a closed subspace of H^1 . To see this, we use the fact that ρ is a minimizer to deduce that, for any $\phi \in H_Q^1$,

$$-\log(\rho_0) \|\phi\|_{L^2}^2 \leq Q(\phi, \phi),$$

which proves that Q is nonnegative and, thus, that

$$\int_{\mathbb{R}^d} \frac{k[\rho](x)}{n_0(x)} |\phi(x)|^2 dx \leq \int_{\mathbb{R}^d} n_0(x) \left| \nabla \left(\frac{\phi(x)}{\sqrt{n_0(x)}} \right) \right|^2 dx + \int_{\mathbb{R}^d} V(x) |\phi(x)|^2 dx.$$

Moreover, we have, thanks to the Cauchy-Schwarz inequality,

$$\begin{aligned} \int_{\mathbb{R}^d} n_0(x) \left| \nabla \left(\frac{\phi(x)}{\sqrt{n_0(x)}} \right) \right|^2 dx &= \|\nabla \phi\|_{L^2}^2 + \left\| \frac{|\nabla \sqrt{n_0}|}{\sqrt{n_0}} \phi \right\|_{L^2}^2 - \int_{\mathbb{R}^d} \frac{\nabla \sqrt{n_0} \cdot \nabla |\phi(x)|^2}{\sqrt{n_0(x)}} dx \\ &\leq \|\nabla \phi\|_{L^2}^2 + \|V^{1/2} \phi\|_{L^2}^2 + 2\|\nabla \phi\|_{L^2} \|V^{1/2} \phi\|_{L^2}, \end{aligned}$$

which finishes to prove that Q is well-posed on H_Q^1 . In the end, we obtain the following result where we introduce

$$H_\rho := \left\{ \phi \in L^2 : -\sum_{j \in \mathbb{N}} \log(\rho_j) |\langle \psi_j, \phi \rangle|^2 < +\infty \right\},$$

which is the domain of self-adjointness of $\sqrt{-\log(\rho)}$.

Theorem 3.12 Let ρ be the unique minimizer of

$$\min_{\sigma \in \mathfrak{E}^+(n_0)} F_T(\sigma),$$

where $n_0 > 0$ a.e. in \mathbb{R}^d is such that $\sqrt{n_0} \in H^1$ and $\|n_0\|_{L^1} = 1$. Then, ρ is full rank and

$$-\log(\rho_j) = \min_{\phi \in \mathcal{X}_j} Q(\phi, \phi) = Q(\psi_j, \psi_j), \quad \forall j \in \mathbb{N},$$

where

$$\mathcal{X}_j := \left\{ \phi \in H_Q^1 : \|\phi\|_{L^2} = 1 \text{ and } \phi \in (\text{Span}(\psi_\ell)_{0 \leq \ell \leq j-1})^\perp \right\},$$

with the convention that $\mathcal{K}_0 = \{\phi \in H_Q^1 : \|\phi\|_{L^2} = 1\}$. Moreover, denoting Q_S the restriction of Q to $S = \text{Span}(\psi_j)_{j \in \mathbb{N}}$, we have that Q_S is densely defined and closable, and that $-\log(\rho)$ is the unique self-adjoint operator associated with the closure of Q_S . Finally, we have $H_Q^1 \subset H_\rho$.

The previous theorem rigorously prove (3.42) but we are not able to show the existence of a unique self-adjoint operator associated to Q . While Q can be shown to be closed in H_Q^1 when $k[\rho] = 0$, we are incapable to prove it in the general case. This is a consequence of $-k[\rho]$ being negative and the fact that it can not be treated as a perturbation since we only know that it belongs in L^1 (and it is not clear if any additional regularity on n_0 could help in this situation).

3.5 The many-body case

Up until now, we considered the entropy minimization problem for a single (mean-field) particle. In [80], the authors derive the Euler equations directly from many-body quantum mechanics through the introduction of the so-called local Gibbs states, which corresponds to the minimizer of the von Neumann entropy with prescribed density, current and energy at each point $x \in \mathbb{R}^d$. Without going into details, the approach is somehow reminiscent of the one from Levermore's strategy and they prove that, for a system which is initially a local Gibbs state, it stays, in some asymptotic limit, a Gibbs state where the local density, current and energy evolve according to Euler equations. The local Gibbs states are assumed to exist and, in [DP4], we rigorously prove their existence.

Before stating our results, we need to introduce the mathematical background of many-body quantum mechanics. In the previous section, the building block of the mathematical theory for quantum mechanics was the Schrödinger equation, corresponding the first quantization. However, this theory can not be applied when considering a system where the particles can be created or destroyed which is the case for an electromagnetic field which is understood as a collection of photons. The second quantization was then introduced in order to take into account the phenomenon of creation and destruction of particles, leading to the quantum field theory. In this theory, the underlying Hilbert space is the so-called Fermionic (resp. Bosonic) Fock space that is used to describe a system where the number of particles is not necessarily fixed. It is given by

$$\mathfrak{F} := \bigoplus_{N=0}^{+\infty} \mathfrak{F}^{(N)},$$

where $\mathfrak{F}^{(N)} := (L^2(\mathbb{R}^d))^{\wedge, N}$ (resp. $(L^2(\mathbb{R}^d))^{\otimes, N}$) is the N -fold anti-symmetric (resp. symmetric) tensor product of $L^2(\mathbb{R}^d)$ and $\mathfrak{F}^{(0)} := \mathbb{C}$. Any element $\Psi \in \mathfrak{F}$ is represented as a sequence $\{\Psi^{(N)}\}_{N \in \mathbb{N}}$ where $\Psi^{(N)} \in \mathfrak{F}^{(N)}$. The space \mathfrak{F} is a Hilbert space endowed with the scalar product

$$\langle \Phi, \Psi \rangle = \sum_{N=0}^{+\infty} \langle \Phi^{(N)}, \Psi^{(N)} \rangle$$

In the sequel, we will consider the space \mathcal{J}_1 of trace class operators on \mathfrak{F} . The trace on \mathfrak{F} will be denoted $\text{Tr}(\cdot)$ whereas the trace on $\mathfrak{F}^{(k)}$ will be denoted $\text{Tr}_{\mathfrak{F}^{(k)}}(\cdot)$, for any $k \geq 1$. The space of density operators, denoted \mathcal{S} , is the set of nonnegative trace class operators on \mathfrak{F} with trace equal to 1. The observables need to be lifted in order to act on \mathfrak{F} . For an operator A acting on $\mathfrak{F}^{(k)}$, $k \geq 1$, we denote \mathbb{A} its second quantization given by

$$\mathbb{A} := \underbrace{0 \oplus \dots \oplus 0}_{k \text{ times}} \oplus \bigoplus_{N=k}^{+\infty} \sum_{1 \leq i_1 < \dots < i_k \leq N} (A)_{i_1, \dots, i_k},$$

where $(A)_{i_1, \dots, i_k}$ is the operator A acting on the variables labeled i_1, \dots, i_k in $\mathfrak{F}^{(k)}$ and leaving the other variables invariant. When $k = 1$, we usually denote $d\Gamma(A) := \mathbb{A}$. A particular case is the

second quantization of the identity on $\mathfrak{F}^{(1)}$ which is called the number operator and denoted \mathcal{N} . It is a positive self-adjoint operator when equipped with the domain

$$D(\mathcal{N}) := \left\{ \Psi = \{\Psi^{(N)}\}_{N \in \mathbb{N}} \in \mathfrak{F} : \sum_{N \in \mathbb{N}} N^2 \|\Psi^{(N)}\|_{L^2}^2 < +\infty \right\}.$$

We remark that, in general, $\mathcal{N}\rho$ need not be positive for $\rho \in \mathcal{S}$. We denote by \mathcal{S}_k the set of density operators with finite average particle number, *i.e.*

$$\mathcal{S}_k := \left\{ \rho \in \mathcal{S} : \text{Tr} \left(\mathcal{N}^{k/2} \rho \mathcal{N}^{k/2} \right) < +\infty \right\}.$$

For a $H_0 = -\Delta$ and $D(H_0) = H^2(\mathbb{R}^d)$, we denote $\mathbb{H}_0 = d\Gamma(H_0)$ and let

$$\mathcal{E}_0 := \left\{ \rho \in \mathcal{S}_1 : \text{Tr} \left(\mathbb{H}_0^{1/2} \rho \mathbb{H}_0^{1/2} < +\infty \right) \right\},$$

which is the set of density operators with finite particle number and finite kinetic energy. We now introduce the reduced density operators: let A be any bounded operator on $\mathfrak{F}^{(k)}$, for $k \geq 1$. For a state $\rho \in \mathcal{S}_k$, the reduced k -particle density operator $\rho^{(k)}$ is the unique nonnegative trace class operator such that

$$\text{Tr}_{\mathfrak{F}^{(k)}} \left(A \rho^{(k)} \right) = \text{Tr} (A \rho). \quad (3.43)$$

These reduced density operators will be useful to define the local density, current and energy in the same way as we did when considering a (mean-field) single-particle system. In a sense, the duality relation (3.43) states that expectation value of a measurement on the system represented by ρ with the observable \mathbb{A} can be viewed as the one of a corresponding k -particles system represented by $\rho^{(k)}$ with the observable A . It can be proved that

$$\text{Tr}_{\mathfrak{F}^{(1)}} \left(H_0^{1/2} \rho^{(1)} H_0^{1/2} \right) = \text{Tr} \left(\mathbb{H}_0^{1/2} \rho \mathbb{H}_0^{1/2} \right).$$

We are now in a position to introduce the local density, current and kinetic energy for a density operator $\rho \in \mathcal{E}_0$:

1. the local (1-particle) density $n[\rho]$ is defined by duality as

$$\int_{\mathbb{R}^d} n[\rho](x) \phi(x) dx = \text{Tr}_{\mathfrak{F}^{(1)}} \left(\rho^{(1)} \phi \right), \quad \forall \phi \in \mathcal{C}_0^{+\infty}(\mathbb{R}^d),$$

2. the local (1-particle) current $u[\rho]$ is defined by duality as

$$\int_{\mathbb{R}^d} u[\rho](x) \cdot \varphi(x) dx = -i \text{Tr}_{\mathfrak{F}^{(1)}} \left(\rho^{(1)} \left(\varphi \cdot \nabla + \frac{1}{2} (\nabla \cdot \varphi) \right) \right), \quad \forall \varphi \in (\mathcal{C}_0^{+\infty}(\mathbb{R}^d))^d,$$

3. the local (1-particle) kinetic energy $k[\rho]$ is defined by duality as

$$\int_{\mathbb{R}^d} k[\rho](x) \phi(x) dx = -\text{Tr}_{\mathfrak{F}^{(1)}} \left(\rho^{(1)} \nabla \cdot (\phi \nabla) \right), \quad \forall \phi \in \mathcal{C}_0^{+\infty}(\mathbb{R}^d).$$

These functions are well-defined in L^1 and verify

$$\|n[\rho]\|_{L^1} = \text{Tr} \left(\mathcal{N}^{1/2} \rho \mathcal{N}^{1/2} \right), \quad \|k[\rho]\|_{L^1} = \text{Tr} \left(\mathbb{H}_0^{1/2} \rho \mathbb{H}_0^{1/2} \right).$$

In [80], the local moments are n , u and a local energy e , additionally to the local kinetic energy, an interaction potential w is taken into account. Here, we define e by adding yet another external potential v leading to an expression of the form

$$e[\rho] = k[\rho] + e_I[\rho] + e_P[\rho],$$

where e_I is the local interaction energy and e_P is the local potential energy. It is assumed that

$$v_+ \in L^1_{\text{loc}}, \quad v_-, w \in L^p + L^\infty,$$

with $p = 1$ when $d = 1$, $p > 1$ when $d = 2$ and $p = d/2$ when $d \geq 3$. Since the density $n[\rho]$ must have sufficient decay at infinity for entropy of ρ to be bounded below, we introduce a nonnegative confining potential $v_c \in L^1_{\text{loc}}$ verifying $v_c(x) \rightarrow +\infty$ as $|x| \rightarrow +\infty$ and such that

$$\forall t > 0, \quad \int_{\mathbb{R}^d} e^{-tv_c(x)} dx < +\infty.$$

Thus, the local potential energy is given by

$$e_P[\rho] = (v + v_c)n[\rho].$$

We remark that, by prescribing e_P and n , we do not change the minimization problem by introducing of the potential v_c . Furthermore, the operator $H_c = H_0 + v_c$, defined in the sense of quadratic forms, is self-adjoint and admits a compact resolvent. Also, by the Golden-Thompson inequality, the operator e^{-tH_c} is trace class for all $t > 0$. The interaction potential w is assumed to be classically stable of the second kind, that is, there exists a constant $C_0 > 0$ such that

$$\forall N \geq 2, \forall x \in (\mathbb{R}^d)^N, \quad \sum_{1 \leq i < j \leq N} w(x_i - x_j) \geq -C_0 N, \quad \text{a.e. on } (\mathbb{R}^d)^N.$$

For instance, the Coulomb potential $w(x) = 1/|x|$ is classically stable of the second kind when $d = 3$. The local interaction energy e_I is formally given in [80] as

$$e_I[\rho] = \int_{\mathbb{R}^d} n[\rho^{(2)}](x, y) w(x - y) dy,$$

where $n[\rho^{(2)}]$ is the 2-particle local density of ρ defined, for any $\rho \in \mathcal{S}_2$, by duality as

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} n[\rho^{(2)}](x, y) \phi(x, y) dx dy = \text{Tr}_{\mathfrak{F}^{(2)}} \left(\rho^{(2)} \phi \right),$$

for any symmetric test function $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^d \times \mathbb{R}^d)$. An issue with $n[\rho^{(2)}]$ is that it requires $\rho \in \mathcal{S}_2$ which is not a natural assumption to add to our minimization problem. To tackle this issue, we remark that the operator $\sum_{1 \leq i < j \leq N} w(x_i - x_j) + r_0 N$ is strictly positive for $r_0 > C_0$. We then consider the operators $\rho \in \mathcal{S}$ such that

$$\text{Tr} \left((\mathbb{W} + r_0 \mathcal{N})^{1/2} \rho (\mathbb{W} + r_0 \mathcal{N})^{1/2} \right) < +\infty,$$

where \mathbb{W} is the second quantization of $w(x_1 - x_2)$ acting on $\mathfrak{F}^{(2)}$, and let

$$\mathbb{B} := 0 \oplus r_0^{1/2} \oplus \bigoplus_{N=2}^{+\infty} N^{-1} \left(\sum_{1 \leq i < j \leq N} w(x_i - x_j) + r_0 N \right)^{1/2}.$$

Then, the operator $\mathbb{B}\rho\mathbb{B}$ belongs in \mathcal{S}_2 and admits a 2-particle local density. Our definition of the local interaction energy is

$$e_I[\rho] := \int_{\mathbb{R}^d} n[\mathbb{B}\rho\mathbb{B}](x, y) dy \geq 0, \quad \text{a.e.}$$

and we remark that

$$\text{Tr} \left((\mathbb{W} + r_0 \mathcal{N})^{1/2} \rho (\mathbb{W} + r_0 \mathcal{N})^{1/2} \right) = \|e_I[\rho]\|_{L^1}.$$

This ends the definition of the local energy e and we now have to define the space of density operators on which e is well-defined. For $N \geq 2$, we consider the symmetric operator H_N on $\mathfrak{F}^{(N)}$ given by

$$H_N := \sum_{j=1}^N (-\Delta_{x_j} + V(x_j) + r_0) + \sum_{1 \leq i < j \leq N} w(x_i - x_j),$$

and

$$H_1 := -\Delta + V + r_0.$$

It follows from the assumptions on v and w that the potential

$$\sum_{j=1}^N v_-(x_j) + \sum_{1 \leq i < j \leq N} w(x_i - x_j),$$

is infinitesimally H_0 -form bounded (see [64]). Hence, there exists $\gamma \in (0, 1)$, independent of N , such that, by choosing r_0 sufficiently large, we have

$$\gamma \left(\sum_{j=1}^N (-\Delta_{x_j} + V(x_j) + 1) \right) \leq H_N, \quad (3.44)$$

in the sense of operators, and, also, H_N is associated with a quadratic form closed in the space of functions $\Psi^{(N)} \in \mathfrak{F}^{(N)}$ such that $\Psi^{(N)} \in H^1((\mathbb{R}^d)^N)$ and

$$\int_{(\mathbb{R}^d)^N} (v_+(x_1) + v_c(x_1)) |\Psi^{(N)}(x)|^2 dx < +\infty.$$

Therefore, we can consider the self-adjoint realization of H_N , $N \geq 1$, with domain $D(H_N)$ of the quadratic form. Our energy space is defined thanks to the self-adjoint operator \mathbb{H} given by

$$\mathbb{H} = 0 \oplus \bigoplus_{N=1}^{+\infty} H_N \quad \text{and} \quad D(\mathbb{H}) = \mathbb{C} \oplus \bigoplus_{N=1}^{+\infty} D(H_N).$$

The energy space is defined by

$$\mathcal{E} = \left\{ \rho \in \mathcal{S} : \text{Tr} \left(\mathbb{H}^{1/2} \rho \mathbb{H}^{1/2} \right) < +\infty \right\}.$$

We note that (3.44) yields

$$\gamma \left(\text{Tr} \left(d\Gamma(H_c)^{1/2} \rho d\Gamma(H_c)^{1/2} \right) + \text{Tr} \left(\mathcal{N}^{1/2} \rho \mathcal{N}^{1/2} \right) \right) \leq \text{Tr} \left(\mathbb{H}^{1/2} \rho \mathbb{H}^{1/2} \right),$$

which implies that $\mathcal{E} \subset \mathcal{E}_0$. Moreover, we remark that

$$\|e[\rho]\|_{L^1} = \text{Tr} \left(\mathbb{H}^{1/2} \rho \mathbb{H}^{1/2} \right).$$

Before turning to the results from [DP4], we define S the von Neumann entropy for any operator $\rho \in \mathcal{S}$ as

$$S(\rho) := \text{Tr}(\rho \log(\rho)) = \sum_{j \in \mathbb{N}} \rho_j \log(\rho_j),$$

where $\{\rho_j\}_{j \in \mathbb{N}}$ is the nonincreasing sequence of eigenvalues of ρ , counted with multiplicity. The feasible set is given by

$$\mathcal{E}(n_0, u_0, e_0) := \{ \rho \in \mathcal{E} : n[\rho] = n_0, u[\rho] = u_0 \text{ and } e[\rho] = e_0 \}.$$

The main result of [DP4] is the following.

Theorem 3.13 Suppose that $(n_0, u_0, e_0) \in \mathfrak{M}$, where

$$\mathfrak{M} := \left\{ (n_0, u_0, e_0) \in L_+^1 \times (L^1)^d \times L_+^1 : n[\rho] = n_0, u[\rho] = u_0, e[\rho] = e_0, \text{ for some } \rho \in \mathcal{E} \right\},$$

and that $v_c n_0 \in L^1$. Then, the constrained minimization problem

$$\min_{\rho \in \mathcal{E}(n_0, u_0, e_0)} S(\rho),$$

admits a unique solution.

To prove the bound of the entropy on \mathcal{E} , the relative entropy F given by, for any $\rho, \sigma \in \mathcal{S}$,

$$F(\rho, \sigma) = \text{Tr}(\rho(\log(\rho) - \log(\sigma))) \geq 0,$$

is used in conjunction with the density operator $\rho_c = e^{\beta d\Gamma(H_c)} / \text{Tr}(e^{\beta d\Gamma(H_c)})$, for any $\beta > 0$, which belongs in \mathcal{S} since $e^{-\beta H_c}$ is trace class. In fact, we have, for any $\rho \in \mathcal{E}$,

$$F(\rho, \rho_c) = S(\rho) + \beta \text{Tr}\left(d\Gamma(H_c)^{1/2} \rho d\Gamma(H_c)^{1/2}\right) + \log \text{Tr}\left(e^{-d\Gamma(H_c)}\right) \geq 0, \quad (3.45)$$

which proves the lower bound

$$S(\rho) \geq -\beta \text{Tr}\left(d\Gamma(H_c)^{1/2} \rho d\Gamma(H_c)^{1/2}\right) - \log \text{Tr}\left(e^{-d\Gamma(H_c)}\right).$$

Furthermore, we know that F is weakly lower semicontinuous (see [69]) and thus, (3.45) yields that S is also lower semicontinuous. Hence, the main difficulty in Theorem 3.13 is to prove that the limit of a minimizing sequence, denoted ρ , is indeed in $\mathcal{E}(n_0, u_0, e_0)$. We consider a minimizing sequence $\{\rho_m\}_{m \in \mathbb{N}}$ such that $\text{Tr}(\mathbb{H}^{1/2} \rho_m \mathbb{H}^{1/2}) \leq C$ for a certain $C > 0$. By a compactness argument, we are able to prove that, for $\mathbb{B} = \mathbb{H}$ or \mathcal{N} ,

$$\begin{aligned} \mathbb{B}^{1/2} \rho_m \mathbb{B}^{1/2} &\xrightarrow{m \rightarrow +\infty} \mathbb{B}^{1/2} \rho \mathbb{B}^{1/2}, \text{ weak-}^* \text{ in } \mathcal{S}_1 \\ \text{and } \text{Tr}\left(\mathbb{B}^{1/2} \rho \mathbb{B}^{1/2}\right) &\leq \liminf_{m \rightarrow +\infty} \text{Tr}\left(\mathbb{B}^{1/2} \rho_m \mathbb{B}^{1/2}\right). \end{aligned}$$

However, unlike in the one-body case, we can not easily obtain the convergence of the first and second local moments directly. This is due to the fact that, for any $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$,

$$\int_{\mathbb{R}^d} n[\rho_m](x) \phi(x) dx = \text{Tr}_{\mathfrak{F}(1)}\left(\rho_m^{(1)} \phi\right) = \text{Tr}\left(\mathcal{N}^{1/2} \rho_m \mathcal{N}^{1/2} \mathcal{N}^{-1} d\Gamma(\phi)\right),$$

where the operator $\mathcal{N}^{-1} d\Gamma(\phi)$ is not compact. Thus, the weak- $*$ convergence in \mathcal{S}_1 of won't yield the strong L^1 convergence of $n[\rho_m]$ to n_0 (and similarly with $u[\rho_m]$ to u_0 and $e[\rho_m]$ to e_0). Like in the one-body case, what is missing is the convergence of the norm $\|n[\rho_m]\|_{L^1}$ to $\|n_0\|_{L^1}$ (resp. $\|u[\rho]\|_{L^1}$ to $\|u_0\|_{L^1}$ and $\|e[\rho]\|_{L^1}$ to $\|e_0\|_{L^1}$) to obtain the strong convergence. It turns out that, obtaining the strong convergence for n and e is enough to deduce the one for u . At that point, we only know that

$$S(\rho) \leq \min_{\sigma \in \mathcal{E}(n_0, u_0, e_0)} S(\sigma), \|n[\rho]\|_{L^1} := N_* \leq N =: \|n_0\|_{L^1} \text{ and } \|e[\rho]\|_{L^1} := W_* \leq W =: \|e_0\|_{L^1}, \quad (3.46)$$

which yields the following inequalities on minimization problems with global constraints

$$\inf_{\sigma \in \mathcal{E}_g(N_*)} F_\beta(\sigma) \leq \inf_{\sigma \in \mathcal{E}_g(N)} F_\beta(\sigma) \quad \text{and} \quad \inf_{\sigma \in \mathcal{E}_{g,e}(W_*)} S_\beta(\sigma) \leq \inf_{\sigma \in \mathcal{E}_{g,e}(W)} S_\beta(\sigma) \quad (3.47)$$

where $F_\beta(\sigma) = \beta^{-1}S(\sigma) + \text{Tr}(\mathbb{H}^{1/2}\sigma\mathbb{H}^{1/2})$ is the free energy at temperature β^{-1} and

$$\mathcal{E}_g(N) := \{\sigma \in \mathcal{E} : \|n[\sigma]\|_{L^1} = N\} \quad \text{and} \quad \mathcal{E}_{g,e}(W) := \{\sigma \in \mathcal{E} : \|e[\sigma]\|_{L^1} = W\}.$$

From here, the strategy is somehow reminiscent of the one from [DP1]: we assume that the inequalities on the L^1 norms in (3.46) are strict and show that this leads to a contradiction in (3.47). We first deal with the energy inequality then the density inequality (note that doing both at the same time would be much more complicated). The arguments can be stated in a physical way: the density operator with the largest energy should have the smallest (mathematical) entropy and, similarly, the density operator with the largest mass should lose a larger amount of energy to thermal fluctuations, *i.e.* it should have a lower free energy. In the end, we conclude that $\|e[\rho]\|_{L^1} = \|e_0\|_{L^1}$ and $\|n[\rho]\|_{L^1} = \|n_0\|_{L^1}$, proving that $\rho \in \mathcal{E}(n_0, u_0, e_0)$.

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